__Original Research Article__

Slope Rotatable Central Composite Designs of Second Type

ABSTRACT

In this paper, second order slope rotatable designs (SOSRD) of second type using central composite designs (CCD) with $2 \leq n_a \leq 4$ are suggested for $2 \leq v \leq 17$. It is observe that the value of level a_2 for the axial points in CCD required for slope rotatability of second type is appreciably larger than the value required for second order rotatable designs (SORD) of second type using CCD. And also noted that if we replicating axial points (n_a) in SOSRD of second type using CCD then the value of a_2 is approximately nearer to SORD of second type.

Keywords: Response surface designs, Second order slope rotatable designs, Slope rotatable central composite designs, Second order slope rotatable designs of second type.

1. INTRODUCTION

The property of rotatability was proposed by Box and Hunter (1957) for response surface designs and constructed second order rotatable central composite designs (CCD). Das and Narasimham (1962) constructed second order rotatable designs using balanced incomplete block designs (BIBD). Draper and Guttman (1988) suggested an index of rotatability. Khuri (1988) introduced a measure of rotatability for response surface designs. Draper and Pukelshein (1990) developed another look at rotatability. Park et al. (1993) suggested measure of rotatability for second order response surface designs. Victorbabu and Vasundaradevi (2005) suggested modified second order response designs, rotatable designs using BIBD. Kim (2002) introduced extended central composite designs with the axial points indicated by two numbers. Chiranjeevi et al. (2021) developed second order rotatable designs of second type using CCD. Chiranjeevi and Victorbabu (2021) studied second order rotatable designs of second type using BIBD.

Hader and Park (1978) introduced slope rotatable central composite designs. Victorbabu and Narasimham (1991a) constructed second order slope rotatable designs (SOSRD) using BIBD. Victorbabu and Narasimham (1991b) studied SOSRD through a pair of incomplete block designs. Victorbabu (2005, 2006) studied modified slope rotatable CCD and modified SOSRD using BIBD. Victorbabu (2007) suggested a review on SOSRD. Park and Kim (1992) developed a measure of slope rotatability for second order response surface experimental designs. Victorbabu and Surekha (2011, 2012) studied measure of SOSRD using CCD and BIBD. Jyostna and Victorbabu (2021) studied measure of modified rotatability for second degree polynomial using BIBD. Jyostna et al. (2021) suggested measure of modified rotatability for second order response surface designs using CCD. Kim and Ko (2004) introduced slope rotatability of CCD of the second type for $2 \le v \le 5$ (v-stands for number of factors). Ravikumar and Victorbabu (2022) developed SOSRD of second type using CCD for $6 \le v \le 17$.

In this paper an attempt is made to construct SRCCD of second type with $2 \le n_a \le 4$ for $2 \le v \le 17$. It is observed that the value of level a_2 required for SOSRD of second type using CCD is appreciably larger than the value required for SORD of second type using CCD. It also can be noted that if we replicate axial points (n_a) in SOSRD of second type using CCD then the value of a_2 is approximately nearer to SORD of second type.

2. CONDITIONS FOR SECOND ORDER SLOPE ROTATABLE DESIGNS

A general second order response surface design $D=((X_{iu}))$ for fitting

$$Y_u = \beta_0 + \sum_{i=1}^{v} \beta_i X_{iu} + \sum_{i=1}^{v} \beta_{ii} X_{iu}^2 + \sum_{i=1}^{v} \sum_{j=1}^{v} \beta_{ij} X_{iu} X_{ju} + e_u \quad (2.1)$$

where X_{iu} denotes the level of the i[th] factor (i=1,2,…,v) in the u[th] run (u=1,2,…,N) of the experiment and e_u 's are uncorrelated random errors with mean zero and variance σ^2. Then D is said to be SOSRD if the variance of the estimate of the first order partial derivative of $Y(X_1, X_2, ..., X_v)$ with respect to each of independent variable X_i is only a function of the distance $\left(d^2 = \sum_{i=1}^{v} X_i^2\right)$ of the point $(X_1, X_2, ..., X_v)$ from the origin (centre) of the design.

The general conditions for second order slope rotatable designs are as follows [cf. Box and Hunter (1957), Hader and Park (1978) and Victorbabu and Narasimham (1991a)].

All odd order moments are zero. In other words when at least one odd power X's equal to zero.

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

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 all $i \ne j$ (2.2) where c, λ_2 and λ_4 are constants.

