Second Order Slope Rotatable Designs of Second Type using Pairwise Balanced designs

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Summary

Kim (2002) and Kim and Ko (2004) proposed second order rotatable designs (SORD) of second type and second order slope rotatable designs (SOSRD) of second type using central composite designs (CCD), in which the positions of axial points are indicated by two numbers (a_1, a_2). In this paper, anew method of construction on SOSRD of second type using pairwise balanced designs (PBD) is suggested. It is shown that the new method sometimes leads to designs with less number of design points compared to designs with the help of SOSRD of second type using balanced incomplete block designs (BIBD).Variance of the estimated response is also obtained for $6 \le v \le 15$.

Keywords: Second order rotatable designs, Second order slope rotatable designs of second type, Incomplete block designs, Pairwise balanced designs.

1. Introduction

Response surface design is a collection of mathematical and statistical techniques useful for analyzing problems where several independent variables influence a dependent variable.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 (SORD) using balanced incomplete block designs (BIBD). Tyagi (1964) constructed SORD using pairwise balanced designs (PBD). Draper and Guttman (1988) suggested an index of rotatability. Khuri (1988) introduced 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. Kim (2002) introduced SORD usingCCD with the axial points indicated by two numbers. Victorbabu (2004) studied second order rotatable designs using pair of partially balanced incomplete block designs. Victorbabuand Vasundharadevi(2005) studiedmodified second order response surface designs using BIBD.Victorbabu (2009)studied modified second order response surface designs, rotatable designs, rotatable designs with equi-spaced doses. Victorbabu andSurekha (2013) developedmeasure of rotatability for second order response surface designs using incomplete block designs.Victorbabu and Surekha (2015)suggested measure of rotatability for second order response surface designs using BIBD.Rajyalakshmi andVictorbabu (2018)developedSORD under tridiagonal correlated structure of errors using 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.Chiranjeevi et al. (2021) developed SORD of second type using CCD. Chiranjeevi and Victorbabu (2021a, 2021b) studied SORD of second type using BIBD and PBD respectively.

Hader and Park (1978) introduced slope rotatable central composite designs(SRCCD). Victorbabu and Narasimham (1991a, 1991b, 1993) studied second order slope rotatable designs (SOSRD) using BIBD, pair of incomplete block designs and PBD respectively. Park and Kim (1992) developed measure of slope rotatability for second order response surface experimental designs.Kim and Ko (2004) introduced slope rotatability for CCD of second type for $2\leq v\leq 5$ (v-stands for number of factors) by taking $n_a = 1$(where n_a denotes the number of replications of axial points), in which the positions of axial points are indicated by two numbers(a_1, a_2). Victorbabu (2005a, 2005b, 2006) introduced modified SOSRD using CCD, PBD and BIBD respectively. Victorbabu (2007) suggested a review on SOSRD. Victorbabu and Surekha (2011, 2012a, 2012b) studied measure of SOSRD using CCD, BIBD and PBD respectively. Rajyalakshmi and Victorbabu (2019) constructed SOSRD under tri-diagonal correlated structure of errors using BIBD. Rajyalakshmi et al. (2020) studied SOSRD under intra-class correlated errors using PBD. Sulochana and Victorbabu (2020a) studied SOSRD under intra-class correlated structure of errors using partially balanced incomplete block type designs. Sulochanaand Victorbabu (2020b) studied SOSRD under tri-diagonal correlation structure of errors using a pair of incomplete block designs. Victorbabu and Jyostna (2021) studied measure of modified slope rotatability for second order response surface designs.Ravikumar and Victorbabu (2022a) extended the work of Kim and Ko (2004) and developed SOSRD of second type using CCD for 6≤v≤17 by taking n_a=1. Ravikumar and Victorbabu (2022b) studied SRCCD of second type for2≤v≤17 with $2 \le n_a \le 4$. Victorbabu and Ravikumar (2022) developed SOSRD of second type using BIBD.

