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MODIFIED SECOND ORDER RESPONSE SURFACE DESIGNS USING CENTRAL COMPOSITE DESIGNS

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ABSTRACT

In this paper, modified second order response surface designs that provide more precise estimates of response surface rotatable designs using central composite designs (CCD) are studied. Construction of modified second order response surface designs using CCD for 2≤v≤17 (v: number of factors) are given. Modified second order rotatable CCD and modified equi-spaced doses second order rotatable CCD are also constructed.

Keywords: Modified second order response surface designs, modified second order rotatable designs (SORD), modified equi-spaced doses SORD.

INTRODUCTION

Investigation of input-output relationship is a useful activity in many situations. Fitting input-output relations to unorganized data involves complex computations and control of precession of estimates of response at desired points is not possible. An alternative is to use for fitting panned data obtained through appropriate designs. The concept of rotatability, which is very important in second order response surface, was introduced by Box and Hunter (1957) with the property that the variances of estimates of response at points equidistant from the centre of the design are all equal. Das and Narasimham (1962) constructed rotatable designs through balanced incomplete block designs (BIBD). Dey (1970) studied response surface designs with equi-spaced doses (levels). Several authors Draper and John (1988), Aggarwal and Bansal (1998) and Wu and Ding (1998) gave some designs for fitting response surface designs. Das *et al*. (1999) introduced modified response surface designs. Victorbabu and Vasundharadevi (2005) suggested modified second order response surface designs using BIBD. Victorbabu *et al*. (2006) suggested modified second order response surface designs, rotatable designs using pairwise balanced design.

In agricultural and other similar experiments any numbers of experimental units are available and any factorial combinations can be applied on them without much restriction. But in industrial experiments machines or some industrial/manufacturing processes are experimental units. The number of such units are limited. There is limitation on the choice of number of levels of factors involved in such experiments. Certain factors may not be allowed to have more than three levels while others also may have restrictions on number of levels. For example, if temperature is factor under study, may be that this factor is not allowed to have more than three levels. Some response surface designs obtained in this paper are suitable for experiments in such situations.

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In this paper, modified second order response surface designs that provide more precise estimates of response surface rotatable designs using central composite designs (CCD) are studied. Construction of modified second order response surface designs using CCD for 2≤v≤17 (v: number of factors) are given. Modified second order rotatable CCD and modified equi-spaced doses second order rotatable CCD are also constructed.

1. Conditions for second order rotatable designs

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

$$Y_u = b_0 + \sum_{i=1}^{v} b_i x_{iu} + \sum_{i=1}^{v} b_{ii} x_{iu}^2 + \sum_{i<j}\sum b_{ij} x_{iu} x_{ju} + e_u \quad (1.1)$$

where x_{iu} denotes the level of the ith factor (i =1,2,…,v) in the uth run (u =1,2,…,N) of the experiment, e_u's are uncorrelated random errors with mean zero and variance σ^2. D is said to be a SORD if the variance of the estimated response of $\hat{Y}_u$ from the fitted surface is only a function of the distance $(d^2 = \sum_i x_{iu}^2)$ of the point $(x_{1u}, x_{2u}, ..., x_{vu})$ from the origin (centre) of the design. Such a spherical variance function for estimation of second order response surface is achieved if the design points satisfy the following conditions [cf. Box and Hunter (1957), Das and Narasimham (1962)].

$$1. \sum_{u=1}^{N} \prod_{i=1}^{v} x_{iu}^{\alpha_i} = 0 \text{ if any } \alpha_i \text{ is odd, for } \sum \alpha_i \le 4 \quad (1.2)$$

$$2.(i) \sum_{u=1}^{N} x_{iu}^2 = \text{constant} = N\lambda_2 ,$$

$$(ii) \sum_{u=1}^{N} x_{iu}^4 = \text{constant} = cN\lambda_4 \text{, for all i} \quad (1.3)$$

3. $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = \text{constant} = N\lambda_4$, for $i \neq j$ (1.4)

4. $\sum_{u=1}^{N} x_{iu}^4 = c\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2$ (1.5)

5. $(c+v-1)\lambda_4 > v\lambda_2^2$ (1.6)

where c, λ_2 and λ_4 are constants and the summation is over the design points.

