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MODIFIED SLOPE ROTATABLE CENTRAL COMPOSITE DESIGNS

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ABSTRACT

In this paper, modified second order slope rotatable designs are introduced and modified slope rotatable central composite designs (SRCCD) are constructed for $2 \leq v \leq 17$ (v: the number of factors). Further, it can be shown for certain values of 'v', the modified SRCCD can be viewed as SRCCD constructed as with the technique of augmentation of second order rotatable design (SORD) using central composite design to SRCCD. These designs are useful in parts to estimate responses and slopes with spherical variance functions.

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1. INTRODUCTION

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, 1987).

Box and Hunter (1957) introduced rotatable designs for the exploration of response surfaces. Das et al. (1999) constructed modified rotatable designs. Hader

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and Park (1978) introduced slope rotatable central composite designs (SRCCD). Victorbabu and Narasimham (1991, 1994, 1994&95), Victorbabu (2002a, 2002b) studied second order slope rotatable designs (SOSRD) and constructed SOSRD using different methods. Park and Kim (1992), Jang and Park (1993) obtained a measure and graphical method for evaluating slope rotatability in response surface designs.

In this paper, some modified second order slope rotatable designs are introduced and modified slope rotatable central composite designs are constructed for $2 \leq v \leq 17$.

2. CONDITIONS FOR MODIFIED SOSRD

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

$$Y_u = b_0 + \sum_{i=1}^{v} b_i x_{iu} + \sum_{i=1}^{v} b_{ii} x_{iu}^2 + \sum\sum_{i<j} b_{ij} x_{iu} x_{ju} + e_u \tag{2.1}$$

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 σ^2.

SOSRD: A second order response surface design D is said to be a SOSRD, if the variance of the estimate of first order partial derivative $(\partial \hat{Y}_u / \partial x_i)$ with respect to each of independent variables (x_i) is only a function of the distance $(d^2 = \sum_i x_{iu}^2)$ of the point $(x_{1u}, x_{2u}, \ldots, x_{vu})$ from the origin (centre) 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 (1991)).

$$\sum_{u=1}^{N} \prod_{i=1}^{v} x_{iu}^{\alpha_i} = 0 \quad if\ any\ \alpha_i\ is\ odd,\ for \sum \alpha_i \leq 4 \tag{2.2}$$

$$(i) \quad \sum_{u=1}^{N} x_{iu}^2 = constant = N\lambda_2, \tag{2.3}$$

$$(ii) \quad \sum_{u=1}^{N} x_{iu}^4 = constant = cN\lambda_4, \quad for\ all\ i$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = constant = N\lambda_4, \quad for\ i \neq j \tag{2.4}$$

$$(c+v-1)\lambda_4 > v\lambda_2^2 \tag{2.5}$$

$$\lambda_4[v(5-c)-(c-3)^2]+\lambda_2^2[v(c-5)+4]=0 \tag{2.6}$$

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

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

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

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

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

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

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

and other covariances are zero.

$$v\left(\frac{\partial\hat{Y}}{\partial x_i}\right) = V(\hat{b}_i)+4x_i^2V(\hat{b}_{ii})+\sum_{j\neq i}x_j^2V(\hat{b}_{ij}) = \frac{1}{N}\left[\frac{\lambda_4+\lambda_2 d^2}{\lambda_2\lambda_4}\right]\sigma^2.$$

The usual method of construction of SOSRD is to take combinations with unknown constants, associate a 2^v factorial combinations or a suitable fraction of it with factors each at ±1 levels to make the level codes equidistant. All such combinations form a design. Generally SOSRD need at least five levels (suitably coded) at $0,\pm1,\pm a$ for all factors $(0,0,\ldots,0$ – chosen center of the design, unknown level 'a' to be chosen suitably to satisfy slope rotatability). Generation of design points this way ensures satisfaction of all the conditions even though the design points contain unknown levels.