In this paper,an attempt is made to develop SOSRD of second type using PBD. It is found that in some cases this new method leads to SOSRD of second type with lesser number of design points compared to designs constructed with the help of SOSRD of second type using BIBD. Specifically for 6, 10 and 15 factors these new designs needs 81, 217 and 573 points whereas corresponding SOSRD of second type using BIBD of Victorbabu and Ravikumar (2022)needs85, 221 and 1021 design points respectively(including one central point).

2. Conditions for Second Order Slope Rotatable Designs

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

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

(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 ’sare uncorrelated random errors with mean zero and varianceσ^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.i.e;

A. $\sum X_{iu}=0, \sum X_{iu}X_{ju}=0, \sum X_{iu}X_{ju}^2=0, \sum X_{iu}X_{ju}X_{ku}=0,$

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

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#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 $V\left(\hat{\beta}_0\right)$ 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)

(2.4)For the second order model (2.1), we have

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

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

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

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

On simplification of (2.7), using (2.3) we get

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. Victorbabu and Narasimham (1991a)] (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)].

On simplification of equation (2.6) we get $V\left(\frac{\partial \hat{Y}}{\partial X_i}\right) = \frac{1}{N}\left[\frac{\lambda_4 + \lambda_2 d^2}{\lambda_2 \lambda_4}\right]\sigma^2$ (2.9)

A New Method of Construction on Second Order Slope Rotatable Designs of Second Type usingPairwise Balanced Designs

Kim (2002) developed second type of rotatable central composite designs (CCD) in which the positions of axial points are indicated by two numbers for $2 \le v \le 8$. Chiranjeevi et al. (2021) extended the results of Kim (2002) and developedSORD of second type using CCD for $9 \le v \le 17$. Chiranjeevi and Victorbabu (2021 a, b) developedSORD of second type using BIBD and PBD respectively.Specifically, Kim and Ko (2004) developed slope rotatability of second type using CCD for $2 \le v \le 5$ by taking $n_a = 1$. Ravikumar and Victorbabu (2022a) extended the results of Kim and Ko (2004)and developed SOSRD of second type using CCD for $6 \le v \le 17$ by taking $n_a = 1$.Ravikumar and Victorbabu (2022b) studied SRCCD of second type for$2 \le v \le 17$ with $2 \le n_a \le 4$. Victorbabu and Ravikumar (2022) developed SOSRD of second type using BIBD.

The design plan of SOSRD of second type using PBD in which the positions of the axial points are indicated by two numbers a_1 and a_2 ($a_2 \ge a_1 > 0$). Let $\left(v,b,r,k_1,k_2,...,k_p,\lambda\right)$ denote a parameters of PBD, $k=\sup.\left(k_1,k_2,...,k_p\right)$ 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 and n_0 be the number of central points in the design.

Let $\left[1-\left(v,b,r,k_1,k_2,...,k_p,\lambda\right)\right]$ denote the design points generated from the transpose of incidence matrix of PBD. Let $\left[1-\left(v,b,r,k_1,k_2,...,k_p,\lambda\right)\right]2^{t(k)}$ are the $b2^{t(k)}$ design points generated from PBD by multiplication (cf.Raghavarao (1971)). We use the additional set of points like $(\pm a_1,0,...,0),(0,\pm a_1,0,...,0),...,(0,0,...,\pm a_1)$; $(\pm a_2,0,...,0),(0,\pm a_2,0,...,0),...,(0,0,...,\pm a_2)$ are two sets of axial points. Here $(a_1,0,...,0)2^1U(a_2,0,...,0)2^1$ denote the 4v axial points generated from $(a_1,0,...,0)$ and $(a_2,0,...,0)$ point sets. Let U denote the union of the design points generated from different sets of points and n_0 denote the number of central points. The new method of construction of SOSRDof second type using PBD is given in the following theorem (cf. Kim and Ko (2004), Ravikumar andVictorbabu (2022a, 2022b)).

