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Construction of Measure of Second Order Slope Rotatable Designs Using Balanced Incomplete Block Designs

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Abstract

In this paper, a new method of construction measure of Second Order Slope Rotatable Designs using Balanced Incomplete Block Designs is suggested which enables us to assess the degree of slope-rotatability for a given Response Surface Design.

Keywords

Second order response surface designs, Second order slope rotatable designs (SOSRD), Measure of second order slope rotatable designs

1. Introduction

Response Surface methodology is a statistical technique that is very useful in design and analysis of scientific experiments. In many experimental situations, the experimenter is concerned with explaining certain aspects of a functional relationship

$$Y=f(x_1,x_2,...,x_v)+e$$

where Y is the response and $x_1,x_2,...,x_v$ are the levels of v-quantitative variables or factors and 'e' is the random error. Response Surface methods are useful where several independent variables influence a dependent variable. The independent variables are assumed to be continued and controlled by the experimenter.

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The response is assumed to be as random variable. For example, if a chemical engineer wishes to find the temperature (x_1) and pressure (x_2) that maximizes the yield (response) of his process then the observed response Y may be written as a function of the levels of the temperature (x_1) and pressure (x_2) as

$$Y=f(x_1,x_2)+e$$

The concept of rotatability, which is very important in Response Surface Designs, was proposed by Box and Hunter (1957). The study of rotatable designs is mainly emphasized on the estimation of differences of yields and its precision. Estimation of differences in responses at two different points in the factor space will often be of great importance. If differences in responses at two points close together are of interest then estimation of local slope (rate of change) of the response is required. Estimation of slopes occurs frequently in practical situations. For instance, there are cases in which we want to estimate rate of reaction in chemical experiment, rate of change in the yield of a crop to various fertilizer doses, rate of disintegration of radioactive material in an animal etc. (Park, 1987).

Hader and Park (1978) introduced Slope Rotatable Central Composite Designs (SRCCD). Victorbabu and Narasimham (1991) studied in detail the conditions to be satisfied by a general Second Order Slope Rotatable Designs (SOSRD) and constructed SOSRD using Balanced Incomplete Block Designs (BIBD). Victorbabu (2007) suggested a review on SOSRD. Park and Kim (1992) suggested a measure of slope rotatability for Second Order Response Surface Designs. Jang and Park (1993) suggested a measure and a graphical method for evaluating slope rotatability in Response Surface Designs. These measures are useful to enable us to assess the degree of slope rotatability for a given Second Order Response Surface Designs.

2. Conditions for Second Order Slope Rotatable Designs

Suppose we want to use the Second Order Response Surface Design D = (x_{iu}) to fit the surface

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

where x_{iu} denotes the level of the i^{th} factor (i =1,2,…,v) in the u^{th} run (u=1,2,…,N) of the experiment, e_u's are uncorrelated Random Errors with mean zero and variance σ^2. The design is said to be SOSRD if the variance of the estimate of first order partial derivative of $Y_u(x_1,x_2,...,x_v)$ 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_v) from the origin (center) of the design. Such a spherical variance function for estimation of slopes in the Second Order Response Surface is achieved if the design points satisfy the following conditions (Hader and Park, 1978; Victorbabu and Narasimham, 1991).

- $\sum x_{iu} = 0$, $\sum x_{iu}x_{ju} = 0$, $\sum x_{iu}x_{ju}^2 = 0$, $\sum x_{iu}\ x_{ju}\ x_{ku} = 0$, $\sum x_{iu}^3 = 0$, $\sum x_{iu}x_{ju}^3 = 0$, $\sum x_{iu}x_{ju}\ x_{ku}^2 = 0$, $\sum x_{iu}x_{ju}x_{ku}x_{lu} = 0$; for $i \neq j \neq k \neq l$;
- (i) $\sum x_{iu}^2 = \text{Constant} = N\lambda_2$; for all i; (ii) $\sum x_{iu}^4 = \text{Constant} = cN\lambda_4$; for all i
- $\sum x_{iu}^2 x_{ju}^2 = \text{Constant} = N\lambda_4$; for $i \neq j$
- $\dfrac{\lambda_4}{\lambda_2^2} > \dfrac{v}{(c+v-1)}$.
- $[v(5-c)-(c-3)^2]\ \lambda_4 + [v(c-5)+4]\ \lambda_2^2 = 0$ (2.2)

where c, λ_2 and λ_4 are constants.

