Optimality of Central Composite Designs Augmented from One-half Fractional Factorial Designs

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Abstract – The central composite design (CCD) is a popular choice for fitting the second-order model. This popularity may be due to the design's flexibility and use in sequential experimentation. CCDs can be constructed by augmenting a full factorial or a fractional factorial design (resolution III and V). This study explored the optimality of CCDs that are augmented from one-half fractional factorial designs. The rotatability and approximate orthogonality of this type of CCDs were investigated. In addition, for specified designs, the alphabetic criterion values based on the D, A, E, and V were calculated. An R script containing functions were developed for this study. The R script was used in determining the rotatability and approximate orthogonality. The D, A, E, and V criteria values were also calculated using the same R script. The conditions for CCDs to be rotatable and approximately orthogonal were presented in the results. Furthermore, the recommended axial distance and center points to achieve reasonable alphabetic criterion values were also given. The results may be used as a reference or guide in choosing an appropriate combination of axial distance and center points in a central composite design.

Index Terms – Central Composite Design, Optimality, One-half Fractional Factorial Design, Orthogonality, Rotatability

1. INTRODUCTION

Experimental designs have enjoyed wide application in different areas of research, be it in agriculture, business, or manufacturing. An experiment is conducted for the purpose of studying the effect of one or more factors on a response variable. The goal is to determine suitable factor levels so that the desired response is achieved. Several designs are available for use in experimentation. The choice of design depends on the design's applicability to the current situation. Resources, facilities, and other relevant conditions can have an impact on a design's effectiveness.

The relationship between the factors and the response variable can usually be described by certain models. The first and second-order model can be fitted depending on the type of design implemented. The central composite design (CCD) is a popular choice for fitting the second-order model.

CCDs have been studied and applied in different areas since its introduction. This class of designs has been used in analytical chemistry [1]. It has also been applied in the area of chemical and biological engineering [3]. A study has been made comparing different types of CCDs [7]. A measure on the degree of rotatability has been proposed [6]. CCDs were also compared under different optimality criteria [5].

Park, Kim, and Cho focused on CCDs that are mostly augmented from full factorials [5]. This study draws idea from their work and explored the optimality of CCDs that are augmented from one-half fractional factorial designs. Additional optimality criteria were also included. Conditions for designs to be rotatable and approximately orthogonal were investigated. The results of this study can be used for choosing an appropriate CCD based on the purpose of the experiment.

2. CENTRAL COMPOSITE DESIGN, ROTATABILITY, ORTHOGONALITY, AND OPTIMALITY

2.1. Central Composite Design

There are experimental situations in which the second-order model given below is appropriate.

$$y = \beta_0 + \sum_{j=1}^{k} \beta_j x_j + \sum_{i<}\sum_{j} \beta_{ij} x_i x_j + \sum_{j=1}^{k} \beta_{jj} x_j^2 + \epsilon \qquad (1)$$

The central composite design is one of the designs that can be used for fitting the second-order model. CCDs can be constructed by augmenting a 2^k factorial or its fraction (resolution V) with 2k axial points [4]. CCDs may also be constructed from resolution III fractional factorial designs. These designs are called small composite designs (SCD). The inclusion of axial points in the design is an effective solution to the problem of parameter estimation encountered when using 2^k designs for second-order models.

Appending the axial points in the design matrix, the central composite design can now be viewed as an experiment containing factorial points, center points, and axial points. The experimenter conducts a 2^k factorial experiment and uses the center points to check for curvature. If curvature is present, the axial points may be used to estimate additional parameters.

As an example, the design matrix for a 2^3 factorial design with 3 center points and 6 axial runs is shown in Table 1. The axial distance (α) for this example is 1.6818.

A	B	C
-1	-1	-1
1	-1	-1
-1	1	-1
1	1	-1
-1	-1	1
1	-1	1
-1	1	1
1	1	1
-1.6818	0	0
1.6818	0	0
0	-1.6818	0
0	1.6818	0
0	0	-1.6818
0	0	1.6818
0	0	0
0	0	0
0	0	0

Table 1 Sample Design Matrix for a Central Composite Design

2.2. Rotatability and Orthogonality

For second-order designs, it is important to have a reasonably stable scaled prediction variance $N\,\mathrm{var}[\hat{y}(\mathbf{x})]/\sigma^2$. In a rotatable design, the value of the scaled prediction variance is equal for any two points whose distance from the design center is equal. The rotatability of a CCD depends on the number of factorial points. A design is rotatable if the following condition holds,

$$\alpha = \sqrt[4]{n_F} \quad (2)$$

where n_F refers to the number of factorial points [4].

