

Some Optimality Variations of Central Composite Designs

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Abstract

Some variations of central composite designs (CCD) under complete and partial replications of cube, axial and center points are studied using A, D and G optimality criteria. The results obtained suggest that complete replication of the cube, axial and center points are better than the partial replication of cube, axial and center points under the A and D optimality criteria studied while it varies under G optimality criterion. The partial replication of the cube, axial and center point for all the CCDs studied, the partial replicated cube point is D optimal but varies under A and G optimality criteria.

Keywords: Central composite design; Cube point; Axial point; Center point; Optimality criteria; Partial replication.



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1. Introduction

In a two level unreplicated factorial design which involves only continuous factor, there is no degree of freedom available to estimate the error sum of squares and hence the model coefficients cannot be statistically tested. In this situation, replication becomes very important for the purpose of obtaining a more precise estimate of experimental error and for modeling curvature; therefore it is necessary to consider the second order design.

According to [Box and Wilson \(1951\)](#), Central Composite Design is the most popular class of second order designs which consists of a number of 2^k factorial (cube) points with n_f (number of replication at each factorial point), $2k$ axial (star) point with n_α (number of replication at each axial point) and n_c (number of replicated center point). A replicated Central Composite Designs are designs in which the cube point, the axial point and the center point are repeated a few or several times in order to obtain a better estimate of all the linear and product term coefficient, squared term coefficient and also estimate pure error respectively. There are two ways of replicating a Central Composite Design:

- (a) Complete replication (b) Partial replication

In this work, the complete replication involves replicating the cube point, the axial point and the center point while Partial replication involves replicating either cube point, the axial point or the center point. Several works have been done by many researchers on replication of Central Composite Designs.

[Chigbu and Ohaegbulem \(2011\)](#), compared two variations of central composite designs under the orthogonal and rotatable restriction using the D optimality criterion and concluded that the replicated cube plus one star variation is better than the replicated star plus one cube variation under both restrictions.

[Nduka and Chigbu \(2014\)](#), in an extended version compared two variation of N point orthogonal and rotatable

$$\sum_{i=1}^k \lambda_i(\xi) \geq \sum_{i=1}^k \lambda_i(\eta); (k = 1, 2, \dots, p)$$

central composite design based on the Schur's ordering of designs which says as well as the D optimality and A optimality criteria. They concluded that the replicated factorial point plus one axial point is better than the one factorial point plus replicated axial point in the sense of Schur's ordering of designs and also showed that the result remained the same for both A optimality and D optimality criteria.

In the presence of complete replication under rotatable and orthogonal design restrictions using the A-, D- and E- optimality criteria, [Ibanga, \(2013\)](#) compared some variations of experimental points of central composite designs. The efficiency values was obtained and the results suggest that replicated cubes plus replicated star points is better than partial replication of cube and star points under the design restrictions of rot at ability and orthogonality.

[Iwundu \(2015\)](#), also examined the optimal partially replicated cube, star and center runs in Face centered central composite designs. The cube points was replicated while the star points and center point were fixed or not replicated, the star points was replicated while the cube points and star points were fixed and not replicated and the center points was replicated while the cube points and the star points were fixed or not replicated. The efficiencies of the designs were assessed using the D and G optimality criteria. The results showed that the Face centered central composite design comprising of two cube portions, one star portion and a center point performed better than other variations under D-optimality criterion as well as G-optimality criterion. It was also observed that replicating only the center points were not as efficient as replicating the cube points. It was suggested that emphasis should shift from replication of only center points, as non-center points performed better.

Earlier and later studies on the partial replication of the response surface central composite designs (CCDs) was examined by Chigbu and Ukaegbu (2017) when the factorial and axial points are replicated and the results showed that the optimum performance of the replicated variations of the CCD depends on the axial distance, α , and also the cuboidal or spherical design region. No particular replicated variation of the CCD is consistently optimum in both design regions studied. They concluded that in most cases replicating the axial points, improves the designs.

2. Methodology

In this work, the effect of complete replication and partial replication for the various central composite designs; Rotatable, Orthogonal, Spherical and Face centered central composite design was studied using the A, D and G optimality criteria and computed using the DESIGN EXPERT software for factors $k=2, \dots, 6$. The full cube portion of the CCDs are employed for factors $k=2, 3$ and 4 while half replicate of the cube portion of the CCDs are employed for factors $k=5$ and 6, also the axial portions and cube portions are replicated and center points increased two and three times.

The variations of CCD studied include:

- Two replicated cube points, two replicated axial points and two replicated center points.
- Two replicated cube points, one axial point and one center point.
- Two replicated axial points, one cube point and one center point.
- Two replicated center points, one cube point and one axial point.
- Three replicated cube points, three replicated axial points and three replicated center points.
- Three replicated cube points, one axial point and one center point.
- Three replicated axial points, one cube point and one center point.
- Three replicated center points, one cube point and one axial point.