The variances and covariances of the estimated Parameters are

$$V(\hat{b}_0) = \frac{\lambda_4(c+v-1)\sigma^2}{N\left[\lambda_4(c+v-1)-v\lambda_2^2\right]}, \quad V(\hat{b}_i)=\frac{\sigma^2}{N\lambda_2}, \quad V(\hat{b}_{ij})=\frac{\sigma^2}{N\lambda_4},$$

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

$$Cov(\hat{b}_{ii},\hat{b}_{jj})=\frac{(\lambda_2^2-\lambda_4)\sigma^2}{(c-1)N\lambda_4[\lambda_4(c+v-1)-v\lambda_2^2]} \quad \text{and other covariances vanish.} \tag{2.3}$$

3. Second Order Slope Rotatable Designs using Balanced Incomplete Block Designs

A Balanced Incomplete Block Design (BIBD) denoted by (v, b, r, k, λ) is an arrangement of ‘v’ treatments in ‘b’ blocks each containing k(<v) treatments, if (i)

every treatment occurs at most once in a block, (ii) every treatment occurs in exactly 'r' blocks, and (iii) every pair of treatments occurs together in λ blocks.

Let (v, b, r, k, λ) denote a Balanced Incomplete Block Design, $2^{t(k)}$ denote a fractional replicate of 2^k in ±1 levels, in which no interaction with less than five factors is confounded. $[1-(v,b,r,k,\lambda)]$ denote the design points generated from the transpose of incidence matrix of BIBD. $[1-(v,b,r,k,\lambda)]2^{t(k)}$ are the 'b' $2^{t(k)}$ design points generated from BIBD by 'multiplication' (Raghavarao, 1971). $(a,0,0,\ldots,0)2^1$ denote the design points generated from (a,0,0...,0) point set, and $\bigcup$ denotes combination of the design points generated from different sets of points. Let (n_a) denote replication of axial points, n_0 denote the number of central points. The method of construction of SOSRD using BIBD is given below (Victorbabu and Narasimham, 1991).

3.1 Result: The design points $[1-(v,b,r,k,\lambda)]2^{t(k)} \bigcup n_a\,(a,0,0,\ldots,0)2^1 \bigcup (n_0)$ will give a v-dimensional SOSRD in $N = b2^{t(k)} + 2vn_a + n_0$ design points, where a^2 is positive real root of the fourth degree polynomial equation

$$
\begin{aligned}
&(8vn_a^3-4Nn_a^2)a^8+8vr2^{t(k)}a^6n_a^2+\\
&\left[2vr^2 2^{2t(k)}n_a+\left\{\left(\left(12n_a-2vn_a\right)\lambda-4r\right)N+\left(16\lambda n_a^2-20v\lambda n_a^2+4vrn_a^2\right)\right\}2^{t(k)}\right]a^4+\\
&\left[4vr^2+\left(16n_a-20vn_a\right)r\lambda\right]2^{2t(k)}a^2+\left[\left(5v-9\right)\lambda^2+\left(6-v\right)r\lambda-r^2\right]N2^{2t(k)}+\\
&\left(vr+4\lambda-5v\lambda\right)r^2 2^{3t(k)}=0
\end{aligned}
$$

Note: Values of SOSRD using BIBD can be obtained by solving the above equation.

