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Research Paper

An approach to measuring rotatability in central composite designs

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Abstract

An approach to measure design rotatability and a measure, that quantifies the percentage of rotatability (from 0 to 100) in the central composite designs are introduced. This new approach is quite different from the ones provided by previous authors which assessed design rotatability by the viewing of tediously obtained contour diagrams. This new approach has no practical limitations, and the measure is very easy to compute. Some examples were used to express this approach.

Keywords: *Central Composite Designs; Design Rotatability; Near Rotatable Designs; Perfectly Rotatable Designs; Second-Order Response-Surface Designs.*

1. Introduction

The concept of rotatability was first introduced in experimental design in Box and Hunter [6], and has since become an important design criterion. Rotatability is a desirable feature of any experimental design (see, for example, [7]); and this is mainly; because the experimenter does not have any prior information or knowledge about the location of the optimum. Therefore, a design that provides equal precision of estimation in all directions would be preferred. Such a design will ensure the experimenter that no matter what direction is taken to search for the optimum, he/she will be able to estimate the response value with equal precision.
As an illustrative example, consider an event where a (linear) response-surface polynomial of order d is fit on k predictor variables, $x_1, x_2, \cdots, x_k$ over a spherical region of interest, R, using a design consisting of n experimental runs; and is written as,

$$y = X\beta + \varepsilon \tag{1}$$

Where,
y is a vector of n observations; X is an $n \times p$ matrix of rank p whose elements are known functions of the design settings of the predictor variables; β is a vector of unknown regression coefficients, which can be estimated approximately by Ordinary Least Squares (OLS), given by

$$\hat{\beta} = (X'X)^{-1}X'y \tag{2}$$

And $\varepsilon \sim N(0, I_n\sigma^2)$, where (σ^2) is unknown and I_n is an $n \times n$ identity matrix.
Now, let D denote the $n \times k$ experimental design matrix whose u^{th} row consists of the settings of the k predictor variables at the u^{th} experimental run, $x_{1u}, x_{2u}, \cdots, x_{ku}; u = 1, 2, \cdots, n$
Also, let $\hat{y}(x)$ denote the predicted response value at a particular point, $x = (x_1, x_2, \cdots, x_k)'$ in the region, R.
The experimental design matrix D is said to be rotatable if the variance of $\hat{y}(x)$, $Var[\hat{y}(x)]$ is a function of only the distance of the point x from the center of the design and not on the direction. That is, if $Var[\hat{y}(x)]$ is a function only of $r^2 = x_1^2 + x_2^2 + \cdots + x_k^2$ (where r is the radius of a circle). Thus, the advantage of the rotatability property in a design is

that the prediction variance, $\mathrm{Var}[\hat{y}(x)]$ remains unchanged under any rotation of the coordinate axes. In addition, if optimization of $\hat{y}(x)$ is desired on concentric hyper-spheres within R, then it would be desirable for the design to be rotatable (see, for example, [3]). Consequently, anything short of this might result in poor estimates of the optimum (see, [2]).

Often times, in practical situations, experimenters encounter designs that may be best described as being "near rotatable". That is, non-rotatable designs, that exhibit surfaces of constant prediction variances that are nearly spherical (see, for example, [1]). This condition of "near rotatable" can occur under the following circumstances:

1) When a perfectly rotatable design is deformed ; because of incorrect settings of some of the predictor variables or; because certain specified levels of the predictor variables may be difficult to employ in practice;
2) When a rotatable design undergoes certain modifications to fit the needs of the experiment; of which might involve in adding new design points or shifting existing design points to gain more information in a certain region of interest.

According to Draper and Pukelsheim [7], it is still a good idea to make the design as rotatable as possible, even if circumstances are such as that exact rotatability is unattainable. Thus, it is important to know if a particular design is rotatable or, if it not, to know how rotatable the design is.

Khuri [1] introduced a measure that quantifies the amount of rotatability in a given response-surface design; a measure which is expressible as a percentage taking the value 100 when the design is rotatable. This measure can also, be useful in the following situations:

1) Comparison of designs on the basis of their degrees of rotatability.
2) Assessment of the extent of departure from rotatability of a "deformed or modified" design.
3) Repairing or improving rotatability, by a proper augmentation, of a non-rotatable design.

It is worthy of note that, generally, assessing the degree of rotatability has been a pretty hard task to carry out with the customary technique of drawing and inspecting the prediction variance contour plots; to see how close they are being completely circular. Most likely, this could be quite subjective too. This practice is somehow manageable for $k = 2$ input variables, but poses some practical limitations for dimensions, $k \geq 3$. The assessment of rotatability has been discussed in published articles by different authors such as [8], [1], and [7]; but the subject matter had always been approached essentially via the drawing of contour plots.