If the above-mentioned conditions are satisfied, the variances and covariances of the estimated parameters become,

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

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

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

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

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

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

and other covariances are zero.

2. Modified second order response surface designs using central composite designs

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 $\frac{1}{2^p}x2^v$ fractional factorial design (here $2^{t(v)} = \frac{1}{2^p}x2^v$ 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 (±a, ±a, … , ±a) and 2v axial points have coordinates of the form (±b, 0, …,0), (0, ±b, …,0), …, (0,0, …, ±b) etc., and n_0 central points. The usual method of construction of SORD 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, SORD need at least five levels (suitably coded) at 0, ±a, ±b for all factors $((0,0,...0)$-chosen centre of the design, unknown level 'a' and 'b' are to be chosen suitably to satisfy the conditions of the 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 $\sum x_{iu}^2 x_{ju}^2$ some equations involving the unknowns are obtained and their solution gives the unknown levels. In SORD the restriction used is $\sum x_{iu}^4 = 3\sum x_{iu}^2 x_{ju}^2$, i.e., c=3. Other restrictions are also possible though, it seems, not exploited well. We shall investigate the restriction $(\sum x_{iu}^2)^2 = N\sum x_{iu}^2 x_{ju}^2$, i.e., $\lambda_2^2 = \lambda_4$ to get another series of symmetrical second order response surface designs, which provide more precise estimates of response at specific points of interest than what is available from the corresponding existing designs. Further, the variances and covariances of the estimated parameters are,

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

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

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

$$V(\hat{b}_{ii}) = \frac{\sigma^2}{(c-1)N\lambda_4}$$

$$Cov(\hat{b}_0, \hat{b}_{ii}) = \frac{-\sigma^2}{N\sqrt{\lambda_4}(c-1)}$$

and other covariances are zero. These modifications of the variances and covariances affect the variance of the estimated response at specific points considerably. Using these variances and covariances, variance of estimated response at any point can be obtained. Let $\hat{y}_u$ denote the estimated response at the point $(x_{1u}, x_{2u}, ..., x_{vu})$. Then,

$$V(\hat{y}_u) = V(\hat{b}_0) + d^2\left[V(\hat{b}_i) + 2Cov(\hat{b}_0, \hat{b}_{ii})\right] + .$$

$$d^4 V(\hat{b}_{ii}) + (\sum x_{iu}^2 x_{ju}^2)\left[(c-3)\sigma^2/(c-1)N\lambda_4\right]$$

Construction of modified response surface designs is the same as for SORD except that instead of taking c=3 the restriction $(\sum x_{iu}^2)^2 = N\sum x_{iu}^2 x_{ju}^2$ is to be used and this condition will provide different values of the unknowns involved.

Theorem 2.1: A central composite design will be a v-dimensional modified second order response surface design in $N = \frac{(2^{t(v)}a^2 + 2b^2)^2}{2^{t(v)}a^4}$ design points, if

$(b/a)^2 = (\sqrt{N2^{t(v)}} - 2^{t(v)})/2.$

Proof: For the design points generated from central composite design the conditions in equations (1.2) to (1.6) are satisfied. The conditions in equations (1.3) and (1.4) are true as follows:

$$\sum x_{iu}^2 = 2^{t(v)}a^2 + 2b^2 = N\lambda_2 \quad (2.1)$$

$$\sum x_{iu}^4 = 2^{t(v)}a^4 + 2b^4 = cN\lambda_4 \quad (2.2)$$

$$\sum x_{iu}^2 x_{ju}^2 = 2^{t(v)}a^4 = N\lambda_4 \quad (2.3)$$

Using the modified condition $\lambda_2^2 = \lambda_4$, from equations (2.1) and (2.3) we get, $N = \frac{(2^{t(v)}a^2 + 2b^2)^2}{2^{t(v)}a^4}$. Alternatively N may be obtained directly as $N = 2^{t(v)} + 2v + n_0$, where $n_0 = \frac{(2^{t(v)}a^2 + 2b^2)^2}{2^{t(v)}a^4} - 2^{t(v)} - 2v$. From equations (2.1) and (2.3) using the modified condition, we have $(2^{t(v)}a^2 + 2b^2)^2 = N2^{t(v)}a^4$, which on simplification lead to $(b/a)^2 = (\sqrt{N2^{t(v)}} - 2^{t(v)})/2.$

