A Note on Second Order Slope Rotatable Designs
Bejjam Re Victorbabu
Department of Statistics, Acharya Nagarjuna University, Guntur-522 510, India.
*Corresponding author; e-mail: victorsugnanam@yahoo.co.in

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Abstract
In this paper, a note on second order slope rotatable designs using a pair of partially balanced incomplete block designs is suggested. It is observed that the method sometimes leads to designs with less number of design points than those available in the literature.

Keywords: Response surface designs, slope rotatability, partially balanced incomplete block designs.

1. Introduction
Box and Hunter (1957) introduced multifactor experimental designs for exploring response surface designs. Das and Narasimham (1962) constructed rotatable designs through balanced incomplete block designs (BIBD). Chowdhury and Gupta (1985) constructed second order rotatable designs associated with partially balanced incomplete block designs. Victorbabu (2004) suggested second order rotatable designs using a pair of partially balanced incomplete block designs.

Hader and Park (1978) introduced slope rotatable central composite designs (SRCCD). Victorbabu and Narasimham (1991a, b) studied in detail the conditions to be satisfied by a general second order slope rotatable designs (SOSRDs). Victorbabu and Narasimham (1993) constructed SOSRD using pairwise balanced designs (PBD). Victorbabu and Narasimham (1996) studied SOSRD using partially balanced incomplete block designs (PBIBD). Victorbabu (2002) constructed SOSRD using symmetrical unequal block arrangements (SUBA) with two unequal block sizes. Victorbabu (2007) suggested a review on SOSRD. Victorbabu and Surekha (2010) studied a new method of construction of SOSRD using PBD. Victorbabu and Surekha (2011) suggested a new method of construction of SOSRD using BIBD. Victorbabu (2013) suggested a bibliography on slope rotatable designs. Victorbabu (2015) studied on second order slope rotatable designs.
2. **Conditions of Second Order Slope Rotatable Designs**

Suppose we want to use the second order response surface design \( D = (x_{iu}) \) to fit the surface,

\[
Y_u = b_0 + \sum_{i=1}^{v} b_i x_{iu} + \sum_{i=1}^{v} b_i^2 x_{iu}^2 + \sum_{i<j} b_{ij} x_{iu} x_{ju} + e_u,
\]

where \( x_{iu} \) denotes the level of the \( i^{th} \) factor \((i=1, 2, \ldots, v)\) in the \( u^{th} \) run \((u=1, 2, \ldots, N)\) of the experiment, \( e_u \)'s are uncorrelated random errors with mean zero and variance \( \sigma^2 \). The design \( D \) is said to be SOSRD if the variance of the estimate of first order partial derivative of \( Y_u(x_1, x_2, \ldots, x_v) \) with respect to each of independent variables \( x_i \) is only a function of the distance (i.e., \( d^2 = \sum_{i=1}^{v} x_i^2 \)) of the point \((x_1, x_2, \ldots, x_v)\) from the origin (center) of the design. Such a spherical variance function for estimation of slopes in the second order response surface is achieved if the design points satisfy the following conditions (cf. Hader and Park 1978, Victorbabu and Narasimham 1991a).

1. \( \sum x_{iu} = 0, \sum x_{iu} x_{ju} = 0, \sum x_{iu}^2 = 0, \sum x_{iu} x_{ju} x_{ku} = 0, \sum x_{iu}^3 = 0, \sum x_{iu} x_{ju}^2 = 0, \sum x_{iu} x_{ju} x_{ku} x_{mu} = 0; \) for \( i \neq j \neq k \neq l; \)
2. (i) \( \sum x_{iu}^2 = \text{constant} = N \lambda_2; \)
   (ii) \( \sum x_{iu}^4 = \text{constant} = cN \lambda_4; \) for all \( i \)
3. \( \sum x_{iu} x_{ju}^2 = \text{constant} = N \lambda_4; \) for \( i \neq j \)

where \( c, \lambda_2 \) and \( \lambda_4 \) are the summation is over the design points. The variances and covariances of the estimated parameters are

\[
V(\hat{b}_0) = \frac{\lambda_4 (c + v - 1) \sigma^2}{N \lambda_4^2 (c + v - 1) - v \lambda_2^2},
\]

\[
V(\hat{b}_i) = \frac{\sigma^2}{N \lambda_4^2},
\]

\[
V(\hat{b}_0) = \frac{\sigma^2}{N \lambda_4^2},
\]

