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On Construction of Three Level Variance-Sum Second Order Slope Rotatable Designs

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Abstract: Response Surface Methodology (RSM) is a collection of mathematical and statistical techniques useful for analyzing experiments where the yield is believed to be influenced by one or more controllable factors. Box and Hunter (1957) introduced rotatable designs in order to explore the response surfaces. The analogue of Box-Hunter rotatability criterion is a requirement that the variance of $\partial\hat{y}(x)/\partial x_i$ be constant on circles (v=2), spheres (v=3) or hyper spheres (v ≥ 4) at the design origin. These estimates of the derivatives would then be equally reliable for all points $(x_1, x_2, \ldots, x_v)$ equidistant from the design origin. This property is called as slope rotatability (Hader and Park (1978)). Anjaneyulu et al (1997) established that SOSRD (OAD) has the additional interesting property that the sum of the variance of estimates of slopes in all axial directions at any point is a function of the distance of the point from the design origin. In this paper we made an attempt to construct Variance-Sum Second Order Slope Rotatable in three levels.
Keywords: Response Surface Methodology. Second Order Slope Rotatable Design (SOSRD); SOSRD (OAD), Variance-Sum Second Order Slope Rotatable Design.

I. INTRODUCTION

Response Surface Methodology (RSM) is a collection of mathematical and statistical techniques useful for analyzing experiments where the yield is believed to be influenced by one or more controllable factors. Experimenters are required to make choices of the experimental designs before the actual experiments to avoid incurring more experimental costs. Therefore, an experimental design must be selected prior to experimentation.

Box and Hunter (1957) suggested that these types of experimental designs are suitable for such experimentations and called them rotatable designs. Several authors studied several experimental designs some of which can be applied in food or chemical companies to test ingredients, prepare and reformulate a new food product or even to optimize the conditions leading to an optimal process and perhaps more important in estimating rate of change of a given response.

Designs for fitting first-degree models are called first-order designs and those for fitting second-degree models are referred to as second-order designs. Some of these designs are; full factorial design, fractional factorial designs, saturated designs; central composite designs, slope rotatable designs etc,. In this context, Box and Hunter (1957) introduced rotatable designs in order to explore the response surfaces.

Bose and Draper (1959) gave a method of constructing second order rotatable designs in three dimensions. There was need to have a general method for construction of second order rotatable designs in four or more dimensions and Draper (1960) provided the method, where he constructed second order rotatable designs in three dimensions and gave the conditions for existence of second order rotatable designs in k-dimensions.

Herzberg (1967) came up with an alternative method of constructing second order rotatable designs in k-dimensions. When comparing Herzberg's method with Draper's method, Herzberg's method gave designs with very large number of points but there were no conditions to be satisfied like the case in Draper's method.

Gardiner et al., (1959) gave both the moments and the non-singularity conditions for third order rotatability. Their work was followed by Patel and Arap Koske (1985) who also gave the moments and the non-singularity conditions for fourth order rotatability. Njui and Patel (1988) gave the moments and non-singularity conditions for fifth order rotatability. Since then, different authors have constructed several second, third and fourth order rotatable designs in different dimensions. Huda (1982a, 1982b) gave an alternative method of constructing some third order rotatable designs. Arap koske and Patel (1986) constructed a fourth order rotatable design in three dimensions.

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II. ROTATABLE DESIGNS

Let v factor affect the yield and suppose the yield Y satisfies the functional relation

$$Y = f\left(x_1, x_2, \ldots, x_v\right) + e$$

Where $x_1, x_2, \ldots, x_v$ are the levels of the 'v' factor used for getting that response. We assume that 'f' can be represented adequately in a small region of interest by polynomial of degree d.

The estimates of the coefficients in the polynomial f1 can be obtained by the method of least squares. It was observed by Box and Hunter (1957) that, instead of considering the variances of individual coefficients, the accuracy of the estimated response at a point ($x_1, x_2, \ldots, x_v$) should provide a criterion of the selection of design.

Definition: A 'v'- dimensional design of order 'd' is said to be a rotatable design if the variance of the estimated response at the point($x_1, x_2, \ldots, x_v$) is function of the square of the distance of the point from a suitable origin, so that variances of all estimated responses at points equidistant from the origin are the same, By using the properties of the spherical distribution Box and Hunter(1957) given conditions for the N-design points to form a second order rotatable design.

