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Construction of Second Order Slope Rotatable Designs Using Supplementary Difference Sets

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Abstract

In this paper, construction of second order slope rotatable designs using supplementary difference sets is suggested. Some illustrative examples are presented. It is observed that the method sometimes leads to designs with less number of design points than those available in the literature.

Keywords: Second order response surface designs, slope rotatability, incomplete block designs.

1. Introduction

The concept of rotatability, which is very important in response surface designs, was proposed by Box and Hunter (1957). Das and Narasimham (1962) constructed rotatable designs through balanced incomplete block designs. Seberry (1973) introduced some remarks on supplementary difference sets. Koukouvinos et al. (2013) suggested a general construction method for five level second order rotatable designs. Mutiso et al. (2016a) constructed five level second order rotatable designs using supplementary difference sets. Mutiso et al. (2016b) studied five level modified second order rotatable designs using supplementary difference sets.

A design is said to be rotatable if the variance of the response estimate is a function only of the distance of the point from the design center. The study of rotatable designs is mainly emphasized on the estimation of differences of yields and its precision. Estimation of differences in responses at two points in the factor space will often be of great importance. If differences in responses at two points close together are of interest then estimation of local slope (rate of change) of the response is required. 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 and rate of disintegration of radioactive material in an animal, etc. (Park 1987).

An analogue of Box and Hunter (1957) rotatability property for second order response surface designs, Hader and Park (1978) proposed slope rotatability for second order response surface designs and constructed slope rotatable central composite designs (SRCCD). Victorbabu and Narasimham (1991) suggested conditions for slope rotatability in any general second order response surface designs and constructed second order slope rotatable designs (SOSRD) using balanced incomplete block designs (BIBD). Victorbabu and Narasimham (1993a) constructed three level SOSRD using balanced incomplete block designs. Victorbabu and Narasimham (1993b) studied SOSRD using pairwise balanced designs (PBD) and pointed out that this method lead to designs with less number of design points than the number required in Victorbabu and Narasimham (1991) in some cases. Victorbabu (2002) constructed SOSRD using symmetrical unequal block arrangements (SUBA) with two unequal block sizes and pointed out that this method lead to designs with less number of design points than the number required in Victorbabu and Narasimham (1991, 1993b) in some cases. Victorbabu (2005, 2006) suggested a new restriction $\sum x_{iu}^4 = N\sum x_{iu}^2 x_{ju}^2$ to get modified slope rotatability for second order response surface designs. Further, they have constructed modified SOSRD using central composite designs and BIBD. Victorbabu (2007a, 2007b) suggested reviews on second order rotatable and slope rotatable designs. The author also studied different methods of construction of second order rotatable designs (SORD) and SOSRD. Further, suggested an optimum SORD and SOSRD with minimum number of design points of different methods. Victorbabu and Surekha (2011) constructed a new method of three level SOSRD using BIBD. Victorbabu (2013) suggested a bibliography on slope rotatable designs. Victorbabu (2015) suggested a review on SOSRD over axial directions, modified SOSRD, SOSRD with equi-spaced levels, modified SOSRD with equi-spaced levels and so on. Victorbabu (2019) suggested new method of construction of SOSRD using a pair of partially balanced incomplete block designs and noted that this method lead to designs with less number of design points in some cases.

In this paper, following Koukouvinos et al. (2013), Mutiso et al. (2016a) and Mutiso et al. (2016b) methods of construction of second order rotatable designs using supplementary difference sets, an attempt is made to construct second order slope rotatable designs using supplementary difference sets. Some illustrative examples are also presented.

2. Conditions for Second Order Slope Rotatable Designs

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

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

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 and e_u's are uncorrelated random errors with mean zero and variance σ^2. Then the design D is said to be second order slope rotatable design (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 $(d^2 = \sum_{i=1}^{v} x_i^2)$ of the point $(x_1, x_2, \ldots, x_v)$ from the origin (center) of the design.

Following Box and Hunter (1957), Hader and Park (1978) and Victorbabu and Narasimham (1991) the general conditions for second order slope rotatability can be obtained as follows. To simplify the fit of the second order polynomial from design points D through the method of least squares we impose the following simple symmetry conditions on D to facilitate easy solutions of the normal equations.

