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Measure of rotatability for second order response surface designs using a pair of partially balanced incomplete block designs

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Abstract

In this paper, measure of rotatability for second order response surface designs using a pair of partially balanced incomplete block designs (PBIBD) is suggested which enables us to assess the degree of rotatability for a given response surface design.

Keywords: second order response surface designs, second order rotatable designs, measure of rotatability.

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 continuous and controlled by the experimenter. 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, the observed response Y may be written as a function of the levels of the temperature (x_1) and pressure (x_2) as $Y=f(x_1,x_2)+e$.

Box and Hunter [1] introduced multifactor experimental designs for exploring response surface designs. Das and Narasimham [2] constructed rotatable designs through balanced incomplete block designs (BIBD). Narasimham et al. [3] constructed second order rotatable designs (SORD) through a pair of BIBD. Chowdhury and Gupta [4], Victorbabu [5] and several others have suggested various methods for the construction of SORD. Draper and Guttman [6] suggested index of rotatability. Khuri [7] suggested a measure of rotatability for response surface designs. Draper and Pukelsheim [8] suggested another look at rotatability. Further, Park et al. [9] introduced a new measure of rotatability for second order response surface designs and illustrated for 3^k factorial and central composite designs. Victorbabu and Surekha [10-11] suggested a measure of rotatability for second order response surface designs using BIBD and incomplete block designs like pairwise balanced designs (PBD) symmetrical unequal block arrangements (SUBA) with two unequal block sizes. In this paper, measure of rotatability for second order response surface designs using a pair of partially balanced incomplete block designs is suggested which enables us to assess the degree of rotatability for a given response surface design.

2. Conditions for second order rotatable designs

Suppose we want to use the second order response surface design D= $((x_{iu}))$ to fit the surface,

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

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, is said to be second order rotatable design (SORD) if the variance of the estimate of $Y_u(x_1,x_2, \dots,x_v)$ 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 ($x_1, x_2, \ldots, x_v$) from the origin (center) of the design. Such a spherical variance function for estimation of responses in the second order response surface is achieved if the design points satisfy the following conditions [1-2].

$$\sum_{u=1}^{N}\prod_{i=1}^{v} x_{iu}^{\alpha_i}=0 \text{ if any } \alpha_i \text{ is odd, for } \sum\alpha_i \le 4, \quad (2)$$

$$\sum x_{iu}^2 = \text{constant} = N\lambda_2, \quad (3)$$

$$\sum x_{iu}^4 = \text{constant} = cN\lambda_4; \text{ for all } i \quad (4)$$

$$\sum x_{iu}^2 x_{ju}^2 = \text{constant} = N\lambda_4; \text{ for } i \neq j \quad (5)$$

$$(c+v-1)\lambda_4 > v\lambda_2^2 \quad (6)$$

$$\sum x_{iu}^4 = c\sum x_{iu}^2 x_{ju}^2 \quad (7)$$

where c, λ_2 and λ_4 are constants.

The variances and covariances of the estimated parameters are

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

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

$$Cov(\hat{b}_{ii},\hat{b}_{jj})=\frac{(\lambda_2^2-\lambda_4)\sigma^2}{(c-1)N\lambda_4[\lambda_4(c+v-1)-v\lambda_2^2]} \text{ and other covariances vanish.} \quad (8)$$

The variances of the estimated response at the point ($x_{10}, x_{20}, \ldots, x_{v0}$) is

$$V(\hat{y}_0)=V(\hat{b}_0)+\left[V(\hat{b}_i)+2cov(\hat{b}_0,\hat{b}_{ii})\right]d^2+V(\hat{b}_{ii})d^4$$
$$+\sum x_{i0}^2x_{j0}^2\left[V(\hat{b}_{ij})+2cov(\hat{b}_{ii},\hat{b}_{jj})-2V(\hat{b}_{ii})\right] \quad (9)$$

The coefficient of $\sum x_{i0}^2x_{j0}^2$ in the above equation (2.9) is simplified to $(c-3)\sigma^2/(c-1)N\lambda_4$.

A second order response surface design D is said to be a SORD, if in this design c=3 and all the conditions (2) to (8) hold.

3. SORD using a pair of PBIBD (cf. Victorbabu, [5])

Take an incomplete block arrangement with constant block size and replication in which some pair of treatments occur λ_{11} times each $(\lambda_{11} \neq 0)$ and some other pairs do not occur at all $(\lambda_{12} = 0)$ (the design need not be PBIBD). Take this as the first design. For the second design take the incomplete block design with all missing pairs (in the first design) once each with $k = 2, \lambda_{21} = 0, \lambda_{22} = 1$. Such pairs of designs can be constructed in a straight forward manner using existing two-associate PBIB designs with one of the $\lambda's$ equal to zero.