In this work, consider the complete replication of cube, axial and center point to as design 1, partial replication of cube point as design 2, partial replication of star point be design 3 and partial replication of center point as design 4.

2.1. Central Composite Design (CCD)

According to Montgomery (2005) the second degree model is written as

$$y_{ij} = \beta_0 + x'b + x'Bx + \varepsilon_{ij} \tag{2.1.1}$$

where y_{ij} is the measured response, $x = (x_1, x_2, \dots, x_k)'$ are the input variables, $b = (\beta_1, \beta_2, \dots, \beta_k)'$ B is a symmetric matrix of order $k \times k$ whose i^{th} diagonal element is β_{ii} ($i=1, 2, \dots, k$) and its $(i, j)^{th}$ diagonal element is

$$B = \begin{bmatrix} b_{11} & b_{12}/2 & \dots & b_{1k}/2 \\ & b_{22} & \dots & b_{2k}/2 \\ & & \ddots & \vdots \\ & & & b_{kk} \end{bmatrix}$$

$\frac{1}{2} \beta_{ij}$ ($i, j = 1, 2, \dots, k; i \neq j$) given as where β_0, b, B are the estimates of the intercept,

linear and quadratic coefficients respectively and ε_{ij} is the random error with mean zero and variance σ^2 .

The axial in a Central composite design specifies the type of central composite design to be used. According to [8], the spherical choice of α is \sqrt{k} , the face centered cube (FCC), choice of $\alpha = 1$, the rotatable choice of α is $f^{\frac{1}{4}}$

$$\alpha = \left(\frac{\sqrt{FN} - F}{2} \right)^{\frac{1}{2}}$$

where f is the number of cube points in the CCD while the orthogonal choice of

2.2. Design Optimality Criteria

2.2.1. A-Optimal Design

This design maximizes the trace of the $X'X$ matrix or minimizes the trace of the inverse of the $X'X$ matrix.

2.2.2. D-Optimal Design

This design maximizes the determinant of the $X'X$ matrix or minimizes the determinant of the inverse of the $X'X$ matrix.

2.2.3. G-Optimal Design

This design minimizes the maximum prediction variance over the region of interest.

3. Illustrations

The derivation for A-, D-, and G- optimality value will be obtained for 2 factors.

i) Derivation of A-optimality value (k=2 factors) when $n_f=1, n_s = 1, n_t = 1$ and $n_0 = 2$

$$X = \begin{matrix} & x_0 & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \\ \begin{matrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{matrix} & \begin{matrix} +1 \\ +1 \\ -1 \\ -1 \\ -\alpha \\ +\alpha \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{matrix} & \begin{matrix} +1 \\ -1 \\ -1 \\ -1 \\ 0 \\ 0 \\ -\alpha \\ +\alpha \\ 0 \\ 0 \\ 0 \end{matrix} & \begin{matrix} 1 \\ 1 \\ 1 \\ 1 \\ \alpha^2 \\ \alpha^2 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{matrix} & \begin{matrix} 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ \alpha^2 \\ \alpha^2 \\ 0 \\ 0 \\ 0 \end{matrix} & \begin{matrix} +1 \\ -1 \\ -1 \\ +1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{matrix} \end{matrix} \tag{3.1}$$

The $X'X$ matrix for a 2 factor CCD is determined by matrix multiplication

$$X'X = \begin{bmatrix} 10 & 0 & 0 & 4+2\alpha^2 & 4+2\alpha^2 & 0 \\ 0 & 4+2\alpha^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4+2\alpha^2 & 0 & 0 & 0 \\ 4+2\alpha^2 & 0 & 0 & 4+2\alpha^4 & 4 & 0 \\ 4+2\alpha^2 & 0 & 0 & 4 & 4+2\alpha^4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{bmatrix} \tag{3.2}$$

In general,

$$X'X = \begin{bmatrix} N & 0 & 0 & x & x & 0 \\ 0 & x & 0 & 0 & 0 & 0 \\ 0 & 0 & x & 0 & 0 & 0 \\ x & 0 & 0 & y & f & 0 \\ x & 0 & 0 & f & y & 0 \\ 0 & 0 & 0 & 0 & 0 & f \end{bmatrix} \tag{3.3}$$

where

$$x = f + 2\alpha^2, y = f + 2\alpha^4 \tag{3.4}$$

According to [9] the inverse of a matrix by partitioning, is given by

$$(X'X)^{-1} = \begin{pmatrix} A^{11} & A^{12} \\ A^{21} & A^{22} \end{pmatrix} \tag{3.5}$$

