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Evaluating Percentage Rotatability For The Small Box – Behnken Design

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ARTICLE INFORMATION	ABSTRACT

Rotatability property for the Small Box-Behnken design is discussed in this paper. This paper aimed at applying a measure of obtaining percentage rotatability on the Small Box-Behnken designs to determine if the Small Box-behnken designs are rotatable or not and investigated the extent of rotatability in terms of percentage. The factors, q, considered range from 3 to 11. The results showed that for factors q, the Small Box-Behnken design is rotatable for q = 3 factors, near rotatable for q = 4, 7 factors and not rotatable for q = 5, 6, 8, 9, 10 and 11 factors.

1. Introduction

Considering the importance of experimental design and modelling of experiments, the Response Surface Methodology (RSM) is a combination of mathematical and statistical procedures that is helpful in the modeling and analysis of problems with the aim of optimizing the response of interest, Montgomery (2005). RSM procedure is basically presented using two important models, the first-degree model of order, r, $(r = 1)$, given in (1),

$$y = \tau_0 + \sum_{j=1}^{q} \tau_j x_j + \varepsilon_{ji}$$

(1)

and the second degree modelof order, r, $(r = 2)$, given in (2),

$$y = \tau_0 + \sum_{j=1}^{q} \tau_j x_j + \sum \sum_{j<i} \tau_{ji} x_j x_i + \sum_{j=1}^{q} \tau_{jj} x_j^2 + \varepsilon_{ji}$$

(2)

Kiwu-Lawrence et al. (2021), in their work, used the second-order response surface model to evaluate and compare the performances of three classes of Central Composite Design: Central Composite Circumscribed Design (CCCD), Central Composite Inscribed Design (CCID) and Central Composite Face-Centered Design (CCFD) using the A-, D-, and G-efficiencies for factors, k, that ranges from 3 to 10, with 0-5 centre points. It was shown from their result that the CCDs (CCCD, CCFD and CCID) are at their best when the G-efficiency is employed for all the factors considered while the CCID, in particular, behaves poorly when using the A- and D-efficiencies. Chigbu and Ohaegbulem (2011), in their study, applied the D-optimality criterion, which is a response

surface design optimality criteria to compare partially replicated cube and star portions of the rotatable and orthogonal CCD. They concluded that when the cube portion is replicated, the D-optimal performance of the CCD is enhanced better than replicating the star portion.

Designs that are based on three-level incomplete factorial designs for effectively fitting response surface model given in (2) were proposed by Box and Behnken (1960). The proposed designs gained popularity because they effectively obtain the maximum amount of information in a short period of time and their wide applications in industrial processes: see, for example, Aslan and Cebeci (2006). The designs proposed by Box and Behnken (1960), are rotatable or near rotatable. Rotatabilty is a property that ensures that from points equidistant from the design centre, the variance of a predicted response at a point remains constant at all such points, Mutai et al. (2013). Given that there is no advanced knowledge on how the response surface will orient itself with respect to its axes, it becomes necessary to adopt the rotatability property to explore the study of response surface design, Onukogu and Chigbu (2002). Since the introduction of the method of assessing rotatability or near-rotatability by Box and Hunter (1957), several efforts have been made at obtaining the rotatability or near-rotatability of the second-order design over a particular region of interest.

In other to obtain design rotatability or near-rotatability, researchers have developed different measures of design rotatability; the most common measures are given by Ekman (1994). In his study, graphical techniques were used to explore the variance function and the study concluded that it is not possible to construct a design with equal variance over the design space. Draper and Pukelsheim (1990), suggested a criterion for rotatability, which is invariant under design rotation. The criterion was provided for central composite designs and it was concluded that the criterion could be extended to higher-degree models. Draper and Guttman (1988) suggested a measure of rotatability for design space, but the measure has the limitations of not providing the extent of design rotatability.

