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A new method of construction of second-order slope-rotatable designs using incomplete block designs with unequal block sizes

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Abstract In this paper, a new method of construction of second-order slope-rotatable designs (SOSRD) using incomplete block designs with unequal block sizes like symmetrical unequal block arrangements (SUBA) with two unequal block sizes and pairwise balanced designs (PBD) is suggested. It is observed that the method sometimes leads to designs with less number of design points than those available in the literature. Modified SOSRD using incomplete block designs with unequal block sizes suggested by Victorbabu [10] is shown to be obtainable using this method.

1 Introduction

Box and Hunter [1] introduced rotatable designs for the exploration of response surfaces. The study of rotatable designs mainly emphasized on the estimation of absolute response. Estimation of differences in response at two different points in the factor space will often be of great importance. If differences at two points close together, estimation of local slope (rate of change) of the response is of interest. Estimation of slopes occurs frequently in practical situations. For instance, there are cases in which we want to estimate rate of reaction in chemical experiment, rate of change in the yield of a crop to various fertilizer doses, rate of disintegration of radioactive material in an animal etc., (cf. Park [4]). Hader and Park [3] introduced slope-rotatable central composite designs (SRCCD). Victorbabu and Narasimham [12, 13] studied SOSRD and constructed SOSRD using balanced incomplete block designs (BIBD) and PBD. Victorbabu [6] suggested the method of construction of SOSRD using SUBA with two unequal block sizes. Different methods of constructions of SOSRDs were suggested by various authors, including Victorbabu [9, 10, 11], Victorbabu and Narasimham [14, 15], and so on. Victorbabu [7] introduced modified SRCCD. Victorbabu [8] suggested modified SOSRD using BIBD. Victorbabu and Surekha [16] constructed a new method of SOSRD using BIBD.

Conditions for second-order slope-rotatable designs

Suppose we want to use the second-order response surface design $D = ((x_{ui}))$ to fit the model,

$$Y_u = b_0 + \sum_{i=1}^{v} b_i x_{ui} + \sum_{i=1}^{v} b_{ii} x_{ui}^2 + \sum\sum_{i<j} b_{ij} x_{ui} x_{uj} + e_u \tag{1.1}$$

where x_{ui} 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 σ^2. The parameters of the model b_o, b_i, b_{ii} and b_{ij} are estimated by the least squares estimation to provide $\hat{b}_o, \hat{b}_i, \hat{b}_{ii}$ and $\hat{b}_{ij}$. It is said to be a SOSRD if the variance of the estimate of first order partial derivative of Y_u with respect to each of independent variables (x_i) is only a function of the distance $(d^2 = \sum_{i=1}^{v} x_i^2)$ 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 (Hader and Park [3]):

1. $\sum x_{ui} = 0$, $\sum x_{ui} x_{uj} = 0$, $\sum x_{ui} x_{uj}^2 = 0$, $\sum x_{ui} x_{uj} x_{uk} = 0$, $\sum x_{ui}^3 = 0$, $\sum x_{ui} x_{uj}^3 = 0$, $\sum x_{ui} x_{uj} x_{uk}^2 = 0$, $\sum x_{ui} x_{uj} x_{uk} x_{ul} = 0$; for $i \neq j \neq k \neq l$;
2. (i) $\sum x_{ui}^2 = \text{constant} = N\lambda_2$;
   (ii) $\sum x_{ui}^4 = \text{constant} = cN\lambda_4$; for all i
3. $\sum x_{ui}^2 x_{uj}^2 = \text{constant} = N\lambda_4$; for $i \neq j$.
4. $\frac{\lambda_4}{\lambda_2^2} > \frac{v}{(c+v-1)}$
5. $$\left[v(5-c) - (c-3)^2\right] \lambda_4 + \left[v(c-5) + 4\right] \lambda_2^2 = 0 \tag{1.2}$$
   where c, λ_2, λ_4 are constants and v denotes the number of factors.