The variances and covariances of the estimated parameters are

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

$$V\left(\hat{\beta}_i\right)=\frac{\sigma^2}{N\lambda_2}$$

$$V\left(\hat{\beta}_{ij}\right)=\frac{\sigma^2}{N\lambda_4}$$

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

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

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

and other covariances vanish. (2.3)

An inspection of the variance of $\hat{\beta}_0$ shows that a necessary condition for the existence of a non singular second order design is

D. $\dfrac{\lambda_4}{\lambda_2^2}>\dfrac{v}{c+v-1}$ (Non Singularity condition) (2.4)

For the second order model

$$\frac{\partial\hat{Y}}{\partial X_i}=\hat{\beta}_i+2\hat{\beta}_{ii}X_{iu}+\sum_{j\neq i}\hat{\beta}_{ij}X_{ju} \tag{2.5}$$

$$V\left(\frac{\partial\hat{Y}}{\partial X_i}\right)=V\left(\hat{\beta}_i\right)+4X_{iu}^2V\left(\hat{\beta}_{ii}\right)+\sum_{j\neq i}X_{ju}^2V\left(\hat{\beta}_{ij}\right) \tag{2.6}$$

The condition for R.H.S of the equation (2.6) to be a function of $d^2=\sum_{i=1}^{v}X_i^2$ alone (for slope rotatability) is

$4V\left(\hat{\beta}_{ii}\right)=V\left(\hat{\beta}_{ij}\right)$ [cf. Hader and Park (1978)] (2.7)

On simplification of (2.7), using (2.3) we get [cf. Victorbabu and Narasimham (1991a)]

E. $\lambda_4\left[v(5\text{-}c)\text{-}(c\text{-}3)^2\right]+\lambda_2^2\left[v(c\text{-}5)+4\right]=0$ [cf. Hader and Park (1978)] (2.8)

Therefore A, B, C of (2.2), (2.4) and (2.8) give a set of conditions for slope rotatability in any general second order response design. [cf. Hader and Park (1978), Victorbabu and Narasimham (1991a)].

3. CONSTRUCTION OF SECOND ORDER ROTATABLE DESIGNS OF SECOND TYPE USING CENTRAL COMPOSITE DESIGNS

Kim (2002) developed second type of rotatable central composite designs (CCD) in which the position of axial points are indicated by two numbers for 2≤v≤8. Chiranjeevi et al. (2021) developed second order rotatable designs (SORD) of second type using CCD for 9≤v≤17. Chiranjeevi and Victorbabu (2021) developed SORD of second type using BIBD.

The design plan of SORD of second type using CCD in which the position of the axial points are indicated by two numbers a_1 and a_2 ($a_2 \geq a_1 \geq 0$). The CCD are constructed by adding suitable fractional combinations to those obtained from $\frac{1}{2^p}\times 2^v$ fractional factorial design, (here $2^{t(v)}=\frac{1}{2^p}\times 2^v$ denotes a suitable fractional replicate of 2^v), in which no interaction with less than five factors are confounded. In coded form CCD has the points of 2^v ($2^{t(v)}$) factorial with coordinates $\left(\pm 1,\pm 1,\ldots,\pm 1\right)$ and 4v axial points with coordinates $(\pm a_1,0,\ldots,0),(0,\pm a_1,\ldots,0),\ldots\ldots.,(0,0,\ldots,\pm a_1)$; $(\pm a_2,0,\ldots,0),(0,\pm a_2,\ldots,0),\ldots\ldots.,(0,0,\ldots,\pm a_2)$ and if necessary n_0 central points may be replicated. Thus the total number of experimental points $N=2^{t(v)}+4v+n_0$.

For the design points generated from CCD, simple symmetry conditions A, B and C of equation (2.2) are true. Condition (A) of equation (2.2) is true obviously, condition (B) and (C) are true as follows.

B. (i) $\sum X_{iu}^2=2^{t(v)}+2a_1^2+2a_2^2=N\lambda_2$

(ii) $\sum X_{iu}^4=2^{t(v)}+2a_1^4+2a_2^4=3N\lambda_4$

C. $\sum X_{iu}^2X_{ju}^2=2^{t(v)}=N\lambda_4$ (3.1)

From B(ii) and C of equation (3.1), we get

$$\begin{aligned}&2^{t(v)}+2a_1^4+2a_2^4=3\left(2^{t(v)}\right)\\ &\Rightarrow a_1^4+a_2^4=2^{t(v)}\end{aligned} \qquad (3.2)$$

Example (3.1):

We illustrate the construction of SORD of second type using CCD for v=6. The design points $\left(\pm1,\pm1,...,\pm1\right)2^{t(6)}\mathrm{U}\left(\pm a_1,0,...,0\right)2^1\mathrm{U}\left(\pm a_2,0,...,0\right)2^1\mathrm{U}(n_0=1)$ will give a SORD of second type in N=57 design points with $a_1=1$.

