CUBIC RESPONSE SURFACE DESIGNS USING BIBD IN FOUR DIMENSIONS

P.Seshu Babu,[2] A.V.Dattatreya Rao[1] , G.V.S.R. Anjaneyulu[1] and K.Srinivas[3]

[1]Department of Statistics, Acharya Nagarjuna University,
Guntur- 522 510.(A.P),INDIA.
[2]Department of Science & Humanities, Sri Vasavi Institute of Engineering & Technology, Nandamuru, Padana Mandal, Krishna District – 521 369 (A.P), INDIA.
[3] Department of Statistics, Andhra Loyola College, Vijayawada-520008.

ABSTRACT

Response Surface Methodology (RSM) has applications in Chemical, Physical, Meteorological, Industrial and Biological fields. The estimation of slope response surface occurs frequently in practical situations for the experimenter. The rates of change of the response surface, like rates of change in the yield of crop to various fertilizers, to estimate the rates of change in chemical experiments etc. are of interest. If the fit of second order response is inadequate for the design points, we continue the experiment so as to fit a third order response surface. Higher order response surface designs are sometimes needed in Industrial and Meteorological applications. Gardiner et al (1959) introduced third order rotatable designs for exploring response surface. Anjaneyulu et al (1994-1995) constructed third order slope rotatable designs using doubly balanced incomplete block designs. Anjaneyulu et al (2001) introduced third order slope rotatable designs using central composite type design points. Seshu babu et al (2011) studied modified construction of third order slope rotatable designs using central composite designs. Seshu babu et al (2014) constructed TOSRD using BIBD. In view of wide applicability of third order models in RSM and importance of slope rotatability, we introduce A Cubic Slope Rotatable Designs Using BIBD in four dimensions.

KEYWORDS AND PHRASES:

Third Order Slope Rotatable Design, Balanced Incomplete Block Designs.

1. INTRODUCTION

Box and Hunter (1957) proved that a necessary and sufficient condition for a design of order d (d =1, 2) to be rotatable is that the moments of the independent variable be the same, through order 2d, as those of a spherical distribution or that these moments be invariant under a rotation around its centre. Gardiner *et al* (1959) obtained some third order rotatable designs for two and three factors. Draper (1960a, b) obtained some further third order rotatable designs in three and four dimensions. Das (1961) also obtained some new Third Order Rotatable Designs (TORD) up to eight factors. Das and Narasimham (1962) constructed TORD both sequential and non sequential, up to fifteen factors, using Doubly Balanced Incomplete Block Designs (BIBD) and complementary BIBD.

Several authors diverted their attention from rotatability to slope rotatability. Hader and Park (1978) introduced slope rotatability for central composite type. Victor Babu and Narasimham (1990) studied Second Order Slope Rotatable Designs (SOSRD) in detail and suggested several methods for construction of SOSRD. Anjaneyulu *et al* (1994-1995) studied construction of TOSRD through Doubly BIBD. Anjaneyulu *et al* (2001) introduced and constructed TOSRD using Central Composite Designs (CCD). Seshu babu *et al* (2011) studied modified construction of TOSRD using CCD. Seshu babu *et al* (2014) constructed TOSRD using BIBD.

As the estimation of response surface occur frequently in practical situations for the experimenter. The rates of change of the response surface, like rates of change in the yields of a crop to various fertilizers, to estimate the rates of change in chemical experiments etc. Higher order response surface designs needed in Chemical, Physical, Meteorological, Industrial and Biological fields. In view of wide applicability of third order models in RSM and importance of slope rotatability we introduce construction of TOSRD using BIBD.

2.1 THIRD ORDER SLOPE ROTATABLE DESIGNS

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

The general Third Order Response surface is

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

…(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 $V\left[\frac{\partial \hat{y}}{\partial x_i}\right]=f(d^2)$; ∀ i=1,2,3,...,N …(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)