III. SECOND ORDER ROTATABLE DESIGN (SORD)

The design points have to be so chosen that they satisfy the following conditions to form SORD.

i) $\sum x_i, \sum x_i x_j, \sum x_i^2 x_j, \sum x_i^3, \sum x_i x_j x_k, \sum x_j x_k, \sum x_i^3 x_j,$

$\sum x_i x_j x_k x_l$ etc., $i \neq j \neq k \neq l$

are equal to zero. That is, all some of products in which at least one of the x's is with an odd power are zero.

(ii) $\sum x_i^2$ = Constant = $N\lambda_2$, say that is same for each factor.

(iii) $\sum x_i^4$ = Constant = $aN\lambda_4$

(iv) $\sum x_i^2 x_j^2$ = Constant = $N\lambda_4$ for $i \neq j$

(v) $\sum x_i^4 = 3\sum x_i^2 x_j^2 \quad (a = 3)$

(vi) $(\lambda_4 / \lambda_2^2) > v/(v+2)$ . . . (2)

All the summations in the above expressions are over the design points. An inspection of the variance of least squares estimate b_0 shows that a necessary condition for the existence of a second order design is $[\lambda_4(v+2) - v\lambda_2^2] > 0.$ this actually leads to the condition above.

IV. SLOPE ROTATABLE DESIGNS

The essence of Box and Hunter rotatability is that by imposing certain restrictions on the moment matrix of the design it is possible to make estimates of the responses equally good for all combinations of the independent variables at the same distance from the design centre. Suppose now that the objective of the analysis is to estimate the first derivatives (slopes) of the second order surface.

$$y(x) = b_0 + \sum b_i x_i + \sum b_i x_i^2 + \sum_{i \neq j}\sum b_{ij} x_i x_j \quad \ldots(3)$$

with respect to each of the independent variables i.e.,

$$\frac{\partial \hat{y}(x)}{\partial x_i} = \hat{b}_i + 2\hat{b}_{ii} x_i + \sum_j \hat{b}_{ij} x_j \quad \ldots(4)$$

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The variance of the derivative is a function of the point $(x_1, x_2, ..., x_v)$ at which the derivative is estimated and is also a function of the experimental design through the familiar relationship Var $(\hat{b}) = \sigma^2 (x'x)^{-1}$, where x is the moment – matrix of the design. The analogue of Box-Hunter rotatability criterion is a requirement that the variance of $\partial\hat{y}(x)/\partial x_i$ be constant on circles (v=2), spheres (v=3) or hyperspheres (v ≥ 4) at the design origin. These estimates of the derivatives would then be equally reliable for all points $(x_1, x_2, ..., x_v)$ equidistant from the design origin. This property is called as slope rotatability (Hader and Park (1978)) and we refer Box-Hunter rotatability property as $\hat{y}$ – rotatability.

V. SECOND ORDER SLOPE ROTATABLE DESIGNS (SOSRD)

The object of the slope rotatability is to estimate the first order partial derivatives of (1) with respect to each of the independent variables with certain desirable properties.

In addition to the symmetry conditions in SORD (Conditions (i), (ii) and (iii) and the non-singularity condition (v)), the following slope-rotatability condition (parallel to condition iv in SORD) should be satisfied.

$$\lambda_4\left[v(5-a)-(a-3)^2\right]+\lambda_2^2\left[v(a-5)+4\right]=0 \qquad ...(5)$$

The symmetry conditions and non-singularity conditions are one and the same in both the cases of rotatability i.e., Box-Hunter (BH) rotatability and Hader-Park (HP) slope rotatability. But the condition a=3 of BH rotatability, condition (iv) of (2) is replaced by the Condition (3) in HP slope rotatability.

