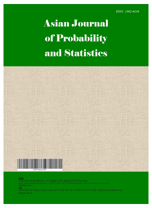

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Second Order Rotatable Designs of Second Type Using Central Composite Designs

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Authors' contributions

This work was carried out in collaboration among all authors. Author PC designed the study, performed the statistical analysis, wrote the protocol, and wrote the first draft of the manuscript. Author KJB and BRVB managed the analyses of the study. Author BRVB managed the literature searches. All authors read and approved the final manuscript.

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Abstract

Kim [1] introduced rotatable central composite designs of second type with two replications of axial points for $2 \leq v \leq 8$ (v: number of factors). In this paper we have extended the work of Kim [1] for second order rotatable designs of second type using central composite designs for $9 \leq v \leq 17$.

Keywords: Response surface methodology; central composite designs; rotatability, orthogonality; efficiency.

1 Introduction

Response surface methodology (RSM) is a collection of statistical and mathematical techniques useful for developing, improving, and optimizing processes. It also has important applications in the design, development, and formulation of new products, as well as in the improvement of existing product designs.

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Box and Hunter [2] introduced rotatable designs. Das and Narasimham [3] constructed rotatable designs using balanced incomplete block designs (BIBD). Draper and Guttman [4] suggested an index of rotatability. Khuri [5] introduced a measure of rotatability for response surface designs. Draper and Pukelshein [6] developed another look at rotatability. Park et al. [7] suggested measure of rotatability for second order response surface designs. Das et al. [8] developed modified response surface designs. Kim and Ko [10] developed slope rotatability of second type of central composite designs. Victorbabu and Vasundharadevi [11] suggested modified second order response surface designs using BIBD. Victorbabu et al. [12] studied modified second order response surface designs using pairwise block designs. Victorbabu [13,14] studied modified second order slope rotatable designs using central composite designs (CCD) and BIBD. Victorbabu [15] suggested a review on second order rotatable designs. Victorbabu and Vasundharadevi [16] studied second order response surface designs using symmetrical unequal block arrangements with two unequal block sizes. Victorbabu et al. [17] suggested modified second order response surface designs using CCD. Park and Park [18] suggested the extension of central composite designs for second order response surface models. Surekha and Victorbabu [19] suggested measure of rotatability for second order response surface designs using CCD. Kim [23] introduced modified slope rotatability using extended central composite designs. Ali et al. [20] studied Evolutionary numerical approach for solving nonlinear singular periodic boundary problems. Baleanu et al. [21] studied the method of lines for solution of the carbon nanotubes engine oil nanofluid over an unsteady rotating disk. Specially, Kim [1] introduced extended central composite designs with replications of axial points and developed these designs using second type CCD for $2 \le v \le 8$.

In this paper, following the work of Kim [1] an attempt is made to study second order rotatable designs of second type using CCD for $9 \le v \le 17$.

2 Stipulations and Formulas for Second Order Rotatable Designs

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

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

where x_{iu} represents the level of i^{th} factor (i=1,2,…,v) in the u^{th} run (u=1,2,…,N) of the experiment and φ_u are uncorrelated random error with mean zero and variance σ^2. Then 'D' is said to be second order rotatable designs (SORD), if the variance of $Y_u(x_1, x_2, \ldots, x_v)$ with respect to each of independent variable (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 responses in the second order polynomial model is achieved if the design points satisfy the following stipulations [2].

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

$$\sum x_{iu} = 0, \sum x_{iu} x_{ju} = 0, \sum x_{iu} x_{ju}^2 = 0, \sum x_{iu} x_{ju} x_{ku} = 0,$$
$$\sum x_{iu}^3 = 0, \sum x_{iu} x_{ju}^3 = 0, \sum x_{iu} x_{ju} x_{ku}^2 = 0, \sum x_{iu} x_{ju} x_{ku} x_{lu} = 0.$$

for $i \ne j \ne k \ne l$; (2.2)

(i) $\sum x_{iu}^2 = \text{constant} = N\mu_2$ (ii) $\sum x_{iu}^4 = \text{constant} = cN\mu_4$ for all i (2.3)

$$\sum x_{iu}^2 x_{ju}^2 = \text{constant} = N\mu_4 \text{ for all } i \neq j \tag{2.4}$$

$$\frac{\mu_4}{\mu_2^2} > \frac{v}{(c+v-1)} \tag{2.5}$$

$$\sum x_{iu}^4 = c \sum x_{iu}^2 x_{ju}^2 \tag{2.6}$$

where c, μ_4 and μ_2 are constants.