Nevertheless, this paper presents a different approach to measuring design rotatability for the Central Composite Designs (CCDs). This approach provides a new measure of rotatability which takes values between 0 and 100, just like the measure provided by [1] and others, but its determination absolutely does not involve the art of drawing any prediction variance contour plots. This approach is devoid of subjectivity, has no practical limitations, and the measure is very easy to compute and provides the most accurate percentage of rotatability.

2. Measuring design rotatability

The concept of rotatability is not restricted to second-order designs, but most of the published works pertaining to design rotatability laid particular emphasis on the second-order model. For instance, Montgomery [4] stated that the preferred class of second-order response-surface designs is the class of rotatable designs. Myers [9] posited that the second-order rotatable response-surface designs which find the most use in practical situations are the rotatable Central Composite Designs (CCDs).Consequently, discussion in this paper on measuring design rotatability will be specifically centered on the Central Composite Designs.

According to Myers [9], a second-order design is rotatable if its moments have the following conditions:

1) All moments that have at least one δ_i odd are zero (where δ is the order of the design moment, such that for k variables, $\sum_{i=1}^{k} \delta_i = \delta$);
2) Pure fourth moments are three times the mixed fourth moments. That is,

$$\sum_{u=1}^{N} x_{iu}^4 = 3 \sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 \quad (3)$$

Now, considering the typical design matrix for the general CCD with respect to the portion containing the second-order terms, $x_1^2, x_2^2, \cdots, x_k^2$ (see, [9]); it can easily be seen that,

$$\sum_{u=1}^{N} x_{iu}^4 = F + 2 \propto^4 \quad (4)$$

and

$$\sum_{u=1}^{N} x_{iu}^2 x_{i'u}^2 = F \quad (5)$$

Where $F = 2^k$ and $i = 1, 2, \cdots, k$.

Of the two conditions given, which must be met in order that a second-order design is rotatable, the first is automatically met by the CCDs (this is verifiable by mere inspection of the entire X matrix of the CCDs).

Now, for the second condition, we recall the information matrix for the general CCD (see, [5]) given as,

$$M = \bar{X}'\bar{X} = \text{diag}\left(M_1 I_k, M_2 I_t, \underline{M_3}\right) \quad (6)$$

Where

$$M_1 = 2^k + 2 \propto^2 \quad (7)$$

$$M_2 = 2^k \quad (8)$$

and

$$\underline{M_3} = (p - q)I_k + qJ_k \quad (9)$$

In similarity to (4) and (5);

$$p = 2^k + 2 \propto^4 \quad (10)$$

and

$$q = 2^k \quad (11)$$

are, respectively, the diagonal and off-diagonal elements of the $\underline{M_3}$ portion of the information matrix, M. Invariably, for the CCD to satisfy the second condition for a second-order design to be rotatable, (3) now implies;

$$p = 3q \quad (12)$$

This is a strict condition for perfectly rotatable CCDs; and looking at the matrix $\underline{M_3}$ from the information matrix of the perfectly rotatable CCD as given (13) below, we obviously see that for $i, j = 1, 2, \cdots, k$; $p_{11} = p_{22} = \cdots = p_{kk} = p$ and $q_{12} = q_{13} = \cdots = q_{1k} = q$ (noting that $q_{ij} = q_{ji}; i \neq j$).

$$\underline{M_3} = \begin{pmatrix} p_{11} & q_{12} & q_{13} & \cdots & q_{1k} \\ & p_{22} & q_{23} & \cdots & q_{2k} \\ & & p_{33} & \cdots & q_{3k} \\ & & & \ddots & \vdots \\ SYM & & & & p_{kk} \end{pmatrix} \quad (13)$$

Now, we involve all the elements of (13) in creating an expression which may be seen as yet a third condition for a central composite design to be rotatable. To do this, we take into consideration the relationship between sum of squares and sum of cross-products as well as the relationship between the trace and off-diagonal elements of (13). In terms of $p_{ij}'s$ and $q_{ij}'s$, an extended expression that could be used to ascertain whether or not a CCD is rotatable can now be written as,

$$(k - 1)\sum_{i=j} p_{ij} = 3\sum_{i \neq j} q_{ij} \quad (14)$$

Just like (12), (14) is a strict condition for perfectly rotatable CCDs; and (14) accommodates (12) in the sense that any matrix in the form of (13) that satisfies the former will equally satisfy the latter.
For a rotatable CCD that has been deformed or modified, and is no longer perfectly rotatable, (14) will not hold. Now, suppose the difference between the left-hand side and the right-hand side of (14) is represented by Δ_R; such that,

$$\Delta_R = (k - 1)\sum_{i=j} p_{ij} - 3\sum_{i \neq j} q_{ij} \quad (15)$$

From (12), we see that p is dependent on q, and as such we can express Δ_R as a percentage of $(k - 1)\sum_{i=j} p_{ij}$ to give the extent to which the design is short of being perfectly rotatable. This expression is given as,

$$\Delta_R^{\blacksquare} = \frac{|\Delta_R|}{(k-1)\sum_{i=j} p_{ij}} \times 100\% \quad (16)$$