A. $\sum x_{iu} = 0, \sum x_{iu} x_{ju} = 0, \sum x_{iu} x_{ju}^2 = 0, \sum x_{iu}\, x_{ju}\, x_{ku} = 0,$
$\sum x_{iu}^3 = 0, \sum x_{iu} x_{ju}^3 = 0, \sum x_{iu} x_{ju} x_{ku}^2 = 0, \sum x_{iu} x_{ju} x_{ku} x_{lu} = 0;$ for $i \neq j \neq k \neq l$, etc

B. (i) $\sum x_{iu}^2 = \text{constant} = N\lambda_2;$

(ii) $\sum x_{iu}^4 = \text{constant} = cN\lambda_4;$ for all i

C. $\sum x_{iu}^2 x_{ju}^2 = \text{constant} = N\lambda_4$; for $i \neq j$, (1)

where c, λ_2 and λ_4 are constants. All the summations are over the design points. The variances and covariances of the estimated parameters are

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

$$V(\hat{b}_i) = \frac{\sigma^2}{N\lambda_2}, \quad V(\hat{b}_{ij}) = \frac{\sigma^2}{N\lambda_4},$$

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

$$Cov(\hat{b}_{ii}, \hat{b}_{jj}) = \frac{(\lambda_2^2 - \lambda_4)\sigma^2}{(c-1)N\lambda_4\left[\lambda_4(c+v-1)-v\lambda_2^2\right]}, \text{ and other covariances vanish.} \quad (2)$$

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

D. $\frac{\lambda_4}{\lambda_2^2} > \frac{v}{(c+v-1)}$ (non-singularity condition). (3)

For the second order model,

$$\frac{\partial \hat{Y}}{\partial x_i} = \hat{b}_i + 2\hat{b}_{ii}x_i + \sum_{i \neq j} \hat{b}_{ij}x_j,$$

$$V\left(\frac{\partial \hat{Y}}{\partial x_i}\right) = V(\hat{b}_i) + 4x_i^2 V(\hat{b}_{ii}) + \sum_{i \neq j} x_j^2 V(\hat{b}_{ij}). \quad (4)$$

The condition for right hand side of (4) to be a function of $d^2 = \sum x_i^2$ alone (for slope rotatability) is clearly (cf. Hader and Park 1978, and Victorbabu and Narasimham 1991),

$$V(\hat{b}_{ii}) = \frac{1}{4}V(\hat{b}_{ij}). \quad (5)$$

Here, (1), (2), and (5) lead to the condition

E. $\lambda_4\left[v(5-c)-(c-3)^2\right] + \lambda_2^2\left[v(c-5)+4\right] = 0.$ (6)

Therefore, A, B, C of (1), D of (3) and E of (6) give a set of conditions for slope rotatability for any general second order response surface design.

3. Second Order Rotatable Designs Using Supplementary Difference Sets

3.1. Supplementary difference sets

Seberry (1973) defined supplementary difference sets and stated that the parameters $[v, k_1, k_2, ..., k_e; \lambda]$ supplementary difference sets (SDS) satisfy

$$\lambda(v-1) = \sum_{i=1}^{e} k_i(k_i - 1). \quad (7)$$

If $k_1 = k_2 = ... = k_e = k$, then $e-[v; k; \lambda]$ to denote the SDS and (7) becomes $\lambda(v-1) = ek(k-1)$.

3.2. Result

1) (cf. Koukouvinos et al. 2013) Let $C_1, C_2, \ldots, C_e$ be 2-subset of Z_v (or any finite abelian group of order v), where $v = n-1 = 2e+1, C_i = \{i, v-i\}, i = 1, 2, \ldots, \frac{(v-1)}{2} = 1, 2, \ldots, e.$ Then the sets $C_1, C_2, \ldots, C_e$ will be an $e-[v;\, 2;\, 1]$ SDS. Based on these SDS, Koukouvinos et al. (2013) constructed second order rotatable designs in m-factors, constitute of a factorial part with level combinations $(-1, 1, 0)$ plus a set of $2m$ axial points at a distance b from the origin, following the steps given below.

- First consider an $e-\{v;\, 2;\, 1\}$, SDS, where $m = \frac{(v-1)}{2}$. Suppose, A is the incidence matrix of the $e-\{v;\, 2;\, 1\}$, SDS and take the mirror image of A, i.e., replace 0 with 1 and 1 with 0.
- Consider the first $\frac{(v-1)}{2}$ columns of A. An array with e rows and e columns, where $e = \frac{(v-1)}{2}$, is obtained, whose every column has one zero element and $e-1$ elements equal to 1.
- Superimpose a 2^{e-r} factorial fraction onto the units of each row of the array, while onto the zero elements superimpose $2^{e-r} \times 1$ vector with all elements zero. In this way, a three level design with e factors and $(e-1) \times 2^{e-r}$ runs is obtained.
- Add an axial point $\pm b$ in every column of the design in order to attain the rotatability of the design; b must be equal to $a^{1/4}$, where $a = (2e-5) \times 2^{e-r-1}$.