The variances and covariances of the estimated parameters are

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

$$
\begin{aligned}
V\left(\hat{b}_{ij}\right) &= \frac{\sigma^2}{N\lambda_4}, \\
V\left(\hat{b}_{ii}\right) &= \frac{\sigma^2}{N\lambda_4}\frac{\lambda_4(c+v-2)-(v-1)\lambda_2^2}{\lambda_4(c+v-1)-v\lambda_2^2}, \\
\text{Cov}\ \left(\hat{b}_0,\hat{b}_{ii}\right) &= \frac{-\lambda_2\sigma^2}{N\left[\lambda_4(c+v-1)-v\lambda_2^2\right]}, \\
\text{Cov}\ \left(\hat{b}_{ii},\hat{b}_{jj}\right) &= \frac{\left(\lambda_2^2-\lambda_4\right)\sigma^2}{(c-1)N\lambda_4\left[\lambda_4(c+v-1)-v\lambda_2^2\right]}, \\
&\text{and other covariances are zero.} \\
V\left(\frac{\partial\hat{Y}_u}{\partial x_i}\right) &= \frac{1}{N}\left[\frac{\lambda_4+\lambda_2 d^2}{\lambda_2\lambda_4}\right]\sigma^2.
\end{aligned}
$$

2 New method of construction of SOSRD using incomplete block designs with unequal block sizes

It is clear from the slope rotatability condition 5 of (1.2) that the solution for design levels (like a, b, etc.,) depend on c and number of central points (n_0). In contrast to rotatable designs, we have to choose the non-zero design levels a, b, etc., in SOSRD depending on the number of central points. The interdependence of the parameters n_0, c and design levels is utilized to evolve a new method of construction of SOSRD using incomplete block designs with unequal block sizes.

In SOSRD using SUBA with two unequal block sizes (Victorbabu [6]) and pairwise balanced designs (Victorbabu and Narasimham [14]) usually the number of central points n_0 is prefixed and design levels are chosen to satisfy the conditions of SOSRD. The parameter c is then evaluated. Alternatively we prefix c and choose n_0 and the design levels suitably such that the design points satisfy the conditions of SOSRD. If such designs exist with integral values of n_0, then this approach leads to a new method of construction of SOSRD using SUBA with two unequal block sizes and pairwise balanced designs.

3 Construction of SOSRD using SUBA with two unequal block sizes

Definition 3.1 *SUBA with two unequal block sizes (c.f. Raghavarao [5]) The arrangement of v-treatments in b blocks where b_1 blocks of size k_1, and b_2 blocks of size k_2 is said to be a symmetrical unequal block arrangement with two unequal block sizes, if* *(i) every treatment occurs* $\frac{b_i k_i}{v}$ *blocks of size* $k_i (i = 1, 2)$, *and*

(ii) every pair of first associate treatments occurs together in u *blocks of size* k_1 *and in* $(\lambda - u)$ *blocks of size* k_2 *while every pair of second associate treatments occurs together in* λ *blocks of size* k_2.

From (i) each treatment occurs in $\left(\frac{b_1 k_1}{v}\right) + \left(\frac{b_2 k_2}{v}\right) = r$ *blocks in all.* $(v, b, r, k_1, k_2, b_1, b_2, \lambda)$ *are known as the parameters of the SUBA with two unequal block sizes. For example, consider the SUBA with two unequal block sizes with parameters* $(v = 6, b = 7, r = 3, k_1 = 2, k_2 = 3, b_1 = 3, b_2 = 4, \lambda = 1)$.

