Construction of Third Order Slope Rotatable Designs Using Symmetrical Unequal Block Arrangements with Two Unequal Block Sizes

P.Seshu Babu and M.Lakshimi Prasanna

Department of Mathematics and Statistics,
Kakaraparti Bhavanarayana College (Autonomous) Kothapeta, Vijayawada – 520 001. (A.P.), INDIA.

ABSTRACT

Response Surface Methodology (RSM) finds utility in various fields, including Chemical, Physical, Meteorological, Industrial, and Biological applications. Estimating the slope of the response surface is a common task for experimenters. Understanding how the response surface changes, such as the effects of different fertilizers on crop yield or variations in chemical experiments, is of great interest. When a second-order response model isn't suitable for the design points, researchers continue the experiment to fit a third-order response surface. In certain Industrial and Meteorological applications, higher-order response surface designs become necessary. Gardiner et al. (1959) introduced third-order rotatable designs to explore response surfaces. Anjaneyulu et al. (1994-1995) developed Third Order Slope Rotatable Designs (TOSRD) using doubly balanced incomplete block designs. Anjaneyulu et al. (2001) introduced TOSRD with central composite type design points. Seshu Babu et al. (2011) investigated modified methods for constructing TOSRD using central composite designs. Seshu Babu et al. (2014) devised TOSRD using balanced incomplete block designs. Recognizing the broad applicability of third-order models in RSM and the significance of slope rotatability, this endeavor focuses on constructing TOSRD using symmetrical unequal block arrangements with two unequal block sizes.

Keywords and phrases: Third Order Slope Rotatable Designs, Symmetrical Unequal Block Arrangements with Two Unequal Block Sizes.

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1.1 INTRODUCTION

In 1957, Box and Hunter established that a design of order d (where d = 1, 2) is rotatable if and only if the moments of the independent variables match those of a spherical distribution up to order 2d or if these moments remain unchanged when rotated around its center. Gardiner et al. (1959) devised some third-order rotatable designs for two and three factors. Draper (1960a, b) expanded upon this by creating additional third-order rotatable designs in three and four dimensions. Das (1961) contributed to the field by producing new Third Order Rotatable Designs (TORD) involving up to eight factors. Das and Narasimham (1962) developed both sequential and non-sequential TORD up to fifteen factors, employing Doubly Balanced Incomplete Block Designs (BIBD) and complementary BIBD.

Several researchers shifted their focus from rotatability to slope rotatability. Hader and Park (1978) introduced slope rotatability for central composite designs. Victor Babu and Narasimham (1990) conducted a comprehensive study of Second Order Slope Rotatable Designs (SOSRD) and proposed various methods for their construction. Anjaneyulu et al. (1994-1995) explored the construction of Third Order Slope Rotatable Designs (TOSRD) using Doubly BIBD. Anjaneyulu et al. (2001) introduced and constructed TOSRD using Central Composite Designs (CCD). Seshu Babu et al. (2011) examined modified techniques for constructing TOSRD using CCD. Seshu Babu et al. (2015) constructed TOSRD using BIBD.

In practical scenarios, estimating the response surface is a crucial task for experimenters. Various methods are employed to estimate the rates of change of the response surface, such as the yield of different crops under various fertilizers and chemical experiments. In the fields of chemical, physical, meteorological, industrial, and biological research, higher-order response surface designs are necessary. Given the wide applicability of third-order models in Response Surface Methodology (RSM) and the significance of slope rotatability, this study suggests the use of symmetrically unequal block arrangements with two different block sizes for constructing TOSRD.

2.1 THIRD ORDER SLOPE ROTATABLE DESIGNS

(*c.f.* Anjaneyulu *et al* (2001))

The general Third Order Response surface is

$$\boldsymbol{y(x) = b_0 + \sum_{i=1}^{v} b_i\, x_i + \sum_{i<}^{v}\sum_{j}^{v} b_{ij}\, x_i\, x_j + \sum_{i=1}^{v} b_{ii}\, x_i^2 + \sum_{i=1}^{v} b_{iii}\, x_i^3 + \sum_{i\neq}^{v}\sum_{j}^{v} b_{ijj}\, x_i x_j^2 + \sum_{i<}^{v}\sum_{j<}^{v}\sum_{k}^{v} b_{ijk}\, x_i\, x_j x_k + e} \qquad \ldots(2.1)$$

where e's are independent random errors with same mean zero and variance σ^2.

Let D=((x_{iu})), i=1,2,3,. . .,v; u=1,2,3,. . .,N be a set of N design points to fit the third order response surface in(2.1).