For a design satisfying the above symmetry assumptions of the normal equations of (2.1) reduce the following

$$\sum y = Nb_0 + N\lambda_2(b_{11} + b_{22} + b_{33} + \cdots + b_{vv})$$
$$= Nb_0 + B_0 N\lambda_2 \quad \text{where } B_0 = (b_{11} + b_{22} + b_{33} + \cdots + b_{vv})$$
$$\sum x_i y = b_i \sum x_i^2 + b_{iii} \sum x_i^4 + \sum_j (b_{ijj} \sum x_i^2 x_j^2)$$
$$= b_i N\lambda_2 + b_{iii} N\lambda_2 + b_{ijj}\, aN\lambda_4$$
$$\sum x_i x_j y = b_i \sum x_i^2 x_j^2$$
$$= b_{ij} N\lambda_4$$
$$\sum x_i^2 y = b_0 + \sum x_i^2 + b_{ii} \sum x_i^4 + \sum (b_{jj} \sum x_i^2 x_j^2)$$
$$= b_0 N\lambda_2 + b_{ii}\, a\, N\lambda_4 + b_{ijj}\, aN\lambda_4 + \sum b_{jj} N\lambda_4$$
$$\sum x_i^4 y = b_i + \sum x_i^4 + b_{iii} \sum x_i^6 + \sum (b_{ijj} \sum x_i^4 x_j^2)$$
$$= b_i N\lambda_4 + b_{iii}\, b\, N\lambda_6 + \sum b_{ijj}\, cN\lambda_6$$
$$\sum x_i x_j^2 y = b_i \sum x_i^2 x_j^2 + b_{iii} \sum x_i^4 x_j^2 + b_{ijj} \sum x_i^4 x_j^2 + b_{ikk} \sum x_i^2 x_j^2 x_k^2$$
$$= b_i N\lambda_2 + b_{iii}\, c\, N\lambda_6 + b_{ijj}\, cN\lambda_6 + b_{ikk} N\lambda_6$$
$$\sum x_i^2 x_j y = b_i \sum x_i^2 x_j^2 + b_{jjj} \sum x_i^2 x_j^4 + b_{iij} \sum x_i^4 x_j^2 + b_{jkk} \sum x_i^2 x_j^2 x_k^2$$
$$= b_j N\lambda_2 + b_{jjj}\, c\, N\lambda_6 + b_{iij}\, cN\lambda_6 + b_{jkk} N\lambda_6$$
$$\sum x_i x_j x_k y = b_{ijk} \sum x_i^2 x_j^2 x_k^2$$
$$= b_{ijk} N\lambda_6 \qquad \ldots(3.2)$$

By solving the above normal equations under the symmetry assumptions, we get,

$\widehat{b_0}$ = [(a+v-1) $\lambda_4 \sum y$ - $\lambda_2 \sum\sum x_i^2 y]/(N\delta)$

$$\widehat{b_\iota} = \frac{\lambda_6\{b(c+v-2)-c^2(v-1)\}\sum x_i y}{N\delta_1} - \frac{\lambda_4\{a(c+v-2)-c(v-1)\}\sum x_i^3 y}{N\delta_1} + \frac{\lambda_4(ac-b)\sum x_i x_j^2 y}{N\delta_1} + \frac{\lambda_4(v-2)(ac-b)\sum\sum x_i x_j^2 y}{N\delta_1}$$

$$\widehat{b_{\iota\iota}} = \frac{\sum x_i^2\, y}{(a-1)N\lambda_4} - \frac{\lambda_2\lambda_4(a-1)\sum y - \sum(\sum x_i^2\, y)(\lambda_2^2-\lambda_4)}{(a-1)N\lambda_4\delta}$$

$$\widehat{b_{\iota J}} = \frac{\sum x_i x_j\;\; y}{N\lambda_4}$$

$$\widehat{b_{\iota\iota\iota}} = \frac{-\lambda_6\{a(c+v-2)-c(v-1)\}\sum x_i y}{N\delta_1} + \frac{\{\lambda_2\lambda_6(c+v-2)-\lambda_2^2(v-1)\sum x_i^3 y}{N\lambda_6\delta_1} - \frac{\{c\lambda_2\lambda_6-a\lambda_4^2\}\sum x_i x_j^2 y}{N\lambda_6\delta_1} - \frac{(v-2)\{c\lambda_2\lambda_6-a\lambda_4^2\}\sum\sum x_i x_k^2 y}{N\lambda_6\delta_1}$$

$$\widehat{b_{\iota JJ}} = \frac{\lambda_4(ac-b)\sum x_i y}{N\delta_1} - \frac{\left(c\lambda_2\lambda_6-a\lambda_4^2\right)\sum x_i^2 y}{N\lambda_6\delta_1} + \frac{\left[\lambda_2\lambda_6\{b(c+v-3)-c^2(v-2)\}-\lambda_4^2\{a^2(c+v-3)-(v-2)(2ac-b)\}\right]\sum x_i x_j^2 y}{N\lambda_6(c-1)\delta_1} - \frac{(v-2)\{\lambda_2\lambda_6(b-c^2)-\;\lambda_4^2(a^2-2ac+b)\}\sum\sum x_i x_j^2 y}{N\lambda_6(c-1)\delta_1}$$