Consequently, the measure of the extent to which a design is rotatable can be expressed as,

$$R^{\vartheta} = (100 - \Delta_{R}^{\blacksquare})\% \quad (17)$$

Now, with (17), every perfectly rotatable CCD will have a measure of 100% rotatability; while for “near rotatable” as well as other non-rotatable CCDs, they will have less than 100% rotatability. This measure (as remarked in [1] on the measure of rotatability introduced), in conjunction with other measures of design efficiency, can be used to select a design that possesses several characteristics of interest to the experimenter.

3. Examples/applications

Some numerical examples of CCDs are presented in this section to illustrate the applications of the measures of rotatability developed in this paper. The main purpose of presenting and discussing these examples is to demonstrate the actual implementation of (17) in measuring design rotatability. These CCDs, which are described in Examples 1 to 3, include some well-known rotatable CCDs as well as two specific non-rotatable CCDs already considered by previous authors using the approaches and measures they derived. The essence of determining the measures of rotatability for these two specific designs is not at all for comparison sake; rather it is to have already existing designs to which references would be made.

NB: These designs are titled in such a way that the first digit is the number of variables; the next two digits are the number of design points. A letter differentiates designs of the same size (see, for example, [1]).

Example1: Consider three CCDs with the following descriptions: a 9-point CCD in two input variables (209) with axial distance, $\propto = 1.414$; a 15-point CCD in three input variables (315) with axial distance, $\propto = 1.682$; and a 26-point CCD in four input variables (426) with axial distance, $\propto = 2.000$. Recall that, given the values of their axial distances, the 209, 315, and 426 CCDs are qualified to be rotatable designs (see, for example, [5]).

Example 2: Consider the non-rotatable 210 design due originally to Hebble and Mitchell [10], which was discussed in [1] and also in [7]. This design is presented in Table 1.

Table 1: The Non-Rotatable 210 CCD (Example 2)

Run No.	x_1	x_2
1	-1	1.35
2	1	-1.25
3	-1.6	-0.85
4	1	1
5	-1.5	0
6	1.55	0
7	0	-1
8	0	1.55
9	0.55	0.30
10	0	0

Repairing the non-rotatable 210 CCD in Example 2 to become as rotatable as possible, Khuri [1] augmented the design with three additional repair points, one at a time, to get the sequence of designs 211A, 212A, and 213A, respectively.

In another attempt to repair the same non-rotatable 210 CCD in Example 2, Draper and Pukelsheim [7] augmented the design with four additional repair points, one at a time, to get the sequence of designs 211B, 212B, 213B, and 214, respectively.

Example 3: Consider the non-rotatable 316 design discussed in [1] and also in [7] as presented in Table 2.

Khuri [1] ventured repairing the non-rotatable 316 CCD in Example 3 by augmenting the design with two additional repair points, one at a time, to get the sequence of designs 317A and 318A, respectively.

In another development, Draper and Pukelsheim [7] went about to repair the same non-rotatable 316 CCD in Example 3 by augmenting the design with three additional repair points, one at a time, to arrive at the sequence of designs 317B, 318B, and 319, respectively.

It is worthy of note also that Khuri [1] and Draper and Pukelsheim [7] used their approaches to determine the measures of rotatability of the respective designs credited to them.

In order to measure the percentages of rotatability of the designs cited in Examples 1 to 3, using our approach, the $\underline{M_3}$ portions of the respective information matrices of these designs are obtained first (these are presented in Table 3). The corresponding measures of rotatability, R^{ϑ} for each of the designs are determined using (17); and the numerical values of these measures are presented in Table 4.

Table 2: The Non-Rotatable 316 CCD (Example 3)

Run No.	x_1	x_2	x_3
1	-1	-1	-1
2	1	-1	-1
3	-1	1	-1
4	1	1	-1
5	-1	-1	1
6	1	-1	1
7	-1	1	1
8	0.48	1	1
9	-1.682	0	0
10	1	0	0
11	0	-1.682	0
12	0	1.682	0
13	0	0	-1.682
14	0	0	1.682
15	0	0	0
16	0	0	0

4. Conclusions

A new approach to measure design rotatability, as it affects the central composite designs, is presented. With the approach, the CCDs (209, 315, and 426) whose design structures show clear rotatability property (i.e., from the respective $\underline{M_3}$ portions of their information matrices; $p = 3q$) have R^{ϑ} values of exactly 100%. On the other hand, the other CCDs in Table 3 that are not rotatable given their design structures (such that $p \neq 3q$) have R^{ϑ} values less than 100%; affirming the non-rotatable statuses of these designs.

