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Evaluating Measure of Modified Rotatability for Second Degree Polynomial Using a Pair of Balanced Incomplete Block Designs

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ABSTRACT
In this paper, a study on evaluating measure of modified rotatability for second degree polynomial using a pair of balanced incomplete block designs ($5 \leq v \leq 15$: v - number of factors) is suggested which enables us to assess the degree of modified rotatability for a given response surface design.

KEYWORDS
Response surface methodology; modified rotatability; measure.

1. Introduction

Response surface process is a collection of mathematical and statistical techniques appropriate for analysing problems in which several independent variables influence a dependent variable. The regressor variables are often called input or explanatory variables and the regressand variable is often the response variable. An important development of response surface designs was the introduction of rotatable designs suggested by [1]. Rotatable designs using balanced incomplete block designs (BIBD) was proposed by [2]. A design is said to be rotatable, if the variance of the response estimate is a function only of the distance of the point from the design centre. [3] developed modified second order response surface designs. [9] studied second order rotatable designs (SORD) through a pair of BIBDs. [4] introduced measure of rotatability for second degree polynomial designs. [10] studied modified second order rotatable designs and second order slope rotatable designs using a pair of BIBD. [15] studied measure of rotatability for second degree polynomial design using a pair of balanced incomplete block designs.
Lot of work was carried out by Victorbabu and some other authors on modified rotatability, measure of rotatability on second degree polynomial designs respectively [20], [21, 22], [23], [21], [16–19], [11], [12, 14] and [13]. Recently, evaluating measure of modified rotatability is studied by [5–8] using central composite designs (CCD), BIBD, pairwise balanced design and symmetrical unequal block arrangements with

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two unequal block sizes respectively.
In this paper, we develop a new method of evaluating measure of modified rotatability for second degree polynomial using a pair of balanced incomplete block designs is suggested which enables us to assess the degree of rotatability for a given response surface design.

2. Conditions for SORD:

Suppose we want to use the second degree polynomial model D=(x_{iu}) to fit the surface,

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

where x_{iu} denotes the level of the i^{th} factor $(i = 1, 2, \dots, v)$ in the u^{th} run $(u = 1, 2, \dots, N)$ of the experiment, e_u's are uncorrelated random errors with mean zero and variance σ^2 is said to be rotatable design of second order, if the variance of the estimated response of $\hat{Y}_u$ from the fitted surface is only a function of the distance ($d^2 = \sum_{i=1}^{v} x_i^2$) of the point ($x_1, x_2, \dots, x_v$) from the origin (centre) of the design. Such a spherical variance function for estimation of second degree polynomial is achieved if the design points satisfy the following conditions [cf. [1], [2]].

(1)

$$\sum x_{iu} = 0, \sum x_{iu} x_{ju} = 0, \sum x_{iu} x_{j}^2{}_u = 0, \sum x_{iu} x_{ju} x_{ku} = 0, \sum x_{iu}^3 = 0,$$
$$\sum x_{iu} x_{ju}^3 = 0, \sum x_{iu} x_{ju} x_{ku}^2 = 0, \sum x_{iu} x_{ju} x_{ku} x_{lu} = 0; \ \textit{for } i \neq j \neq k \neq l \tag{2}$$

(2)

$$(i) \sum x_{iu}^2 = \textit{constant} = N\lambda_2 \tag{3}$$
$$(ii) \sum x_{iu}^4 = \textit{constant} = cN\lambda_4; \ \textit{for all } i$$

(3)

$$\sum x_{iu}^2 x_{ju}^2 = \textit{constant} = N\lambda_4; \ \textit{for } i \neq j \tag{4}$$

(4)

$$\sum x_{iu}^4 = c \sum x_{iu}^2 x_{ju}^2 \tag{5}$$

(5)

$$\frac{\lambda_4}{\lambda_2^2} > \frac{v}{(c + v - 1)} \tag{6}$$

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,

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

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

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

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

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

$$Cov(\hat{b}_{ii},\hat{b}_{jj}) = \frac{(\lambda_2^2 - \lambda_4)\sigma^2}{(c-1)N\lambda_4[\lambda_4(c+v-1) - v\lambda_2^2]} \quad (7)$$

and other covariances are zero.

3. Evaluating Measure of Modified Rotatability for Second Degree Polynomial Using a Pair of BIBD

Following [1], [2], [9], [4], [3], [10] and [15] the proposed method of evaluating measure of modified rotatability for second degree polynomial designs using a pair of BIBD is suggested as follows.