For the design points generated from SOSRD of second type using CCD, simple symmetry conditions A of equation (2.2) are true.

Here B and C of equation (3.1) are

B. (i) $\sum X_{iu}^2=32+2a_1^2+2a_2^2=N\lambda_2$

(ii) $\sum X_{iu}^4=32+2a_1^4+2a_2^4=3N\lambda_4$

C. $\sum X_{iu}^2X_{ju}^2=32=N\lambda_4$ (3.3)

From B (ii) and C of equation (3.3), we get

$32+2a_1^4+2a_2^4=3\left(32\right)$

$\Rightarrow a_1^4+a_2^4=32$

$\Rightarrow a_2^4=31$ (taking $a_1=1$)

$\Rightarrow a_2=2.3596$

4. A NEW METHOD ON CONSTRUCTION OF SLOPE ROTATABLE CENTRAL COMPOSITE DESIGNS OF SECOND TYPE

Kim and ko (2004) developed slope rotatability of second type using CCD for 2≤v≤5 by taking n_a=1. Ravikumar and Victorbabu (2022) developed SOSRD of second type using CCD for 6≤v≤17 with n_a=1.

The design plan of SOSRD of second type using CCD in which the position of the axial points are indicated by two numbers a_1 and a_2 ($a_2\geq a_1\geq0$). The CCD are constructed by adding suitable fractional combinations to those obtained from $\frac{1}{2^p}\times2^v$ fractional factorial design, (here $2^{t(v)}=\frac{1}{2^p}\times2^v$ denotes a suitable fractional replicate of 2^v), in which no interaction with less than five factors are confounded. In coded form CCD has the points of 2^v ($2^{t(v)}$) factorial with coordinates $(\pm1,\pm1,...,\pm1)$ and 4v axial points are replicated n_a times with coordinates $(\pm a_1,0,...,0),(0,\pm a_1,...,0),.......,(0,0,...,\pm a_1)$; $(\pm a_2,0,...,0),(0,\pm a_2,...,0),.......,(0,0,...,\pm a_2)$ and if necessary n_0 central points may be replicated. Thus the total number of experimental points $N=2^{t(v)}+4n_a v+n_0$.

For CCD simple symmetry conditions A, B and C of equation (2.2) are true for any n_a. Condition (A) of equation (2.2) is true obviously, condition (B) and (C) are true as follows.

B. (i) $\sum X_{iu}^2=2^{t(v)}+2n_a a_1^2+2n_a a_2^2=N\lambda_2$

(ii) $\sum X_{iu}^4=2^{t(v)}+2n_a a_1^4+2n_a a_2^4=cN\lambda_4$

C. $\sum X_{iu}^2 X_{ju}^2=2^{t(v)}=N\lambda_4$ (4.1)

From B(ii) and C of equation (4.1), we have $c=\dfrac{2^{t(v)}+2n_a a_1^4+2n_a a_2^4}{2^{t(v)}}$

Substituting for the values of λ_2, λ_4 and c in equation (2.8), we get the following biquadratic equation

$$\left[2N(n_a)^2-4v(n_a)^3\right]\left(a_1^8+a_2^8\right)-8v(n_a)^3\left(a_1^6a_2^2+a_1^2a_2^6\right)+4\left[N(n_a)^2-2v(n_a)^3\right]a_1^4a_2^4$$
$$-2^{t(v)+2}v(n_a)^2\left[a_1^6+a_1^4a_2^2+a_1^2a_2^4+a_2^6\right]-2^{t(v)}\left[v(n_a)2^{t(v)}+8(1-v)(n_a)^2+N(4-v)(n_a)\right]\left(a_1^4+a_2^4\right)$$
$$+2^{t(v)+4}(v-1)(n_a)^2a_1^2a_2^2+2^{2t(v)+3}(v-1)(n_a)\left(a_1^2+a_2^2\right)-2^{2t(v)+1}(1-v)\left(2^{t(v)}-N\right)=0$$

(4.2)

The design exists, if at least one positive real root exists for the above equation (4.2). Given the values of v, n_a and n_0 there are countless combinations of a_1 and a_2 that satisfy the equation (4.2).

Example (4.1):

We illustrate the construction of SOSRD of second type using CCD for v=6. The design points $\left(\pm1,\pm1,...,\pm1\right)2^{t(6)}Un_a\left(\pm a_1,0,...,0\right)2^1Un_a\left(\pm a_2,0,...,0\right)2^1U(n_0=26)$ will give a SOSRD of second type in N=106 design points with $n_a=2,\ a_1=1.$

For the design points generated from SOSRD of second type using CCD, simple symmetry condition A of equation (2.2) are true for any n_a.