$$\widehat{b_{\iota Jk}} = \frac{\sum x_i x_j\; x_k y}{N\lambda_4} \qquad \ldots(3.3)$$

where $\delta = [\;(a+v-1)\lambda_4 - v\lambda_2^2\;]$>0

$\delta_1 = [\lambda_2\lambda_6\{b(c+v-2)-c^2(v-1)\}-\lambda_4^2\{a^2(c+v-2)-(2ac-b)(v-1)\}] > 0$

Now it follows that variance of estimate of any parameter, say $\widehat{b_{\iota\iota}}$ is given by σ^2 times the coefficient of $\sum x_i^2 y$, in the solution $\widehat{b_{\iota\iota}}$. similarly, the covariance between any two estimates say $Cov(\widehat{b_{\iota\iota}}\;\;,\widehat{b_{JJ}})$ is σ^2 times of the coefficient of $\sum x_j^2 y$, in the solution $\widehat{b_{\iota\iota}}$ or σ^2 times the coefficient of $\sum x_i^2 y$ in the solution $\widehat{b_{JJ}}$, here σ^2 is the error variance.

Applying the above principle we get the expressions for variances and covariances of b's are as follows

$$V(\hat{b}_0) = \frac{(a+v-1)\lambda_4}{N\delta}\sigma^2$$

$$V(\hat{b}_i) = \frac{\lambda_6[b(c+v-2)-c^2(v-1)]}{N\delta_1}\sigma^2$$

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

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

$$V(\hat{b}_{iii}) = \frac{[\lambda_2\lambda_6(c+v-2)-\lambda_4^2(v-1)]}{N\lambda_6\delta_1}\sigma^2$$

$$V(\hat{b}_{ijj}) = \frac{[\lambda_2\lambda_6\{b(c+v-3)-c^2(v-2)\}-\lambda_4^2\{a^2(c+v-3)-(2ac-b)(v-2)\}]}{N\lambda_6(c-1)\delta_1}\sigma^2$$

$$V(\hat{b}_{ijk}) = \frac{1}{N\lambda_6}\sigma^2$$

$$Cov = (\hat{b}_0, \hat{b}_{ii})\frac{-\lambda_2}{N\delta}$$

$$Cov\,(\hat{b}_{ii}, \hat{b}_{jj}) = \frac{1}{N\delta}$$

$$Cov\,(\hat{b}_i, \hat{b}_{ijj}) = \frac{\lambda_4(ac-b)}{N\delta_1}$$

$$Cov\,(\hat{b}_i, \hat{b}_{iii}) = \frac{-\lambda_4\{a(c+v-2)-c(v-1)\}}{N\delta_1}$$

$$Cov\,(\hat{b}_{iii}, \hat{b}_{ijj}) = \frac{-[c\lambda_2\lambda_6 - a\lambda_4^2]}{N\delta_1\lambda_6}$$

$$Cov\,(\hat{b}_{ijj}, \hat{b}_{ikk}) = \frac{-[\lambda_2\lambda_6(b-c^2)-\lambda_4^2(a^2-2ac+b)]}{N\delta_1\lambda_6(c-1)} \qquad \ldots(3.4)$$

Other covariances are zero.

$$V\left[\frac{\partial \hat{y}}{\partial x_i}\right] = V(\hat{b}_i) + d^2 V(\hat{b}_{ij}) + d^2\{V(\hat{b}_{ijj}) + 2Cov(\hat{b}_i, \hat{b}_{ijj})\} + d^4 V(\hat{b}_{ijj}) = f(d^2) \qquad \ldots(3.5)$$

Slope Rotatability Conditions:

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

$\Rightarrow$ $(c-3)\,\delta_1 = 0$ where $\delta_1 \neq 0$

$\because$ $c = 3$

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

$$\Rightarrow \quad \delta_1[\lambda_4[v(5-a)-(a-3)^2]+\lambda_2^2[v(a-5)+4]]$$
$$-\delta[2(a-1)\lambda_4^2[9a(v+1)-9(v-1)+3a-b]]=0$$