Alternatively by putting some restrictions indicating some relation among $\sum x_{iu}^2$, $\sum x_{iu}^4$ and $\sum x_{iu}^2x_{ju}^2$ some equations involving the unknown levels are obtained and their solution gives the unknown levels. In SOSRD the restrictions used are $V(b_{ij}) = 4V(b_{ii})$ and $c=\sum x_{iu}^4/\sum x_{iu}^2x_{ju}^2$. Other restrictions are also possible though, it seems, not yet exploited. We shall investigate the restriction $(\sum x_{iu}^2)^2 = N\sum x_{iu}^2x_{ju}^2$ *i.e.*, $(N\lambda_2)^2 = N(N\lambda_4)$ *i.e.*, $\lambda_2^2=\lambda_4$ to get modified SOSRD (Das *et al.*, 1999). By applying this new restriction $\lambda_2^2=\lambda_4$ in equation

(2.6), we get $c = 1$ or $c = 5$. The non-singularity condition (2.5) leads to $c = 5$. It may be noted $\lambda_2^2 = \lambda_4$ and $c = 5$ are equivalent conditions. Further,

$$V(\hat{b}_0) = \frac{(v+4)\sigma^2}{4N}$$
$$V(\hat{b}_i) = \frac{\sigma^2}{N\sqrt{\lambda_4}}$$
$$V(\hat{b}_{ij}) = \frac{\sigma^2}{N\lambda_4}$$
$$V(\hat{b}_{ii}) = \frac{\sigma^2}{4N\lambda_4}$$
$$Cov(\hat{b}_0, \hat{b}_{ii}) = \frac{-\sigma^2}{4N\sqrt{\lambda_4}} \quad \textit{and other covariances are zero.}$$
$$V\left(\frac{\partial \hat{Y}}{\partial x_i}\right) = \left[\frac{\sqrt{\lambda_4} + d^2}{N\lambda_4}\right]\sigma^2.$$

3. Construction of Modified SRCCD

The most widely used design for fitting a second order model is the central composite design. Central composite designs are constructed by adding suitable factorial combinations to those obtained from $(1/2^p) \times 2^v$ fractional factorial design (here $2^{t(v)} = (1/2^p) \times 2^v$ denotes a suitable fractional replicate of 2^v, in which no interaction with less than five factors is confounded). In coded form the points of $2^v(2^{t(v)})$ factorial have coordinates $(\pm1, \pm1, \ldots, \pm1)$ and $2v$ axial points have coordinates of the form $(\pm a, 0, \ldots, 0)$, $(0, \pm a, \ldots, 0)$,..., $(0, 0, \ldots, \pm a)$ *etc.*, and n_0 central points. The axial points may be replicated n_a times and central points to be replicated n_0 times. The method of construction of modified SRCCD is given in the following Theorem 3.1.

THEOREM 3.1. *A central composite design will be a v-dimensional modified SRCCD in* $N = \left(2^{t(v)} + 2n_a a^2\right)^2 / 2^{t(v)}$ *design points, if* $a^4 = 2^{t(v)+1}/n_a$.

PROOF. For the design points generated from central composite design the conditions in equation (2.2) are satisfied. The conditions in equations (2.3) and (2.4) are true as follows:

$$\sum x_{iu}^2 = 2^{t(v)} + 2n_a a^2 = N\lambda_2 \tag{3.1}$$
$$\sum x_{iu}^4 = 2^{t(v)} + 2n_a a^4 = cN\lambda_4 \tag{3.2}$$
$$\sum x_{iu}^2 x_{ju}^2 = 2^{t(v)} = N\lambda_4 \tag{3.3}$$

TABLE 3.1 *A list of modified SRCCD for* $2 \leq v \leq 17$

No. of factors (v)	$t(v)$	n_a	a^2	n_0	N	$V(\hat{b}_i)\sigma^{-2}$	$V(\frac{\delta\hat{y}}{\delta x_i})\sigma^{-2}$
2	2	2	2	24	36	0.0833	$0.0833+0.2500d^2$
3	3	1	4	18	32	0.0625	$0.0625+0.1250d^2$
4	4	2	4	32	64	0.0313	$0.0313+0.0625d^2$
5	4	2	4	28	64	0.0313	$0.0313+0.0625d^2$
6	5	1	8	28	72	0.0208	$0.0208+0.0313d^2$
7	6	2	8	52	144	0.0104	$0.0104+0.0156d^2$
8	6	2	8	48	144	0.0104	$0.0104+0.0156d^2$
9	7	1	16	54	200	0.0063	$0.0063+0.0078d^2$
10	7	1	16	52	200	0.0063	$0.0063+0.0078d^2$
11	7	1	16	50	200	0.0031	$0.0063+0.0078d^2$
12	8	2	16	96	400	0.0031	$0.0031+0.0039d^2$
13	8	2	16	92	400	0.0031	$0.0031+0.0039d^2$
14	8	2	16	88	400	0.0031	$0.0031+0.0039d^2$
15	8	2	16	84	400	0.0031	$0.0031+0.0039d^2$
16	8	2	16	80	400	0.0031	$0.0031+0.0039d^2$
17	8	2	16	76	400	0.0031	$0.0031+0.0039d^2$