Khuri (1988), introduced a measure that quantifies rotatability in percentage. That is, presenting the extent of rotatability for a design space in terms of percentage. The proposed measures have some desirable advantages. Hence, in this study, the proposed measure of rotatability by Khuri (1988) was used to ascertain the extent of rotatability in terms of percentage for the Small Box-Behnken designs. The Small Box-Behnken designs which fits the second-order response surface model with only a much smaller run size and with reasonably high D-efficiencies was developed by Zhang et al. (2011) as an alternative to the Box-Behnken design, since the Box Behnken designs have the limitation of a rapid increase in design run size as the number of factors, k, increases. The Orthogonality property of the original Box-Behnken design is preserved in the Small Box-Behnken designs, as pointed by Zhang et al. (2011). However, their work was silent on whether the rotatability property of the Box-Behnken designs is preserved in the Small Box-Behnken designs or not and that form the basis of this study. In this study, our aim is to evaluate the rotatability property of the Small Box-Behnken design in terms of percentage and recommend the design that is rotatable or not based on the percentage.

2. Methods and Materials
2.1. Condition for Rotatability
Rotatability is characterized by the information matrix, $X'X$. where, $X'X$, is called esign moments. In general, a design moment for a model such as equation (2) of order r and in q input variables is denoted by $\left[1^{\delta 1}, 2^{\delta 2}, ..., q^{\delta q}\right]$ and is equal to equation (3), where $\delta_i, i = 1, ..., q,$ are non-negative numbers and x_{ui} represents the level for the ith factor used in the uth experimental runs, $(i = 1, 2, ..., q; u = 1, 2, ..., n)$. Given that the design matrix, (X), for q factors is represented by $x_1, x_2, ..., x_q$ as an $N \times q$ matrix whose u_{th} row; $x_u' = (x_{u1}, x_{u2}, ..., x_{uq})$ represents the coded factor levels to be which is be used in the u_{th} row of the design space as in (2). $\left[1^{\delta 1}, 2^{\delta 2}, ..., q^{\delta q}\right]$ is used to denote the general design moment of (2) where;

$$\left[1^{\delta 1}, 2^{\delta 2}, ..., q^{\delta q}\right] = \sum_{u=1}^{n} X_{ui}^{\delta 1}, X_{u2}^{\delta 2}, ..., q_{uq}^{\delta q} \tag{3}$$

According to [2], for model such as (2) the necessary and sufficient condition for fitting such model of order r and in q factor so as to achieve rotatablility is that the general design moment of order $\delta (\delta = 0, 1, 2, ..., 2r)$ must be of the form;

$$\left[1^{\delta 1}, 2^{\delta 2}, ..., k^{\delta q}\right]$$

where,

$$\left[1^{\delta_1}, 2^{\delta_2}, ..., k^{\delta_k}\right] = 0; \text{ if any } \delta_i \text{ is odd}$$

$$= \frac{\theta_\delta \prod_{i=1}^{k} \delta_i!}{2^{\delta/2} \prod_{i=1}^{k} (\delta_i/2)!}; \text{if any } \delta_i \text{ are even} \tag{4}$$

Where, θ_δ, depends on r, δ and n; Box and Hunter (1957).

3. Second-Order Requirement for Rotatability

The general requirement for (2) rotatable is that the even moments must have the following form:

$$\left[j^2\right] = \frac{1}{N} \sum_{u=1}^{N} x_{uj}^2 = \lambda_2$$

$$\left[j^2 i^2\right] = \frac{1}{N} \sum_{ui}^{N} x_{uj}^2 x_{ui}^2 = \lambda_4$$

$$\left[j^4\right] = \frac{1}{N} \sum_{u=1}^{N} x_{uj}^4 = 3\lambda_4 \; (j^4) = 3\lambda_4 \tag{5}$$

where, $j = (1, 2, ..., q)$, $j = (1, 2, ..., q)$, $(j \neq i)$, q is the number of factors, λ_2 and λ_4 are the second-order of the design moments and fourth-order of the design moments, respectively, for any second-order design. Here, the odd moments of the order less than or equal to four is set to zero. Adding centre points to the design matrix X, does not change the general form of the design moments once design moments of X, satisfies the rotatability condition, Box and Behnken (1959).