Further, Koukouvinos et al. (2013) stated that, it was convenient to choose to use the smallest fraction of 2^e factorial, so the resulting design has the minimum possible number of runs. However, for more than three factors, it is necessary to use fractions of resolution V in order to attain the rotatability of the design.

2) Let a supplementary difference set with parameters $e-\{v;\, 2;\, 1\}$, where $e = \frac{(v-1)}{2}$. Then, Koukouvinos et al. (2013) suggested second order rotatable designs with $m = \frac{(v-1)}{2}$ factors at five levels $(\pm 1, 0, \pm b)$ and $N = m.2^{t(m)} n_a$ design points, where $2^{t(m)}$ denotes resolution-V fractional factorial design replicate of 2^m in ± 1 levels, and n_a is number of axial points.

4. Proposed Method of Construction of SOSRD Using Supplementary Difference Sets

Following Koukouvinos et al. (2013), Mutiso et al. (2016a) methods of construction of second order rotatable designs using supplementary difference sets, here a new method of construction of second order slope rotatable designs using supplementary difference sets is suggested. Let a supplementary difference set with parameters $e-\{v;\, 2;\, 1\}$, where $e = \frac{(v-1)}{2}$. Then, we can construct a second order slope rotatable designs with $m = \frac{(v-1)}{2}$ factors at five levels $(\pm 1, 0, \pm \text{b})$ and $N = m2^{t(m)} + n_a + n_0$ design points, where $2^{t(m)}$ denotes a resolution-V fractional factorial design replicate of 2^m in ± 1 levels, n_a denotes axial points, n_0 denotes the number of central points and U denotes the combination of the design points generated from different sets of points.

Theorem 1 *The design points,* $\left[1-(v,k,\lambda)\right]2^{t(m)}U\left(b,0,0,\ldots,0\right)2^1U(n_0)$ *will give a* v*- dimensional second order slope rotatable designs using supplementary difference sets in* $N = m2^{t(m)} + n_a + n_0$ *design points, where* b^2 *is a positive real root of the biquardratic equation,*

$$(8m-4N)b^8 + 8m(e-1)2^{t(m)}b^6 + [2m(e-1)^2 2^{2t(m)} +$$
$$\{(12-2m)(e-2)-4(e-1))N + (16(e-2)-20m(e-2)+4m(e-1)\}2^{t(m)}]b^4$$
$$+[4m(e-1)^2 + (16-20m)(e-1)(e-2)]2^{2t(m)}b^2 + [(5m-9)(e-2)^2 +$$
$$(6-m)(e-1)(e-2)-(e-1)^2]N2^{2t(m)} + (m(e-1)+4(e-2)-5m(e-2))(e-1)^2 2^{3t(m)} = 0, \quad (8)$$

If at least one positive real root for b^2 *exists in (8) then the design exists, and* c *can be obtained from*

$$c = \frac{(e-1)2^{t(m)} + 2b^4}{(e-2)2^{t(m)}}. \quad (9)$$

(Evaluation of (8) is explained below)

Proof: For the design points generated from the SDS, simple symmetry conditions A, B and C of (1) are true. Condition A of (1) is true obviously. Conditions B and C of (1) are true as follows:

B. (i) $\sum x_{iu}^2 = 2^{t(m)}(e-1) + 2b^2 = N\lambda_2$;

(ii) $\sum x_{iu}^4 = 2^{t(m)}(e-1) + 2b^4 = cN\lambda_4$.

C. $\sum x_{iu}^2 x_{ju}^2 = 2^{t(m)}(e-2) = N\lambda_4$. (10)

These expressions follow easily from the definition of points sets generated from SDS and their consequent multiplication with factorial combinations as explained in Koukouvinos et al. (2013).