Example: We illustrate the construction of the modified response surface design for v=4 factors in N=25 (here $n_0 = 1$) design points with the help of a central composite design. We have,

$$\sum x_{iu}^2 = 2^{t(v)}a^2 + 2b^2 = 16a^2 + 2b^2 = N\lambda_2$$

$$\sum x_{iu}^4 = 2^{t(v)}a^4 + 2b^4 = 16a^4 + 2b^4 = cN\lambda_4$$

$$\sum x_{iu}^2 x_{ju}^2 = 2^{t(v)}a^4 = 16a^4 = N\lambda_4$$

Using the modified condition $(\sum x_{iu}^2)^2 = N\sum x_{iu}^2 x_{ju}^2$, we have, $(16a^2 + 2b^2)^2 = 25x16a^4 = 400a^4$. Therefore $b^2 = 2a^2$. Now fixing 'a' conveniently 'b' is obtained. Thus the design as combinations of level codes is obtained along with $\sum x_{iu}^2$, $\sum x_{iu}^4$ and $\sum x_{iu}^2 x_{ju}^2$. For a=1, b=1.4142 and c=1.5. For a SORD, i.e., for c=3, $b^4 = 16a^4$. For a=1, b=2.00. It may be observed that as N changes for a modified response surface design, the ratio b/a also changes. Taking a=1 the variances of estimated responses at the central and axial points of interest for modified second order response surface design and SORD using central composite designs are presented in table 2.1 for 2≤v≤17. It is observed from table 2.1 that the variance of the estimated response at the central and axial points for modified second order response surface design is less than the variance of the estimated response for the second order rotatable central composite designs.

It can be seen that for this modified design both the conditions namely c=3 and $(\sum x_{iu}^2)^2 = N\sum x_{iu}^2 x_{ju}^2$ cannot be satisfied simultaneously. These can be a further series of designs which are both modified in the above sense and rotatable using both the restrictions c=3 and $(\sum x_{iu}^2)^2 = N\sum x_{iu}^2 x_{ju}^2$ together for fixed N design points.

3. Modified second order rotatable central composite designs

Consider the following set of points: (i) $2^{t(v)}$ (where $2^{t(v)}$ is Resolution V fraction of 2^v) points on cube viz., coordinates (±a, ±a, … , ±a)-repeated y_1 times, (ii) 2v axial points, viz., (±b, 0, …,0), (0, ±b, …,0), …, (0,0, …, ±b))-repeated y_2 times, (iii) n_0 central points, where y_1 and y_2 are chosen to satisfy the criterion of modified rotatability.

Theorem (3.1): The design points, $y_1(\pm a,\pm a,...,\pm a)2^{t(v)} \cup y_2(\pm b,0,0,...,0)2^1 \cup n_0$, will give a v-dimensional modified second order rotatable central composite design in $N = (2^{t(v)}a^2y_1 + 2b^2y_2)^2 / 2^{t(v)}a^4y_1$ design points, if

$$(b/a)^4 = (2^{t(v)}y_1 / y_2), \quad (3.1)$$

$$n_0 = \{(2^{t(v)}a^2y_1 + 2b^2y_2)^2 / 2^{t(v)}a^4y_1\} - y_1 2^{t(v)} - 2vy_2 \quad (3.2)$$