4. Rotatability property

In many cases, the scaled prediction variance $N\left(\dfrac{\text{var}\left[(X)\right]}{\delta^2}\right)$ of a response surface design is the general property in experimental design used to show how the design points are distributed within the region of interest. The distribution of design points in the experimental region is characterized by the design moments and the design moment is a function of the model being fitted. The design moment comes from the moment matrix, M, given by

$$M = \frac{X'X}{N}, \text{ where, } (X'X), \text{ is referred to as the information matrix and } N \text{ is number of runs.}$$

For a second-degree model, where q = 3, the moment matrix is given by;

$$M = \begin{bmatrix} x_0 & x_1 & x_2 & x_3 & x_1 x_2 & x_1 x_3 & x_2 x_3 & x_1^2 & x_2^2 & x_3^2 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_2 & \sigma_2 & \sigma_2 \\ 0 & \sigma_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sigma_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sigma_{22} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sigma_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sigma_{22} & 0 & 0 & 0 \\ \sigma_2 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_4 & \sigma_{22} & \sigma_{22} \\ \sigma_2 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_{22} & \sigma_4 & \sigma_{22} \\ \sigma_2 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_{22} & \sigma_{22} & \sigma_4 \end{bmatrix}$$

(see Borkowski 2003),

5. Rotatability Measure

According to Montgomery (2005), the model in (2) of order r, with q factors $(x_1, x_2, ..., x_q)$. If the factors are codes as in (6) and the model is fitted in a spherical region, we have the following representation, $\sum_{u=1}^{n} Z_{uj} = 0; \quad j = 1, 2, ..., q$

$$\sum_{u=1}^{n} Z_{uj}^2 = \lambda_2; \quad j = 1, 2, ..., q \tag{6}$$

So that, Z_{uj} represents the coded value of x_{uj}, and λ_2 is some positive constant. By adapting the notion described in equation (4) to the coding variables (factors), the equalities described in equation (6) is hence, in the form of (7);

$$\sum_{u=1}^{n} Z_{uj} = (j) = 0; \quad j = 1, 2, ..., q$$

$$\sum_{u=1}^{n} Z_{uj}^2 = (j^2) = \lambda_2; \quad j = 1, 2, ..., q \tag{7}$$

6. Rotatable Design and the Canonical Representation of the information matrix (Z'Z)

Let Z_r denote the Z matrix when the design is rotatable. In this case, the vector $v(Z_r' Z_r)$ is given by

$$v(Z'Z) = \theta_0 w_0 + \theta_2 w_2 + ... + \theta_{2d} w_{2d} \tag{8}$$

where, w_δ $(\delta = 0, 2, ..., 2r)$, represents a vector, with dimension, $h^* \times 1$, $h^* = \dfrac{h(h+1)}{2}$ and h, is the number of parameters in (2). The quantity in (9) represents scale-free quantities;

$$Av(Z'Z) = u(Z'Z) \tag{9}$$

Where, the elements of, $A = 1/\gamma^\delta$, corresponds one-to-one with the elements of $v(Z'Z)$ and the elements of A corresponds to design moments of order, δ; (10) shows the canonical expression for $u(Z'Z)$ and it is obtained from (12) and (8)

$$u(Z'Z) = \frac{\sum_{m=0}^{r} \theta_{2m} w_{2m}}{\gamma^{2m}}$$

$$= nw_0 + w_2 + \sum_{m=2}^{r} q_{2m} w_{2m} \tag{10}$$

where,

$$q_{2m} = \frac{\theta_{2m}}{\gamma^{2m}}, \qquad m = 2, 3, ..., r \tag{11}$$

Supposed that the N-point design, X, for the fitting model in the (1) and (2), with the input variables (factors), coded as in equation (7). The corresponding vector, u(Z'Z), in equation (9) is given by

$$u(Z'Z) = nw_0 + w_2 + u*(Z'Z), \tag{12}$$

where, w_0 and w_2 are the same as in equation (10), and for a design with an equal number of runs, n, (12) holds for a rotatable design. Except for those that correspond to design moments of order, $\delta = 0$, and even design moments of order, $\delta = 2$, which are equal to 0, the elements of $u*(Z'Z)$ are equal to the corresponding elements of u(ZZ). The percentage rotatability measure is represented in (13), Khuri (1988).

$$\phi_n(X) = 100 \times \left\{ \sum_{m=2}^{r} \left[\mathbf{u} *' (\mathbf{Z'Z}) \mathbf{w}_{2m} \right]^2 / \|w_{2m}\|^2 \right\} / \|\mathbf{u} * (\mathbf{Z'Z})\|^2 \qquad (13)$$