Let $D_1 = (v, b_1, r_1, k_1, \lambda_{11} \neq 0, \lambda_{12} = 0)$ be an incomplete block design with constant replication in which only some pair of treatments occur a constant number of times $\lambda_{11}(\lambda_{12} = 0)$, $2^{t(k_1)}$ denote a fractional replicate of 2^{k_1} in +1 and -1 levels, in which no interaction with less than five factors is confounded. Let $[(1-(v, b_1, r_1, k_1, \lambda_{11}, \lambda_{12} = 0)]$ denote the design points generated from the transpose of the incidence matrix of incomplete block design D_1. $[(1-(v, b_1, r_1, k_1, \lambda_{11}, \lambda_{12} = 0)]2^{t(k_1)}$ are the $b_1 2^{t(k_1)}$ design points generate from D_1 by "multiplication" (see, Das and Narasimham, [2]).

Let $D_2 = (v, b_2, r_2, k_2 = 2, \lambda_{21} = 0, \lambda_{22} = 1)$ be the associated second design containing only the missing pairs of treatments of above design D_1. $[a-(v, b_2, r_2, k_2 = 2, \lambda_{21} = 0, \lambda_{22} = 1)]2^2$ are the $b_2 2^2$ design points generated from

D_2 by “multiplication”, with levels +a and –a. The method of construction of SORD using a pair of PBIBD is given in the following result (cf. Victorbabu, [5]).

Result: The design points,

$$\left[1-\left(v,b_1,r_1,k_1,\lambda_{11},\lambda_{12}\right)\right]2^{t(k_1)} \cup \left[a-\left(v,b_2,r_2,k_2=2,\lambda_{21},\lambda_{22}\right)\right]2^2$$

give a v-dimensional SORD in $N = b_1 2^{t(k_1)} + b_2 2^2$ design points, with

$$a^4 = \frac{-(r_1-3\lambda_{11})2^{t(k_1)-2}}{(r_2-3\lambda_{21})}.$$

4. Conditions of measure of rotatability for second order response surface designs

Following Box and Hunter [1], Das and Narasimham [2] , Park et al. [9], equations from (2) to (8) give the necessary and sufficient conditions for measure of 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 $i \neq j \neq l$. (10)

Park et al [9] suggested that if the conditions in (2) to (8) and (10) are met, then the following measure $(P_v(D))$ given below asses the degree of measure of rotatability for any general second order response surface design (cf. Park et al. [9], page 661).

$$P_v(D) = \frac{1}{1+R_v(D)}. \qquad (11)$$

where $R_v(D)=\left[\frac{N}{\sigma^2}\right]^2 \frac{6v\left[V(\hat{b}_{ij})+2cov(\hat{b}_{ii},\hat{b}_{jj})-2V(\hat{b}_{ii})\right]^2 (v-1)}{(v+2)^2(v+4)(v+6)(v+8)g^8}$ (12)

and g is the scaling factor (cf. Park et al. [9], page 658).

On simplification of $[V(\hat{b}_{ij})+2cov(\hat{b}_{ii},\hat{b}_{jj})-2V(\hat{b}_{ii})]$ becomes $\frac{(c-3)\sigma^2}{(c-1)N\lambda_4}$.

Thus, (4.3) becomes

$$R_v(D)=\left[\frac{N}{\sigma^2}\right]^2 \frac{6v\left[(c-3)\sigma^2\right]^2 (v-1)}{[(c-1)N\lambda_4]^2(v+2)^2(v+4)(v+6)(v+8)g^8} \quad (13)$$

5. Measure of rotatability for second order response surface designs using a pair of PBIBD

In this section the proposed measure of rotatability for second order response surface designs using a pair of PBIBD is suggested.