Proof: For the design points generated from central composite design the conditions in equations (1.2) to (1.6) are satisfied. The conditions in equations (1.3) and (1.4) are true as follows:

$$\sum x_{iu}^2 = 2^{t(v)}y_1a^2 + 2y_2b^2 = N\lambda_2 \quad (3.3)$$

$$\sum x_{iu}^4 = 2^{t(v)}y_1a^4 + 2y_2b^4 = 3N\lambda_4 \quad (3.4)$$

$$\sum x_{iu}^2 x_{ju}^2 = 2^{t(v)}y_1a^4 = N\lambda_4 \quad (3.5)$$

From equations (3.4) and (3.5), we have $2^{t(v)}y_1a^4 + 2y_2b^4 = 3x2^{t(v)}y_1a^4$, which on simplification lead to equation (3.1). Using the modified condition $\lambda_2^2 = \lambda_4$, from equations (3.3) and (3.5) we have, $(2^{t(v)}y_1a^2 + 2y_2b^2)^2 = Nx2^{t(v)}y_1a^4$, which leads to $N = (2^{t(v)}a^2y_1 + 2b^2y_2)^2 / 2^{t(v)}a^4y_1$. Alternatively N may be obtained directly as $N = 2^{t(v)}y_1 + 2vy_2 + n_0$, where $n_0 = \{(2^{t(v)}a^2y_1 + 2b^2y_2)^2 / 2^{t(v)}a^4y_1\} - y_1 2^{t(v)} - 2vy_2$. The modified second order rotatable central composite designs are presented in table 3.1 for 2≤v≤17 (taking a=1).

Table 2.1. Variances of estimated responses at the central and axial points for modified second order response surface design and SORD using central composite designs.

No. of factors v	t(v)	Number of design points (N)	Nature of points	Variance of the estimated response $(V(\hat{y})/\sigma^2)$	
				Modified design	SORD
2	2	9 ($n_0 = 1$)	Central Axial	0.555556 0.555556	1.000000 0.625000
3	3	14 ($n_0 = 0$)	Central Axial	0.585310 0.622036	84.926679 0.707102
4	4	25 ($n_0 = 1$)	Central Axial	0.360000 0.560000	0.999999 0.583333
5	4	26 ($n_0 = 0$)	Central Axial	0.356893 0.607768	3.499999 0.666666
6	5	44 ($n_0 = 0$)	Central Axial	0.308801 0.573599	33.970272 0.630602
7	6	78 ($n_0 = 0$)	Central Axial	0.272260 0.547089	4.500158 0.600000
8	6	80 ($n_0 = 0$)	Central Axial	0.236803 0.543210	8.388608 0.550000
9	7	146 ($n_0 = 0$)	Central Axial	0.215148 0.531835	1.027419 0.575111
10	7	148 ($n_0 = 0$)	Central Axial	0.192998 0.535010	3.476366 0.575108
11	7	150 ($n_0 = 0$)	Central Axial	0.174887 0.538128	66.078682 0.575124
12	8	280 ($n_0 = 0$)	Central Axial	0.163015 0.521909	0.437506 0.555556
13	8	282 ($n_0 = 0$)	Central Axial	0.150214 0.523607	0.833334 0.555556
14	8	284 ($n_0 = 0$)	Central Axial	0.139245 0.525287	1.999991 0.555555
15	8	286 ($n_0 = 0$)	Central Axial	0.129740 0.526950	8.502214 0.555556
16	8	289 ($n_0 = 1$)	Central Axial	0.114189 0.525952	0.999999 0.527778
17	8	290 ($n_0 = 0$)	Central Axial	0.114091 0.530224	9.499990 0.555556

4. Modified equi-spaced doses second order rotatable central composite designs

The modified SORD available is not generally available with equi-spaced levels. Though designs with equi-spaced levels are not necessary, they are likely to be preferred in view of the case in handling the doses. Further in modified SORD, the calculation of the actual doses often requires approximations and hence actual dose levels can not be applied in practice. For example, in Agriculture experiments, the factors may have equi-spaced doses (levels). The response surface designs with v-factors each having equi-spaced doses may be obtained using central composite type designs as follows.

Consider the following set of points: (i) $2^{t(v)}$ (where $2^{t(v)}$ is Resolution V fraction of 2^v) points on cube viz., coordinates (±a, ±a, … , ±a)-repeated y_1 times, (ii) 2v axial points, viz., (±b, 0, …,0), (0, ±b, …,0), …, (0,0, …, ±b)). The corresponding equi-spaced design of the composite type is obtained by changing the axial points from (±b, 0, …,0) etc., to (±2a, 0, …,0)-repeated y_2 times, (iii) n_0 central points, where y_1 and y_2 are chosen to satisfy the criterion of modified equi-spaced rotatable central composite type designs. Let the equi-spaced doses be –2, -1, 0, 1, 2.