Here B and C of equation (4.1) are

B. (i) $\sum X_{iu}^2=32+4a_1^2+4a_2^2=N\lambda_2$

(ii) $\sum X_{iu}^4=32+4a_1^4+4a_2^4=cN\lambda_4$

C. $\sum X_{iu}^2X_{ju}^2=32=N\lambda_4$ (4.3)

From B (ii) and C of equation (4.1), we have $c=\dfrac{32+4a_1^4+4a_2^4}{32}$

Substituting for the values of λ_2, λ_4 and c in equation (2.8) and on simplification we get the biquadratic equation in a_2^2

$$656(a_1^8+a_2^8)+1312a_1^4a_2^4-384(a_1^6a_2^2+a_1^2a_2^6)-3072(a_1^6+a_1^4a_2^2+a_1^2a_2^4+a_2^6)+6400(a_1^4+a_2^4)+10240a_1^2a_2^2+81920(a_1^2+a_2^2)-757760=0$$

Let us fix $a_1=1$, solving the above equation we get

$$656a_2^8-3456a_2^6+4640a_2^4+88704a_2^2-671856=0 \qquad (4.4)$$

Equation (4.4) has only one positive real root $a_2^2=5.5686 \Rightarrow a_2=2.3598$.

From the examples of (3.1) and (4.1) it can be noted that the value of $a_2=2.3598$ in SOSRD of second type using CCD which is approximately nearer to the value of $a_2=2.3596$ in SORD of second type using CCD.

5. CONCLUSION

In this paper, second order slope rotatable designs (SOSRD) of second type using central composite designs (CCD) with $2 \leq n_a \leq 4$ are suggested for $2 \leq v \leq 17$. It is observe that the value of level a_2 for the axial points in CCD required for slope rotatability of second type is appreciably larger than the value required for second order rotatable designs (SORD) of second type using CCD. And also noted that if we replicating axial points (n_a) in SOSRD of second type using CCD then the value of a_2 is approximately nearer to SORD of second type.

The table gives the appropriate SRCCD values of the parameters a_2 with $a_1 = 1$ for designs using second type of CCD with $2 \leq n_a \leq 4$ for $2 \leq v \leq 17$ given in the Appendix.

APPENDIX

Values of a_2 for SOSRD of second type using CCD for $2 \leq v \leq 17$ with $2 \leq n_a \leq 4$

v=2, p=0, a_1=1, a_2^*=1.3161

N	n_0	n_a	a_2
21	1	2	1.7347
25	5	2	1.5803
30	10	2	1.4738
35	15	2	1.4134
40	20	2	1.3755
45	25	2	1.3499
50	30	2	1.3315
55	35	2	1.3178
56	36	2	1.3154
29	1	3	1.6205
33	5	3	1.4818
38	10	3	1.3700
41	13	3	1.3238
42	14	3	1.3108
37	1	4	1.5473
41	5	4	1.4213
45	9	4	1.3276
46	10	4	1.3081

v=3, p=0, a_1=1, a_2^*=1.6266

N	n_0	n_a	a_2
33	1	3	1.9110
37	5	3	1.8060
42	10	2	1.7321
47	15	2	1.6894
52	20	2	1.6624
57	25	2	1.6439
62	30	2	1.6304
63	31	2	1.6282
64	32	2	1.6260
45	1	3	1.7469
49	5	3	1.6554
50	6	3	1.6380
51	7	3	1.6222
57	1	4	1.6397
58	2	4	1.6165

v=4, p=0, a_1=1, a_2^*=1.9680

N	n_0	n_a	a_2
49	1	2	2.1666
53	5	2	2.0991
58	10	2	2.0482
63	15	2	2.0167
68	20	2	1.9956
73	25	2	1.9806
78	30	2	1.9694
79	31	2	1.9675
65	1	3	1.9500
81	1	4	1.8046

v=5, p=1, a_1=1, a_2^*=1.9680

N	n_0	n_a	a_2
57	1	2	2.0781
61	5	2	2.0368
66	10	2	2.0061
71	15	2	1.9868
76	20	2	1.9736
78	22	2	1.9694
79	23	2	1.9675
86	30	2	1.9567
77	1	3	1.8507
97	1	4	1.7009

v=6, p=1, a_1=1, a_2^*=2.3596

N	n_0	n_a	a_2
81	1	2	2.4579
85	5	2	2.4269
90	10	2	2.4012
95	15	2	2.3837
100	20	2	2.3710
105	25	2	2.3614
106	26	2	2.3598
107	27	2	2.3582
105	1	3	2.1923
129	1	4	2.0191