Given the model matrix X, a design is said to be orthogonal if $X'X$ is a diagonal matrix [4]. Khuri and Cornell (1987) suggested a method for designs to be rotatable and approximately orthogonal [2]. The experimenter must first choose an α for rotatability using equation (2). Center points (n_o) are then added so that

$$n_o \approx 4\sqrt{n_F} + 4 - 2k \quad (3)$$

2.3. D-Optimality

D-Optimality is a criterion that focuses on model parameter estimation. It is the most popular alphabetic optimality criterion. The measure is based on the control of the inverse of the moment matrix $\mathbf{M} = \mathbf{X}'\mathbf{X}/\mathrm{N}$. A design is said to be D-optimal if the determinant given in (4)

$$|\boldsymbol{M}| = \frac{|\boldsymbol{X}'\boldsymbol{X}|}{N^P} \quad (4)$$

is maximized or similarly $\mathrm{N}^{\mathrm{P}}|(\mathbf{X}'\mathbf{X})^{-1}|$ is minimized where $\mathbf{X}$ is the model matrix, N is the number of runs, and p is the number of model parameters [4].

2.4. A-Optimality

The A-Optimality is another criterion that measures how well model parameters are estimated. A-Optimality is concerned with the variances of each regression coefficient. A design is A-Optimal if

$$tr\boldsymbol{M}^{-1} = tr(N(\boldsymbol{X}'\boldsymbol{X})^{-1}) \quad (5)$$

is minimized, where tr represents the trace of the inverse of the moment matrix **M** [4].

2.5. E-Optimality

The determinant of $\mathbf{X}'\mathbf{X}$ can be expressed in terms of eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_p$, specifically, $|\mathbf{X}'\mathbf{X}| = \prod_{i=1}^{p} \frac{1}{\lambda_i}$. The measure is a minimax approach and a design is said to be E-optimal if for all designs in the set

$$E = Max\,\lambda_i \quad for\ i = 1,2,\dots,p \quad (6)$$

is minimized [5].

2.6. V-Optimality

Previous measures of optimality have been concerned with the estimation of model parameters. Experimenters may also be interested on how well a design performs in the aspect of prediction. The scaled prediction variance given by

$$v(\boldsymbol{x}) = \frac{N\,\mathrm{var}[\hat{y}(\boldsymbol{x})]}{\sigma^2} = N\boldsymbol{x}^{(m)\prime}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}^{(m)} \quad (7)$$

is measure of prediction accuracy at a point $\mathbf{x}^{(\mathrm{m})}$ in the design space.

The V-criterion takes into account the prediction variance on a specific set of points within the design space. The set of points may be selected based on its practical importance to the experimenter. The design is V-Optimal if it minimizes the average prediction variance [4].

3. METHODOLOGY

This study dealt with the optimality of central composite designs that are augmented from one-half fractional factorial designs. The fractional factorial designs are of resolution III and V. In addition, the principal fraction was used. That is, the fractional factorial designs were generated using a positive word in the defining relation. The designs were produced by varying the number of factors (3, 4, 5, and 6 factors), the axial distance (from 0.5 to 5 with increments of 0.5), and the number of center points (from 3 to 7 center points).

In computing the V values, the design points are considered as the set of particular importance. Hence, the average scaled prediction variance is determined using this set of points.

The general procedure that was employed in determining the rotatability, orthogonality, and alphabetic criteria values are shown in the succeeding figure.