4. Conditions of Measure of Second Order Slope Rotatable Designs

Following Hader and Park (1978), Park and Kim (1992), Victorbabu and Narasimham (1991), equations 1, 2, 3, 4, 5 of (2.2), and (2.3) give the necessary and sufficient conditions for a measure of slope rotatability for any general Second Order Response Surface Designs. Further we have

$V(b_i)$ are equal for i,

$V(b_{ii})$ are equal for i,

$V(b_{ij})$ are equal for i, j, where $i \neq j$,

$Cov(b_i, b_{ii}) = Cov(b_i, b_{ij}) = Cov(b_{ii}, b_{ij}) = Cov(b_{ij}, b_{il}) = 0$ for all $i \neq j \neq l$. (4.1)

Park and Kim (1992) proposed that if the conditions in (2.2) together with (2.3) and (4.1) are met, then the following measure ($Q_v(D)$) given below assess the degree of slope rotatability for any general Second Order Response Surface Design 'D' with v-independent variables.

$$Q_v(D)=\frac{1}{2(v-1)\sigma^4}\left\{(v+2)(v+4)\sum_{i=1}^{v}\left[(v(b_i)-\frac{1}{v}\sum_{i=1}^{v}v(b_i))+\frac{(4v(b_{ii})+\sum\limits_{\substack{j=1\\j\neq i}}^{v}v(b_{ij}))-\frac{1}{v}\sum\limits_{i=1}^{v}(4v(b_{ii})+\sum\limits_{\substack{j=1\\j\neq i}}^{v}v(b_{ij}))}{v+2}\right]^2\right.$$

$$+\frac{4}{v(v+2)}\sum_{i=1}^{v}((4v(b_{ii})+\sum_{\substack{j=1\\j\neq i}}^{v}v(b_{ij}))-\frac{1}{v}\sum_{i=1}^{v}(4v(b_{ii})+\sum_{\substack{j=1\\j\neq i}}^{v}v(b_{ij})))^2+2\sum_{i=1}^{v}\left[\left[4v(b_{ii})-\frac{(4v(b_{ii})+\sum\limits_{\substack{j=1\\j\neq i}}^{v}v(b_{ij}))}{v}\right]^2+\sum_{\substack{j=1\\j\neq i}}^{v}\left[v(b_{ij})-\frac{(4v(b_{ii})+\sum\limits_{\substack{j=1\\j\neq i}}^{v}v(b_{ij}))}{v}\right]^2\right]$$

$$\left.+4(v+4)\left[4cov^2(b_i,b_{ii})+\sum_{\substack{j=1\\j\neq i}}^{v}cov^2(b_i,b_{ij})\right]+4\sum_{i=1}^{v}\left[4\sum_{\substack{j=1\\j\neq i}}^{v}cov^2(b_{ii},b_{ij})+\sum_{\substack{j<l\\j,l\neq i}}^{v}\sum cov^2(b_{ij},b_{il})\right]\right\}$$

Further, it is simplified to $Q_V(D)=\frac{1}{\sigma^4}\left[4V(b_{ii})-V(b_{ij})\right]^2$.

5. Construction of Measure of Second Order Slope Rotatable Design (SOSRD) Using Balance Incomplete Block Design (BIBD)

In this section, the proposed new method of construction of measure of SOSRD using BIBD is given below.

Let (v, b, r, k, λ) denote a BIBD. For the design points, $[1-(v,b,r,k,\lambda)]2^{t(k)} \cup n_a$ $(a,0,0,\ldots,0)2^1 \cup (n_0)$ generated from BIBD in $N = b2^{t(k)} + 2vn_a + n_0$ design points, simple symmetry conditions 1, 2, 3 of (2.2) are true. Condition 1 of (2.2) is true obviously. Conditions 2 and 3 of (2.2) are true as follows