Let $(v, b, r, k_1, k_2, b_1, b_2, \lambda)$, $k = \sup(k_1, k_2)$ *denote a SUBA with two unequal block sizes, and* $2^{t(k)}$ *denote a fractional replicate of* 2^k *in* ± 1 *level, in which no interaction with less than five factors is confounded. Let* $[1 - (v, b, r, k_1, k_2, b_1, b_2, \lambda)]$ *denote the design points generated from the transpose of incidence matrix of SUBA with two unequal block sizes. Consider* $[1-(v, b, r, k_1, k_2, b_1, b_2, \lambda]$ $2^{t(k)}$ *are the* $b2^{t(k)}$ *design points generated from SUBA with two unequal block sizes by "multiplication" (c.f. Das and Narasimham [2], Raghavarao [5, pp. 298–300]). Let* $(a, 0, 0, \ldots, 0)2^1$ *denote the design points generated from* $(a, 0, 0 \ldots, 0)$ *point set. Repeat this set of additional design points say '*n_a*' times when* $r < c\lambda$. *Let* $(a, a, \ldots, a)2^{t(v)}$ *denote the design points generated from* $(a, a, \ldots, a)$ *point set. Repeat this set of additional design points say '*n_a*' times when* $r > c\lambda$, *and* $\cup$ *denotes combination of the design points generated from different sets of points. It is observed that replication of axial points* (n_a) *rather than replication of central points provide appreciable advantage in terms of efficiency of the estimates of the parameters of the model.*

Theorem 3.1
Method I *If* $r < c\lambda$, *then the design points,* $[1 - (v, b, r, k_1, k_2, b_1, b_2, \lambda)]$ $2^{t(k)}$ $\cup n_a(a, 0, \ldots, 0)2^1$ $\cup (n_0)$ *will give a* v*-dimensional SOSRD with* $N = b2^{t(k)} + 2n_a v + n_0$ *design points if,*

$$a^4 = \frac{(c\lambda - r)2^{t(k)-1}}{n_a}, \tag{3.1}$$

$$n_0 = \frac{-(r2^{t(k)} + 2n_a a^2)^2 [v(c-5)+4]}{\lambda 2^{t(k)}[v(5-c)-(c-3)^2]} - b2^{t(k)} - 2vn_a. \tag{3.2}$$

Proof. For the design points generated from SUBA with two unequal block sizes the conditions in equation 1 of (1.2) are satisfied. The conditions in equations 2 and 3 of (1.2) are true as follows:

$$\sum x_{ui}^2 = r2^{t(k)} + 2n_a a^2 = N\lambda_2 \tag{3.3}$$

$$\sum x_{ui}^4 = r2^{t(k)} + 2n_a a^4 = cN\lambda_4 \tag{3.4}$$

$$\sum x_{ui}^2 x_{uj}^2 = \lambda 2^{t(k)} = N\lambda_2. \tag{3.5}$$

Solving equations (3.4) and (3.5), we get a^4 given in equation (3.1). Substituting λ_2 and λ_4 in equation 5 of (1.2) and on simplification, we get n_0 given in equation (3.2).

Method II If $r > c\lambda$, then the design points, $[1-(v,b,r,k_1,k_2,b_1,b_2,\lambda)]\ 2^{t(k)}$ $\cup n_a(a,a,a,\ldots,a)2^{t(v)}$ $\cup(n_0)$ give a v-dimensional SOSRD with $N = b2^{t(k)} + n_a 2^{t(v)} + n_0$ design points if,

$$a^4 = \frac{(r-c\lambda)2^{t(k)-t(v)}}{(c-1)n_a}, \tag{3.6}$$

$$n_0 = \frac{-\left(r2^{t(k)} + 2^{t(v)}a^2\right)^2 [v(c-5)+4]}{(\lambda 2^{t(k)} + n_a 2^{t(v)}a^4)\,[v(5-c)-(c-3)^2]} - \left(b2^{t(k)} + n_a 2^{t(v)}\right). \tag{3.7}$$

Proof. For the design points generated from SUBA with two unequal block sizes the conditions in equation 1 of (1.2) are satisfied. The conditions in equations 2 and 3 of (1.2) are true as follows:

$$\sum x_{ui}^2 = r2^{t(k)} + n_a 2^{t(v)}a^2 = N\lambda_2 \tag{3.8}$$

$$\sum x_{ui}^4 = r2^{t(k)} + n_a 2^{t(v)}a^4 = cN\lambda_4 \tag{3.9}$$

$$\sum x_{ui}^2 x_{uj}^2 = \lambda 2^{t(k)} + n_a 2^{t(v)}a^4 = N\lambda_4. \tag{3.10}$$

Solving equations (3.9) and (3.10), we get a^4 given in equation (3.6). Substituting λ_2 and λ_4 in equation 5 of (1.2) and on simplification, we get n_0 given in equation (3.7).