The variances and covariances of the estimated parameters are

$$V(\hat{b}_0) = \frac{\mu_4(c+v-1)\sigma^2}{N[\mu_4(c+v-1)-v\mu_2^2]},$$

$$V(\hat{b}_i) = \frac{\sigma^2}{N\mu_2},$$

$$V(\hat{b}_{ij}) = \frac{\sigma^2}{N\mu_4},$$

$$V(\hat{b}_{ii}) = \frac{\sigma^2}{(c-1)N\mu_4}\left[\frac{\mu_4(c+v-2)-(v-1)\mu_2^2}{\mu_4(c+v-1)-v\mu_2^2}\right],$$

$$Cov(\hat{b}_0, \hat{b}_{ii}) = \frac{-\mu_2\sigma^2}{N[\mu_4(c+v-1)-v\mu_2^2]},$$

$$Cov(\hat{b}_{ii}, \hat{b}_{jj}) = \frac{(\mu_2^2-\mu_4)\sigma^2}{(c-1)N\mu_4[\mu_4(c+v-1)-v\mu_2^2]} \text{ and other covariances vanish.} \tag{2.7}$$

The variance of the estimated response at the point ($x_{10}, x_{20}, \ldots, x_{v0}$) is

$$\begin{aligned} V(\hat{y}_0) = V(\hat{b}_0) + \left[V(\hat{b}_i) + 2Cov(\hat{b}_0, \hat{b}_{ii})\right] d^2 + V(\hat{b}_{ii}) d^4 + \\ \sum x_{i0}^2 x_{j0}^2 \left[V(\hat{b}_{ij}) + 2Cov(\hat{b}_{ii}, \hat{b}_{jj}) - 2V(\hat{b}_{ii})\right] \end{aligned} \tag{2.8}$$

The coefficient of $\sum x_{i0}^2 x_{j0}^2$ in the above equation (2.8) is simplified to $(c-3)\sigma^2/(c-1)N\mu_4$.

A second order response surface design D is said to be rotatable design, if in this design c=3 and all the other conditions (2.2) to (2.7) hold.

3 Construction of Second Order Rotatable Designs of Second Type Using Central Composite Designs [1]:

3.1 Central composite designs

The central composite designs are widely used for estimating second order response surfaces. Box and Wilson (1951) introduced the central composite designs (CCD). Box and Hunter (2) introduced rotatable central composite designs For notational convenience, the Box and Hunter (2) CCD, will be called as first-type of CCD. This design consists of:

1. a complete (or a $\frac{1}{2^p}\times 2^v$ fractional) factorial design, where 0≤m<p, and the design levels are coded to the usual ±1 values;
2. m_0 central points ($m_0 \geq 1$);
3. Two axial points on the axis of each independent variable at a distance of from the design center.
4. For example v=2 factors the plan of first -type of CCD is as follows.

X_1	X_2
1	1
1	-1
-1	1
-1	-1
a	0
-a	0
0	a
0	-a
0	0

The total number of experimental points in the first -type of CCD plan is $M=2^{t(v)}+2v+m_0$, where $2^{t(v)}$ is the fractional factorial designs, 2v is the number of axial points and m_0 number of central points.

The design become an orthogonal system, then

From (i) of (2.3), we have $\sum x_{iu}^2=2^{t(v)}+2a^2=N\mu_2$

For the conviene let us consider N=M.

$$\sum x_{iu}^2=2^{t(v)}+2a^2=M\mu_2$$

$$\text{where}\, M\mu_2=\sqrt{2^{t(v)}M}$$

$$2^{t(v)}+2a^2=\sqrt{2^{t(v)}M}$$

by simplification then we can obtained

$$a=\left(\frac{\sqrt{2^{t(v)}M}-2^{t(v)}}{2}\right)^{\frac{1}{2}} \tag{3.1}$$

and the condition for the design become an rotatability

From (ii) of (2.3) and (2.4), we have

$$\sum x_{iu}^{4}=2^{t(v)}+2a^{4}=3M\mu_{4}$$

$$\sum x_{iu}^{2}x_{ju}^{2}=2^{t(v)}=M\mu_{4}$$

Then the rotatability condition equation (2.6)

$$\sum x_{iu}^{4}=c\sum x_{iu}^{2}x_{ju}^{2}$$

$\Rightarrow 2^{t(v)}+2a^{4}=3(2^{t(v)})$ and on simplification, we get

$$a=(2^{t(v)})^{1/4} \tag{3.2}$$

3.2 The central composite designs with the two replications of axial points

The design plan of second type of CCD in which the position of the axial points are indicated by two numbers a and a is as follows same way v=2 factors the plan of second type of CCD is as follows.