2. (i) $\sum x_{iu}^2 = r2^{t(k)} + 2n_a a^2 = N\lambda_2$

   (ii) $\sum x_{iu}^4 = r2^{t(k)} + 2n_a a^4 = cN\lambda_4$

3. $\sum x_{iu}^2 x_{ju}^2 = \lambda 2^{t(k)} = N\lambda_4$

Measure of SOSRD using BIBD can be obtained by

$$Q_v(D) = \left[\frac{\sum x_{iu}^2}{N}\right]^4 \left[4e - V(b_{ij})\right]^2$$

$$\text{where } e = V(b_{ii}) = \frac{(v-1)\left[2^{t(k)}\lambda n_0 + 2^{t(k)+1}\lambda v\, n_a - 2^{t(k)+2} r\, n_a\, a^2 - r^2\, 2^{2t(k)} + b\lambda 2^{2t(k)}\right] + \left[2^{t(k)+1} b\, n_a + 2n_a n_0 + 4n_a^2\right] a^4 + (r-\lambda)\left[2^{t(k)+1} v n_a + 2^{t(k)} n_0 + b2^{2t(k)}\right]}{\left[2^{t(k)}(r-\lambda) + 2n_a a^4\right]\left[\begin{array}{l} v2^{t(k)}\left(\lambda n_0 - 4r n_a a^2\right) + 2^{t(k)+1} n_a\left(v^2\lambda + b a^4\right) + \\ 2n_a n_0\, a^4 + (r-\lambda)\left(b2^{2t(k)} + 2^{t(k)+1} v n_a + 2^{t(k)} n_0\right) + 2^{2t(k)} v\left(b\lambda - r^2\right) \end{array}\right]}$$

Table 1 gives the values of $Q_v(D)$ for SOSRD using various Parameters of BIBD, n_0 and the value of 'a' which make SOSRD using BIBD. It can be verified that $Q_v(D)$ is zero, if and only if, a design 'D' is slope-rotatable. $Q_v(D)$ becomes larger as 'D' deviates from a Slope Rotatable Design.

6. Conclusion

In this paper, general measure has been proposed which enables us to assess the degree of slope rotatability for a given Second Order Response Surface Design using BIBD. This measure, $Q_v(D)$ has the value zero, if and only if, the design 'D' is SOSRD, and $Q_v(D)$ becomes larger as 'D' deviates from a Slope Rotatable Design. It may be used to compare the degree of slope rotatability for the same 'v'. It can be generally used to increase the degree of slope rotatability of SOSRD by the addition of experimental runs. We also point out here that this measure of SOSRD using BIBD has 71 design points for 7-factors, whereas the corresponding measure of SRCCD obtained by Park and Kim (1992) needs 79 design points. Thus the new method leads to a 7-factor measure of SOSRD in less number of design points than the corresponding measure of Slope Rotatable Central Composite Designs (SRCCD). Further, 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.

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Table 1: Values of measure of SOSRD using BIBD ($n_a = 1$)