Where

$$A^{11} = (A_{11} - A_{12}A_{22}^{-1}A_{21})^{-1} \tag{3.6}$$

$$A^{12} = -A_{11}^{-1}A_{12}A_{22} \tag{3.7}$$

$$A^{21} = -A_{22}^{-1}A_{21}A^{11} \tag{3.8}$$

$$A^{22} = (A_{22} - A_{21}A_{11}^{-1}A_{12})^{-1} \tag{3.9}$$

Given that

$$A_{11} = \begin{pmatrix} N & 0 & 0 \\ 0 & f + 2\alpha^2 & 0 \\ 0 & 0 & f + 2\alpha^2 \end{pmatrix}, A_{12} = \begin{pmatrix} f + 2\alpha^2 & f + 2\alpha^2 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, A_{21} = \begin{pmatrix} f + 2\alpha^2 & 0 & 0 \\ f + 2\alpha^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$A_{22} = \begin{pmatrix} f + 2\alpha^4 & f & 0 \\ f & f + 2\alpha^4 & 0 \\ 0 & 0 & f \end{pmatrix} \tag{3.10}$$

$$A_{11}^{-1} = \begin{bmatrix} \frac{1}{N} & 0 & 0 \\ 0 & \frac{1}{x} & 0 \\ 0 & 0 & \frac{1}{x} \end{bmatrix} \tag{3.11}$$

$$(A_{11} - A_{12}A_{22}^{-1}A_{21})^{-1} = \begin{bmatrix} \frac{y+f}{N(y+f)-2x^2} & 0 & 0 \\ 0 & \frac{1}{x} & 0 \\ 0 & 0 & \frac{1}{x} \end{bmatrix} \tag{3.12}$$

$$-A_{11}^{-1}A_{12}A^{22} = \begin{bmatrix} \frac{-xf}{N(y+f)-2x^2} & \frac{-xf}{N(y+f)-2x^2} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{3.13}$$

$$-A_{22}^{-1}A_{21}A^{11} = \begin{bmatrix} \frac{-xf}{N(y+f)-2x^2} & 0 & 0 \\ \frac{-xf}{N(y+f)-2x^2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{3.14}$$

$$(A_{22} - A_{21}A_{11}^{-1}A_{12})^{-1} = \begin{bmatrix} \frac{Ny-x^2}{(y-f)[N(y+f)-2x^2]} & \frac{x^2-Nf}{(y-f)[N(y+f)-2x^2]} & 0 \\ \frac{x^2-Nf}{(y-f)[N(y+f)-2x^2]} & \frac{Ny-x^2}{(y-f)[N(y+f)-2x^2]} & 0 \\ 0 & 0 & \frac{1}{f} \end{bmatrix} \tag{3.15}$$

$$(X'X)^{-1} = \begin{bmatrix} \frac{y+f}{N(y+f)-2x^2} & 0 & 0 & \frac{-xf}{N(y+f)-2x^2} & \frac{-xf}{N(y+f)-2x^2} & 0 \\ 0 & \frac{1}{x} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{x} & 0 & 0 & 0 \\ \frac{-xf}{N(y+f)-2x^2} & 0 & 0 & \frac{Ny-x^2}{(y-f)[N(y+f)-2x^2]} & \frac{x^2-Nf}{(y-f)[N(y+f)-2x^2]} & 0 \\ \frac{-xf}{N(y+f)-2x^2} & 0 & 0 & \frac{x^2-Nf}{(y-f)[N(y+f)-2x^2]} & \frac{Ny-x^2}{(y-f)[N(y+f)-2x^2]} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{f} \end{bmatrix} \tag{3.16}$$

The A-optimality value is given by

$$tr(X'X)^{-1} = \sum_{i=1}^p \lambda_i, \text{ for } i=1, 2, \dots, 6$$

$$tr(X'X)^{-1} = \frac{y+f}{N(y+f)-2x^2} + \frac{2}{x} + \frac{2(Ny-x^2)}{(y-f)[N(y+f)-2x^2]} + \frac{1}{f} \tag{3.17}$$

(Ibanga, 2013)

ii) Derivation of D-optimality value (k=2 factors)

For factor k= 2 when , $n_f = 1, n_s = 1$ and $n_0 = 2$; where $N = 10, x = f + 2\alpha^2, y = f + 2\alpha^4$

$$X'X = \begin{bmatrix} N & 0 & 0 & x & x & 0 \\ 0 & x & 0 & 0 & 0 & 0 \\ 0 & 0 & x & 0 & 0 & 0 \\ x & 0 & 0 & y & f & 0 \\ x & 0 & 0 & f & y & 0 \\ 0 & 0 & 0 & 0 & 0 & f \end{bmatrix} \tag{3.18}$$