X_1	X_2
1	1
1	-1
-1	1
-1	-1
a_1	0
$-a_1$	0
0	a_1
0	$-a_1$
a_2	0
$-a_2$	0
0	a_2
0	$-a_2$
0	0

Here the number of central points are integers greater than or equal to 1, and the axial points a_1 and a_2 are $a_2 \geq a_1 > 0$. Even if v=3 or more factors creating the same way, then the total numbers of experimental points are $N=2^{t(v)}+4v+n_0$, where $2^{t(v)}$ is the fractional factorial designs and $4v+n_0$ is sum of the axial points and central points.

The central composite designs are widely used for fitting of second order model. The central composite designs are constructed by adding suitable fractional combinations to those obtained from $\frac{1}{2^p}\times 2^v$ fractional factorial design (here $\frac{1}{2^p}\times 2^v$ denotes a suitable fractional replicates of 2^v), in which no interaction with less than five factors are confounded. In coded from the points of 2^v ($2^{t(v)}$ factorial have coordinates ($(\pm 1,\pm 1,...,\pm 1)$ and 4v axial points have coordinates of the form $(\pm a_1,0,...,0),(0,\pm a_1,0,...,0),...,(0,0,...,\pm a_1)$ and $(\pm a_2,0,...,0),(0,\pm a_2,0,...,0),...,(0,0,...,\pm a_2)$ etc, and if necessary n_o central points may be replicated. It is pointed out 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. Thus we have the total number of experimental points $N=2^{t(v)}+4v+n_0$ and

$$\sum X_{iu}^2=2^{t(v)}+2a_1^2+2a_2^2=N\mu_2 \tag{3.3}$$

$$\sum x_{iu}^4=2^{t(v)}+2a_1^4+2a_2^4=3N\mu_4 \tag{3.4}$$

$$\sum x_{iu}^2 x_{ju}^2=2^{t(v)}=N\mu_4 \tag{3.5}$$

From equation (3.3)

$$2^{t(v)}+2a_1^2+2a_2^2=\sqrt{2^{t(v)}N}$$

$$\text{where } N\mu_2=\sqrt{2^{t(v)}N} \text{ (cf. Kim (2002))}$$

$$a_1^2+a_2^2=\frac{\sqrt{2^{t(v)}N}-2^{t(v)}}{2} \tag{3.6}$$

From equations (3.4) and (3.5) we get

$$2^{t(v)}+2a_1^4+2a_2^4=3(2^{t(v)}) \tag{3.7}$$

$$a_1^4+a_2^4=2^{t(v)}$$

$$a_1+a_2=(2^{t(v)})^{1/4} \tag{3.8}$$

4 Study of Orthogonality Using Second Type of Central Composite Designs [1]

An orthogonal design is one in which the terms in the fitted model are uncorrelated with one another and thus the parameter estimates are uncorrelated. In this case, the variance of the predicated response at any point x in the experimental region, is expressible as a weighted sum of the variance of the parameter estimates in the model. For second order moments $\sum x_{iu}^2$ and $\sum x_{iu}^2 x_{ju}^2$ is impossible to obtain. This is because the moments $\sum x_{iu}^2$ and $\sum x_{iu}^2 x_{ju}^2$ are necessarily positive. Hence, we consider the model with the pure quadratic terms correlated for their means. In regard to orthogonality, this model is often used for the sake of simplicity in the calculation. The condition that second type of CCDs orthogonal design is $\mu_2^2=\mu_4$.

$$a_1^2+a_2^2=\frac{\sqrt{N(2^{t(v)})}-2^{t(v)}}{2} \tag{4.1}$$

It must be established the equation (4.1) makes second type of CCD an orthogonal system. However $N=2^{t(v)}+4v+n_0$, the value of (4.1) depends on v, n_0 and the design points of second type of CCD. The following table 1 gives the values of orthogonality of second order response surface methodology using various parameters of second type of CCD and n_0, the value of '$a_1^2+a_2^2$' makes orthogonal second order response surface designs by using second type of CCD. Table 1 gives the values of the orthogonal of second type of CCD.