Table 3.1. Modified second order rotatable central composite designs.

No. of factors v	t(v)	y_1	y_2	b^2	n_0	N
2	2	1	1	2.00	8	16
3	3	1	2	2.00	12	32
4	4	1	1	4.00	12	36
5	4	1	1	4.00	10	36
6	5	1	2	4.00	16	72
7	6	1	1	8.00	22	100
8	6	1	1	8.00	20	100
9	7	1	2	8.00	36	200
10	7	1	2	8.00	32	200
11	7	1	2	8.00	28	200
12	8	1	1	16.00	44	324
13	8	1	1	16.00	42	324
14	8	1	1	16.00	40	324
15	8	1	1	16.00	38	324
16	8	1	1	16.00	36	324
17	8	1	1	16.00	34	324

Table 4.1. Modified equi-spaced doses second order rotatable central composite designs.

No. of factors v	t(v)	y_1	y_2	n_0	N
2	2	4	1	16	36
3	3	2	1	14	36
4	4	1	1	12	36
5	4	1	1	10	36
6	5	1	2	16	72
7	6	1	4	24	144
8	6	1	4	16	144
9	7	1	8	16	288
10	7	1	8	0	288

Theorem (4.1): The design points, $y_1(\pm a,\pm a,...,\pm a)2^{t(v)} \cup y_2(\pm 2a,0,0,...,0)2^1 \cup n_0$, will give a v-dimensional modified equi-spaced doses second order rotatable central composite type design in $N = (2^{t(v)}y_1 + 8y_2)^2 / 2^{t(v)}y_1$ design points, if

$$(y_2 / y_1) = 2^{t(v)-4}\ , \qquad (4.1)$$

$$n_0 = \{(2^{t(v)}y_1 + 8y_2)^2 / 2^{t(v)}y_1\} - 2^{t(v)}y_1 - 2vy_2 \qquad (4.2)$$

Proof: For the design points generated from central composite design the conditions in equations (1.2) to (1.6) are satisfied. The conditions in equations (1.3) and (1.4) are true as follows:

$$\sum x_{iu}^2 = 2^{t(v)}y_1a^2 + 8y_2a^2 = N\lambda_2 \qquad (4.3)$$

$$\sum x_{iu}^4 = 2^{t(v)}y_1a^4 + 32y_2a^4 = 3N\lambda_4 \qquad (4.4)$$

$$\sum x_{iu}^2 x_{ju}^2 = 2^{t(v)}y_1a^4 = N\lambda_4 \qquad (4.5)$$

From equations (4.4) and (4.5), we have $2^{t(v)}y_1a^4 + 32y_2a^4 = 3x2^{t(v)}y_1a^4$, which on simplification lead to equation (4.1). Using the modified condition $\lambda_2^2 = \lambda_4$, from equations (4.3) and (4.5) we have, $(2^{t(v)}y_1a^2 + 2y_2a^2)^2 = Nx2^{t(v)}y_1a^4$, which leads to $N = (2^{t(v)}y_1 + 8y_2)^2 / 2^{t(v)}y_1$. Alternatively N may be obtained directly as $N = 2^{t(v)}y_1 + 2vy_2 + n_0$, where $n_0 = \{(2^{t(v)}y_1 + 8y_2)^2 / 2^{t(v)}y_1\} - 2^{t(v)}y_1 - 2vy_2$. The modified equi-spaced doses rotatable central composite designs are presented in table 4.1 for $2 \le v \le 10$.

CONCLUSIONS

This article gives some modified second order response surface designs that provide more precise estimates of response surface rotatable designs using central composite designs. Construction of modified second order response surface designs using central composite designs for $2 \leq v \leq 17$ are suggested. Further, modified second order rotatable central composite designs and modified equi-spaced doses second order rotatable central composite designs are constructed. The results obtained are provided in Tables 2.1, 3.1, and 4.1 respectively.

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