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

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

(iv) $V(\hat{b}_{ijj}) + 3\mathrm{Cov}(\hat{b}_{iii}, \hat{b}_{ijj}) = 0$

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

Non-Singularity Conditions:

D: **(i)** $\delta > 0 \quad \Rightarrow$

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

(ii) $\delta_1 > 0 \quad \Rightarrow$

$$\frac{\lambda_2\lambda_6}{\lambda_4^2} > \frac{a^2\{(v+1)-(6a-b)(v-1)\}}{\{b(v+1)-9(v-1)\}} \qquad \ldots(3.6)$$

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

4.1 CUBIC SLOPE ROTATABLE DESIGNS USING BALANCED INCOMPLETE BLOCK DESIGNS

Let (v, b, r, k, λ) denote a BIBD, $2^{t(k)}$ denote a fractional replicate of 2^k in ±1 levels, in which no interaction with less than five factors is confounded.

[1 - (v,b,r,k,λ)] denote the design points generated from the transpose of incidence matrix of BIBD , [1- (v,b,r,k,λ)] $2^{t(k)}$ are the $b2^{t(k)}$ design points generated from BIBD by "multiplication" . We choose additional unknown combinations (α, α, α, . . . , α) and multiply with $2^{t(v)}$ associate combinations (or a suitable fraction of 2^v associate combinations) to obtain $2^{t(v)}$ additional design points. From these deign points generated through BIBD, we construct cubic designs using BIBD.

The design points,[1- (v,b,r,k,λ)] $2^{t(k)} \cup$ (α , α, α, . . . , α)$2^{t(v)}$ give a v- dimensional third order slope rotatable designs using BIBD in the total number of design points

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

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

Construction of TOSRD in 4 dimensions using Balanced Incomplete Block Design, consider the following design points

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

Thus we get $N = b2^{t(k)} + 2^{t(v)} = 48$ design points.
The 48 design points are given below

1- (4,4,3,3,2)] $2^{t(3)}$

1	1	1	0
-1	-1	-1	0
-1	1	1	0
1	-1	1	0
1	1	-1	0
-1	-1	1	0
1	-1	-1	0
-1	1	-1	0
1	1	0	1
-1	1	0	1
1	-1	0	1
1	1	0	-1
-1	-1	0	1
1	-1	0	-1
-1	1	0	-1
-1	-1	0	-1
1	0	1	1
-1	0	1	1
1	0	-1	1
1	0	1	-1
-1	0	-1	1
1	0	-1	-1
-1	0	1	-1

-1	0	-1	-1
0	1	1	1
0	-1	1	1
0	1	-1	1
0	1	1	-1
0	-1	-1	1
0	1	-1	-1
0	-1	1	-1
0	-1	-1	-1

$(\alpha, \alpha, \alpha, \alpha) 2^{t(4)}$

α	α	α	α
-α	α	α	α
α	-α	α	α
α	α	-α	α
α	α	α	-α
-α	-α	α	α
α	-α	-α	α
α	α	-α	-α
-α	α	α	-α
α	-α	α	-α
-α	α	-α	α
-α	-α	-α	α
α	-α	-α	-α
-α	α	-α	-α
-α	-α	α	-α
-α	-α	-α	- α

For the above design points we have

(i) $\sum x_i^2 = 16\alpha^2 + 24 = N\lambda_2$
(ii) $\sum x_i^4 = 16\alpha^4 + 24 = aN\lambda_4$
(iii) $\sum x_i^6 = 16\alpha^6 + 24 = bN\lambda_6$
(iv) $\sum x_i^2 x_j^2 = 16\alpha^4 + 16 = N\lambda_4$
(v) $\sum x_i^2 x_j^4 = 16\alpha^6 + 16 = cN\lambda_6$
(vi) $\sum x_i^2 x_j^2 x_k^2 = 16\alpha^6 = N\lambda_6$ …(4.3)

By solving the TOSRD conditions C(i) to C(iv) of (3.5) using (4.3), we get
$\alpha = 0.8908971814$
From (i),(iv) and (vi) of (4.3) we will get λ_2, λ_4 and λ_6
$\lambda_2 = 0.76456684199$, $\lambda_4 = 0.54332017498$ and $\lambda_6 = 0.16666666667$
From (ii,iv), (iii,vi) and (v,vi) of (4.3) we have a, b and c
a = 1.30675589522, b = 4 and c = 3.

It can be verified that non-singularity conditions (i) and (ii) of (3.6) is satisfied.

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