Estimation of Parameters and Optimality of Second-Order Spherical Designs Using Quadratic Function Relative to Non-Spherical Face centered CCD

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

Original Research Article

Abstract

The study presented the estimation of parameters and optimality of second-order spherical designs using quadratic model in comparison to the non-spherical face centered CCD for varying axial distances. The designs considered were equiradial design of axial distances of 1.0 and 1.414, inscribed CCD of axial distance of 1.0 and circumscribed CCD of axial distance of 1.414, the study employed sum of square error, variance estimation, D-, A-, and T-optimality criteria as well as Grand mean of these designs for quadratic model and 1 to 10 center runs were considered. The study observed that the sum of square error of the non-spherical face centred CCD is zero (0) for radial point of n=5 with 1 centre point and this result is seen to be a misleading result, because, no process is 100%. While the sum of square error of the spherical designs with axial distance of 1.0 gave minimal sum of square errors and the spherical designs with axial distance of 1.414 gave very large sum of square error. The Grand mean of the spherical and the non-spherical designs were equal or approximately equal for radial point of n=5 for centre points 1-10 inclusive. But as the radial distance increases above 5, the Grand mean of the non-spherical CCD differs significantly from those of the spherical designs. The study suggests that the non-spherical second order design is inferior to their spherical second order design counterparts. The spherical designs with axial distance of 1.414 (equiradial and circumscribed CCD) have better D-optimality, A-optimality and T-optimality than the non-spherical face

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centred CCD, while, the spherical designs with axial distance of 1.0 (equiradial and inscribed) has inferior D-optimality, A-optimality and T-optimality compared to the non-spherical face centred CCD with axial distance of 1.0.

1 Introduction

Equiradial design is a second-order design that can be alternatively used in place of some other second-order designs, such as the central composite designs (inscribed, circumscribed and face centered) and the 3^k complete factorial designs. See Iwundu & Onu [1] and Iwundu [2] the design is used as an alternative second-order design to the popular central composite designs. It consists of sets of points arranged such that each point in a set has an equal distance from the design center [3,2,1] (Hundson 1972). Myer et al. [4] considered equiradial design as a special and interesting design that is always in two factors, such design has its points found on a common spherical region. Khuri and Cornell [3], stated that equiradial design is used in modeling second-order response functions. Wu and Hamada (2021) studied central composite designs, Box-Behnken designs and uniform shell designs, by sequentially moving from a first order model to a second order model using iterative search method of the design regions. The equiradial design is a k-factor design, usually k=2 factors and it has five points in one set for radius $\rho \geq 1$ from the center of the design in two dimensions. Among the k-factor designs, the general 3^k factorial design is always affected by the size of the factor k. That is to say, as k increases the design appears to be too tedious to apply because of the large number of experimental runs. As a result of this, more efficient designs have been introduced to help reduce the problems associated with large number of experimental runs [5,6].

Central Composite Design is a second- order design developed by Box and Wilson [7] which can also be called Box-Wilson design. This design is seen as an alternative to the complete 3^k design. It was developed by the combinations of the 2^k factorial or fractional factorial design points having factor level of -1, 1 with axial points of $\{(\pm1, 0, \ldots, 0), (0, \pm1, \ldots, 0), \ldots, (0, 0, \ldots, \pm1)\}$ and then the center point(s) c given as (0, 0, . . . , 0). This process is called the augmentation of the first-order design. The factorial portion as stated above contains the 2^k factorial points or the fractions of it, while the axial portion contains the $2k$ design points properly arranged such that two points are selected on each axis of the explanatory variables with axial distance of α taken from the design center. (Khuri & Mukhopadhyay 2010) [7].