Theorem (3.1):

The design points,

$[1-(v,b,r,k_1,k_2,...,k_p,\lambda)]2^{t(k)}U(a_1,0,...,0)2^1U(a_2,0,...,0)2^1U(n_0)$, k=sup.$\left(k_1,k_2,...,k_p\right)$ will give a v-dimensional SOSRD of second type using PBD in $N=b2^{t(k)}+4v+n_0$ design points with the following biquadratic equation

$$[8v-4N](a_1^8+a_2^8)+[16v-8N]a_1^4a_2^4+16v(a_1^6a_2^2+a_1^2a_2^6)+8vr2^{t(k)}(a_1^6+a_1^4a_2^2+a_1^2a_2^4+a_2^6)$$
$$+[-2vN\lambda-4N(r-3\lambda)+4vr+2vr^2 2^{t(k)}-20v\lambda+16\lambda]2^{t(k)}(a_1^4+a_2^4)+[4vr^2-20rv\lambda+16r\lambda]2^{2t(k)}(a_1^2+a_2^2)$$
$$+[8vr+32\lambda-40v\lambda]2^{t(k)}a_1^2a_2^2+[5v\lambda^2-vr\lambda-(r-3\lambda)^2]N2^{2t(k)}+[vr^3-5v\lambda r^2+4r^2\lambda]2^{3t(k)}=0 \quad (3.1)$$

If at least one positive real root exists for the above equation (3.1), then the design exists. (Evolution of (3.1) is explained in (3.4) below)

Proof: For the design points generated from PBD, 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) of (2.2) are true as follows.

B. (i) $\sum X_{iu}^2=r2^{t(k)}+2a_1^2+2a_2^2=N\lambda_2$

(ii) $\sum X_{iu}^4=r2^{t(k)}+2a_1^4+2a_2^4=cN\lambda_4$

C. $\sum X_{iu}^2 X_{ju}^2 = \lambda 2^{t(k)} = N\lambda_4$ (3.2)

From B(ii) and C of (3.2), we have $c=\dfrac{r2^{t(k)}+2a_1^4+2a_2^4}{\lambda 2^{t(k)}}$. Substituting λ_2, λ_4 and c in equation (2.8) and on simplification, we get

$$\frac{\lambda 2^{t(k)}}{N}\left[v\left(5-\frac{r2^{t(k)}+2a_1^4+2a_2^4}{\lambda 2^{t(k)}}\right)-\left(\frac{r2^{t(k)}+2a_1^4+2a_2^4}{\lambda 2^{t(k)}}-3\right)^2\right]+\left(\frac{r2^{t(k)}+2a_1^2+2a_2^2}{N}\right)^2\left[v\left(\frac{r2^{t(k)}+2a_1^4+2a_2^4}{\lambda 2^{t(k)}}-5\right)+4\right]=0$$

(3.3)

On simplification (3.3) leads to the biquadratic equation given in (3.1).

Example:

We illustrate the use of theorem (3.1)by constructinga SOSRD of second type for 6-factors with the help of the PBD $(v=6, b=7, r=3, k_1=3, k_2=2, \lambda=1)$. The design points,

$[1-(6,7,3,3,2,1)]2^{t(3)}U(a_1,0,...,0)2^1U(a_2,0,...,0)2^1U(n_0=1)$, k=sup.(3,2) will give a SOSRD of second type using PBD in N=81 design points with $n_0=1$ and $a_1=1$.

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

Here B and C of equation (3.2) are

B. (i) $\sum X_{iu}^2 = 24+2a_1^2+2a_2^2 = N\lambda_2$

(ii) $\sum X_{iu}^4 = 24+2a_1^4+2a_2^4 = cN\lambda_4$

C. $\sum X_{iu}^2 X_{ju}^2 = 8 = N\lambda_4$ (3.4)

From B (ii) and C of equation (3.5), we have $c=\dfrac{24+2a_1^4+2a_2^4}{8}$

Substituting λ_2, λ_4 and c in equation (2.8) and on simplification, we get the following biquadratic equation.

$$-276(a_1^8+a_2^8)-552a_1^4a_2^4+96(a_1^6a_2^2+a_1^2a_2^6)+1152(a_1^6+a_1^4a_2^2+a_1^2a_2^4+a_2^6)-1120(a_1^4+a_2^4)-6144(a_1^2+a_2^2)$$

$$-512a_1^2a_2^2+25344=0$$

Substitute $a_1=1$ in the above equation and on simplification, we get

$$-276a_2^8+1248a_2^6-520a_2^4-5408a_2^2+18956=0 \quad (3.5)$$

Equation (3.5) has only one positive real root a_2^2=3.9074 ⇒ a_2=1.9767. It can be verified that non singularity condition D of (2.4) is satisfied.