Theorem (5.1): The design points,

$$\left[1-\left(v,b_1,r_1,k_1,\lambda_{11},\lambda_{12}\right)\right]2^{t(k_1)} \cup \left[a-\left(v,b_2,r_2,k_2=2,\lambda_{21},\lambda_{22}\right)\right]2^2$$

give a v-dimensional measure of rotatability for second order response surface designs using a pair of PBIBD in N design points, with level ‘a’ pre-fixed and

$$c=\frac{r_1 2^{t(k_1)}+r_2 2^2 a^4}{\lambda_{11}2^{t(k_1)}+\lambda_{21}2^2 a^4}.$$

Proof: For the design points generated from a pair of PBIBD, simple symmetry conditions are true. Further we have,

$$\sum x_{iu}^2 = r_1 2^{t(k_1)}+r_2 2^2 a^2 = N\lambda_2 \quad (14)$$

$$\sum x_{iu}^4 = r_1 2^{t(k_1)}+r_2 2^2 a^4 = cN\lambda_4 \quad (15)$$

$$\sum x_{iu}^2 x_{ju}^2 = \lambda_{11} 2^{t(k_1)}+\lambda_{21} 2^2 a^4 = N\lambda_4 \quad (16)$$

From (15) and (16), we get $c=\frac{r_1 2^{t(k_1)}+r_2 2^2 a^4}{\lambda_{11} 2^{k_1}+\lambda_{21} 2^2 a^4}$. From (11) we can obtain the measure of rotatability values for second order response surface designs using a pair of PBIBD. From (4.4) we have

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

$$\text{where } g=\begin{cases} \frac{1}{a}, \text{ if } a<\sqrt{\frac{(b_1-r_1)2^{t(k_1)-2}}{r_2}+\frac{b_2}{r_2}}; \\ \frac{1}{\sqrt{\frac{(b_1-r_1)2^{t(k_1)-2}}{r_2}+\frac{b_2}{r_2}}}, \quad \text{if } a\geq\sqrt{\frac{(b_1-r_1)2^{t(k_1)-2}}{r_2}+\frac{b_2}{r_2}} \end{cases}$$

Example 1: Consider two PBIB designs, D_1=(v=10, b_1=8, r_1=4, k_1=5, λ_{11}=2, λ_{12}=0), and D_2=(v=10, b_2=5, r_2=1, k_2=2, λ_{21}=0, λ_{22}=1). The design points, $[1-(10,8,4,5,2,0)]2^4$ U $[a-(10,5,1,2,0,1)]2^2$ give a measure of rotatability for second order response surface design in N=148 design points for 10 factors.

For v=10 factors, we may point out here that measure of rotatability for second order response surface design using central composite designs of Park et al. [9], Victorbabu and Surekha [10-11] using BIBD (v=10, b=18, r=9, k=5, λ=4), PBD (v=10, b=11, r=5, k_1=5, k_2=4, λ=2), SUBA with two unequal block sizes (v=10, b=11, r=5, k_1=4, k_2=5, b_1=5, b_2=6, λ=2) need 149, 309, 197, 197 design points respectively.

Example 2: Consider two PBIB designs, D_1=(v=12, b_1=8, r_1=4, k_1=6, λ_{11}=2, λ_{12}=0), and D_2=(v=12, b_2=6, r_2=1, k_2=2, λ_{21}=0, λ_{22}=1). The design points, $[1-(12,8,4,6,2,0)]2^5$ U $[a-(12,6,1,2,0,1)]2^2$ give a measure of rotatability for second order response surface design in N=280 design points for 12 factors.

For v=12 factors, this new method needs 280 design points, whereas the corresponding measure of rotatability for second order response surface design constructed using central composite design, BIBD (v=12, b=22, r=11, k=6, λ=5), SUBA with two unequal block sizes (v=12, b=15, r=7, k_1=4, k_2=6, b_1=3, b_2=9, λ=3) need 281, 729, 505 design points respectively.

Example 3: Consider two PBIB designs, D_1=(v=6, b_1=4, r_1=2, k_1=3, λ_{11}=1, λ_{12}=0), and D_2=(v=6, b_2=3, r_2=1, k_2=2, λ_{21}=0, λ_{22}=1). The design points, $[1\text{-}(6,4,2,3,1,0)]2^3$ U $[a\text{-}(6,3,1,2,0,1)]2^2$ give a measure of rotatability for second order response surface design in N=44 design points for 6 factors.

In case of 6-factors, this new method needs 44 design points, whereas the corresponding measure of rotatability for second order response surface design constructed using central composite design, BIBD (v=6, b=10, r=5, k=3, λ=2), SUBA with two unequal block sizes (v=6, b=11, r=7, k_1=3, k_2=4, b_1=2, b_2=9, λ=4) need 45, 93, 189 design points respectively.

Thus the new method sometimes leads to designs with less number of design points than those available in the literature.

The Table 1 gives the values of measure of rotatability for second order response surface design using a pair of PBIBD. It can be verify that $P_v(D)$ is 1 if and only if the design is rotatable.