Over the years, researchers have worked on the optimality of designs, and stated that a design with maximum D-optimality of the normalized information matrix, is best in estimating model parameters. Estimating model parameters for equiradial designs and doehlert designs for quadratic model is not pronounced in the literature, though, the estimations of model parameters using second-order central composite design have been considered as seen in Box & Wilson [7], Khuri & Cornel [3] and Hundson (1972). Iwundu & Onu [1] worked on the preferences of equiradial designs with changing design sizes, axial distances and increased centered point in relationship to the N-point central composite designs. The work did not estimate the parameters of quadratic function. Just recently, Onu et al. [8] studied the Effects of Changing Design Size, Axial Distances and Increased Center Points for Equiradial Design with Variation in Model Parameters, the study compared equiradial designs for axial distances of 1.0 with that of 1.414 with variation in model parameters. Comparisons of Spherical and Non-Spherical Designs using quadratic model with varying axial distance on the basis of their grand mean, sum of square errors, variances and the optimality criteria have not been so visible in the literature. It was against this backdrop this work is presented to relate the parameters of these designs with some alphabetic criteria.

The aim of the work is to estimate parameters and optimality of second-order designs using quadratic model and compare the spherical second-order designs with the non-spherical face centered design.

Wu & Hamada (2021) described two methods of iterative search of the region of the design which are steepest ascent and rectangular grid search. In their work, they first considered first order experiment and then advanced

to second-order experiment. The second-order designs used were central composite designs, Box-Behnken designs and uniform shell designs.

Chigbu et al. [9] compared the prediction variances of some Central Composite Designs in spherical regions with radius α = √k where k is the number of explanatory variables. Their results showed that Central Composite Designs, Small Composite Designs and Minimum-run resolution (MinRes) V designs are not uniformly superior under G- and I-optimality criteria as well using Variance Dispersion graphs.

Iwundu & Otaru [10] considered imposing D-Optimality criterion on the design regions supported by points of the Central Composite Designs. For the second order polynomial model used, results showed that the D-optimal designs defined over the rotatable Circumscribed Central Composite Design region had better determinant values than those defined over the Face-centered Central Composite Design region and the Inscribed Central Composite Design region.

Ukaegbu & Chigbu [11] considered the prediction capabilities of partially replicated rotatable Central Composite Designs. Their results showed that the replicated cube designs with higher replications are more efficient and have better prediction capabilities than the replicated star designs.

Iwundu [12] studied the optimal partially replicated cube, star and center runs on design region supported by points of the Face-centered Central Composite Design, using quadratic models. With variations involving replicating the cube points while the star points and center point are held fixed, replicating the star points while the cube points and the center point are held fixed and replicating the center point while the cube points and the star points are held fixed, results showed that for the quadratic models considered, 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- and G-optimality criteria [13,14]. When compared with the traditional method of replicating only the center point, the variation involving two cube portions, one-star portion and a center point was relatively better in terms of design efficiencies. The D-optimality is given as:

$$\phi\big(M(\xi)\big) = Max\{det\big(M(\xi)\big) = Min\{det(M^{-1}(\xi)\} \tag{1.1}$$

It has been made clear from the works done by some eminent scholars like Myers et al. (2009), Rady et al. [15], Myers and Montgomery (2002), Chigbu et al. [9], Onukogu & Iwundu [16], Iwundu [17,18] and Iwundu & Onu [1] that obtaining the maximum determinant of the normalized information matrix is equivalent to obtaining the minimum determinant of the inverse of the normalized information matrix.

Oyejola & Nwanya [18] studied the performance of five varieties of Central Composite Design when the axial portions are replicated and the center point increased one and three times. An excellent review of literature on some earlier works involving Central Composite Designs in spherical regions have been documented by Chigbu et al. [9]. Spherical designs are useful in constructing rotatable designs in the field of combinatorics. However, it is important to obtain designs that reflect other important properties. The notions of design optimality and efficiency are paramount in assessing the quality of experimental designs. In particular, the D-optimality and D-efficiency play major roles in design optimality. They have been most studied and are also available in most statistical software.

Chigbu et al. [9] gave various properties of the D-optimality and D-efficiency of designs under varying design conditions. It is worth noting that second-order models are important in process optimization and are very reliable low-order approximating polynomials to the true unknown response functions relating a response with several controllable variables which may be natural or coded.