According to Powell (2011) the determinant of block matrix yields

$$|XX| = |A_{11}| |A_{22} - A_{21}A_{11}^{-1}A_{12}| \tag{3.20}$$

$$A_{11}^{-1} = \begin{bmatrix} \frac{1}{N} & 0 & 0 \\ 0 & \frac{1}{x} & 0 \\ 0 & 0 & \frac{1}{x} \end{bmatrix}, \quad A_{22} - A_{21}A_{11}^{-1}A_{12} = \begin{bmatrix} \frac{Ny - x^2}{N} & \frac{Nf - x^2}{N} & 0 \\ \frac{Nf - x^2}{N} & \frac{Ny - x^2}{N} & 0 \\ 0 & 0 & f \end{bmatrix} \tag{3.21}$$

$$|A_{22} - A_{21}A_{11}^{-1}A_{12}| = \frac{f}{N} (y - f) [N(y + f) - 2x^2] \tag{3.22}$$

$$|XX| = Nx^2 \frac{f}{N} (y - f) [N(y + f) - 2x^2]$$

According to [4], the D optimality value is given by

$$|XX| = fx^2 (y - f) [N(y + f) - 2x^2] \tag{3.23}$$

iii) Derivation of G-optimality value (k=2 factors)

For factor k= 2 when $n_f = 1, N = 10, n_s = 1$ and $n_0 = 2$;

The G-optimality value is given by $Nx'(XX)^{-1}x$ where

$$x = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_2^2 \\ x_1x_2 \end{bmatrix}, \quad x' = [1 \quad x_1 \quad x_2 \quad x_1^2 \quad x_2^2 \quad x_1x_2]$$

In general,

$$X'X = \begin{bmatrix} N & 0 & 0 & x & x & 0 \\ 0 & x & 0 & 0 & 0 & 0 \\ 0 & 0 & x & 0 & 0 & 0 \\ x & 0 & 0 & y & f & 0 \\ x & 0 & 0 & f & y & 0 \\ 0 & 0 & 0 & 0 & 0 & f \end{bmatrix}$$

where

$$x = f + 2\alpha^2, \quad y = f + 2\alpha^4$$

$$(X'X)^{-1} = \begin{bmatrix} \frac{y+f}{N(y+f)-2x^2} & 0 & 0 & \frac{-xf}{N(y+f)-2x^2} & \frac{-xf}{N(y+f)-2x^2} & 0 \\ 0 & \frac{1}{x} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{x} & 0 & 0 & 0 \\ \frac{-xf}{N(y+f)-2x^2} & 0 & 0 & \frac{Ny-x^2}{(y-f)[N(y+f)-2x^2]} & \frac{x^2-Nf}{(y-f)[N(y+f)-2x^2]} & 0 \\ \frac{-xf}{N(y+f)-2x^2} & 0 & 0 & \frac{x^2-Nf}{(y-f)[N(y+f)-2x^2]} & \frac{Ny-x^2}{(y-f)[N(y+f)-2x^2]} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{f} \end{bmatrix} \quad (3.24)$$

Let

$$p = \frac{y+f}{N(y+f)-2x^2}, \quad q = \frac{-xf}{N(y+f)-2x^2}, \quad r = \frac{1}{x}, \quad s = \frac{Ny-x^2}{(y-f)[N(y+f)-2x^2]},$$

$$t = \frac{x^2-Nf}{(y-f)[N(y+f)-2x^2]}, \quad u = \frac{1}{f}$$

Then

$$Nx'(X'X)^{-1}x = N \begin{bmatrix} 1 & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{bmatrix} \begin{bmatrix} p & 0 & 0 & q & q & 0 \\ 0 & r & 0 & 0 & 0 & 0 \\ 0 & 0 & r & 0 & 0 & 0 \\ q & 0 & 0 & s & t & 0 \\ q & 0 & 0 & t & s & 0 \\ 0 & 0 & 0 & 0 & 0 & u \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_2^2 \\ x_1x_2 \end{bmatrix}$$

The G-optimality value is given by

$$Nx'(X'X)^{-1}x = N \left[P + 2qx_1^2 + rx_1^2 + rx_2^2 + (q+sx_1^2+tx_2^2)x_1^2 + (q+tx_1^2+sx_2^2)x_2^2 + (ux_1x_2)x_1x_2 \right] \quad (3.25)$$

4. Results

The optimality criteria values were obtained for the complete and partial replication of cube, axial and center points using the four varieties of Central Composite Design.

Table-4.1. Optimality criteria values for Rotatable Central Composite Design

Factors	No of rep.	n_f	n_α	n_c	N	α	A-opt	D-opt	G-opt
2	2	2	2	2	18	1.4142	1.094	4.768×10^{-7}	9.000
		2	1	1	13	1.6818	1.381	9.746×10^{-7}	9.685
		1	2	1	13	1.1892	1.932	1.559×10^{-5}	9.685
		1	1	2	10	1.4142	1.438	1.526×10^{-5}	6.250
2	3	3	3	3	27	1.4142	0.729	4.186×10^{-8}	8.991
		3	1	1	17	1.8612	0.884	9.745×10^{-8}	10.591
		1	3	1	17	1.0746	1.554	7.894×10^{-6}	10.591
		1	1	3	11	1.4142	1.188	1.017×10^{-5}	6.875
3	2	2	2	2	30	1.6818	1.039	7.228×10^{-14}	14.82
		2	1	1	23	2.000	1.295	1.540×10^{-13}	16.422
		1	2	1	21	1.4142	1.535	2.587×10^{-11}	13.86
		1	1	2	16	1.6818	1.416	3.722×10^{-11}	10.72
3	3	3	3	3	45	1.6818	0.693	1.253×10^{-15}	14.805
		3	1	1	31	2.2134	0.771	2.775×10^{-15}	18.724
		1	3	1	27	1.2779	1.185	1.043×10^{-11}	17.631
		1	1	3	17	1.6818	1.193	2.486×10^{-11}	11.39