It may be point out here that this SOSRD of second type using PBD has only 81 design points for 6 factors, whereas the corresponding SOSRD of second type obtained using BIBD for 6 factors of Victorbabu and Ravikumar (2022)need 85 design points.Thus the new method SOSRD of second type using PBD sometimes leads to lesser number of design points than the SOSRD of second type obtained through BIBD.

The Appendix table 1 gives the appropriate slope rotatability values of the parameter a_2 with $a_1 = 1$ for designs using a PBD and star points and for different number of central points (n_0) for 6≤v≤15. And table 2 gives the variance of the estimated response of first order derivative of SOSRD of Second type using PBD for factors 6≤v≤15.

Appendix

Table 1: Values of a_2 for SOSRD of second type using PBD for 6≤v≤15

[These are SOSRD of second type using PBD with design points $[1- (v,b,r,k_p k_2,...,k_p,\lambda)]2^{t(k)}$ $U(a_1,0,...,0)2^1U(a_2,0,...,0)2^1U(n_0)]$

(6, 7, 3, 3, 2, 1)

n_0	N	a_2
0	80	2.0032
1	81	1.9767
5	85	1.8856
10	90	1.8035
15	95	1.7480
20	100	1.7095
25	105	1.6817

(8, 15, 6, 4, 3, 2, 2)

n_0	N	a_2
0	272	2.6424
1	273	2.6348
5	277	2.6065
10	282	2.5749
15	287	2.5473
20	292	2.5231
25	297	2.5020

(9, 15, 6, 4, 3, 2)

n_0	N	a_2
0	276	2.6672
1	277	2.6580
5	281	2.6236
10	286	2.5858
15	291	2.5534
20	296	2.5256
25	301	2.5018

(9, 11, 5, 5, 4, 3, 2)

n_0	N	a_2
0	212	2.7196
1	213	2.7103
5	217	2.6768
10	222	2.6426
15	227	2.6151
20	232	2.5929
25	237	2.5748

(10, 11, 5, 5, 4, 2)

n_0	N	a_2
0	216	2.7222
1	217	2.7115
5	221	2.6739
10	226	2.6366
15	231	2.6077
20	236	2.5851
25	241	2.5670

(12, 16, 6, 6, 5, 4, 3, 2

n_0	N	a_2
0	560	3.0286
1	561	3.0242
5	565	3.0075
10	570	2.9885
15	575	2.9715
20	580	2.9562
25	585	2.9425

(13, 16, 6, 6, 5, 4, 3, 2)

n_0	N	a_2
0	564	3.0391
1	565	3.0340
5	569	3.0149
10	574	2.9934
15	579	2.9744
20	584	2.9575
25	589	2.9425

(13, 15, 7, 7, 6, 5, 3)

n_0	N	a_2
0	1012	4.1640
1	1013	4.1619
5	1017	4.1540
10	1022	4.1445
15	1027	4.1357
20	1032	4.1273
25	1037	4.1195

(14, 16, 6, 6, 5, 4, 2)

n_0	N	a_2
0	568	3.0495
1	569	3.0436
5	573	3.0217
10	578	2.9975
15	583	2.9764
20	588	2.9579
25	593	2.9417

(14, 15, 7, 7, 6, 3)

n_0	N	a_2
0	1016	4.1729
1	1017	4.1705
5	1021	4.1615
10	1026	4.1509
15	1031	4.1409
20	1036	4.1316
25	1041	4.1229

(15, 16, 6, 6, 5, 2)

n_0	N	a_2
0	572	3.0594
1	573	3.0527
5	577	3.0278
10	582	3.0006
15	587	2.9774
20	592	2.9573
25	597	2.9400

Note: For all designs we have taken a_1=1.