Definition of TOSRD:

A general Third Order Response Surface Design D is said to be a Third Order Slope Rotatable Design (TOSRD) if from this design D, the variance of the estimate of first order partial derivative of y(x) with respect to each of independent variables (x_i) is only a function of the distance ($d^2=\sum_{i=1}^{v} x_i^2$) of the point ($x_1,x_2,x_3,\ldots,x_v$) from the origin(center), *i.e.*, a third order response surface design is a TOSRD if

$$V\left[\frac{\partial \hat{y}}{\partial x_i}\right] = f(d^2); \forall \ i=1,2,3,\ldots,v \qquad \ldots(2.2)$$

3.1 CONDITIONS FOR THIRD ORDER SLOPE ROTATABILITY

Symmetry Assumptions

A: All sums of products in which at least one of the x's with an odd power are zero.

B: (i) $\sum x_i^2 = N\lambda_2$ = Constant

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

(iii) $\sum x_i^6 = bN\lambda_6$ = Constant

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

(v) $\sum x_i^2 x_j^4 = cN\lambda_6$ = Constant for $i \neq j$

(vi) $\sum x_i^2 x_j^2 x_k^2 = N\lambda_6$ = Constant for $i \neq j \neq k$ …(3.1)

Slope Rotatability Conditions

C: **(i)** $V(\hat{b}_{ijk}) + 2\, Cov(\hat{b}_{iij}, \hat{b}_{jkk}) - 2\, V(\hat{b}_{iij}) = 0$

$\Rightarrow (c-3)\,\Delta_1 = 0$ where $\Delta_1 \neq 0$

$\therefore c = 3$

(ii) $\{4\, V(\hat{b}_{iii}) + 6\, Cov(\hat{b}_{i}, \hat{b}_{ijj})\} = V(\hat{b}_{ij}) + 2Cov(\hat{b}_{i}, \hat{b}_{ijj})$

$$\Rightarrow \Delta_1[\lambda_4[v(5-a) - (a-3)^2] + \lambda_2^2[v(a-5) + 4]]$$

$$-\Delta[2(a-1)\lambda_4^2[9a(v+1) - 9(v-1) + 3a - b]] = 0$$

Where $\Delta = [(a+v-1)\lambda_4 - v\lambda_2^2] > 0$

$$\Delta_1 = [\lambda_2\lambda_6\{b(v+1) - 9(v-1)\} - \lambda_4^2\{a^2(v+1) - (6a-b)(v-1)\}] > 0$$

(iii) $V(\hat{b}_{iij}) = 9\, V(\hat{b}_{iii})$

$$\Rightarrow [\lambda_2\lambda_6\{v(b-27)\} - \lambda_4^2\{a^2v - 6a(v-2) + b(v-2) - 18(v-1)\}] = 0$$

(iv) $V(\hat{b}_{iij}) + 3Cov(\hat{b}_{iij}, \hat{b}_{jkk}) = 0$

$$\Rightarrow [\lambda_2\lambda_6\{v(b-9)\} - \lambda_4^2\{a^2v - 6a(v-2) + b(v-2) - 6a\}] = 0 \qquad \ldots(3.5)$$

Non-Singularity Conditions

D: **(i)**

$$\frac{\lambda_4}{\lambda_2^2} > \frac{v}{(a+v-1)}$$

(ii)

$$\frac{\lambda_2\lambda_6}{\lambda_4^2} > \frac{a^2\{(v+1) - (6a-b)(v-1)\}}{\{b(v+1) - 9(v-1)\}}$$

…(3.6)

Where a,b,c, λ_2, λ_4 and λ_6 are constants and the summation is over the design points.

4.1 TOSRD USING SYMMENTRICAL UNEQUAL BLOCK ARRANGEMENTS (SUBA) WITH TWO UNEQUAL BLOCK SIZES

The arrangement of v- treatments in b blocks where b_1 blocks of size k_1 and b_2 blocks of size k_2 is said to be a symmetrical unequal block arrangement with two unequal block sizes , if

(i) Every treatment occurs b_ik_i/v blocks of size k_i (i = 1,2) and (ii)Every pair of first-associate treatments occurs together in u blocks of size k_1 and in (λ - u) sets of size k_2 and every pairof second-associate treatments occurs together in λ blocks of size k_2.

(ii) From (i) each treatment occurs $[(b_1k_1)/v]+[(b_2k_2)/v] = r$ blocks in all. Note that are known as the parameters of the SUBA with two unequal block sizes. (c.f. Raghavarao 1971).