6. Conclusions

In this paper, measure of rotatability for second order response surface designs using a pair of PBIBD has been proposed which enables us to assess the degree of rotatability for a given second order response surface design. This measure, $P_v(D)$ has the value one if and only if the design D is rotatable, and it is smaller than one for a non-rotatable design. It is observed that the new method sometimes leads to designs with less number of design points than those available in the literature.

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Table 1. Values of measure of rotatability for second order response surface designs using pair of PBIBD**.**

D_1=(v=6,b_1=4,r_1=2,k_1=3,λ_{11}=1,λ_{12}=0), D_2=(v=6,b_2=3,r_2=1,k_2=2,λ_{21}=0,λ_{22}=1), N=44, a* = 1.1892				
a	c	g	$R_v(D)$	$P_v(D)$
1.1	2.73	0.9091	2.5980×10^{-3}	0.9974
1.1892	3.00	0.8409	0	1.0000
1.2	3.04	0.8333	7.1082×10^{-5}	0.9999
1.3	3.43	0.7692	0.0128	0.9873
1.6	5.28	0.6250	0.6164	0.6186
1.9	8.52	0.5263	4.6325	0.1775
2.2	13.71	0.4545	19.7339	0.0482
2.5	21.53	0.4000	62.9517	0.0156
2.8	32.73	0.3780	106.7470	9.2810×10^{-3}
3.1	48.18	0.3780	111.4998	8.8889×10^{-3}
3.4	68.82	0.3780	114.5248	8.6561×10^{-3}
3.7	95.71	0.3780	116.5096	8.5099×10^{-3}
4.0	130.00	0.3780	117.8498	8.4140×10^{-3}
4.3	172.94	0.3780	118.7786	8.3487×10^{-3}
4.6	225.87	0.3780	119.4376	8.3031×10^{-3}
4.9	290.24	0.3780	119.9151	8.2703×10^{-3}
D_1=(v=10,b_1=8,r_1=4,k_1=5,λ_{11}=2,λ_{12}=0), D_2=(v=10,b_2=5,r_2=1,k_2=2,λ_{21}=0,λ_{22}=1), N=148, a* = 1.6818				
a	c	g	$R_v(D)$	$P_v(D)$
1.3	2.36	0.7692	0.0364	0.9648
1.6	2.82	0.6250	8.4398×10^{-3}	0.9916
1.6818	3.00	0.5946	0	1.0000
1.9	3.63	0.5263	0.1934	0.8379
2.2	4.93	0.4545	2.6305	0.2754
2.5	6.88	0.4000	13.2244	0.0703
2.8	9.68	0.3571	44.5254	0.0220
3.1	13.54	0.3226	119.8855	8.2723×10^{-3}
3.4	18.70	0.2941	279.5404	3.5645×10^{-3}
3.7	25.43	0.2703	589.0473	1.6948×10^{-3}
4.0	34.00	0.2500	1150.5610	8.6839×10^{-4}
4.3	44.74	0.2326	2117.5050	4.7203×10^{-4}
4.6	57.97	0.2182	3602.2134	2.7753×10^{-4}
4.9	74.06	0.2182	3660.1802	2.7314×10^{-4}

a* indicates exact SORD using a pair of PBIBD.

Table 1. (Continued).

$D_1=(v=12,b_1=8,r_1=4,k_1=6,\lambda_{11}=2,\lambda_{12}=0)$, $D_2=(v=12,b_2=6,r_2=1,k_2=2,\lambda_{21}=0,\lambda_{22}=1)$, N=280, a* = 2.0000				
a	c	g	$R_v(D)$	$P_v(D)$
1.3	2.18	0.7692	0.0532	0.9495
1.6	2.41	0.6250	0.1012	0.9081
1.9	2.81	0.5263	0.0238	0.9767
2.0	3.00	0.5000	0	1.0000
2.2	3.46	0.4545	0.2614	0.7928
2.5	4.44	0.4000	3.5944	0.2178
2.8	5.84	0.3571	17.4749	0.0541
3.1	7.77	0.3226	56.8674	0.0173
3.4	10.35	0.2941	148.1967	6.7026×10^{-3}
3.7	13.71	0.2703	334.9262	2.9768×10^{-3}
4.0	18.00	0.2500	685.1211	1.4575×10^{-3}
4.3	23.37	0.2326	1301.3406	7.6785×10^{-4}
4.6	29.98	0.2174	2333.2519	4.2840×10^{-4}
4.9	38.03	0.2041	3993.4131	2.5035×10^{-4}

a* indicates exact SORD using a pair of PBIBD.

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