Table 2: The Variance of the estimated response of SOSRD of Second type using PBD for different factors $6 \leq v \leq 15$

[These are SOSRDs of second type with design points,$[1-(v,b,r,k_1,k_2,...,k_p,\lambda)]2^{t(k)}U(a_1,0,...,0)2^1U(a_2,0,...,0)2^1U(n_0=1)$]

$(v,b,r,k_1,k_2,\ldots,k_p,\lambda)$	N	a_2	λ_4	λ_2	c	$\sigma^{-2}V(\hat{\beta}_0)$	$\sigma^{-2}V(\hat{\beta}_i)$	$\sigma^{-2}V(\hat{\beta}_{ij})$	$\sigma^{-2}V(\hat{\beta}_{ii})$	$\sigma^{-2}Cov(\hat{\beta}_0,\hat{\beta}_{ii})$	$\sigma^{-2}Cov(\hat{\beta}_{ii},\hat{\beta}_{ij})$	$V\left(\frac{\partial \hat{Y}}{\partial X_i}\right)$
(6,7,3,3,2,1)	81	1.9767	0.0988	0.4175	7.0668	0.1006	0.0296	0.1250	0.0312	-0.0352	0.0106	$(0.029570+0.124956d^2)\ \sigma^{-2}$
(8,15,6,4,3,2,2)	273	2.6348	0.1172	0.4098	6.0746	0.0297	0.0089	0.0313	0.0078	-0.0079	0.0017	$(0.008939+0.031254d^2)\ \sigma^{-2}$
(9,15,6,4,3,2)	277	2.6580	0.1155	0.4048	6.1821	0.0362	0.0089	0.0313	0.0078	-0.0090	0.0018	$(0.008918+0.031256d^2)\ \sigma^{-2}$
(9,11,5,5,4,3,2)	213	2.7103	0.1502	0.4540	5.9350	0.0413	0.0103	0.0313	0.0078	-0.0090	0.0015	$(0.010341+0.031257d^2)\ \sigma^{-2}$
(10,11,5,5,4,2)	217	2.7115	0.1475	0.4456	5.9410	0.0465	0.0103	0.0312	0.0078	-0.0094	0.0015	$(0.010342+0.031243d^2)\ \sigma^{-2}$
(12,16,6,6,5,4,3,2)	561	3.0242	0.1141	0.3784	5.6452	0.0187	0.0047	0.0156	0.0039	-0.0037	0.0005	$(0.004711+0.015623d^2)\ \sigma^{-2}$
(13,16,6,6,5,4,3,2)	565	3.0340	0.1133	0.3759	5.6792	0.0213	0.0047	0.0156	0.0039	-0.0040	0.0006	$(0.004708+0.015621d^2)\ \sigma^{-2}$
(13,15,7,7,6,5,3)	1013	4.1619	0.1895	0.4784	5.4691	0.0098	0.0021	0.0052	0.0013	-0.0014	0.0001	$(0.002063+0.005209d^2)\ \sigma^{-2}$
(14,16,6,6,5,4,2)	569	3.0436	0.1125	0.3735	5.7129	0.0243	0.0047	0.0156	0.0039	-0.0043	0.0006	$(0.004705+0.015622d^2)\ \sigma^{-2}$
(14,15,7,7,6,3)	1017	4.1705	0.1888	0.4767	5.4950	0.0111	0.0021	0.0052	0.0013	-0.0015	0.0001	$(0.002063+0.005208d^2)\ \sigma^{-2}$
(15, 16, 6, 6, 5, 2)	573	3.0527	0.1117	0.3711	5.7451	0.0275	0.0047	0.0156	0.0039	-0.0046	0.0006	$(0.004703+0.015624d^2)\ \sigma^{-2}$

*For all designs we have taken $a_1=1$.

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