From B (ii) and C of (10) we get c given in (9). Substituting for λ_2, λ_4 and c in (6) we get

$$\frac{(e-2)2^{t(m)}}{N}\left[m\left(5-\frac{(e-1)2^{t(m)}+2b^4}{(e-2)2^{t(m)}}\right)-\left(\frac{(e-1)2^{t(m)}+2b^4}{(e-2)2^{t(m)}}-3\right)\right]$$
$$+\frac{((e-1)2^{t(m)}+2b^2)^2}{N^2}\left[m\left(\frac{(e-1)2^{t(m)}+2b^4}{(e-2)2^{t(m)}}-5\right)+4\right] = 0, \quad (11)$$

Simplification of (11) leads to the fourth degree equation in b^2 as given in (8).

Example 1 We illustrate Theorem 1 for 4 factors with the help of a SDS. The design points,

$$\left[4-(9,\,2,\,1)\right]2^{t(m)}U\left(b,\,0,\,0,\,\ldots,0\right)2^1U\left(n_0=1\right),$$

will give a SOSRD using SDS in $N = 41$ design points for 4 factors (taking one central point). From B and C of (10), we have

B. (i) $\sum x_{iu}^2 = 24 + 2b^2 = N\lambda_2$;

(ii) $\sum x_{iu}^4 = 24 + 2b^4 = cN\lambda_4$.

C. $\sum x_{iu}^2 x_{ju}^2 = 16 = N\lambda_4$. (12)

From B (ii) and C of (12) we get c as, $c=\dfrac{24+2b^4}{16}$. Substituting for λ_2, λ_4 and c in (8) and on simplification, we get the biquardratic equation in b^2 (viz.)

$$132b^8-768b^6-2656b^4+15360b^2-31168=0, \quad (13)$$

This can be alternatively written directly from (8). Equation (13) has only one positive real root $b^2=7.006106688.$ It can be verified that the non-singularity condition D of (3) is satisfied.

5. Conclusions

In this paper, construction of second order slope rotatable designs using supplementary difference sets is studied for $3 \le m \le 16$ factors and the results are as shown in Table 1. We may point out here that this SOSRD using Supplementary difference sets has 217 design points for 12-factors, whereas the corresponding SRCCD of Hader and Park (1978), SOSRD using BIBD of Victorbabu and Narasimham (1991), SOSRD using PBD of Victorbabu and Narasimham (1993b), SOSRD using SUBA with two unequal block sizes of Victorbabu (2002), SOSRD using a pair of partially balanced incomplete block designs of Victorbabu (2019) need 281, 377, 537, 233 and 281 design points respectively. Thus the new method of construction of SOSRD using supplementary difference sets leads to a 12-factor SOSRD in less number of design points and same is the case in some other cases also (see Table 2).

Table 1 Values of 'b' in SOSRD using SDS

3-(7, 2, 1)				4-(9, 2, 1)			
n_0	N	b	c	n_0	N	b	c
0	18	2.078872911	11.33859981	0	40	2.681667039	7.964417973
1	19	2.000000000	10.00000000	1	41	2.646905115	7.635691362
5	23	1.789428463	7.126575627	5	45	2.536334806	6.672926874
10	28	1.668427760	5.874356975	10	50	2.447353401	5.984321684
15	33	1.611673217	5.373478600	15	55	2.391881388	5.591368253
20	38	1.580132480	5.117051696	20	60	2.352460249	5.352460249

5-(11, 2, 1)				6-(13, 2, 1)			
n_0	N	b	c	n_0	N	b	c
0	50	2.962456889	7.751735267	0	60	3.570714561	11.410160200
1	51	2.945488248	7.605938208	1	61	3.540819062	11.074149340
5	55	2.926959646	7.449589876	5	65	3.434481064	9.946099410
10	60	2.813238331	6.553025109	10	70	3.337310344	9.002939510
15	65	2.735591806	6.000184285	15	75	3.243243232	8.165095031
20	70	2.658806499	5.797860319	20	80	3.176760384	7.615284949

7-(15, 2, 1)				8-(17, 2, 1)			
n_0	N	b	c	n_0	N	b	c
0	126	3.795683527	6.389194976	0	144	3.975498166	6.370519336
1	127	3.780798112	6.308271344	1	145	3.959993676	6.289812666
5	131	3.728496870	6.031423863	5	149	3.90558219	6.013988878
10	136	3.677267450	5.771312159	10	154	3.852556635	5.756055874
15	141	3.638296022	5.580585232	15	159	3.812545054	5.568349044
20	146	3.608352889	5.438147083	20	164	3.782063315	5.429260406

Table 1 (Continued)

9-(19, 2, 1)

n_0	N	b	c
0	162	4.135958917	6.368224619
1	163	4.119669273	6.286388385
5	167	4.062582578	6.007161931
10	172	4.007273823	5.747628287
15	177	3.965922206	5.560481022
20	182	3.934718602	5.423083009