VI. VARIANCE-SUM SECOND ORDER SLOPE ROTATABLE DESIGNS

Anjaneyulu et al(1997) established that SOSRD(OAD) has the additional interesting property that the sum of the variance of estimates of slopes in all axial directions at any point is a function of the distance of the point from the design origin

i.e $$\sum V\left[\frac{\partial \hat{y}}{\partial X_i}\right] = f(\rho^2) \text{ where } \rho^2 = \sum_{i=1}^{u} X_{iu}^2 \qquad ......(6)$$

proof: In any general v-factor symmetric second order response surface design D=((Xij))i=1,2,…N, j=1,2,…v satisfying the conditions defined by park (1987), we have from VictorBabu and Narasimham(1991).

$$V\left[\frac{\partial \hat{y}}{\partial x_i}\right] = V(\hat{b}_i) + 4x_i^2 V(\hat{b}_{ii}) + \lim_{x\to\infty}\sum\left[\sum x_j^2 V(\hat{b}_{ij})\right]$$

$$......(7)$$

$$\sum_{i=1}^{v} V\left[\frac{\partial \hat{y}}{\partial x_i}\right] = \sum V(\hat{b}_i) + 4\sum_{i=1}^{v} x_i^2\left[V(\hat{b}_{ii})\right] + \sum\left[\sum x_j^2 V(\hat{b}_{ij})\right]$$

$$= V(V(\hat{b}_i)) + 4\left[V(\hat{b}_{ii})\right]\sum x_i^2 + \left[V(\hat{b}_{ij})\right](V-1)\sum x_i^2$$

$$= V(V(\hat{b}_i)) + 4\left[V(\hat{b}_{ii})\right]\rho^2 + \left[V(\hat{b}_{ij})\right](V-1)\rho^2$$

$$= f(\rho^2)$$

The sum of the variances of the slopes in axial directions at any point is a function of the distance of the point from the design origin.

Any symmetric second order response surface design is a SOSRD (OAD). Hence every SOSRD (OAD) has the additional property that the trace of the dispersion matrix estimates of slopes in all directions has a type of variance – sum second order slope rotatability property. Hence we may also call these designs as VARIANCE SUM SOSRDs

VII. CONSTRUCTION OF VARIANCE SUM SECOND ORDER SLOPE ROTATABLE DESIGNS

The Consider design Points are

$$\left[\frac{1}{2}S(\pm\beta,\pm\beta,0)+S(\gamma_{1,}0,0)+S(\gamma_2,0,0)\right]$$

β	β	0
–β	β	0
β	0	β
β	0	– β
0	β	β
0	β	– β
$+\gamma_1$	0	0
$-\gamma_1$	0	0
0	$+\gamma_1$	0
0	$-\gamma_1$	0
0	0	$+\gamma_1$
0	0	$-\gamma_1$
γ_2	0	0
$-\gamma_2$	0	0
0	$+\gamma_2$	0
0	$-\gamma_2$	0
0	0	$+\gamma_2$
0	0	$-\gamma_2$

.............(8)

The above design points are formed as three level design points. The moment condition of a Variance-Sum Second Order Slope Rotatable Designs are

(i) $\sum_{u=1}^{18} x_{iu}^2 = 4\beta^2 + 2\gamma_1^2 + 2\gamma_2^2 = 18\lambda_2$ …………(9)

(ii) $\sum_{u=1}^{18} x_{iu}^4 = 4\beta^4 + 2\gamma_1^4 + 2\gamma_2^4 = 54\lambda_4$ ………..(10)

(iii) $\sum_{u=1}^{18} x_{iu}^2 x_{ju}^2 = 2\beta^4 = 18\lambda_4$ ……(11)

Such that

Let $\gamma_1^2 = x\beta^2 \; and \gamma_2^2 = y\beta^2$ …..(12)

$$x^2 + y^2 - 1 = 0$$

$$\Rightarrow y = \sqrt{1 - x^2},$$

Where,

$$-1 \le x \le 1,$$

Let x = 0.5 then y = 0.866025. ……(13)

The value of x is chosen such that it lies with in the design existence interval.

Substituting the values of x=0.5 and y = 0.866025 to (9) which gives

γ_1=0.25β and γ_2= 0.930604β where β =1.