Using the condition $\lambda_2^2 = \lambda_4$, from equations (3.1) and (3.3) we get, $N = \left(2^{t(v)} + 2n_a a^2\right)^2 / 2^{t(v)}$. (Alternatively N may be obtained directly as $N = 2^{t(v)} + 2vn_a + n_0$, where $n_0 = \left(2^{t(v)} + 2n_a a^2\right)^2 / 2^{t(v)} - 2^{t(v)} - 2vn_a$).
From equations (3.2) and (3.3), we have $2^{t(v)} + 2n_a a^4 = 5 \times 2^{t(v)}$. This condition leads to $a^4 = 2^{t(v)+1}/n_a$. □

In particular, if $n_a = 1$, then $a^2 = 2^{(t(v)+1)/2}$, a^2 is an integer if $t(v)$ is odd. If $n_a = 2$, then $a^2 = 2^{t(v)/2}$, a^2 is an integer if $t(v)$ is even.

We note that for the existence of the modified SRCCD, 'n_a' should be chosen such that 'a^2' is an integer. A list of modified SRCCD for $2 \leq v \leq 17$ is given in Table 3.1.

Alternatively it can be shown for certain values of 'v', the modified SRCCD can be viewed as SRCCD constructed as with the technique of augmentation of SORD using central composite design to SRCCD. This is established in Section 4.

4. AUGMENTED SECOND ORDER ROTATABLE DESIGN AS SECOND ORDER SLOPE ROTATABLE DESIGN

Hader and Park (1978) noted that the value of level 'a' for the axial points in central composite design required for slope rotatability is appreciably larger than the value required for Box and Hunter (1957) rotatability. Now we obtain second order slope rotatable design (with Hader and Park (1978) slope rotatability) by augmenting Box and Hunter (1957) second order rotatable design (SORD) with additional axial points and central points. These designs are useful in parts to estimate responses and slopes with spherical variance functions. These augmented SOSRD are obtained by suitably selecting some additional number of replications for the axial points (n_a) in a SORD. More specifically, in this work SORD constructed using central composite designs are augmented with additional axial points and central points to form SOSRD.

If $D_1(a)$ denotes a Box and Hunter (BH) SORD, $D_2(0)$ are some addition central points and $D_3(a)$ are some additional axial points, we augment the SORD $D_1(a)$ to the SOSRD $D_1(a) \cup D_2(0) \cup D_3(a)$ to obtain an augmented design such that $D_1(a)$ or $D_1(a) \cup D_2(0)$ can be used as BHSORD for estimating responses [here we may mention that $D_1(a)$ is enough for BHSORD but to get pure error we may take additional central points $D_2(0)$] and the augmented design $D_1(a) \cup D_2(0) \cup D_3(a)$ can be used as Hader and Park SOSRD for estimating the slopes. We note that we choose the level $\pm a$ in the axial points to be same in both the designs SORD $D_1(a) \cup D_2(0)$ and SOSRD $D_1(a) \cup D_2(0) \cup D_3(a)$. The exploration of responses surface can be carried sequentially with these augmented designs for estimation of responses and slopes.

The method of construction of augmented second order rotatable central composite design as slope rotatable central composite design is established in the following Theorem 4.1.