\[
V(\hat{b}_i) = \frac{\sigma^2}{(c-1)N \lambda_4} \left[ \frac{\lambda_4 (c + v - 2) - (v - 1) \lambda_2^2}{\lambda_4 (c + v - 1) - v \lambda_2^2} \right],
\]

\[
Cov(\hat{b}_0, \hat{b}_i) = \frac{-\lambda_2 \sigma^2}{N \lambda_4 (c + v - 1) - v \lambda_2^2},
\]

\[
Cov(\hat{b}_i, \hat{b}_j) = \frac{(\lambda_2^2 - \lambda_4) \sigma^2}{(c-1)N \lambda_4 [\lambda_4 (c + v - 1) - v \lambda_2^2]} \quad \text{and other covariances vanish.}
\]

An inspection of the variance of \( \hat{b}_0 \) shows that a necessary condition for the existence of a non-singular second order design is
\[
\frac{\lambda_3}{\lambda_2^2} > \frac{\nu}{(c+\nu-1)} \quad \text{(non-singularity condition)}.
\]

For the second order model
\[
\frac{\partial\hat{Y}}{\partial x_i} = \hat{b}_i + 2\hat{b}_i x_{iu} + \sum_{j \neq i} \hat{b}_{ij} x_{ju},
\]
\[
V\left(\frac{\partial\hat{Y}}{\partial x_i}\right) = V(\hat{b}_i) + 4x_i^2 V(\hat{b}_i) + \sum_{j \neq i} x_{ju}^2 V(\hat{b}_{ij}).
\]

The condition for right hand side of (4) to be a function of \(d^2 = \sum x_i^2\) alone (for slope rotatability) is
\[
V(\hat{b}_i) = \frac{1}{4} V(\hat{b}_j).
\]

Therefore, conditions (1), (2), and (5) lead to the condition
\[
[v(5-c) - (c-3)^2] \lambda_4 + [v(c-5) + 4] \lambda_2^2 = 0.
\]

3. Method of Construction of SOSRD Using a Pair of PBIB Designs

Following the methods of construction of Chowdhury and Gupta (1985), Victorbabu and Narasimham (1991b), Victorbabu and Narasimham (1996), Victorbabu (2004), a new method of construction of SOSRD using a pair of PBIBD is suggested.

Take an incomplete block arrangement with constant block size and replication in which some pairs of treatments occur \(\lambda_{11}\) times each \((\lambda_{11} \neq 0)\), some other pairs do not occur at all \((\lambda_{12} = 0)\). Take this as the first design. For the second design take the incomplete block design with all missing pairs (in the first design) once each with \(k = 2\), \(\lambda_{21} = 0\), \(\lambda_{22} = 1\). Such pair of PBIB designs can be constructed in a straightforward manner in particular using existing two-associate PBIB designs with one of the \(\chi_i\)'s equal to zero. The method of constructing SOSRD using the above two PBIB designs is given below.

Let \(D_1 = (v, b_1, r_1, k_1, \lambda_{11} \neq 0, \lambda_{12} = 0)\) be an incomplete block design with constant replication in which only some pair of treatments occur a constant number of times \(\lambda_{11}\) \((\lambda_{12} = 0)\), \(2^{v(k_i)}\) denote a fractional replicate of \(2^{h}\) in \(\pm 1\) levels, in which no interaction with less than five factors is confounded. Let \([(1-(v,b_1,r_1,k_1,\lambda_{11},\lambda_{12} = 0))\] denote the design points generated from the transpose of the incidence matrix of incomplete block design \(D_1\). \([(1-(v,b_1,r_1,k_1,\lambda_{11},\lambda_{12} = 0))2^{v(k_i)}\] are the \(b_12^{v(k_i)}\) design points generated from \(D_1\) by “multiplication” (cf. Das and Narasimham 1962).