(3,3,2,2,1)					
a	**n_0=1,N=19**	**n_0=2,N=20**	**n_0=3,N=21**	**n_0=4,N=22**	**n_0=5,N=23**
1.0	4.8818×10^{-2}	2.5511×10^{-2}	1.5748×10^{-2}	1.0672×10^{-2}	7.6753×10^{-3}
1.3	1.4991×10^{-1}	3.8709×10^{-2}	1.6675×10^{-2}	8.9508×10^{-3}	5.4362×10^{-3}
1.6	8.1146×10^{-2}	1.7971×10^{-2}	6.1608×10^{-3}	2.5693×10^{-3}	1.1949×10^{-3}
1.9	2.7449×10^{-3}	1.4684×10^{-4}	4.4386×10^{-5}	2.6517×10^{-4}	4.5620×10^{-4}
2.2	7.3135×10^{-3}	7.9415×10^{-3}	7.7606×10^{-3}	7.2278×10^{-3}	6.5697×10^{-3}
2.5	3.8942×10^{-2}	3.3665×10^{-2}	2.8907×10^{-2}	2.4785×10^{-2}	2.1276×10^{-2}
2.8	9.8970×10^{-2}	8.2321×10^{-2}	6.8826×10^{-2}	5.7874×10^{-2}	4.8951×10^{-2}
3.1	2.0378×10^{-1}	1.6755×10^{-1}	1.3888×10^{-1}	1.1601×10^{-1}	9.7604×10^{-2}
*	2.0000	1.9330	1.8764	1.8290	1.7894
(4,6,3,2,1)					
a	**n_0=1,N=33**	**n_0=2,N=34**	**n_0=3,N=35**	**n_0=4,N=36**	**n_0=5,N=37**
1.0	7.9676×10^{-3}	4.3725×10^{-3}	2.7504×10^{-3}	1.8819×10^{-3}	1.3630×10^{-3}
1.3	4.0823×10^{-2}	1.0456×10^{-2}	4.3642×10^{-3}	2.2584×10^{-3}	1.3209×10^{-3}
1.6	1.9950×10^{-2}	4.7914×10^{-3}	1.6367×10^{-3}	6.4547×10^{-4}	2.6887×10^{-4}
1.9	8.5114×10^{-5}	1.1294×10^{-5}	1.0811×10^{-4}	2.1175×10^{-4}	2.9080×10^{-4}
2.2	2.8300×10^{-3}	2.8377×10^{-3}	2.7609×10^{-3}	2.6380×10^{-3}	2.4921×10^{-3}
2.5	9.9660×10^{-3}	9.0715×10^{-3}	8.2475×10^{-3}	7.4967×10^{-3}	6.8171×10^{-3}
2.8	2.1792×10^{-2}	1.9277×10^{-2}	1.7292×10^{-2}	1.5546×10^{-2}	1.4010×10^{-2}
3.1	3.9976×10^{-2}	3.5606×10^{-2}	3.1810×10^{-2}	2.8500×10^{-2}	2.5606×10^{-2}
*	1.9348	1.8833	1.8352	1.7909	1.7504
(5,10,4,2,1)					
a	**n_0=1,N=51**	**n_0=2,N=52**	**n_0=3,N=53**	**n_0=4,N=54**	**n_0=5,N=55**
1.0	1.7567×10^{-3}	9.6797×10^{-4}	5.9534×10^{-4}	3.9368×10^{-4}	2.7409×10^{-4}
1.3	1.4342×10^{-2}	3.5871×10^{-3}	1.4176×10^{-3}	6.8471×10^{-4}	3.6975×10^{-4}
1.6	6.1878×10^{-3}	1.5446×10^{-3}	5.0685×10^{-4}	2.4158×10^{-4}	6.1112×10^{-5}
1.9	6.4166×10^{-6}	2.1626×10^{-5}	1.1067×10^{-4}	1.5654×10^{-4}	1.9092×10^{-4}
2.2	1.2470×10^{-3}	1.2302×10^{-3}	1.1998×10^{-3}	1.1609×10^{-3}	1.1169×10^{-3}
2.5	3.4563×10^{-3}	3.2407×10^{-3}	3.0379×10^{-3}	2.8478×10^{-3}	2.6702×10^{-3}
2.8	6.7001×10^{-3}	6.2262×10^{-3}	5.7919×10^{-3}	5.3936×10^{-3}	5.0280×10^{-3}
3.1	1.1547×10^{-2}	1.0703×10^{-2}	9.9344×10^{-3}	9.2327×10^{-3}	8.5913×10^{-3}
*	1.8836	1.8393	1.7955	1.7525	1.7104
(6,15,5,2,1)					
a	**n_0=1,N=73**	**n_0=2,N=74**	**n_0=3,N=75**	**n_0=4,N=76**	**n_0=5,N=77**
1.0	4.5787×10^{-4}	2.4479×10^{-4}	1.4189×10^{-4}	8.6686×10^{-5}	5.4870×10^{-5}