Iwundu [2] saw equiradial design as alternative to the popular N-point spherical central composite design. The work considered equiradial designs for design radius ρ=1.0 and the circumscribed, inscribed and face centered central composite designs, it was observed that these designs are comparable with the standard second-order Central Composite Designs. D-efficiencies of the equiradial designs are evaluated with respect to the D-optimal exact designs, furthermore, the D-efficiencies of the equiradial designs are evaluated with respect to the spherical Central Composite Designs defined on the design regions of the Circumscribed Central Composite Design, the Inscribed Central Composite Design and the Face-centered Central Composite Design. The D-efficiency values show that the alternative second-order N-point spherical equiradial designs are better than the

Inscribed Central Composite Design though inferior to the Circumscribed Central Composite Design with efficiency values less than 50% in the cases so far studied.

Iwundu & Onu [1] proposed two alternative measures of design optimality and efficiency when trying to study the preferences of equiradial designs under changing axial distance and design size and increased center points, known as D-absolute Deviation (D-AD) and G-absolute Deviation (G-AD).

2 Materials and Methods

According to Khuri & Mukhopadyay (2010) RSM is mathematically defined as

$$y = \phi(x_1, \ x_2, \ \ldots, x_n, \boldsymbol{\beta}) \tag{2.1}$$

It is a general form of a statistical model. The quadratic and cubic models having all the parameters represented will be applied in this study and the quadratic model is given as seen in Iwundu [2], and Iwundu & Onu [1] generally as seen

$$y = \beta_0 + \left(\sum_{i=1}^k \beta_i X_i\right) + \left(\sum_{j=1}^k \beta_j X_j\right) + \left(\sum_{i=1}^k \sum_{i<j}^k \beta_{ij} X_i X_j\right) + \left(\sum_{i=1}^k \beta_{ii} X_i^2\right) + \left(\sum_{j=1}^k \beta_{jj} X_i^2\right) + \varepsilon \tag{2.2}$$

It can be written in a reduced form as seen

$$y = X\beta + \varepsilon \tag{2.3}$$

Where X is an $N \times P$ matrix, y is an $N \times 1$ vector of observed responses, $\boldsymbol{\beta}$ is the $P \times 1$ vector of unknown parameters and $\boldsymbol{\varepsilon} \sim N(0, \delta^2)$ is the error term which is randomly distributed. From (2.1) ϕ is not known and represents real functional relationship between the response y and the explanatory variables $(x_1, x_2, \ \ldots, x_n)$.

The model in (2.2) will be applied throughout this study in obtaining design matrices for both equiradial designs for radius ρ=1.0 and 1.414 and central composite designs, face centered, inscribed, circumscribed and doehlert design for two variables. The parameters of this model will be estimated alongside their alphabetic optimality criteria. The least square equation which will be used in the estimation of the parameters for the model is given as:

$$\underline{\hat{\beta}} = \left(\frac{X'X}{N}\right)^{-1} X'Y \tag{2.4}$$

Where $\underline{\hat{\beta}}$ is an $N \times 1$ vector, given as $(\beta_0, \ \beta_1, \ \beta_2, \ \beta_{12}, \ \beta_{11}, \ \beta_{22})'$ and $\left(\frac{X'X}{N}\right)^{-1}$ is the inverse of the normalized information matrix and N is the number of design size. The design matrix X is obtained from the quadratic model in (2.2) as seen in Iwundu [2,1], Oyejola & Nwanya [18] and Iwundu & Onu [19] from the design points of equiradial design for ρ=1.0 which starts with a pentagon (n=5) given the radial points as shown

The design will be obtained as:

$$D_5 =$$

$$\begin{pmatrix} 1 & 0 \\ 0.309 & 0.951 \\ -0.81 & 0.587 \\ -0.808 & -0.589 \\ 0.311 & -0.95 \end{pmatrix}$$

This was obtained from (2.2) as seen in Khuri & Cornel [3] and Iwundu & Onu [19].

By the addition of one centre point, givs the Design measure given as

$\xi_6 =$

$$\begin{pmatrix} 1 & 0 \\ 0.309 & 0.951 \\ -0.81 & 0.587 \\ -0.808 & -0.589 \\ 0.311 & -0.95 \\ 0 & 0 \end{pmatrix}$$

The design size is given as $N = n + c$ where n is the number of points of the design or the radial point and c is the number of centre points.