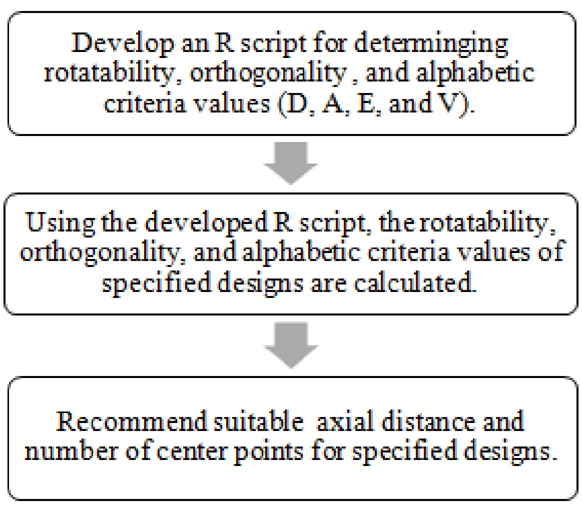

Figure 1 General Procedure of the Study

4. RESULTS AND DISCUSSIONS

4.1. Rotatability and Orthogonality of Specified Designs

The axial distance and number of center points are shown in Table 2. Designs with three or four factors are augmented from resolution III fractional factorial designs. These are small composite designs and lack the characteristic of rotatability. For five factors, an axial distance of 2 and 10 center points are required to achieve rotatability and approximate orthogonality. Similarly, for six factors, an axial distance of 2.3784 and 15 center points are needed.

Number of Factors	Axial Distance (α)	Number of Center Points
3 (1/2)	-	-
4 (1/2)	-	-
5 (1/2)	2.0000	10
6 (1/2)	2.3784	15

Table 2 CCD for Rotatability and Approximate Orthogonality

4.2. Alphabetic Criterion Values for a Three-Factor Small Composite Design

The subsequent analyses are based on the range of α and number of center points as specified in the methodology of this study. Thus, all conclusions are limited to the stated range as observed from the tables and plots.

The D values for a three-factor SCD are shown in Table 3. The values generally increase as the axial distance gets larger. The increase becomes large for an axial distance of 3.0 and above. The same pattern can be observed in the plot of D values. Considering the number of center points, for an axial distance of roughly between 0.5 and 2.5, D values do not differ by large amounts. However, for an axial distance of 3.0 and above, large values of D are apparent for small number of center points.

Axial Distance (α)	Number of Center Points				
	3	4	5	6	7
0.5	8.7839E-11	4.7104E-11	2.6256E-11	1.5149E-11	9.0139E-12
1.0	1.0993E-06	6.2306E-07	3.6226E-07	2.1607E-07	1.3206E-07
1.5	3.0737E-04	1.9223E-04	1.1936E-04	7.4631E-05	4.7265E-05
2.0	3.4076E-02	2.1345E-02	1.3267E-02	8.3008E-03	5.2595E-03
2.5	1.9640	1.1737	0.708	0.4339	0.2707
3.0	57.5545	33.3229	19.6709	11.8668	7.3175
3.5	996.7783	566.5446	330.0734	197.1769	120.6648
4.0	11,660.41	6,553.25	3,786.7490	2,248	1,368.94
4.5	101,161	56,439.72	32,437.32	19,176.28	11,638.97
5.0	694,371.4	385,473.5	220,714.3	130,103.2	78,782.48

Table 3 D Values for a Three-Factor SCD

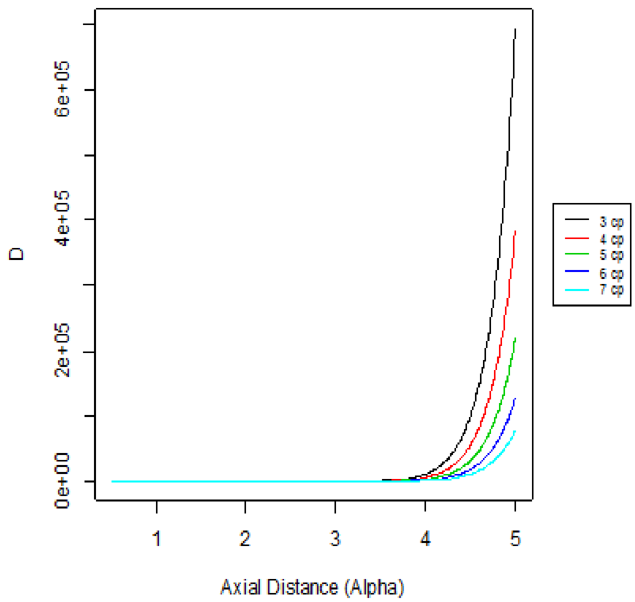

Figure 2 Plot of D Values for a Three-Factor SCD

In Table 4, it can be observed that the A values generally decrease as the axial distance gets larger. From an axial distance of 3.0 onwards, the amount of decrease becomes minimal. For an axial distance between 0.5 and 1.0, a small number of center points can be used. The number of center points ceases to be much of a factor for a large axial distance.