In fact that the approach involves the use of the diagonal and the off-diagonal elements of the $\underline{M_3}$ portion of the information matrix of the design, it can be used to determine the percentage rotatability of central composite designs of any dimension. The most interesting aspect of the new approach is that it does not involve contour plots - which are quite tedious to go about, and it has no practical limitations. It is very easy to apply.

Table 3: The $\underline{M_3}$ Portions of the Information Matrices of the Designs in Examples 1 to 3

S/N	Design	The $\underline{M_3}$ Portion	S/N	Design	The $\underline{M_3}$ Portion
1	209	$\begin{pmatrix} 12 & 4 \\ 4 & 12 \end{pmatrix}$	9	212B	$\begin{pmatrix} 20.4813 & 6.2907 \\ 6.2907 & 19.1531 \end{pmatrix}$
2	315	$\begin{pmatrix} 24 & 8 & 8 \\ & 24 & 8 \\ SYM & & 24 \end{pmatrix}$	10	213B & 214	$\begin{pmatrix} 20.4814 & 6.2907 \\ 6.2907 & 19.1531 \end{pmatrix}$
3	426	$\begin{pmatrix} 48 & 16 & 16 & 16 \\ & 48 & 16 & 16 \\ & & 48 & 16 \\ SYM & & & 48 \end{pmatrix}$	11	316	$\begin{pmatrix} 16.0570 & 7.2304 & 7.2304 \\ & 24.0079 & 8.0000 \\ SYM & & 24.0079 \end{pmatrix}$
4	210	$\begin{pmatrix} 20.4796 & 6.2618 \\ 6.2618 & 14.0650 \end{pmatrix}$	12	317A	$\begin{pmatrix} 16.5270 & 7.4060 & 7.4060 \\ & 24.0735 & 8.0655 \\ SYM & & 24.0735 \end{pmatrix}$
5	211A	$\begin{pmatrix} 20.4798 & 6.3105 \\ 6.3105 & 26.0158 \end{pmatrix}$	13	318A	$\begin{pmatrix} 17.3979 & 7.4273 & 7.4273 \\ & 24.0740 & 8.0660 \\ SYM & & 24.0740 \end{pmatrix}$
6	212A	$\begin{pmatrix} 20.9533 & 6.3106 \\ 6.3106 & 26.0158 \end{pmatrix}$	14	317B	$\begin{pmatrix} 16.8715 & 7.2868 & 7.2868 \\ & 24.0118 & 8.0039 \\ SYM & & 24.0118 \end{pmatrix}$
7	213A	$\begin{pmatrix} 20.9537 & 6.3122 \\ 6.3122 & 26.0216 \end{pmatrix}$	15	318B	$\begin{pmatrix} 17.8715 & 7.2868 & 7.2868 \\ & 24.0118 & 8.0039 \\ SYM & & 24.0118 \end{pmatrix}$
8	211B	$\begin{pmatrix} 20.4796 & 6.2843 \\ 6.2843 & 26.0158 \end{pmatrix}$	16	319	$\begin{pmatrix} 18.0011 & 7.3012 & 7.3012 \\ & 24.0134 & 8.0055 \\ SYM & & 24.0134 \end{pmatrix}$

Table 4: Summary of the Measures of Rotatability for the Designs in Examples 1 to 3

S/N	Design	$(k-1)\sum_{i=j} p_{ij}$	$3\sum_{i\neq j} q_{ij}$	R^{ϑ}
1	209	24	24	100
2	315	144	144	100
3	426	576	576	100
4	210	34.5446	37.5708	91.24
5	211A	46.4956	37.8630	81.43
6	212A	46.9691	37.8636	80.61
7	213A	46.9753	37.8732	80.62
8	211B	39.6071	37.7058	95.20
9	212B	39.6344	37.7442	95.23
10	213B	39.6345	37.7442	95.23
11	214	39.6345	37.7442	95.23
12	316	128.1456	134.7648	94.83
13	317A	129.3480	137.2650	93.88
14	318A	131.0918	137.5236	95.09
15	317B	129.7902	135.4650	95.63
16	318B	131.7902	135.4650	97.21
17	319	132.0558	135.6474	97.28

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