This study considers center points from 1 to 10 inclusive, in each case the variance-covariance matrix is evaluated. MATHLAB software was used in obtaining the parameters. The least square in (2.4) was applied to obtain the parameters of the second-order model.

The alphabetic optimality criteria to be employed in this research are

2.1 D-optimality

which is given as

$$\text{D-optimality} = Min \, det(M^{-1}) \equiv Max \, det(M) \tag{2.5}$$

The design that has the highest determinant of the normalized information matrix is considered the best design under this criterion. This is obtained using the MATHLAB software, by entering the values of the design matrix in the software which starts from n=5 with c=1 and transposing it, the multiply the transpose by the matrix, to obtain the information matrix, for the purpose of unequal design sizes, we normalize by dividing the information matrix by the number of design size. Then we obtain determinant of the normalized information matrix. This processes continues for radial points n=6, 7, 8, with c=1-10 center points in each radial point.

2.2 A-optimality

$$\text{A-optimality} = Min \, tr(M^{-1}) \tag{2.6}$$

In the MATHLAB software, when you obtain the inverse of the normalized information matrix then you obtain the trace of the inverse. The design with the smallest trace is seen as the best design under this criterion. Note that trace is the addition of the diagonal elements of a design.

2.3 T-optimality

$$\text{T-optimality} = Max \, tr(M) \tag{2.7}$$

Where tr represents the trace and Max represents maximum. From the normalized information matrix $M = \left(\frac{X'X}{n}\right)$, we obtain the trace of this which is obtained by adding the diagonal elements. The design that has the highest trace is the best under this criterion. Minimizing the A-optimality is equivalent to maximizing the T-optimality.

2.4 E-optimality

$$\text{E-optimality} = Max \, \chi_{min}(M) \equiv Min \, \chi_{max}(M)^{-1} \tag{2.8}$$

Where χ_{min} represents the minimum Eigen value of M and χ_{max} represents the maximum Eigen value of $(M)^{-1}$. The results of these alphabetic optimality are tabulated in table.

2.5 Evaluation of the error sum of squares for the second-order designs with $c = 1 - 10$ center points for quadratic model

From each of these designs with each centre point, we obtain the estimate of the regression sum of square errors.

Let the estimate of y be given as $\hat{y}$ then from models (2.2) which is the quadratic model respectively we have the error by making ε the subject in (2.2), we obtain

$\varepsilon = (y - \hat{y})$, for different values of y given as y_i and corresponding values of $\hat{y}$ given as $\hat{y}_i$ we obtain

$$\varepsilon_i = (y_i - \hat{y}_i) \tag{2.9}$$

Summing and squaring (3.10), we obtain the error sum of square for both the quadratic and cubic models and it is given as

$$\sum \varepsilon_i^2 = \sum(y_i - \hat{y}_i)^2 \tag{2.10}$$

In obtaining this error sum of square of the regression equations, we applied EXCEL software package.

We apply sum of square error, Akaike and Schwarz Bayesian Criterion to the quadratic model, as seen.

$\min \sum \varepsilon_i^2$ among sets of designs for the two models, is preferred. That is to say, we search for designs that will give us the minimum value for each point estimate. Which is to say, a design having the smallest difference between each of the raw response and the estimated response.

Let y_i be the raw response from 1- ith responses and $\hat{y}_i$ be the estimated response from 1- ith estimated responses, then

$\min(y_i - \hat{y}_i)$ is a good estimate, we square it to overcome the effect of negative difference in the process. Also, the smaller the variance, the better the model for that design.

The variance is given as

$$\sigma^2 = \frac{1}{N}\left(\sum(y_i - \hat{y}_i)^2\right) \tag{2.11}$$
$$= \frac{1}{N}\left(\sum(\varepsilon_i)^2\right)$$

Where N is the number of design size.

We also employ Akaike Information Criterion (AIC) and Schwarz Bayesian Criterion (SBC) to investigate model specification for specialized designs, they are given as seen in Kutner et al. [20] as:

$$\text{AIC} = n \ln \text{SS}_{\text{Error}} - n \ln n + 2p \tag{2.12}$$

See Akaike [21]

And

$$\text{SBC} = n \ln \text{SS}_{\text{Error}} - n \ln n + [\ln n]p \tag{2.13}$$

See Schwarz [22].