(6,15,5,2,1)					
a	**n_0=1,N=73**	**n_0=2,N=74**	**n_0=3,N=75**	**n_0=4,N=76**	**n_0=5,N=77**
1.3	5.9767×10^{-3}	1.4593×10^{-3}	5.4323×10^{-4}	2.4142×10^{-4}	1.1701×10^{-4}
1.6	2.2530×10^{-3}	5.7160×10^{-4}	1.7637×10^{-4}	5.3795×10^{-5}	1.2973×10^{-5}
1.9	3.3626×10^{-5}	6.4681×10^{-5}	9.1377×10^{-5}	1.1251×10^{-4}	1.2853×10^{-4}
2.2	6.2158×10^{-4}	6.1172×10^{-4}	5.9885×10^{-4}	5.8391×10^{-4}	5.6761×10^{-4}
2.5	1.4678×10^{-3}	1.4012×10^{-3}	1.3375×10^{-3}	1.2767×10^{-3}	1.2189×10^{-3}
2.8	2.6276×10^{-3}	2.4947×10^{-3}	2.3698×10^{-3}	2.2524×10^{-3}	2.1420×10^{-3}
3.1	4.2785×10^{-3}	4.0560×10^{-3}	3.8477×10^{-3}	3.6524×10^{-3}	3.4693×10^{-3}
*	1.8419	1.8015	1.7599	1.7170	1.6728
(7,7,3,3,1)					
a	**n_0=1,N=71**	**n_0=2,N=72**	**n_0=3,N=73**	**n_0=4,N=74**	**n_0=5,N=75**
1.0	3.6876×10^{-4}	3.0765×10^{-4}	2.6256×10^{-4}	2.2798×10^{-4}	2.0065×10^{-4}
1.3	7.4243×10^{-4}	4.7849×10^{-4}	3.3952×10^{-4}	2.5641×10^{-4}	2.0223×10^{-4}
1.6	3.9307×10^{-3}	1.1486×10^{-3}	5.2055×10^{-4}	2.8787×10^{-4}	1.7848×10^{-4}
1.9	2.2780×10^{-3}	5.9303×10^{-4}	2.1790×10^{-4}	9.2232×10^{-5}	4.1254×10^{-5}
2.2	6.1415×10^{-6}	6.7524×10^{-7}	8.5695×10^{-6}	1.8867×10^{-5}	2.8393×10^{-5}
2.5	2.3610×10^{-4}	2.4443×10^{-4}	2.4834×10^{-4}	2.4904×10^{-4}	2.4740×10^{-4}
2.8	7.2031×10^{-4}	6.9292×10^{-4}	6.6562×10^{-4}	6.3872×10^{-4}	6.1243×10^{-4}
3.1	1.3742×10^{-3}	1.3064×10^{-3}	1.2423×10^{-3}	1.1817×10^{-3}	1.1245×10^{-3}
*	2.2305	2.1872	2.1449	2.1039	2.0647
(8,28,7,2,1)					
a	**n_0=1,N=129**	**n_0=2,N=130**	**n_0=3,N=131**	**n_0=4,N=132**	**n_0=5,N=133**
1.0	3.7574×10^{-5}	1.6291×10^{-5}	6.6546×10^{-6}	2.2986×10^{-6}	5.0686×10^{-7}
1.3	1.4462×10^{-3}	3.3949×10^{-4}	1.1237×10^{-4}	4.1305×10^{-5}	1.4865×10^{-5}
1.6	4.0998×10^{-4}	1.0270×10^{-4}	2.6345×10^{-5}	4.7726×10^{-6}	6.9811×10^{-8}
1.9	3.8057×10^{-5}	4.6409×10^{-5}	5.3162×10^{-5}	5.8542×10^{-5}	6.2773×10^{-5}
2.2	2.0258×10^{-4}	1.9991×10^{-4}	1.9697×10^{-4}	1.9380×10^{-4}	1.9047×10^{-4}
2.5	3.8978×10^{-4}	3.7929×10^{-4}	3.6910×10^{-4}	3.5919×10^{-4}	3.4956×10^{-4}
2.8	6.2432×10^{-4}	6.0601×10^{-4}	5.8834×10^{-4}	5.7130×10^{-4}	5.5485×10^{-4}
3.1	9.3614×10^{-4}	9.0806×10^{-4}	8.8103×10^{-4}	8.5498×10^{-4}	8.2988×10^{-4}
*	1.7782	1.7417	1.7023	1.6587	1.6093

* Values of SOSRD using BIBD.

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