Method III If $r = c\lambda$, then the design points, $[1-(v,b,r,k_1,k_2,b_1,b_2,\lambda)]\ 2^{t(k)}$ $\cup n_0$ give a v-dimensional SOSRD with $N = b2^{t(k)} + n_0$ design points if,

$$n_0 = \frac{-(r2^{t(k)})^2\,[v(c-5)+4]}{\lambda 2^{t(k)}[v(5-c)-(c-3)^2]} - b2^{t(k)}. \tag{3.11}$$

Proof. For the design points generated from SUBA with two unequal block sizes the conditions in equation 1 of (1.2) are satisfied. The conditions in equations 2 and 3 of (1.2) are true as follows:

$$\sum x_{ui}^2 = r2^{t(k)} = N\lambda_2 \tag{3.12}$$

$$\sum x_{ui}^4 = r2^{t(k)} = cN\lambda_4 \tag{3.13}$$

$$\sum x_{ui}^2 x_{uj}^2 = \lambda 2^{t(k)} = N\lambda_4. \tag{3.14}$$

From equations (3.13) and (3.14), we get $r = c\lambda$. Substituting λ_2 and λ_4 in equation 5 of (1.2) and on simplification, we get n_0 given in equation (3.11). However the case with $r = c\lambda$ obviously give designs with $0, \pm 1$ levels and do not need 'a' and n_a.

Example 3.1

We illustrate the method of construction of SOSRD using SUBA with two unequal block sizes ($v = 12, b = 13, r = 4, k_1 = 3, k_2 = 4, b_1 = 4, b_2 = 9, \lambda = 1$) with $c = 5$ and $n_a = 2$ with $N = 324$ design points. We have,

$$\sum x_{ui}^2 = r2^{t(k)} + 2n_a a^2 = 64 + 4a^2 = N\lambda_2 \tag{3.15}$$

$$\sum x_{ui}^4 = r2^{t(k)} + 2n_a a^4 = 64 + 4a^4 = 5N\lambda_4 \tag{3.16}$$

$$\sum x_{ui}^2 x_{uj}^2 = \lambda 2^{t(k)} = 16 = N\lambda_4. \tag{3.17}$$

From equations (3.16) and (3.17), we get $a^4 = 4$. From equation (3.2) we get $n_0 = 68$.

We may point out here that this SOSRD has only 324 design points for 12-factors, whereas the corresponding SOSRD obtained by using BIBD suggested by Victorbabu and Narasimham [12] needs 377 design points and SOSRD constructed by using PBD suggested by Victorbabu and Narasimham [14] needs 537 design points. Thus this new method leads to a 12-factor SOSRD in less number of design points than those available in the literature.

Example 3.2

Consider the SUBA with two unequal block sizes ($v = 6, b = 7, r = 3, k_1 = 2, k_2 = 3, b_1 = 3, b_2 = 4, \lambda = 1$) will give a new SOSRD using SUBA with two unequal block sizes with $c = 6, n_a = 3, a_4 = 4$ and $n_0 = 16$ with $N = 108$ design points.

A list of new method of construction of SOSRD using SUBA with two unequal block sizes for $6 \leq v \leq 16$ is given in Table 1 in the Appendix.