7. Evaluating the percentage rotatability for the Small Box-Behnken Design

The expanded design matrix for Small Box-Behnken design for q = 3 is given by

$$Z = \begin{bmatrix}
X_0 & X_1 & X_2 & X_3 & X_1X_2 & X_1X_3 & X_2X_3 & X_1^2 & X_2^2 & X_3^2 \\
1 & -1 & -1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\
1 & 1 & -1 & 0 & -1 & 0 & 0 & 1 & 1 & 0 \\
1 & -1 & 1 & 0 & -1 & 0 & 0 & 1 & 1 & 0 \\
1 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\
1 & -1 & 0 & -1 & 0 & 1 & 0 & 1 & 0 & 1 \\
1 & 1 & 0 & -1 & 0 & -1 & 0 & 1 & 0 & 1 \\
1 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & 1 \\
1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\
1 & 0 & -1 & -1 & 0 & 0 & 1 & 0 & 1 & 1 \\
1 & 0 & 1 & -1 & 0 & 0 & -1 & 0 & 1 & 1 \\
1 & 0 & -1 & 1 & 0 & 0 & -1 & 0 & 1 & 1 \\
1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1
\end{bmatrix}.$$

$$Z'Z = \begin{bmatrix}
x_0 & x_1 & x_2 & x_3 & x_1x_2 & x_1x_3 & x_2x_3 & x_1^2 & x_2^2 & x_3^2 \\
12 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 8 & 8 \\
 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 & & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 & & & 8 & 0 & 0 & 0 & 0 & 0 & 0 \\
 & & & & 4 & 0 & 0 & 0 & 0 & 0 \\
 & & & & & 4 & 0 & 0 & 0 & 0 \\
 & & & & & & 4 & 0 & 0 & 0 \\
 & & & & & & & 8 & 4 & 4 \\
 & & & & & & & & 8 & 4 \\
 & & & & & & & & & 8
\end{bmatrix}.$$

For the average of all even design moments of order 2, γ^2 is given as;

$$\gamma = \left[\sum_{j=1}^{q} j^2 / q \right]^{1/2}$$

Where, $j^2 = \sum_{j=1}^{q} x_j^2 = 8.$

Therefore, $\gamma = \left[\dfrac{8+8+8}{3} \right]^{1/2} = 8^{1/2}.$

$A = \gamma^{\delta}$

The following steps from 1 to 5 were used to calculate the values of $w_0, w_2, \text{and } w_4$ entries in Table 1:

1. W_0, W_2, W_4, can be obtained from equation (8) through equation (11), given that; $u(Z'Z) = \dfrac{\sum_{m=0}^{r} \theta_{2m} w_{2m}}{\tau^{2m}}$, we

   shall use this notation to obtain the values of W_0, W_2, W_4, for *m = 0, 1, 2.*

2. If *m = 0,* we have that $u(Z_r'Z_r) = \dfrac{\theta_0 w_0}{\gamma^0}$; recall that, from equation (8), the elements of $W_0 = 1$ for only the first

   entry, all other entries are 0. From (4), it can be seen that θ_0 = n. Since for q = 3, n = 12, $u(Z'Z) = 12$, therefore, $\text{w}_o = 1$.

3. $W_{2m} = 0$, except for those elements that corresponding to even design moments of order $2m$. Also note that, θ_2 = λ_2 by the coding scheme of equation (7). Hence, by equation (11), $\theta_2 = \gamma^2$.

   If *m =1,* we have that $w_2 = \dfrac{\gamma^2 (u(Z'Z))}{\theta_2} = 1$; that is, $\theta_2 = \tau^2 = 8$ and $u(Z'Z) = 1$.

4. If *m = 2,* we have a case of the second pure moment and second mixed moment.

5. For the second pure moment, we have that; $W_4 = \dfrac{2\left[(u(Z'Z))\gamma^4\right]}{\theta_4}$, and for the second mixed moment, we have;

   $\text{W}_4 = \dfrac{\left[(u(Z'Z))\gamma^4\right]}{\theta_4}$.

Table 1: Computation of percentage rotatability for factor k = 3.