Axial Distance (α)	Number of Center Points				
	3	4	5	6	7
0.5	377.1216	405.8555	434.6091	463.3771	492.1559
1.0	66.4932	70.9546	75.5147	80.1379	84.8039
1.5	36.0939	37.3703	39.0501	40.9383	42.9480
2.0	25.6054	26.2880	27.3191	28.5294	29.8442
2.5	20.1005	20.8542	21.7807	22.8053	23.8909
3.0	17.2451	18.0143	18.8834	19.8132	20.7826
3.5	15.6279	16.3839	17.2090	18.0780	18.9765
4.0	14.6258	15.3641	16.1566	16.9842	17.8360
4.5	13.9604	14.6831	15.4514	16.2498	17.0692
5.0	13.4952	14.2051	14.9553	15.7324	16.5284

Table 4 A Values for a Three-Factor SCD

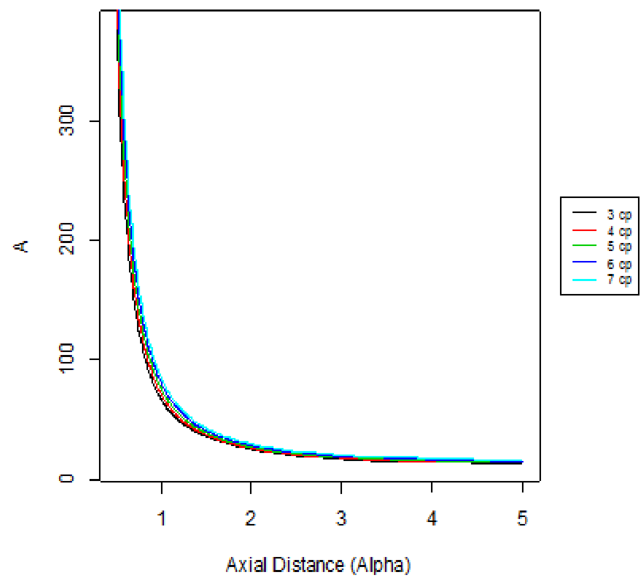

Figure 3 Plot of A Values for a Three-Factor SCD

The E values shown in Table 5 are equal regardless of the design's center points. It can also be observed that E values decrease as the axial distance increases. The change in E values is minimal for an axial distance of 1.5 and above.

Axial Distance (α)	Number of Center Points				
	3	4	5	6	7
0.5	8.0000	8.0000	8.0000	8.0000	8.0000
1.0	1.1404	1.1404	1.1404	1.1404	1.1404
1.5	0.6022	0.6022	0.6022	0.6022	0.6022
2.0	0.4268	0.4268	0.4268	0.4268	0.4268
2.5	0.3534	0.3534	0.3534	0.3534	0.3534
3.0	0.3173	0.3173	0.3173	0.3173	0.3173
3.5	0.2973	0.2973	0.2973	0.2973	0.2973
4.0	0.2851	0.2851	0.2851	0.2851	0.2851
4.5	0.2771	0.2771	0.2771	0.2771	0.2771
5.0	0.2716	0.2716	0.2716	0.2716	0.2716

Table 5 E Values for a Three-Factor SCD

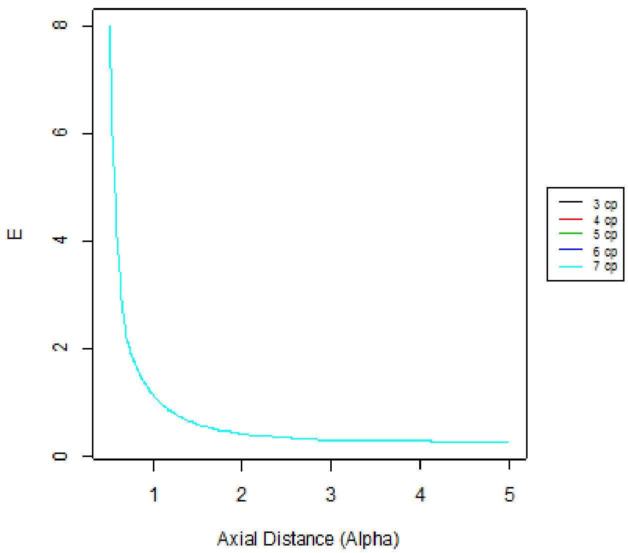

Figure 4 Plot of E Values for a Three-Factor SCD

An increase in the axial distance does not have a large effect on the V values (see Table 6). But a small dip in the values can be observed in the axial distance of 1.5 to 2.0. Therefore, a suitable choice for the design considering this criterion is an axial range of 1.5 to 2.0 combined with a small number of center points.