Factors	No of rep.	n_f	n_α	n_c	N	α	A-opt	D-opt	G-opt
4	2	2	1	1	41	2.3784	0.960	2.745×10^{-24}	24.067
		1	2	1	33	1.6818	1.317	1.778×10^{-20}	18.909
		1	1	2	26	2.000	1.217	2.856×10^{-20}	15.158
4	3	3	3	3	75	2.000	0.531	3.980×10^{-27}	24.975
		3	1	1	57	2.6322	0.632	5.681×10^{-27}	33.63
		1	3	1	41	1.5197	0.973	1.681×10^{-21}	23.206
		1	1	3	27	2.000	1.063	1.904×10^{-20}	15.741
5(Half)	2	2	2	2	54	2.000	0.962	3.607×10^{-34}	23.814
		2	1	1	43	2.3784	1.552	1.380×10^{-33}	38.27
		1	2	1	37	1.6818	1.293	1.379×10^{-28}	32.042
		1	1	2	28	2.000	1.505	4.255×10^{-28}	24.64
5(Half)	3	3	3	3	81	2.000	0.641	7.232×10^{-38}	23.814
		3	1	1	59	2.6322	0.901	2.890×10^{-37}	38.27
		1	3	1	47	1.5197	1.115	4.531×10^{-29}	32.042
		1	1	3	29	2.000	1.341	2.960×10^{-28}	24.64
6(Half)	2	2	2	2	90	2.3784	0.914	5.277×10^{-53}	43.74
		2	1	1	77	2.8284	0.924	8.758×10^{-53}	43.813
		1	2	1	57	2.000	1.079	2.624×10^{-45}	35.45
		1	1	2	46	2.3784	1.267	7.186×10^{-45}	29.026
6(Half)	3	3	3	3	135	2.3784	0.482	6.192×10^{-58}	43.74
		3	1	1	109	3.1302	0.609	8.377×10^{-58}	62.239
		1	3	1	69	1.8072	0.855	7.726×10^{-46}	42.435
		1	1	3	47	2.3784	1.076	4.814×10^{-45}	29.657

A design is said to be A- optimal if it satisfies the criterion $A = \text{mintrace}[(X'X)^{-1}]$. From Table 4.1 for $k=2$, when replicated two times, we observed the traces to be $\min\{1.094, 1.381, 1.932, 1.438\} = 1.094$. This shows clearly that complete replication at cube, axial and center point is A-optimal and performed better than the partial replication of cube, axial and center points. Also, when replicated three times, we observed the traces to be $\min\{0.729, 0.884, 1.554, 1.188\} = 0.729$. This also shows clearly that complete replication at cube, axial and center point is A-optimal and performed better than the partial replication of cube, axial and center point for all factors. But when judging only on the partial replication of the cube, axial and center point for all factors, partial replication of the cube point is preferred than that of axial and center points.

Table 4.1 also shows the D-optimality values. A design is said to be D- optimal if it satisfies the criterion $D = \min |(X'X)^{-1}|$. For $k=2$, when replicated two times, we observed the determinants to be $\min\{4.768 \times 10^{-7}, 9.746 \times 10^{-7}, 1.559 \times 10^{-5}, 1.526 \times 10^{-5}\} = 4.768 \times 10^{-7}$. This shows clearly that full replication at cube, axial and center points is D-optimal and performed better than the partial replication of cube, axial and center points.

When replicated three times, it also shows clearly that complete replication at cube, axial and center point is D-optimal and performed better than the partial replication of cube, axial and center point. The partial replication of the cube, axial and center point for all factors, partial replication of the cube point is preferred than that of axial and center points. The G-optimality values in Table 4.1 show that for all factors except factor $k=5$, the partial replication of the center points is better than the complete replication of cube, axial and center points.