Where p is the number of model parameters, for the quadratic model used, p=6. The smaller the value of AIC and SBC the better the model for that design. Negative value of these criteria shows how more the model suits the design.

3 Results

3.1 Spherical Equiradial designs

Variance-Covariance Matrix for spherical Equiradial Design for ρ=1.0 and centre point c=1

The variance-covariance matrix is as shown;

$$\square^{-1} =$$

6	-0.003	-0.001	-0.007	-5.997	-6.003
-0.003	2.399	0.001	0.003	0.002	0.003
-0.001	0.001	2.402	-0.003	0.003	0
-0.007	0.003	-0.003	9.590	0.017	0.001
-5.997	0.002	0.003	0.017	9.597	4.795
-6.003	0.003	0	0.001	4.795	9.614

Using the above variance- covariance matrix $\square^{-1}$ obtained from equiradial designs with ρ=1.0 and c=1 centre point from a second-order model given as

$$y(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \varepsilon$$

We proceed to obtaining the estimates of the model parameters, $\beta_0, \beta_1, \beta_2, \beta_{12}, \beta_{11}, \beta_{22}$ respectively using the formula

$$\beta = \square^{-1} X'y$$

where y is the response or the output variable and X is the design matrix generated from the design points of the equiradial designs or the central composite designs. The response is given as

$$y_6 = \begin{bmatrix} 20 \\ 50 \\ 40 \\ 80 \\ 30 \\ 70 \end{bmatrix}$$

And

X' is the transpose of the design matrix X given as;

$$X' =$$

1	1	1	1	1	1
1	0.309	-0.81	-0.808	0.311	0
0	0.951	0.587	-0.589	-0.95	0
0	0.294	-0.475	0.476	-0.295	0
1	0.095	0.656	0.653	0.097	0
0	0.904	0.345	0.347	0.903	0

To obtain $X'y$ we multiply X' by y as shown;

$X'y =$

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0.309 & -0.81 & -0.808 & 0.311 & 0 \\ 0 & 0.951 & 0.587 & -0.589 & -0.95 & 0 \\ 0 & 0.294 & -0.475 & 0.476 & -0.295 & 0 \\ 1 & 0.095 & 0.656 & 0.653 & 0.097 & 0 \\ 0 & 0.904 & 0.345 & 0.347 & 0.903 & 0 \end{pmatrix} \begin{pmatrix} 20 \\ 50 \\ 40 \\ 80 \\ 30 \\ 70 \end{pmatrix}$$

$=$

$$\begin{pmatrix} 290 \\ -52.26 \\ -4.59 \\ 24.93 \\ 104.3 \\ 113.85 \end{pmatrix}$$

Applying equation (2.2) to get the parameters of the second-order model, we have;

$\beta = \quad \square^{-1} X'y =$

$$\begin{pmatrix} 6 & -0.003 & -0.001 & -0.007 & -5.997 & -6.003 \\ -0.003 & 2.399 & 0.001 & 0.003 & 0.002 & 0.003 \\ -0.001 & 0.001 & 2.402 & -0.003 & 0.003 & 0 \\ -0.007 & 0.003 & -0.003 & 9.590 & 0.017 & 0.001 \\ -5.997 & 0.002 & 0.003 & 0.017 & 9.597 & 4.795 \\ -6.003 & 0.003 & 0 & 0.001 & 4.795 & 9.614 \end{pmatrix} \begin{pmatrix} 290 \\ -52.26 \\ 4.59 \\ 24.93 \\ 104.3 \\ 113.85 \end{pmatrix}$$

$$\begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_{12} \\ \beta_{11} \\ \beta_{22} \end{pmatrix} = \begin{pmatrix} 420.024 \\ -125.618 \\ -11.124 \\ 238.824 \\ -174.288 \\ -137.507 \end{pmatrix}$$

$$\hat{y} = 420.024 - 125.618x_1 - 11.124x_2 + 238.824x_1x_2 - 174.288x_1^2 - 137.507 + \varepsilon$$