4.1 Example

Let us consider v = 9 factors

Here the total number of experimental plots N=165
From equation (3.6), we have

$$a_1^2+a_2^2=\frac{\sqrt{2^{t(v)}N}-2^{t(v)}}{2} \quad \Rightarrow a_1^2+a_2^2=\frac{\sqrt{(128)\times(165)}-128}{2} =8.6636.$$

The values of orthogonality using second type of CCD for 9≤v≤17 with central points are given in the following Table 1

Table 1. values of orthogonality using second type of CCD

(v,p) / **n_0**	**(9,2)**	**(10,3)**	**(11,4)**	**(12,4)**	**(13,5)**	**(14,6)**	**(15,7)**	**(16,8)**	**(17,9)**
1	8.6636	9.5391	10.4043	11.7139	12.6272	13.5344	14.4359	15.3318	16.2221
2	8.8835	9.7564	10.6190	11.9428	12.8545	13.76604	14.6604	15.5549	16.4438
3	9.1027	9.9729	10.8331	12.1713	13.0815	13.9859	14.8846	15.7776	16.6652
4	9.3212	10.1889	11.0467	12.3994	13.3082	14.2111	15.1084	16.0000	16.8862
5	9.5391	10.4043	11.2596	12.6272	13.5344	14.4359	15.3318	16.2221	17.1069

5 Efficiency Comparison for CCD 2 with CCD1 [1]

In this section, second type of CCD is used as the basis for estimating specific coefficient in the response surface model, second type of CCD is compared with first type of CCD. This comparison criterion is based on the precision at which the coefficient is estimated. It is consider that the numbers of experimental plots are required at same way.

For example in terms of estimating mixed quadratic coefficient b_{ij} (i≠j), two experimental designs, let's try to compare D_1 and D_2. The number of experimental plots required in D_1 and D_2 are N_1 and N_2 respectively. The relative efficiency of D_1 and D_2 is given by the following equation (see Myers [22], section 7.2).

$$E\left(D_1/D_2\right)=\frac{\{Var(b_{ij})\,in\,D_2\}\,N_2}{\{Var(b_{ij})\,in\,D_1\}\,N_1} \tag{5.1}$$

In this case, in order to compare fairly, the experimental system should make the second product equal to value of $\frac{\sum x_{iu}^2}{N}$. It must be scaled and for this the following scaling criteria is used.

$$\begin{aligned}&(i)\frac{1}{N}\sum x_{iu}=0\\&(ii)\frac{1}{N}\sum x_{iu}^2=1,\ (i=1,2,...,v)\end{aligned} \tag{5.2}$$

5.1 Comparison in mixed quadratic coefficient $b_{ij}\,(i \neq j)$

According to equation (2.7) $V(\hat{b}_{ij})=\frac{\sigma^2}{N\mu_4}$, but this before scaling equation (5.2) will be write in second type of CCD $(ii)=\frac{(2^{t(v)}+2a_1^2+2a_2^2)}{N}$ each time making equation (5.2) will be is equal to 1, i.e. (ii) =1, then the scaling factor g

$$g=\left\{\left(\frac{2^{t(v)}+4v+n_0}{2^{t(v)}+2a_1^2+2a_2^2}\right)\right\}^{1/2} \tag{5.3}$$

However the $V(b_{ij})$ is multiplied by with the scaling factor 'g' than the $V(b_{ij})=\frac{\sigma^2}{N\lambda_4}.\frac{1}{g^4}$ that is

$$V(b_{ij})=\frac{\sigma^2}{N\lambda_4}\left\{\left[\frac{2^{t(v)}+2a_1^2+2a_2^2}{2^{t(v)}+4v+n_0}\right]\right\}^2$$

According to equation (5.1) the relative efficiency of second type of CCD versus first type of CCD in the mixed quadratic coefficient b_{ij} is obtained as follows

$$E\left(\frac{\text{second type of CCD}}{\text{first type of CCD}}\right)=\frac{\frac{\sigma^2}{N\lambda_4}\left(\frac{2^{t(v)}+2a^2}{2^{t(v)}+2v+m_0}\right)^2(2^{t(v)}+2v+m_0)}{\frac{\sigma^2}{N\lambda_4}\left(\frac{2^{t(v)}+2a_1^2+2a_2^2}{2^{t(v)}+4v+n_0}\right)^2(2^{t(v)}+4v+n_0)}$$

$$=\frac{(2^{t(v)}+2a^2)^2(2^{t(v)}+4v+n_0)}{(2^{t(v)}+2a_1^2+2a_2^2)^2(2^{t(v)}+2v+m_0)} \tag{5.4}$$

From equation (5.4) the condition that $E\left(\frac{\text{second type of CCD}}{\text{first type of CCD}}\right)$>1, than the second type of CCD is more efficient than first type of CCD

$$a_1^2+a_2^2<\frac{1}{2}\left\{(2^{t(v)}+2a^2)\sqrt{\frac{2^{t(v)}+4v+n_0}{2^{t(v)}+2v+n_0}}-2^{t(v)}\right\} \tag{5.5}$$