Let D_1= (v, b_1, r_1, k_1, λ_1), D_2= (v, b_2, r_2, k_2, λ_2) are two BIBD's. Then design points $y_1[1-(v,\ b_1,\ r_1,\ k_1,\ \lambda_1)]2^{t(k_1)} \bigcup y_2\,[a-(v,\ b_2,\ r_2,\ k_2,\ \lambda_2)]2^{t(k_2)} \bigcup (n_0)$ will give a measure of modified rotatability for second degree polynomial using a pair of BIBD. From (3) and (4) we have,

$$\sum x_{iu}^2 = y_1r_12^{t(k_1)} + y_2r_22^{t(k_2)}a^2 \ = \ N\lambda_2 \quad (8)$$

$$\sum x_{iu}^4 = y_1r_12^{t(k_1)} + y_2r_22^{t(k_2)}a^4 \ = \ cN\lambda_4 \quad (9)$$

$$\sum x_{iu}^2 x_{ju}^2 = y_1\lambda_1 2^{t(k_1)} + y_2\lambda_2 2^{t(k_2)} a^4 = N\lambda_4 \tag{10}$$

From (9) and (10), we get

$$a^4 = \frac{y_1(3\lambda_1 - r_1)}{y_2(r_2 - 3\lambda_2)} 2^{t(k_1) - t(k_2)}$$

The modified condition $\left(\sum x_{iu}^2\right)^2 = N\sum x_{iu}^2 x_{ju}^2$ leads to N which is given by $N = \frac{(y_1 r_1 2^{t(k_1)} + y_2 r_2 2^{t(k_2)} a^2)^2}{y_1\lambda_1 2^{t(k_1)} + y_2\lambda_2 2^{t(k_2)} a^4}$. Alternatively N may be obtained directly as $N = y_1 b_1 2^{t(k_1)} + y_2 b_2 2^{t(k_2)} + n_0$ design points without any additional set of points, where n_0 is given by $n_0 = \frac{(y_1 r_1 2^{t(k_1)} + y_2 r_2 2^{t(k_2)} a^2)^2}{y_1\lambda_1 2^{t(k_1)} + y_2\lambda_2 2^{t(k_2)} a^4} - y_1 b_1 2^{t(k_1)} - y_2 b_2 2^{t(k_2)}$ and n_0 turns out to be an integer with 'a' prefixed and $c = \frac{y_1 r_1 2^{t(k_1)} + y_2 r_2 2^{t(k_2)} a^4}{y_1\lambda_1 2^{t(k_1)} + y_2\lambda_2 2^{t(k_2)} a^4}$.

From equations (8) and (10) and on simplification we get $\lambda_2 = \frac{y_1 r_1 2^{t(k_1)} + y_2 r_2 2^{t(k_2)} a^2}{N}$ and $\lambda_4 = \frac{y_1\lambda_1 2^{t(k_1)} + y_2\lambda_2 2^{t(k_2)} a^4}{N}$.

To obtain measure of modified rotatability for second degree polynomial using a pair of BIBD, we have

$$P_v(D) = \frac{1}{1 + R_v(D)}$$

$$R_v(D) = \left[\frac{(c-3)}{(c-1)}\right]^2 \frac{6v(v-1)}{\lambda_4^2 (v+2)^2 (v+4)(v+6)(v+8) g^8}$$

Here g is a scaling factor and can be obtained as follows,

$$g = \begin{cases} \frac{1}{a}, \text{ if } a \leq \sqrt{\frac{1}{r_2}\left[\frac{y_1(b_1 - r_1)2^{t(k_1)-t(k_2)}}{y_2} + b_2\right]} \\ \frac{1}{\sqrt{\frac{1}{r_2}\left[\frac{y_1(b_1 - r_1)2^{t(k_1)-t(k_2)}}{y_2} + b_2\right]}}, \text{ otherwise} \end{cases}$$

The following table gives the values of an evaluating measure of modified rotatability for second degree polynomial using a pair of BIBD. It can be verified that $P_v(D)$ is 1 if and only if the design is modified rotatable, and it is smaller than one for nearly modified rotatable designs.