4 Construction of SOSRD using pairwise balanced designs

Let $(v, b, r, k_1, k_2, \ldots, k_p, \lambda)$, $k = \sup \cdot (k_1, k_2, \ldots, k_p)$ denote a pairwise balanced design, and $2^{t(k)}$ denote a fractional replicate of 2^k in ± 1 levels, in which no interaction with less than five factors is confounded. Let $[1 - (v, b, r, k_1, k_2, \ldots, k_p, \lambda)]$ denote the design points generated from the transpose of incidence matrix of PBD. Consider $[1 - (v, b, r, k_1, k_2, \ldots, k_p, \lambda)]2^{t(k)}$ are the $b2^{t(k)}$ design points generated from PBD by "multiplication". Let $(a, 0, 0, \ldots, 0)2^1$ denote the design points generated from $(a, 0, 0 \ldots, 0)$ point set. Repeat this set of additional design points say 'n_a' times when $r < c\lambda$. Let $(a, a, \ldots, a)2^{t(v)}$ denote the design points generated from $(a, a, \ldots, a)$ point set. Repeat this set of additional design points say 'n_a' times when $r > c\lambda$. It is observed that replication of axial points (n_a) rather than replication of central points provide appreciable advantage in terms of efficiency of the estimates of the parameters of the model.

Theorem 4.1 ***Method I*** *If $r < c\lambda$, then the design points, $[1-(v,b,r,k_1,k_2,\ldots,k_p,\lambda)]2^{t(k)} \cup n_a(a,0,\ldots,0)2^1 \cup (n_0)$ will give a v-dimensional SOSRD with $N = b2^{t(k)} + 2n_a v + n_0$ design points if,*

$$a^4 = \frac{(c\lambda - r)2^{t(k)-1}}{n_a}, \tag{4.1}$$

$$n_0 = \frac{-\left(r2^{t(k)} + 2n_a a^2\right)^2 [v(c-5)+4]}{\lambda 2^{t(k)}[v(5-c)-(c-3)^2]} - \left(b2^{t(k)} + 2vn_a\right). \tag{4.2}$$

Method II *If $r > c\lambda$, then the design points, $[1-(v,b,r,k_1,k_2,\ldots,k_p,\lambda)]2^{t(k)} \cup n_a(a,a,a,\ldots,a)2^{t(v)} \cup (n_0)$ will give a v-dimensional SOSRD with $N = b2^{t(k)} + n_a 2^{t(v)} + n_0$ design points if,*

$$a^4 = \frac{(r - c\lambda)2^{t(k)-t(v)}}{(c-1)n_a}, \tag{4.3}$$

$$n_0 = \frac{-\left(r2^{t(k)} + n_a 2^{t(v)} a^2\right)^2 [v(c-5)+4]}{(\lambda 2^{t(k)} + n_a 2^{t(v)} a^4)\,[v(5-c)-(c-3)^2]} - \left(b2^{t(k)} + n_a 2^{t(v)}\right). \tag{4.4}$$

Method III *If $r = c\lambda$, then the design points, $[1-(v,b,r,k_1,k_2,\ldots,k_p,\lambda)]2^{t(k)} \cup (n_0)$ will give a v-dimensional SOSRD with $N = b2^{t(k)} + n_0$ design points if,*

$$n_0 = \frac{-\left(r2^{t(k)}\right)^2 [v(c-5)+4]}{\lambda 2^{t(k)}[v(5-c)-(c-3)^2]} - b2^{t(k)}. \tag{4.5}$$

Proof. Follows by verifying the conditions to be satisfied by a SOSRD.

Example 4.1

We illustrate the method of construction of SOSRD using PBD ($v = 6, b = 7, r = 3, k_1 = 3, k_2 = 2, \lambda = 1$) with $c = 11$ and $n_a = 2$ with $N = 80$ design points. We have,

$$\sum x_{ui}^2 = r2^{t(k)} + 2n_a a^2 = 24 + 4a^2 = N\lambda_2 \tag{4.6}$$

$$\sum x_{ui}^4 = r2^{t(k)} + 2n_a a^4 = 24 + 4a^4 = 11N\lambda_4 \tag{4.7}$$

$$\sum x_{ui}^2 x_{uj}^2 = \lambda 2^{t(k)} = 8 = N\lambda_4. \tag{4.8}$$

From equations (4.7) and (4.8), we get $a^4 = 16$. From equation (4.2) we get $n_0 = 0$.