10-(21, 2, 1)

n_0	N	b	c
0	180	4.605545712	8.154823398
1	181	4.590582541	8.063909584
5	185	4.534460469	7.730755674
10	190	4.472313195	7.375990861
15	195	4.418298918	7.079432879
20	200	4.37144044	6.830822909

11-(23, 2, 1)

n_0	N	b	c
0	198	4.416478878	6.395224576
1	199	4.382752379	6.235655274
5	203	4.334370816	6.013093626
10	208	4.273310725	5.742650851
15	213	4.228604594	5.551855880
20	218	4.195587061	5.414776061

12-(25, 2, 1)

n_0	N	b	c
0	216	4.542032194	6.419990365
1	217	4.522597207	6.329517899
5	221	4.454742617	6.022667245
10	226	4.390279348	5.743854798
15	231	4.343620548	5.549564727
20	236	4.309564001	5.411648536

13-(27, 2, 1)

n_0	N	b	c
0	234	5.229178594	10.00190820
1	235	5.215611573	9.499791690
5	239	5.164010617	9.171922619
10	244	5.105288923	8.810577183
15	249	5.052571846	8.496629619
20	254	5.005348432	8.223619431

14-(29, 2, 1)

n_0	N	b	c
0	252	4.772257959	6.486201998
1	253	4.750155589	6.386803214
5	257	4.673063733	6.050807114
10	262	4.600802316	5.750604778
15	267	4.549777323	5.546975114
20	272	4.513465493	5.406174443

15-(31, 2, 1)

n_0	N	b	c
0	270	4.879169421	6.526342744
1	271	4.855575336	6.421698327
5	275	4.773262779	6.068388148
10	280	4.696611594	5.755408107
15	285	4.643197930	5.546181314
20	290	4.605696730	5.403535685

16-(33, 2, 1)

n_0	N	b	c
0	288	4.981713166	6.570594840
1	289	4.956525939	6.460221686
5	293	4.868587710	6.087849500
10	298	4.787217275	5.760798925
15	303	4.731292223	5.545480986
20	308	4.692576832	5.400826906

Table 2 Comparison of different methods of construction of SOSRD

No. of factors	SOSRD using					
	SRCCD (1978)	BIBD (1991)	PBD (1993b)	SUBA with two unequal block sizes (2002)	A pair of PBIBD (2019)	SDS
(m)	N	N	N	N	N	N
2	9	−	−	−	−	−
3	15	19 (3, 3, 2, 2, 1)	−	−	−	19
4	25	33 (4, 6, 3, 2, 1)	−	−	−	41
5	27	51 (5, 10, 4, 2, 1)	−	−	−	51
6	45	73 (6,15, 5, 2, 1)	69 (6, 7, 3, 3, 2, 1)	69 (6, 7, 3, 2, 3, 3, 4,1)	45	61
7	79	71 (7, 7, 3, 3, 1)	−	−	−	127
8	81	129 (8, 28, 7, 2,1)	257 (8, 15, 6, 4, 3, 2, 2)	113 (8, 12, 4, 2, 3, 4, 8, 1)	81	145
9	147	115 (9, 12, 4, 3, 1)	195 (9, 11, 5, 5, 4, 3, 2)	163 (9, 18, 5, 2, 3, 9, 9, 1)	−	163
10	149	201 (10, 45, 9, 2, 1)	197 (10, 11, 5, 5, 4, 2)	197 (10, 11, 5, 4, 5, 5, 6, 2)	149	181
11	151	199 (11, 11, 5, 5, 2)	−	−	−	191
12	281	377 (12, 44, 11, 3, 2)	537 (12, 16, 6, 6, 5, 4, 3, 2	233 (12, 13, 4, 3, 4, 4, 9, 1)	281	217
13	283	235 (13, 13, 4, 4, 1)	538 (13, 16, 6, 6, 5, 4, 3, 2)	−	−	235
14	285	−	541 (14,16, 6, 6,5, 4, 2)	309 (14, 35, 7, 2, 3, 7, 28, 1)	−	253
15	287	311 (15, 35, 7, 3, 1)	543 (15, 16, 6, 6, 5, 2)	351 (15, 20, 5, 3, 4, 5,15, 1)	−	271
16	289	353 (16, 20, 5, 4, 1)	−	481 (16, 28, 6, 4, 3, 12, 16, 1)	−	289

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