3.2 Non spherical face centered central composite designs

For n=5, c=1, we have the design matrix given as

$X =$

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The transpose of X is given as

$X' =$

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 0 \\ 1 & -1 & 1 & -1 & 0 & 0 \\ 1 & -1 & -1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \end{pmatrix}$$

The information matrix is given as

$$X'X =$$

$$\begin{pmatrix} 6 & 1 & 0 & 0 & 5 & 4 \\ 1 & 5 & 0 & 0 & 1 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 \\ 5 & 1 & 0 & 0 & 5 & 4 \\ 4 & 0 & 0 & 0 & 4 & 4 \end{pmatrix}$$

Normalizing, we have

$$\left(\frac{X'X}{6}\right) =$$

$$\begin{pmatrix} 1.0000 & 0.1667 & 0 & 0 & 0.8333 & 0.6667 \\ 0.1667 & 0.8333 & 0 & 0 & 0.1667 & 0 \\ 0 & 0 & 0.6667 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.6667 & 0 & 0 \\ 0.8333 & 0.1667 & 0 & 0 & 0.8333 & 0.6667 \\ 0.6667 & 0 & 0 & 0 & 0.6667 & 0.6667 \end{pmatrix}$$

The determinant is obtained as

$$\left|\frac{X'X}{6}\right| = 0.0055$$

The variance-covariance matrix is given as

$$\square^{-1} =$$

$$\begin{pmatrix} 6.0000 & -0.0000 & 0 & 0 & -6.0000 & -0.0000 \\ 0 & 1.5000 & 0 & 0 & -1.5000 & 1.5000 \\ 0 & 0 & 1.5000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.5000 & 0 & 0 \\ -6.0000 & -1.5000 & 0 & 0 & 13.5000 & -7.5000 \\ 0 & 1.5000 & 0 & 0 & -7.5000 & 9.0000 \end{pmatrix}$$

The response variables are as shown

$$y =$$

$$\begin{pmatrix} 20 \\ 50 \\ 40 \\ 80 \\ 30 \\ 70 \end{pmatrix}$$

We obtain $X'y$ as seen

$$X'y=\begin{bmatrix} 290 \\ -20 \\ -70 \\ 10 \\ 220 \\ 190 \end{bmatrix}$$

The parameters are estimated as seen

$$\underline{\hat{\beta}} = \square^{-1}X'y = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_{12} \\ \beta_{11} \\ \beta_{22} \end{bmatrix} = \begin{bmatrix} 420.00 \\ -75.00 \\ -105.00 \\ 15.00 \\ -165.00 \\ 30.00 \end{bmatrix}$$

The results of other second-order designs for 1-10 centre points are seen in the tables below.

Table 1. Comparison of sum of square errors and variance estimates of non-spherical Face centered CCD and spherical Equiradial design for axial distance of 1.0

N	Non-Spherical Design (Face centered CCD)			Spherical Designs (Equiradial design 1.0)		
	$\sum \varepsilon^2$	Det(M)	VAR	$\sum \varepsilon^2$	Det(M)	VAR
6	0	0.0055	0	**0.0031**	**0.00026**	**0.00052**
7	481.67	0.0082	68.81	2011.90	0.00019	287.41
8	438	0.0088	54.8	1959.87	0.00025	244.98
9	987	0.0098	109.7	1548.93	0.00024	172.10

Table 2. Comparison of sum of square errors and variance estimates of non-spherical Face centered CCD and spherical Equiradial design for axial distance of 1.414

N	Non-Spherical Design (Face centered CCD)			Spherical Designs (Equiradial design 1.414)		
	$\sum \varepsilon^2$	Det(M)	VAR	$\sum \varepsilon^2$	Det(M)	VAR
6	**0**	**0.0055**	**0**	2250.79	0.067	375
7	481.67	0.0082	68.81	2073.47	0.066	296.21
8	438	0.0088	54.8	1965.95	0.065	245.74
9	987	0.0098	109.7	3541.97	0.062	393.55