Table-4.2. Optimality criteria values for Orthogonal Central Composite Design

Factors	No of rep.	n_f	n_α	n_c	N	α	A-opt	D-opt	G-opt
2	2	2	2	2	18	1.000	1.069	3.014×10^{-6}	7.254
		2	1	1	13	1.0483	1.735	1.584×10^{-5}	7.618
		1	2	1	13	0.8960	1.619	5.565×10^{-5}	9.854
		1	1	2	10	1.0781	1.703	8.562×10^{-5}	7.66
2	3	3	3	3	27	1.000	0.713	4.186×10^{-8}	7.263
		3	1	1	17	1.0684	1.592	9.745×10^{-8}	10.217
		1	3	1	17	0.8413	1.374	7.894×10^{-6}	12.376
		1	1	3	11	1.1474	1.429	1.017×10^{-5}	8.063
3	2	2	2	2	30	1.2154	0.855	1.164×10^{-12}	11.49
		2	1	1	23	1.2616	1.391	1.156×10^{-11}	11.822
		1	2	1	21	1.1137	1.327	1.833×10^{-10}	15.246
		1	1	2	16	1.2872	1.522	5.093×10^{-10}	12.00
3	3	3	3	3	45	1.2154	0.590	2.018×10^{-14}	11.475
		3	1	1	31	1.2799	1.259	7.437×10^{-13}	15.128
		1	3	1	27	1.0565	1.136	5.456×10^{-11}	18.873
		1	1	3	17	1.3531	1.349	2.403×10^{-10}	12.495

Factors	No of rep.	n_f	n_α	n_c	N	α	A-opt	D-opt	G-opt
4	2	2	2	2	50	1.4142	0.717	1.110×10^{-22}	15.90
		2	1	1	41	1.4529	1.122	2.093×10^{-21}	21.074
		1	2	1	33	1.3208	1.067	2.950×10^{-19}	20.13
		1	1	2	26	1.4826	1.278	1.520×10^{-18}	16.354
4	3	3	3	3	75	1.4142	0.478	2.535×10^{-25}	15.9
		3	1	1	57	1.4674	1.014	2.59×10^{-23}	28.272
		1	3	1	41	1.2657	0.917	6.006×10^{-20}	24.272
		1	1	3	27	1.5467	1.161	6.891×10^{-19}	16.821
5(Half)	2	2	2	2	54	1.5467	0.799	2.108×10^{-32}	23.002
		2	1	1	43	1.5960	1.143	7.992×10^{-31}	23.22
		1	2	1	37	1.4432	1.270	1.833×10^{-27}	32.967
		1	1	2	28	1.6072	1.486	1.807×10^{-26}	25.732
5(Half)	3	3	3	3	81	1.5467	0.533	4.225×10^{-36}	25.029
		3	1	1	59	1.6150	0.986	1.312×10^{-33}	30.621
		1	3	1	47	1.3798	1.137	2.566×10^{-28}	40.843
		1	1	3	29	1.6644	1.397	7.937×10^{-27}	26.477
6(Half)	2	2	2	2	90	1.7244	0.615	2.398×10^{-50}	29.61
		2	1	1	77	1.7606	0.905	1.740×10^{-48}	40.271
		1	2	1	57	1.6362	0.954	1.379×10^{-43}	36.48
		1	1	2	46	1.7842	1.149	2.603×10^{-42}	30.13
6(Half)	3	3	3	3	135	1.7244	0.410	2.814×10^{-55}	29.565
		3	1	1	109	1.7739	0.794	2.448×10^{-52}	55.481
		1	3	1	69	1.5806	0.845	1.292×10^{-44}	43.263
		1	1	3	47	1.8414	1.083	1.120×10^{-42}	30.691

Table 4.2, clearly shows that an Orthogonal Central Composite Design when cube, axial and center points is completely replicated performed better than the partial replication of cube, axial and center points for all factors studied under the three bases of comparison. The partial replication of the cube, axial and center points; partial replication of the cube is D optimal while it varies under A and G optimality criteria.

Table-4.3. Optimality criteria values for Spherical Central Composite Design

Factors	No of rep.	n_f	n_α	n_c	N	α	A-opt	D-opt	G-opt
2	2	2	2	2	18	1.4142	1.094	4.768×10^{-7}	9.000
		2	1	1	13	1.4142	1.958	4.521×10^{-6}	13.000
		1	2	1	13	1.4142	2.021	4.521×10^{-6}	13.000
		1	1	2	10	1.4142	1.438	1.526×10^{-5}	6.250
2	3	3	3	3	27	1.4142	0.729	4.186×10^{-8}	8.991
		3	1	1	17	1.4142	1.865	1.272×10^{-6}	17.000
		1	3	1	17	1.4142	1.948	1.272×10^{-6}	17.000
		1	1	3	11	1.4142	1.188	1.017×10^{-5}	0.872
3	2	2	2	2	30	1.7321	1.029	5.108×10^{-14}	15.00
		2	1	1	23	1.7321	1.783	1.072×10^{-12}	23.00
		1	2	1	21	1.7321	1.931	3.140×10^{-12}	21.00
		1	1	2	16	1.7321	1.391	2.615×10^{-11}	10.576
3	3	3	3	3	45	1.7321	0.686	8.858×10^{-16}	14.985
		3	1	1	31	1.7321	1.681	9.188×10^{-14}	31.00
		1	3	1	27	1.7321	1.874	4.886×10^{-13}	27.00
		1	1	3	17	1.7321	1.169	1.744×10^{-11}	11.237
4	2	2	2	2	50	2.000	0.948	1.743×10^{-24}	25.00
		2	1	1	41	2.000	1.637	6.939×10^{-23}	41.00
		1	2	1	33	2.000	1.805	1.694×10^{-21}	33.00
		1	1	2	26	2.000	1.271	2.856×10^{-20}	15.158
4	3	3	3	3	75	2.000	0.632	3.980×10^{-27}	24.975
		3	1	1	57	2.000	1.545	1.133×10^{-24}	57.000
		1	3	1	41	2.000	1.762	1.645×10^{-22}	41.000
		1	1	3	27	2.000	1.063	1.904×10^{-20}	15.741
5(Half)	2	2	2	2	54	2.2361	1.053	4.492×10^{-35}	27.000
		2	1	1	43	2.2361	1.716	5.178×10^{-33}	43.000
		1	2	1	37	2.2361	2.009	8.556×10^{-31}	37.000