Axial Distance (α)	Number of Center Points				
	3	4	5	6	7
0.5	11.5224	12.3025	13.0904	13.8837	14.6812
1.0	11.3710	12.1198	12.8877	13.6677	14.4559
1.5	11.0803	11.8189	12.5881	13.3731	14.1673
2.0	11.0753	11.8142	12.5837	13.3690	14.1634
2.5	11.2179	11.9540	12.7177	13.4972	14.2863
3.0	11.3104	12.0521	12.8168	13.5954	14.3832
3.5	11.3630	12.1107	12.8781	13.6578	14.4459
4.0	11.3946	12.1470	12.9168	13.6978	14.4866
4.5	11.4149	12.1708	12.9425	13.7247	14.5142
5.0	11.4287	12.1871	12.9603	13.7435	14.5336

Table 6 V Values for a Three-Factor SCD

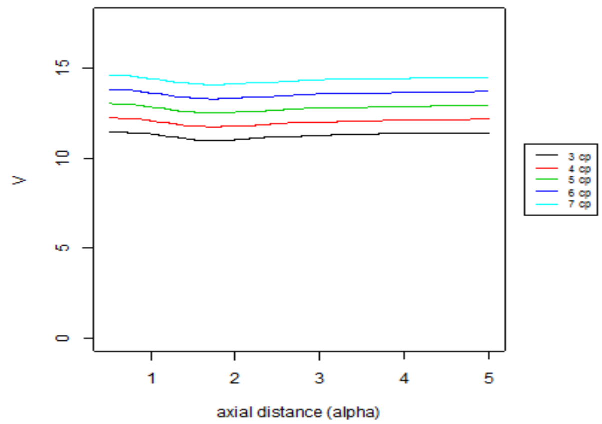

Figure 5 Plot of V Values for a Three-Factor SCD

Results for four, five, and six-factor designs are summarized in the succeeding section.

5. SUMMARY AND CONCLUSIONS

5.1. Summary of Results

In terms of alphabetic optimality, the designs were investigated by varying the axial distance ($0.5 \leq \alpha \leq 5.0$) and number of center points ($3 \leq n_0 \leq 7$). The results and findings of the study are summarized as follows:

1. The five-factor CCD must have an axial distance of 2 and should contain 10 center points so as to achieve rotatability and approximate orthogonality. Similarly, for a six-factor CCD, an axial distance of 2.3784 and 15 center points are needed. The three and four factor SCDs are not rotatable.
2. The following designs with the given combination of axial distance and number of center points have good alphabetic criteria values.

Alphabetic Criteria	Three Factor	Four Factor	Five Factor	Six Factor
D Optimality	α ≥ 3.5 small number of center points	α ≥ 3.5 small number of center points	α ≥ 3.5 small number of center points	α ≥ 4.0 small number of center points
A Optimality	α ≥ 3.0 any number of center points	α ≥ 3.5 any number of center points	α ≥ 3.5 any number of center points	α ≥ 3.5 any number of center points
E Optimality	α ≥ 1.5 any number of center points	α ≥ 1.5 any number of center points	α ≥ 1.0 any number of center points	α ≥ 1.0 any number of center points
V Optimality	1.5 ≤ α ≤ 2.0 small number of center points	1.5 ≤ α ≤ 2.5 small number of center points	2.0 ≤ α ≤ 2.5 small number of center points	2.0 ≤ α ≤ 3.0 small number of center points

Table 7 Suitable α and n_0 for CCDs Augmented from One-Half Fractional Factorials

5.2. Conclusions

Rotatability and approximate orthogonality can be achieved using the five and six-factor designs. Moreover, it is possible to have a rotatable design while maintaining reasonable E and V values. For the CCDs included in this study, the axial distance has an effect on all the alphabetic criteria. The choice of center point is essential for two alphabetic criteria namely, D and V-optimality.

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