Table 3. Comparison of sum of square errors and variance estimates of non-spherical Face centered CCD and spherical Inscribed CCD for axial distance of 1.0

N	Non-Spherical Design (Face centered CCD)			Spherical Designs (Inscribed CCD 1.0)		
	$\sum \varepsilon^2$	Det(M)	VAR	$\sum \varepsilon^2$	Det(M)	VAR
6	**0**	**0.0055**	**0**	**0.069**	**0.00012**	**0.012**
7	481.67	0.0082	68.81	161.63	0.00014	23.09
8	438	0.0088	54.8	813.19	0.00017	101.65
9	987	0.0098	109.7	1894.72	0.00022	210.52

Table 4. Comparison of sum of square errors and variance estimates of non-spherical Face centered CCD and spherical Circumscribed CCD for axial distance of 1.414

N	Non-Spherical Design (Face centered CCD)			Spherical Designs (Circumscribed CCD 1.414)		
	$\sum \varepsilon^2$	Det(M)	VAR	$\sum \varepsilon^2$	Det(M)	VAR
6	**0**	**0.0055**	**0**	1275.26	0.032	212.54
7	481.67	0.0082	68.81	4096.63	0.038	585.23
8	438	0.0088	54.8	1626.44	0.047	203.31
9	987	0.0098	109.7	1722.68	0.062	191.41

Table 5. Comparison of Non-Spherical Face centered CCD and Spherical Equiradial Designs of radius 1.0 for Quadratic Model on the basis of their Grand Mean and Optimality Criteria

			Non-Spherical Design (Face centered CCD)				Spherical Designs (Equiradial design 1.0)			
n	C	N	GM	D-opt	A-opt	T-opt	GM	D-opt	A-opt	T-opt
5	1	6	420	0.0055	33	4.667	420.024	2.61e-4	39.601	2.562
	2	7	560	0.0044	31.50	4.143	560.035	2.07e-4	35.701	2.339
	3	8	632	0.0029	33.33	3.750	632.150	1.40e-4	36.801	2.172
6	1	7	550.7	0.0082	22.75	4.429	630.529	1.94e-4	44.411	2.607
	2	8	632.69	0.0063	22.00	4	668.309	1.74e-4	38.755	2.406
	3	9	675	0.0045	22.93	3.667	705.22	1.29e-4	39.099	2.250
7	1	8	704	0.0088	21	4.250	616.2	2.50e-4	44.577	2.640
	2	9	720	0.0072	19.50	3.889	652.62	2.47e-4	36.649	2.458
	3	10	840	0.0054	19.70	3.600	796.8	1.97e-4	35.721	2.312
8	1	9	684	0.0098	19.25	4.111	611.7	2.42e-4	47.211	2.668
	2	10	824.298	0.0081	17.98	3.800	809.8	2.57e-4	37.462	2.501
	3	11	830.211	0.0061	18.00	3.546	799.2	2.18e-4	35.710	2.364

Table 6. Comparison of Non-Spherical Face centered CCD and Spherical Equiradial Designs of radius 1.414 for Quadratic Model on the basis of their Grand Mean and Optimality Criteria

			Non-Spherical Design (Face centered CCD)				Spherical Designs (Equiradial design 1.414)			
n	C	N	GM	D-opt	A-opt	T-opt	GM	D-opt	A-opt	T-opt
5	1	6	420	0.0055	33	4.667	419.94	0.0668	15.604	5.580
	2	7	560	0.0044	31.50	4.143	560.203	0.0529	12.954	4.926
	3	8	632	0.0029	33.33	3.750	632.254	0.0356	12.805	4.435
6	1	7	550.7	0.0082	22.75	4.429	629.803	2.58e-4	41.990	2.607
	2	8	632.69	0.0063	22.00	4	668.097	2.32e-4	35.989	2.406
	3	9	675	0.0045	22.93	3.667	704.999	1.72e-4	35.987	2.250
7	1	8	704	0.0088	21	4.250	607.305	0.0647	18.318	5.809
	2	9	720	0.0072	19.50	3.889	647.620	0.0638	13.833	5.275
	3	10	840	0.0054	19.70	3.600	793.037	0.0508	12.860	4.847
8	1	9	684	0.0098	19.25	4.111	611.782	0.0615	19.692	5.887
	2	10	824.3	0.0081	17.98	3.800	809.879	0.0654	14.378	5.398
	3	11	830.2	0.0061	18.00	3.546	799.244	0.0554	13.066	4.998