"(v, b, r, k_1, k_2, b_1, b_2, λ)" represents a SUBA (Symmetrically Unequal Block Arrangement) design with two unequal block sizes.

"$2^{t(k)}$" denotes a fractional replicate of 2^k in ±1 levels, where no interaction with fewer than five factors is confounded.

"[1- (v,b,r,k_1,k_2 ,b_1,b_2, λ)] " represents the design points generated from the transpose of the incidence matrix of the SUBA with two unequal block sizes.

[1- (v,b,r,k_1,k_2 ,b_1,b_2, λ)] $2^{t(k)}$ are the $b2^{t(k)}$design points generated from the SUBA with two unequal block sizes through "multiplication."

The text mentions choosing additional unknown combinations (α, α, α, α, α, α) and multiplying them by $2^{t(v)}$ associated combinations (or a suitable fraction of 2^{v} associated combinations) to obtain $2^{t(v)}$ additional design points.

These design points generated through the SUBA with two unequal block sizes are then used to construct third-order slope rotatable designs using the same SUBA with two unequal block sizes.

The design points,

$$[1- (v,b,r,k_1,k_2 ,b_1,b_2, \lambda)]\ 2^{t(k)} \cup (\alpha , \alpha, \alpha, \alpha, \alpha , \alpha)2^{t(v)}$$

Indeed create a v-dimensional third-order slope rotatable design using a SUBA (Symmetrically Unequal Block Arrangement) with two unequal block sizes, the total number of design points (N) is calculated as:

$$N = b2^{t(k)} + 2^{t(v)} \qquad \ldots(4.1)$$

For these design points

(i) $\sum x_i^2 = 2^{t(v)}\alpha^2 + r2^{t(k)} = N\lambda_2$

(ii) $\sum x_i^4 = 2^{t(v)}\alpha^4 + r2^{t(k)} = aN\lambda_4$

(iii) $\sum x_i^6 = 2^{t(v)}\alpha^6 + r2^{t(k)} = bN\lambda_6$

(iv) $\sum x_i^2 x_j^2 = 2^{t(v)}\alpha^4 + \lambda\, 2^{t(k)} = N\lambda_4$

(v) $\sum x_i^2 x_j^4 = 2^{t(v)}\alpha^6 + \lambda\, 2^{t(k)} = cN\lambda_6$

(vi) $\sum x_i^2 x_j^2 x_k^2 = 2^{t(v)}\alpha^6 + (\lambda -1)\, 2^{t(k)} = N\lambda_6 \qquad \ldots(4.2)$

The design points satisfy all the symmetry assumptions (A) and (B) in (3.1). We solve the equations C(i) to C(iv) in (3.5) subject to (3.6).

Example (4.1)

To construct the TOSRD with SUBA blocks of unequal sizes, the following design points must be considered:

$$[1- (6,7,3,2,3,3,4,1)\ ]\ 2^{t(6)} \cup (\alpha , \alpha, \alpha, \alpha, \alpha , \alpha)2^{t(3)}$$

Thus we get $N = b2^{t(k)} + 2^{t(v)} = 88$ design points.

For the above design points we have

(i) $\sum x_i^2 = 32\alpha^2 + 24 = N\lambda_2$

(ii) $\sum x_i^4 = 32\alpha^4 + 24 = aN\lambda_4$

(iii) $\sum x_i^6 = 32\alpha^6 + 24 = bN\lambda_6$

(iv) $\sum x_i^2 x_j^2 = 32\alpha^4 + 8 = N\lambda_4$

(v) $\sum x_i^2 x_j^4 = 32\alpha^6 + 8 = cN\lambda_6$

(vi) $\sum x_i^2 x_j^2 x_k^2 = 32\alpha^6 = N\lambda_6$ …(4.3)

By solving the TOSRD conditions C(i) to C(iv) of (3.5) using (4.3), we get

$\alpha^2 = 0.5$

From (i),(iv) and (vi) of (4.3) we will get λ_2, λ_4 and λ_6

$\lambda_2 = 0.454545$, $\lambda_4 = 0.181818$ and $\lambda_6 = 0.045455$

From (ii,iv), (iii,vi) and (v,vi) of (4.3) we have a, b and c

a = 2, b = 7 and c = 3.

The statement "It can be verified that non-singularity conditions (i) and (ii) of (3.6) are satisfied" implies that conditions (i) and (ii) as specified in equation (3.6) have been assessed and found to be met.

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