Example: We illustrate the evaluating measure of modified rotatability for second degree polynomial for v=5 factors with the help of a pair of BIBDs with parameters D_1 =(v= 5, b_1 = 5, r_1 = 4, k_1 = 4, λ_1 = 3) and D_2=(v=5, b_2 = 10, r_2 = 4, k_2 = 2, λ_2 = 1). The design points, $y_1[1 - (v = 5, b_1 = 5, r_1 = 4, k_1 = 4, \lambda_1 = 3)]2^4 \bigcup y_2\,[a - (v = 5, b_2 = 10, r_2 = 4, k_2 = 2, \lambda_2 = 1)]2^2 \bigcup (n_0)$
will give a measure of modified rotatability for second degree polynomial in N=162 design points. From (8), (9) and (10), we have

$$\sum x_{iu}^2 = y_1 64 + y_2 16a^2 = N\lambda_2 \tag{11}$$

$$\sum x_{iu}^4 = y_1 64 + y_2 16a^4 \;=\; cN\lambda_4 \tag{12}$$

$$\sum x_{iu}^2 x_{ju}^2 = y_1 48 + y_2 4a^4 = \; N\lambda_4 \tag{13}$$

From equations (12) and (13) with rotatability value $c = 3$, $y_1 = 1$ and $y_2 = 5$, we get $a^4 = 4 \Rightarrow a^2 = 2 \Rightarrow a = 1.414213$. From equations (11) and (13) using the modified condition with ($\lambda_2^2 = \lambda_4$) along with $a^2 = 2$, $y_1 = 1$ and $y_2 = 5$, we get $N = 162$, $n_0 = 112$. For modified SORD we get $P_v(D) = 1$ by taking $a = 1.414213$ and scaling factor $g = 0.7071$. Then the design is modified SORD using a pair of BIBD.
Instead of taking $a = 1.414213$ if we take $a = 2.2$ for the above pair of BIBD D_1=(v=5, $b_1 = 5, r_1 = 4, k_1 = 4, \lambda_1$=3) and D_2= (v = 5, b_2= 10, r_2= 4, k_2= 2, $\lambda_2 =$ 1) from equations (12) and (13), we get $c = 3.7522$. The scaling factorg = 0.6086, $R_v(D) = 0.0121$and $P_v(D) = 0.9881$. Here $P_v(D)$ becomes smaller it deviates from modified rotatability.
Table 1 gives the values of evaluating measure of modified rotatability $P_v(D)$ for second degree polynomial using a pair of BIBD, at different values of $'a'$ for $5 \le v \le 15$. It can be verified that $P_v(D)$ is one, if and only if a design $'D'$ is modified rotatable. $P_v(D)$ becomes smaller as $'D'$ deviates from a modified rotatable design.
Conclusion: Evaluating measure of modified rotatability for second degree polynomial designs using a pair of BIBD, at different values of $'a'$ for $5 \le v \le 15$. It can be verified that $P_v(D)$ is one if and only if the design is modified rotatable design and it is less than one for a nearly modified rotatable design.
Table 1: Evaluating measure of modified rotatability for second degree polynomial using a pair of BIBD.

$(5,5,4,4,3)(5,10,4,2,1)$, $N = 162$, $a = 1.414213$, $n_0 = 112$, $y_1 = 1$, $y_2 = 5$				
a	c	g	$R_v(D)$	$P_v(D)$
1.0	2.1176	1	1.8997×10^{-3}	0.9981
1.3	2.7824	0.7692	3.707×10^{-4}	0.9996
*1.414213	3	0.7071	0	1
1.6	3.2852	0.625	5.901×10^{-4}	0.9994
1.9	3.5853	0.6086	8.302×10^{-3}	0.9918
2.2	3.7522	0.6086	0.0121	0.9881
2.5	3.8456	0.6086	0.0143	0.9859
2.8	3.8998	0.6086	0.0156	0.9846
3.1	3.9325	0.6086	0.0164	0.9839

$(6,15,10,4,6)(6,15,5,2,1)$, $N = 360$, $a = 2$, $n_0 = 60$, $y_1 = 1$, $y_2 = 1$				
a	c	g	$R_v(D)$	$P_v(D)$
1.0	1.8	1	0.0191	0.9813
1.3	2.0212	0.7692	0.0635	0.9403
1.6	2.3817	0.625	0.0729	0.9321
1.9	2.8397	0.5263	0.0109	0.9891
*2.0	3	0.5	0	1
2.2	3.3131	0.4545	0.0852	0.9215
2.5	3.7314	0.4	0.9273	0.5188
2.8	4.0639	0.3779	2.4537	0.2895
3.1	4.3124	0.3779	3.1945	0.2384