Let \(D_2 = (v, b_2, r_2, k_2 = 2, \lambda_{21} = 0, \lambda_{22} = 1)\) be the associated second design containing only the missing pairs of treatments of above design \(D_1\). \([(a-(v,b_2,r_2,k_2 = 2,\lambda_{21} = 0,\lambda_{22} = 1))2^{2}\] are the \(b_22^{2}\) design points generated from \(D_2\) by “multiplication”, with levels \(\pm a\) (cf. Victorbabu and Narasimham 1996). Let \(n_0\) be the number of central points in the design.

\[
\chi_1 > \frac{\nu}{(c+\nu-1)} \quad \text{(non-singularity condition)}.
\]

For the second order model
\[
\frac{\partial\hat{Y}}{\partial x_i} = \hat{b}_i + 2\hat{b}_i x_{iu} + \sum_{j \neq i} \hat{b}_{ij} x_{ju},
\]
\[
V\left(\frac{\partial\hat{Y}}{\partial x_i}\right) = V(\hat{b}_i) + 4x_i^2 V(\hat{b}_i) + \sum_{j \neq i} x_{ju}^2 V(\hat{b}_{ij}).
\]
Theorem 1 The design points,

$$[1-(v,b_1,r_1,k_1,\lambda_{11},\lambda_{12})]2^{(l_1)} \cup [a-(v,b_2,r_2,k_2 = 2,\lambda_{21},\lambda_{22})]2^2 \cup n_0$$

will give a v-dimensional SOSRD in \( N = b_12^{(l_1)} + b_22^4 + n_0 \) design points, where \( a^2 \) is a positive real root of the biquadratic equation given below:

$$\left\{ \begin{array}{l} 4v_r^3 - N_r^2 2^4 a^8 + vr_l^2 2^{(l_1)+5} a^6 + \\
N[(v-6)\lambda_{11}r_2 + 2r_2r_12^{(l_1)+2} + \\
vr_l^2r_22^{2(l_1)+1} + [vr_l^2 - (5v-4)r_2^2\lambda_{11}]2^{4(l_1)+4} \right \}a^4 + r_2[vr_l - (5v-4)\lambda_{11}]2^{2(l_1)+3} a^2 + \\
N[5v\lambda_{11}^2 - (v-6)r_1\lambda_{11} - r_2^2 - 9\lambda_{11}^3] + r_1^2[vr_l - (5v-4)\lambda_{11}]2^{4(l_1)} = 0. \\
\end{array} \right.$$ (7)

If at least one positive real root for \( a^2 \) exists in (7) then the design exists.

Proof: We need to find constant \( c \) satisfying the condition (6). For the design points generated from designs \( D_1 \) and \( D_2 \), simple symmetry conditions 1, 2, 3 of (1) are true. Condition 1 of (1) is true obviously. Conditions 2 and 3 of (1) are true as follows:

2. (i) \( \sum x_m^{2} = r_12^{(l_1)} + r_22^2 a^2 = N\lambda_{2} \),

(ii) \( \sum x_m^{4} = r_12^{(l_1)} + r_22^2 a^4 = cN\lambda_{4} \),

3. \( \sum x_m^{3}x_m^{2} = \lambda_{11}2^{(l_1)} + \lambda_{21}2^2 a^2 = N\lambda_{4} \). (8)

From 2(ii) and 3 of (8), we get \( c \). Substituting for \( \lambda_{2}, \lambda_{4} \) and \( c \) in (6), we get

\[
\frac{\lambda_{11}2^{(l_1)} + \lambda_{21}2^2 a^2}{N^2} \left[ v(5 - \frac{r_12^{(l_1)} + r_22^2 a^4}{\lambda_{11}2^{(l_1)} + \lambda_{21}2^2 a^2} - \frac{r_12^{(l_1)} + r_22^2 a^4}{\lambda_{11}2^{(l_1)} + \lambda_{21}2^2 a^2} - 3) \right] + \\
\frac{(r_12^{(l_1)} + r_22^2 a^4)^2}{N^2} \left[ v\left( \frac{r_12^{(l_1)} + r_22^2 a^4}{\lambda_{11}2^{(l_1)} + \lambda_{21}2^2 a^2} - 5 \right) + 4 \right] = 0. \\
\] (9)

On simplification of (9) leads to the fourth degree equation in \( a^2 \) given in (7).

Example: We illustrate Theorem 1 with the construction of SOSRD for 8-factors with the help of a pair of PBIBD. The design points,

\[
[1-(v = 8, b_1 = 8, r_1 = 3, k_1 = 3, \lambda_{11} = 1, \lambda_{12} = 0)]2^3 \cup \\
[a-(v = 8, b_2 = 4, r_2 = 1, k_2 = 2, \lambda_{21} = 0, \lambda_{22} = 1)]2^2 \cup n_0,
\]

will give a SOSRD in \( N = 81 \) design points for eight factors (taking one central point \( n_0 = 1 \)).