δ	v(Z'Z)	$\delta/2$	A	u(Z'Z)	$u*(Z'Z)$	w_0	w_2	w_4
0	12	0	1	12	0	1	0	0
1	0	0.5	0.3535534	0	0	0	0	0
1	0	0.5	0.3535534	0	0	0	0	0
1	0	0.5	0.3535534	0	0	0	0	0
2	0	1	0.125	0	0	0	0	0
2	0	1	0.125	0	0	0	0	0
2	0	1	0.125	0	0	0	0	0
2	8	1	0.125	1	0	0	1	0
2	8	1	0.125	1	0	0	1	0

2	8	1	0.125	1	0	0	1	0
2	8	1	0.125	1	0	0	1	0
2	0	1	0.125	0	0	0	0	0
2	0	1	0.125	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
2	8	1	0.125	1	0	0	1	0
2	0	1	0.125	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
2	8	1	0.125	1	0	0	1	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
3	0	1.5	0.0441942	0	0	0	0	0
4	4	2	0.015625	0.0625	0.0625	0	0	1
4	0	2	0.015625	0	0	0	0	0
4	0	2	0.015625	0	0	0	0	0
4	0	2	0.015625	0	0	0	0	0
4	0	2	0.015625	0	0	0	0	0
4	0	2	0.015625	0	0	0	0	0
4	4	2	0.015625	0.0625	0.0625	0	0	1
4	0	2	0.015625	0	0	0	0	0
4	0	2	0.015625	0	0	0	0	0

4	0	2	0.015625	0	0	0	0	0
4	0	2	0.015625	0	0	0	0	0
4	4	2	0.015625	0.0625	0.0625	0	0	1
4	0	2	0.015625	0	0	0	0	0
4	0	2	0.015625	0	0	0	0	0
4	0	2	0.015625	0	0	0	0	0
4	8	2	0.015625	0.125	0.125	0	0	4
4	4	2	0.015625	0.0625	0.0625	0	0	1
4	4	2	0.015625	0.0625	0.0625	0	0	1
4	8	2	0.015625	0.125	0.125	0	0	4
4	4	2	0.015625	0.0625	0.0625	0	0	1
4	8	2	0.015625	0.125	0.125	0	0	4

Let, $[u*(Z'Z)] = a$, $[w_4] = b$, $(a \times b') = c$, $norm(a) = d$, $norm(b) = e$

$$\phi_n(X) = 100 \times \left\{ \sum_{m=2}^{d} \left[u*' (Z'Z) w_{2m} \right]^2 / \|w_{2m}\|^2 \right\} / \|u*(Z'Z)\|^2$$

$$\phi_n(X) = 100 \times \left\{ \left(c^2 / e^2 \right) \right\} / d^2$$

$$\phi_n(X) = 92.59\%$$

Same procedure was used to obtain the percentage rotatability for other factors shown in table 2.

Table 2: Result of percentage Rotatability for factor q = 3 to 11.

No. of factors (q)	No. of Parameters (h)	No. of Runs (N)	Percentage Rotatability values
3	10	12	92.59
4	15	16	50.63
5	21	24	39.12
6	28	32	44.86
7	36	40	47.93
8	45	56	39.50
9	55	60	36.15
10	66	76	28.20
11	78	96	33.01

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8. Results and Discussion

Rotatability is an important criterion to be considered when selecting a response surface design. The Small Box-Behnken design is rotatable for factor, q = 3 at 92.59 percent, near rotatable for factors, q = 4, 7 at 50.63 and 47.93 percent respectively and not rotatable for factors, q = 5, 6, 8, 9, 10 and 11 at 39.12, 44.86, 39.50, 36.15, 28.20 and 33. 01.

9. Conclusion

This paper aimed at applying a measure of obtaining percentage rotatability on the Small Box-Behnken designs to determine if the Small Box-behnken designs are rotatable or not and investigated the extent of rotatability in terms of percentage. The factors, q, considered range from 3 to 11. In conclusion, results showed that for factors q, the Small Box-Behnken design is rotatable for q = 3 factor, near rotatable for q = 4, 7 factors and not rotatable for q = 5, 6, 8, 9, 10 and 11 factors. However, it is therefore recommended that, where it is possible, q = 3 factors, should be used in response surface exploration using the Small Box-Behnken design, but where it is not possible to use only q = 3 factors, the q = 4 and 7 factors, should be considered since they have more 47 percent rotatability. For future research work, we suggest that a diagnostic check be carried out on Small Box-Behnken design for factors, q = 5, 6, 8, 9, 10 and 11 and recomputed the percentage rotatability.

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