From the values of (3.1) and (4.1) substitute in (5.4) and then we get the value of greater than 1. From this orthogonal second type of CCD has the same degree of efficiency as orthogonal first type of CCD, and consider the efficiency of second type of CCD is giving the better efficiency than first type of CCD. Now, the efficiency comparison of second type of CCD versus first type of CCD with rotatability. Substituting the values of (3.2) into (5.5) and we evaluated that the second type of CCD will be more efficient than the previous first type of CCD with rotatability.

$$a_1^2+a_2^2<\frac{1}{2}\left\{(2^{t(v)}+2\sqrt{2^{t(v)}})\sqrt{\frac{2^{t(v)}+4v+n_0}{2^{t(v)}+2v+m_0}}-2^{t(v)}\right\} \tag{5.6}$$

For example, in first type of CCD when v=9 and m_0=1 then we get M =147 then a=3.3636 and n_0=1, then the equation (5.6)

$$a_1^2+a_2^2<15.7916 \tag{5.7}$$

Among the rotatability of second type of CCD, it is easy to find an experimental plan that satisfies the equation (5.7). For example in second type of CCD with a_1=1, a_2=3.3569 satisfy the rotatability property equation (3.7), and $a_1^2+a_2^2=12.2688$ as it satisfies the equation (5.7) as well, it is more efficient than the rotatability first type of CCD. Then the relative efficiency of second type of CCD versus first type of CCD equation (5.4) is as follows.

$$\frac{(128+2(11.3137))^2(128+36+1)}{\{128+(2)(12.2694)\}^2(128+18+1)}=1.0945$$

5.2 Comparison in the pure quadratic coefficient b_{ii}

Now this time in terms of estimating the pure quadratic coefficient b_{ii}, the efficiency of second type of CCD is comparing with first type of CCD, here the scaling factor the equation (4.2) is applied. The relative efficiency of second type of CCD versus first type of CCD is as follows based on the equation (5.1)

$$E\left(\frac{\text{second type of CCD}}{\text{first type of CCD}}\right)=\frac{\sigma^2 e_1\left(\frac{2^{t(v)}+2a^2}{2^{t(v)}+2v+m_0}\right)^2\left(2^{t(v)}+2v+m_0\right)}{\sigma^2 e_2\left(\frac{2^{t(v)}+2a_1^2+2a_2^2}{2^{t(v)}+4v+n_0}\right)^2\left(2^{t(v)}+4v+n_0\right)}$$

$$=\frac{e_1\left(2^{t(v)}+2a^2\right)^2\left(2^{t(v)}+4v+n_0\right)}{e_2\left(2^{t(v)}+2a_1^2+2a_2^2\right)^2\left(2^{t(v)}+2v+m_0\right)} \tag{5.8}$$

Where $e_1=v(b_{ii})$ in first type of CCD and $e_2=v(b_{ii})$ in second type of CCD

For example, in second type of CCD v=9, n_o=1, a_1=1, a_2=3.3569, e_2=0.0039 and in first type of CCD m_0=1, a=3.3636. e_1= 0.0093, lets us compare the relative efficiency of second type of CCD versus first type of CCD, if you get the equation (5.8) as 2.6099, then we conclude that the second type of CCD is more efficient than first type of CCD

5.3 Comparison in terms estimating the first order coefficient b_i

It can be discussed in the same process of the $V(b_i)$ by multiplying the scaling factor then $V(b_i)=\frac{\sigma^2}{(2^{t(v)}+2a_1^2+2a_2^2)}$ is to be multiplied by $1/g^2$ then we get $V(b_i)=\frac{\sigma^2}{(2^{t(v)}4v+n_0)}$ similarly the $V(b_i)$ is multiplied by scaling factor in first type of CCD the we obtained $V(b_i)=\frac{\sigma^2}{(2^{t(v)}+2v+n_0)}$ so finally we compare the relative efficiency of $E\left(\frac{\text{second type of CCD}}{\text{first type of CCD}}\right)$ and it obtained 1, then the efficiency of second type of CCD is more efficient than first type of CCD

6 Conclusion

In this paper, we have extended the results of for $9\leq v\leq 17$ using Kim [1] CCD plan in which the axial points are indicated by two numbers a_1 and a_2 and it is called as second type of CCD. The variance covariance of the estimated parameters are studied and we evaluated for the second type of CCD is most orthogonal for second order response surface designs and the results of the orthogonality are given in the Table 1.

The comparison between the second type of CCD versus first type of CCD for different coefficients are studied then we conclude that the second type of CCD is more efficient than first type of CCD. It is convenient to use the practical situations and give the more efficiency when compared to first type of CCD.

Competing Interests

Authors have declared that no competing interests exist.

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