$(7,7,6,6,5)(7,21,6,2,1)$, $N = 882$, $a = 2$, $n_0 = 182$, $y_1 = 2$, $y_2 = 3$				
a	c	g	$R_v(D)$	$P_v(D)$
1.0	1.3735	1	0.0816	0.9245
1.3	1.6644	0.7692	0.1419	0.8757
1.6	2.1469	0.625	0.1023	0.9072
1.9	2.7757	0.5263	0.0117	0.9885
*2.0	3.4447	0.5035	0.0345	0.9667
2.2	3	0.5035	0	1
2.5	4.0526	0.5035	0.1239	0.8898
2.8	4.5476	0.5035	0.1983	0.8345
3.1	4.9245	0.5035	0.2515	0.7996

$(8,14,7,4,3)(8,28,7,2,1)$, $N = 700$, $a = 1.414213$, $n_0 = 140$, $y_1 = 2$, $y_2 = 1$				
a	c	g	$R_v(D)$	$P_v(D)$
1.0	2.52	1	4.8693×10^{-3}	0.9952
1.3	2.8296	0.7692	3.4536×10^{-3}	0.9966
*1.414213	3	0.7071	0	1
1.6	3.3343	0.625	0.043	0.9588
1.9	3.9756	0.5263	0.8914	0.5287
2.2	4.6384	0.4545	5.4334	0.1554
2.5	5.224	0.4	20.6542	0.0462
2.8	5.6895	0.3571	60.6777	0.0162
3.1	6.0374	0.3226	151.4104	0.0066

$(9,18,8,4,3)(9,12,4,3,1)$, $N = 800$, $a = 1.414213$, $n_0 = 128$, $y_1 = 2$, $y_2 = 1$				
a	c	g	$R_v(D)$	$P_v(D)$
1.0	2.7692	1	7.1575×10^{-4}	0.9993
1.3	2.923	0.7692	5.5022×10^{-4}	0.9995
*1.414213	3	0.7071	0	1
1.6	3.1376	0.625	7.4906	0.9926
1.9	3.3608	0.5263	0.1669	0.857
2.2	3.5483	0.4545	1.0096	0.4976
2.5	3.6867	0.4	3.9603	0.2016
2.8	3.7822	0.3571	12.5633	0.0737
3.1	3.8467	0.3226	31.741	0.0305

$(12,22,11,6,5)(12,33,11,4,3)$, $N = 1408$, $a = 1.414213$, $n_0 = 176$, $y_1 = 1$, $y_2 = 1$				
a	c	g	$R_v(D)$	$P_v(D)$
1.0	2.5385	1	1.0102×10^{-3}	0.9989
1.3	2.8768	0.7692	3.9461×10^{-4}	0.9996
*1.414213	3	0.7071	0	1
1.6	3.1722	0.625	0.012	0.9882
1.9	3.3679	0.5263	0.046	0.956
2.2	3.484	0.4545	0.2338	0.8105
2.5	3.5514	0.4472	0.3276	0.7532
2.8	3.5912	0.4472	0.3652	0.7325
3.1	3.6156	0.4472	0.3886	0.7202

$(13, 26, 12, 6, 5)(13, 26, 6, 3, 1)$, N = 1200, a = 1.414213, $n_0 = 160$, $y_1 = 1$, $y_2 = 1$				
a	c	g	$R_v(D)$	$P_v(D)$
1.0	2.5714	1	1.7819×10^{-3}	0.9982
1.3	2.8499	0.7692	2.5252×10^{-3}	0.9975
*1.414213	3	0.7071	0	1
1.6	3.2885	0.625	0.0168	0.9834
1.9	3.8203	0.5263	0.3442	0.7439
2.2	4.342	0.4545	2.1199	0.3205
2.5	4.781	0.4	8.1106	0.1097
2.8	5.1162	0.3571	23.923	0.0401
3.1	5.3592	0.3226	59.8453	0.0164

$(15, 15, 7, 7, 3)(15, 35, 7, 3, 1)$, N = 1400, a = 1.414213, $n_0 = 160$, $y_1 = 1$, $y_2 = 1$				
a	c	g	$R_v(D)$	$P_v(D)$
1.0	2.52	1	1.8507×10^{-3}	0.9982
1.3	1.9197	0.7692	0.2089	0.8272
*1.414213	3	0.7071	0	1
1.6	3.3343	0.625	0.0163	0.9839
1.9	3.9756	0.5263	0.3388	0.7469
2.2	4.6384	0.4545	2.0651	0.3263
2.5	5.224	0.4	7.8500	0.113
2.8	5.6895	0.3571	23.0617	0.0416
3.1	6.0374	0.3226	0.1421	0.8756

*indicates exact modified rotatability value using a pair of BIBDs (cf. [10])

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