2. (i) \( \sum x_m^{2} = 24 + 4a^2 = N\lambda_{2} \),

(ii) \( \sum x_m^{4} = 24 + 4a^4 = cN\lambda_{4} \),

3. \( \sum x_m^{3}x_m^{2} = 8 = N\lambda_{4} \). (10)

From 2(ii) and 3 of (10) we get \( c \) as \( c = \frac{24 + 4a^4}{8} \).

Substituting for \( \lambda_{2}, \lambda_{4} \) and \( c \) in (6) and on simplification, we get the biquadratic equation in \( a^2 \),

\[
784a^8 - 6144a^6 + 3840a^4 + 18432a^2 - 27648 = 0,
\]

(This can be alternatively written directly from (7) of Theorem 1).
Equation (7) has only one positive real root \( a^2 = 6.6988 \). It can be verified that the nonsingularity condition (3) is satisfied.

We may point out here that this SOSRD using a pair of PBIBD has only 81 design points for 8-factors, whereas the corresponding SRCCD of Hader and Park (1978), SOSRD using BIBD of Victorbabu and Narasimham (1991a), SOSRD using PBD of Victorbabu and Narasimham (1993), SOSRD using SUBA with two unequal block sizes of Victorbabu (2002), SOSRD using a pair of BIBD of Victorbabu and Narasimham (1991b), SOSRD using pair of PBIBD of Victorbabu and Narasimham (1996) need 81, 129, 257, 113, 337 and 97 design points respectively. Thus the new method leads to a 8-factor SOSRD in less number of design points and same is the case in some other cases also.

Table 1 gives the appropriate slope ratability values of the parameter ‘a’ for designs using a pair of PBIBD and for different number of central points \( n_0 \) for \( \nu = 6, 8, 10 \) and 12 factors.

| Values of SOSRD Using a Pair of PBIB Designs |
|---------------------------------------------|
| \( D_1 = (\nu = 6, b_1 = 4, r_1 = 2, k_1 = 3, \lambda_{11} = 1, \lambda_{12} = 0) \); |
| \( D_2 = (\nu = 6, b_2 = 3, r_2 = 1, k_2 = 2, \lambda_{21} = 0, \lambda_{22} = 1) \) |
| \( n_0 \) | \( N \)   | \( a \)  |
|---|---|---|
| 1  | 45 | 2.8436 |
| 2  | 46 | 2.7537 |
| 3  | 47 | 2.6667 |
| 4  | 48 | 2.5821 |
| 5  | 49 | 2.4991 |

| \( D_1 = (\nu = 8, b_1 = 8, r_1 = 3, k_1 = 3, \lambda_{11} = 1, \lambda_{12} = 0) \); |
| \( D_2 = (\nu = 8, b_2 = 4, r_2 = 1, k_2 = 2, \lambda_{21} = 0, \lambda_{22} = 1) \) |
| \( n_0 \) | \( N \)   | \( a \)  |
|---|---|---|
| 1  | 81 | 2.5882 |
| 2  | 82 | 2.5438 |
| 3  | 83 | 2.4992 |
| 4  | 84 | 2.4543 |
| 5  | 85 | 2.4089 |

| \( D_1 = (\nu = 10, b_1 = 8, r_1 = 4, k_1 = 5, \lambda_{11} = 2, \lambda_{12} = 0) \); |
| \( D_2 = (\nu = 10, b_2 = 5, r_2 = 1, k_2 = 2, \lambda_{21} = 0, \lambda_{22} = 1) \) |
| \( n_0 \) | \( N \)   | \( a \)  |
|---|---|---|
| 1  | 149 | 3.1058 |
| 2  | 150 | 3.0730 |
| 3  | 151 | 3.0399 |
| 4  | 152 | 3.0064 |
| 5  | 153 | 2.9724 |

| \( D_1 = (\nu = 12, b_1 = 8, r_1 = 4, k_1 = 6, \lambda_{11} = 2, \lambda_{12} = 0) \); |
| \( D_2 = (\nu = 12, b_2 = 6, r_2 = 1, k_2 = 2, \lambda_{21} = 0, \lambda_{22} = 1) \) |
| \( n_0 \) | \( N \)   | \( a \)  |
|---|---|---|
| 1  | 281 | 3.2453 |
| 2  | 282 | 3.2240 |
| 3  | 283 | 3.2026 |
| 4  | 284 | 3.1813 |
| 5  | 285 | 3.1599 |

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