The considered design Points forms Variance-sum Second Order Slope Rotatable arrangement for the constant values given in (4) in three dimensions. Thus, substituting the variables in (10) to (12) gave;

$$\lambda_2 = 0.325392\beta^2 \text{ and } \lambda_4 = 0.111111\beta^4 \quad \text{….(14)}$$

Substituting the above values in slope rotatable conditions are gave;

$$\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2} = 0.6 \quad \text{….. (15)}$$

Therefore, the non-singularity condition is also satisfied. Therefore the considered design points are Variance-Sum Second Order Slope Rotatable design in three dimensions.

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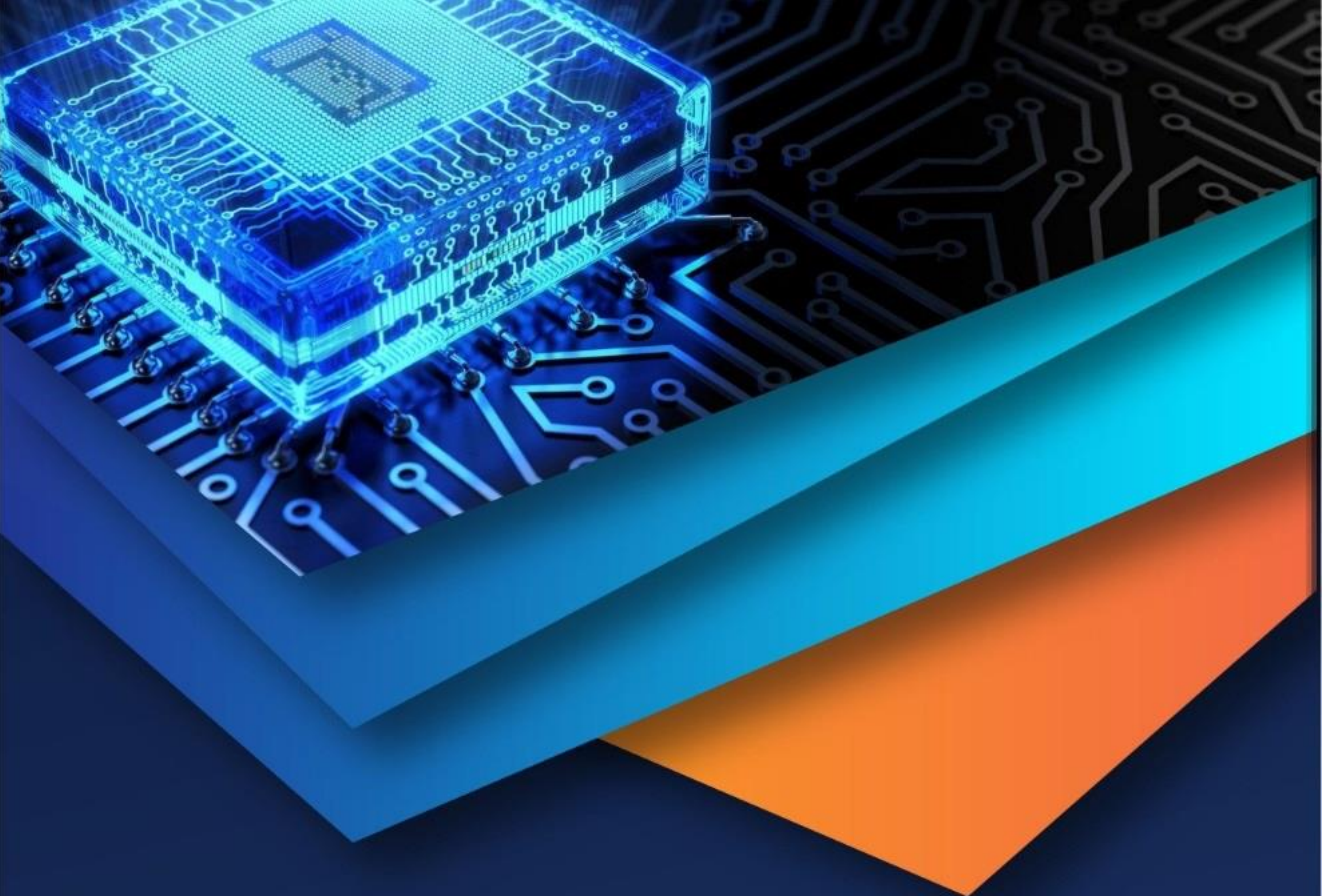

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