		1	1	2	28	2.2361	1.505	4.711×10^{-29}	23.968
5(Half)	3	3	3	3	81	2.2361	0.702	9.007×10^{-39}	26.973
		3	1	1	59	2.2361	1.578	1.295×10^{-35}	59.000
		1	3	1	47	2.2361	1.965	3.792×10^{-32}	47.000
		1	1	3	29	2.2361	1.305	3.140×10^{-29}	24.824

Factors	No of rep.	n_f	n_α	n_c	N	α	A-opt	D-opt	G-opt
6(Half)	2	2	2	2	90	2.4495	0.923	4.751×10^{-51}	77.000
		2	1	1	77	2.4495	1.552	2.660×10^{-53}	45.000
		1	2	1	57	2.4495	1.780	4.125×10^{-47}	57.000
		1	1	2	46	2.4495	1.262	3.571×10^{-45}	28.888
6(Half)	3	3	3	3	135	2.4495	0.410	3.122×10^{-58}	44.955
		3	1	1	109	2.4495	0.794	9.272×10^{-55}	109.000
		1	3	1	69	2.4495	0.845	1.396×10^{-48}	69.000
		1	1	3	47	2.4495	1.083	2.380×10^{-45}	29.516

From Table 4.3 for k=2 to 6, when replicated two and three times for a Spherical Central Composite Design, we observed clearly that complete replication at cube, axial and center points is A and D optimal and performed better than the partial replication of cube, axial and center points. The G-optimality values in Table 4.3 show that for all factors the partial replication of the center points is better than the complete replication of cube, axial and center points. The partial replication of the cube, axial and center points; partial replication of the center point is A and G optimal while partial replication of the cube is D optimal.

Table-4.4. Optimality criteria values for Face Centered Central Composite Design

Factors	No of rep.	n_f	n_α	n_c	N	α	A-opt	D-opt	G-opt
2	2	2	2	2	18	1.0000	1.069	3.014×10^{-6}	7.254
		2	1	1	13	1.0000	1.737	1.838×10^{-5}	6.877
		1	2	1	13	1.0000	1.643	3.488×10^{-5}	9.282
		1	1	2	10	1.0000	1.798	1.240×10^{-4}	7.980
2	3	3	3	3	27	1.0000	0.713	2.646×10^{-7}	7.260
		3	1	1	17	1.0000	1.586	4.252×10^{-6}	8.840
		1	3	1	17	1.0000	1.432	1.096×10^{-5}	11.237
		1	1	3	11	1.0000	1.636	9.137×10^{-5}	8.734
3	2	2	2	2	30	1.0000	1.065	5.298×10^{-12}	11.97
		2	1	1	23	1.0000	1.764	5.880×10^{-11}	11.735
		1	2	1	21	1.0000	1.439	4.528×10^{-10}	15.687
		1	1	2	16	1.0000	2.037	4.209×10^{-9}	12.736
3	3	3	3	3	45	1.0000	0.710	9.188×10^{-14}	11.97
		3	1	1	31	1.0000	1.635	3.868×10^{-12}	15.283
		1	3	1	27	1.0000	1.179	8.906×10^{-11}	19.197
		1	1	3	17	1.0000	1.978	3.439×10^{-9}	13.515