A list of new method of construction of SOSRD using PBD for $6 \le v \le 16$ is given in Table 2 in the Appendix.

Note: If in particular $c = 5$, we get another series of symmetrical response surface designs (modified) which provide more precise estimates of response at specific points of interest than what is available from the corresponding existing designs. The method of construction of modified SOSRD using incomplete block designs with unequal block sizes which was suggested by Victorbabu [10] may be obtained as special case when $c = 5$.

Appendix

Table 1: List of SOSRD using SUBA with two unequal block sizes for $6 \leq v \leq 16$

$(v, b, r, k_1, k_2, b_1, b_2, \lambda)$	c	n_a	a^2	n_0	N
$(6, 7, 3, 2, 3, 3, 4, 1)$	5	2	2.00	48	128
	6	3	2.00	16	108
$(8, 12, 4, 2, 3, 4, 8, 1)$	5	1	2.00	50	162
$(8, 24, 9, 2, 4, 12, 12, 3)$	5	3	4.00	156	588
$(9, 15, 6, 3, 4, 6, 9, 2)$	5	2	4.00	116	392
	6	3	4.00	31	325
$(9, 18, 5, 2, 3, 9, 9, 1)$	5	–	–	56	200
$(10, 15, 8, 4, 6, 5, 10, 4)$	5	3	8.00	182	722
	7	5	8.00	8	588
$(10, 25, 8, 4, 3, 5, 20, 2)$	5	1	4.00	158	578
	5	4	2.00	168	648
$(12, 13, 4, 3, 4, 4, 9, 1)$	5	2	2.00	68	324
$(12, 19, 5, 4, 3, 3, 16, 1)$	5	–	–	96	400
$(12, 21, 5, 2, 4, 12, 9, 1)$	5	–	–	64	400
$(15, 16, 6, 5, 6, 6, 10, 2)$	5	1	8.00	134	676
	5	4	4.00	152	784
$(15, 20, 5, 3, 4, 5, 15, 1)$	5	–	–	80	400
	9	2	4.00	4	384
$(15, 33, 9, 5, 4, 3, 30, 2)$	5	2	2.00	134	722
	9	2	6.00	0	588
$(16, 36, 7, 4, 3, 4, 32, 1)$	7	–	–	12	588
	9	1	4.00	4	612

Table 2: List of SOSRD using PBD for $6 \leq v \leq 15$

$(v, b, r, k_1, k_2, \ldots, k_p, \lambda)$	c	n_a	a^2	n_0	N
$(6, 7, 3, 3, 3, 2, 1)$	5	2	2.00	48	128
	6	3	2.00	16	108
	11	2	4.00	0	80
$(8, 15, 6, 4, 3, 2, 2)$	5	2	4.00	120	392
	7	4	4.00	16	320
$(9, 15, 6, 4, 3, 2)$	5	2	4.00	116	392
	6	3	4.00	31	325
$(12, 16, 6, 6, 5, 4, 3, 2)$	5	1	8.00	140	676
	5	4	4.00	176	784
$(13, 16, 6, 6, 5, 4, 3, 2)$	5	1	8.00	138	676
	5	4	4.00	168	784
$(13, 15, 7, 7, 6, 5, 3)$	5	1	16	214	1200
$(14, 16, 6, 6, 5, 4, 2)$	5	1	8.00	136	676
	5	4	4.00	160	784
$(14, 15, 7, 7, 6, 3)$	5	1	16	212	1200
$(15, 16, 6, 6, 5, 2)$	5	1	8.00	134	676
	5	4	4.00	152	784

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