THEOREM 4.1. *A central composite design in 'N' design points, with Box and Hunter (1957) rotatability level $a^4 = 2^{t(v)}$ will give a particular type of augmented SRCCD with $c = 5$, if*

$$n_0 = \frac{\left(2^{t(v)} + 2n_a a^2\right)^2}{2^{t(v)}} - 2^{t(v)} - 2vn_a. \tag{4.1}$$

TABLE 4.1 *A list of augmented SORD as SOSRD using CCD for* $2 \leq v \leq 17$

No. of factors (v)	$t(v)$	n_a	a^2	n_0	N	$V(\hat{b}_i)\sigma^{-2}$	$V(\frac{\delta\hat{y}}{\delta x_i})\sigma^{-2}$
2	2	2	2	24	36	0.0833	$0.0833+0.2500d^2$
4	4	2	4	32	64	0.0313	$0.0313+0.0625d^2$
5	4	2	4	28	64	0.0313	$0.0313+0.0625d^2$
7	6	2	8	52	144	0.0104	$0.0104+0.0156d^2$
8	6	2	8	48	144	0.0104	$0.0104+0.0156d^2$
12	8	2	16	96	400	0.0031	$0.0031+0.0039d^2$
13	8	2	16	92	400	0.0031	$0.0031+0.0039d^2$
14	8	2	16	88	400	0.0031	$0.0031+0.0039d^2$
15	8	2	16	84	400	0.0031	$0.0031+0.0039d^2$
16	8	2	16	80	400	0.0031	$0.0031+0.0039d^2$
17	8	2	16	76	400	0.0031	$0.0031+0.0039d^2$

PROOF. For the design points generated from central composite design the conditions in equation (2.2) are satisfied. The conditions in equations (2.3) and (2.4) are true as follows:

$$\sum x_{iu}^2 = 2^{t(v)} + 2n_a a^2 = N\lambda_2 \tag{4.2}$$

$$\sum x_{iu}^4 = 2^{t(v)} + 2n_a a^4 = 5N\lambda_4 \tag{4.3}$$

$$\sum x_{iu}^2 x_{ju}^2 = 2^{t(v)} = N\lambda_4 \tag{4.4}$$

From equations (4.3) and (4.4) we have, $2^{t(v)} + 2n_a a^4 = 5 \times 2^{t(v)}$. The condition leads to $a^4 = 2^{t(v)+1}/n_a$. Here specifically $n_a = 2$ leads to Box and Hunter (1957) rotatability. The modified condition $\lambda_2^2 = \lambda_4$ leads to n_0 given in equation (4.1). □

A list of augmented SORD as SOSRD using central composite design for $2 \leq v \leq 17$ is given in Table 4.1. We note that augmented designs do not exist for $v = 3, 6, 9, 10, 11$ factor with the modified condition $\lambda_2^2 = \lambda_4$.

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REFERENCES

BOX, G.E.P. AND HUNTER, J.S. (1957), "Multifactor experimental designs for exploring response surfaces", *Annals of Mathematical Statistics*, **28**, 195–241.

DAS, M.N., RAJENDRA PRASAD, AND MANOCHA, V.P. (1999). "Response surface designs, symmetrical and asymmetrical, rotatable and modified", *Statistics and Applications*, **1**, 17–34.

HADER, R.J. AND PARK, S.H. (1978). "Slope rotatable central composite designs", *Technometrics*, **20**, 413–417.

JANG, D.H. AND PARK, S.H. (1993). "A measure and graphical method for evaluating slope rotatability in response surface designs", *Communications in Statistics – Theory and Methods*, **22**,1849–1863.

PARK, S.H. (1987). "A class of multifactor designs for estimating the slope of response surfaces", *Technometrics*, **29**, 449–453.

PARK, S.H. AND KIM, H.J. (1992). "A measure of slope rotatability for second order response surface experimental designs", *Journal of Applied Statistics*, **19**, 391–404.

VICTOR BABU. B.RE. (2002a). "A note on the construction of four and six level second order slope rotatable designs", *Statistical Methods*, **4**, 11–20.

VICTOR BABU. B.RE. (2002b). "Construction of second order slope rotatable designs using symmetrical unequal block arrangements with two unequal block sizes", *Journal of the Korean Statistical Society*, **31**, 153–161.

VICTOR BABU, B. RE. AND NARASIMHAM, V.L. (1991). "Construction of second order slope rotatable designs through balanced incomplete block designs", *Communications in Statistics -Theory and Methods*, **20**, 2467–2478.

VICTOR BABU. B. RE. AND NARASIMHAM, V.L. (1994). "A new type of slope rotatable central composite design", *Journal of the Indian Society of Agricultural Statistics*, **46**, 315–317.

VICTOR BABU. B. RE. AND NARASIMHAM, V.L. (1994&95). "Augmented second order rotatable design as second order slope rotatable design", *Gujarat Statistical Review*, **21** & **22**, 31–36.