v=7, p=1, a_1=1, a_2^*=2.8173

N	n_0	n_a	a_2
121	1	2	2.9250
125	5	2	2.8989
130	10	2	2.8750
135	15	2	2.8574
140	20	2	2.8439
145	25	2	2.8334
150	30	2	2.8249
155	35	2	2.8179
156	36	2	2.8166
149	1	3	2.6158
177	1	4	2.4127

v=8, p=2, a_1=1, a_2^*=2.8173

N	n_0	n_a	a_2
129	1	2	2.8858
133	5	2	2.8674
138	10	2	2.8505
143	15	2	2.8380
148	20	2	2.8283
153	25	2	2.8205
155	27	2	2.8179
156	28	2	2.8166
161	1	3	2.5789
193	1	4	2.3811

v=9, p=2, a_1=1, a_2^*=3.3570

N	n_0	n_a	a_2
201	1	2	3.4518
205	5	2	3.4342
210	10	2	3.4166
215	15	2	3.4026
220	20	2	3.3913
230	30	2	3.3742
235	35	2	3.3676
240	40	2	3.3619
245	45	2	3.3570
237	1	3	3.0929
273	1	4	2.8574

v=10, p=3, a_1=1, a_2^*=3.3570

N	n_0	n_a	a_2
209	1	2	3.4253
213	5	2	3.4114
218	10	2	3.3976
223	15	2	3.3866
228	20	2	3.3777
233	25	2	3.3703
238	30	2	3.3641
243	35	2	3.3589
245	37	2	2.3570
249	1	3	3.0673
289	1	4	2.8358

v=11, p=4, a_1=1, a_2^*=3.3570

N	n_0	n_a	a_2
217	1	2	3.4026
221	5	2	3.3922
226	10	2	3.3818
231	15	2	3.3735
236	20	2	3.3666
241	25	2	3.3609
245	29	2	3.3570
261	1	3	3.0487
305	1	4	2.8213

v=12, p=4, a_1=1, a_2^*=3.9961

N	n_0	n_a	a_2
353	1	2	4.0763
357	5	2	4.0650
362	10	2	4.0530
367	15	2	4.0430

v=13, p=5, a_1=1, a_2^*=3.9961

N	n_0	n_a	a_2
361	1	2	4.0592
365	5	2	4.0497
370	10	2	4.0396
375	15	2	4.0311

372	20	2	4.0344
377	25	2	4.0270
382	30	2	4.0149
387	35	2	4.0205
392	40	2	4.0099
397	45	2	4.0055
402	50	2	4.0015
407	55	2	3.9979
412	60	2	3.9947
401	1	3	3.6589
449	1	4	3.3857

380	20	2	4.0238
385	25	2	4.0175
390	30	2	4.0121
395	35	2	4.0073
400	40	2	4.0031
405	45	2	3.9993
409	49	2	3.9966
410	50	2	3.9959
413	1	3	3.6422
465	1	4	3.3718

v=14, p=6, a_1=1, a_2^*=3.9961

N	n_0	n_a	a_2
369	1	2	4.0437
373	5	2	4.0359
378	10	2	4.0276
383	15	2	4.0205
388	20	2	4.0145
393	25	2	4.0093
398	30	2	4.0048
403	35	2	4.0008
408	40	2	3.9972
409	41	2	3.9966
410	42	2	3.9959
425	1	3	3.6289
481	1	4	3.3615

v=15, p=7, a_1=1, a_2^*=3.9961

N	n_0	n_a	a_2
377	1	2	4.0303
381	5	2	4.0240
386	10	2	4.0173
391	15	2	4.0116
396	20	2	4.0066
401	25	2	4.0024
406	30	2	3.9986
409	33	2	3.9966
410	34	2	3.9959
437	1	3	3.6186
497	1	4	3.3540

v=16, p=8, a_1=1, a_2^*=3.9961

N	n_0	n_a	a_2
385	1	2	4.0191
389	5	2	4.0141
394	10	2	4.0087
399	15	2	4.0041
404	20	2	4.0001
409	25	2	3.9966
410	26	2	3.9959
449	1	3	3.6107
513	1	4	3.3485

v=17, p=9, a_1=1, a_2^*=3.9961

N	n_0	n_a	a_2
393	1	2	4.0099
397	5	2	4.0059
402	10	2	4.0016
407	15	2	3.9979
409	17	2	3.9966
410	18	2	3.9959
461	1	3	3.6048
529	1	4	3.3445

a_2^* indicates the value of a_2 in SORD of second type

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