Factors	No of rep.	n_f	n_α	n_c	N	α	A-opt	D-opt	G-opt
4	2	2	2	2	50	1.0000	1.177	6.119×10^{-21}	16.50
		2	1	1	41	1.0000	2.047	1.234×10^{-19}	20.787
		1	2	1	33	1.0000	1.482	9.038×10^{-18}	21.021
		1	1	2	26	1.0000	2.316	1.690×10^{-16}	17.134
4	3	3	3	3	75	1.0000	0.785	1.397×10^{-23}	16.50
		3	1	1	57	1.0000	1.942	1.546×10^{-21}	28.329
		1	3	1	41	1.0000	1.176	1.261×10^{-18}	25.379
		1	1	3	27	1.0000	2.289	1.460×10^{-16}	17.793
5(Half)	2	2	2	2	54	1.0000	1.543	2.415×10^{-29}	26.082
		2	1	1	43	1.0000	2.632	1.030×10^{-27}	22.188
		1	2	1	37	1.0000	1.984	1.002×10^{-24}	34.669
		1	1	2	28	1.0000	3.065	4.450×10^{-23}	27.02
5(Half)	3	3	3	3	81	1.0000	1.029	4.842×10^{-33}	26.082
		3	1	1	59	1.0000	2.478	1.733×10^{-30}	29.913
		1	3	1	47	1.0000	1.601	8.395×10^{-26}	43.005
		1	1	3	29	1.0000	3.049	3.969×10^{-23}	27.985

6(Half)	2	2	2	2	90	1.0000	1.039	1.112×10^{-45}	30.42
		2	1	1	77	1.0000	2.954	8.517×10^{-44}	38.962
		1	2	1	57	1.0000	1.960	3.497×10^{-39}	38.019
		1	1	2	46	1.0000	3.266	2.693×10^{-37}	31.096
6(Half)	3	3	3	3	135	1.0000	1.093	1.305×10^{-50}	30.375
		3	1	1	109	1.0000	2.845	1.210×10^{-47}	54.609
		1	3	1	69	1.0000	1.513	2.262×10^{-40}	45.402
		1	1	3	47	1.0000	3.256	2.454×10^{-37}	31.772

A design is said to be A- optimal if it satisfies the criterion $A = \text{mintrace}[(X'X)^{-1}]$. From Table 4.4 for $k=2$, when replicated two times, we observed the traces to be $\min\{1.069, 1.737, 1.643, 1.798\} = 1.069$. This shows clearly that complete replication at cube, axial and center points are A-optimal and performed better than the partial replication of cube, axial and center points. When replicated three times, we observed the traces to be $\min\{0.713, 1.586, 1.432, 1.636\} = 0.713$. This also shows clearly that complete replication at cube, axial and center point is A-optimal and performed better than the partial replication of cube, axial and center point for all factors. The partial replication of the cube, axial and center points for all factors, partial replication of the axial point is preferred than that of cube and center points. For $k=2$, when replicated two times, we observed the determinants to be $\min\{3.014 \times 10^{-6}, 1.838 \times 10^{-5}, 3.488 \times 10^{-5}, 1.240 \times 10^{-4}\} = 3.014 \times 10^{-6}$. This shows clearly that complete replication at cube, axial and center points is D-optimal and performed better than the partial replication of cube, axial and center points. When replicated three times, it also shows clearly that complete replication at cube, axial and center point is D-optimal and performed better than the partial replication of cube, axial and center point. The partial replication of the cube, axial and center point for all factors, partial replication of the cube point is preferred than that of axial and center points.

A design is said to be G-optimal if out of the maximum prediction variance values the design have a minimum prediction variance, in Table 4.4 we observed that $\min \{ N \hat{\sigma}_{\max}^2 \} = \min\{7.254, 6.877, 9.282, 7.980\} = 6.877$ shows that for factors $k=2$ and 3, when replicated twice, the complete replication at cube, axial and center points of Face centered CCD failed to be G optimal. The partial replication of the cube, axial and center point for all factors, the results varies.

5. Discussion of Findings

The results showed that complete replication of cube, axial and center points is A and D optimal for Rotatable CCD and G-optimal for all factors except factor $k=5$, where the partial replication of the center points is better than the complete replication of cube, axial and center points. The Orthogonal CCD showed that when cube, axial and center points is completely replicated, it performed better than the partial replication of cube, axial and center points for all factors studied under the three criteria for comparison. The results also showed that complete replication of cube, axial and center points is A and D optimal for Spherical CCD and G-optimal for all factors where the partial replication of the center points is better than the complete replication of cube, axial and center points. The Face centered CCD is also A and D optimal when completely replicated but failed to be G optimal.

6. Conclusion

The results obtained suggest that complete replication of the cube, axial and center points are better than the partial replication of cube, axial and center points under the A and D optimality criteria studied while it varies under G optimality criterion. But when judging only on the partial replication of the cube, axial and center point for all the CCDs studied, the partial replicated cube point is D optimal but varies under A and G optimality criteria.

Recommendation

After studying the four varieties of CCDs in the presence of complete and partial replication of cube, axial and center points using the A, D and G optimality criteria the results have shown that complete replication of cube, axial and center points is A and D optimal, hence when we wish to carry out replication in a Central Composite Design, the replication should be on the cube, axial and center points as the design will be A and D optimal. When we have limited resources, the replication should be on the cube point as the design will be D optimal.

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