4 Discussion

4.1 Discussion based on Sum of Square Errors and Variance

From Table 1-4, the non-spherical face centered CCD was compared with the spherical designs on the basis of their sum of square errors, variance estimation and D-optimality criterion. It was observed that the sum of square error of the non-spherical face centered CCD with axial distance of 1.0 for radial point n=5 with 1 centre point is zero (0), while its spherical equiradial design counterpart with axial distance of 1.0 has a sum of square error of 0.0031 and variance of 0.00052, equiradial design with axial distance of 1.414 has a sum of square error

of 2250.79 and variance of 375, inscribed central composite design with axial distance of 1.0 has a sum of square error of 0.069 and variance 0.012 and circumscribed central composite design with axial distance of 1.414 has sum of square error of 1275.26 and variance 212.54. This shows that designs with equal axial distances behave alike, also, it shows that non-spherical designs have higher variance in estimation of model parameters in relation to the spherical designs than it is between two spherical designs. The sum of square error of zero (0) for non-spherical face centred CCD is a misleading result, because, no result is 100%. As a result, the non-spherical face centred CCD is said to have misbehaved in the presence of the spherical designs counterpart. It was also observed that as the radial points increases from 5 the sum of square errors and variances also increases for both the non-spherical and spherical designs.

Table 7. Comparison of non-spherical face centered CCD and spherical inscribed CCD of radius 1.0 for quadratic model on the basis of their grand mean and optimality criteria

			Non-Spherical Design (Face centered CCD)				Spherical Designs (Inscribed CCD 1.0)			
n	C	N	GM	D-opt	A-opt	T-opt	GM	D-opt	A-opt	T-opt
5	1	6	420	0.0055	33	4.667	419.99	1.17e-4	51.170	2.567
	2	7	560	0.0044	31.50	4.143	559.99	9.25e-5	49.079	2.343
	3	8	632	0.0029	33.33	3.750	632.15	6.23e-5	52.044	2.175
6	1	7	550.7	0.0082	22.75	4.429	631.299	1.38e-4	48.378	2.586
	2	8	632.69	0.0063	22.00	4	668.882	1.24e-4	43.127	2.388
	3	9	675	0.0045	22.93	3.667	705.522	9.20e-5	43.957	2.233
7	1	8	704	0.0088	21	4.250	612.968	1.67e-4	47.617	2.600
	2	9	720	0.0072	19.50	3.889	650.805	1.65e-4	39.836	2.422
	3	10	840	0.0054	19.70	3.600	795.398	1.31e-4	39.174	2.280
s8	1	9	684	0.0098	19.25	4.111	604.9	2.22e-4	48.051	2.645
	2	10	824.298	0.0081	17.98	3.800	806.0	2.36e-4	38.208	2.480
	3	11	830.211	0.0061	18.00	3.546	796.4	2.00e-4	36.459	2.346

Table 8. Comparison of non-spherical face centered CCD and spherical circumscribed CCD of radius 1.414 for quadratic model on the basis of their grand mean and optimality criteria

			Non-Spherical Design (Face centered CCD)				Spherical Designs (Circumscribed CCD 1.414)			
n	C	N	GM	D-opt	A-opt	T-opt	GM	D-opt	A-opt	T-opt
5	1	6	420	0.0055	33	4.667	420	0.0319	17.73	5.50
	2	7	560	0.0044	31.50	4.143	560	0.0253	15.43	4.86
	3	8	632	0.0029	33.33	3.750	632	0.017	15.64	4.37
6	1	7	550.7	0.0082	22.75	4.429	630	0.0384	18.66	5.71
	2	8	632.69	0.0063	22.00	4	668.05	0.0344	15.32	5.12
	3	9	675	0.0045	22.93	3.667	705.04	0.0255	14.99	4.67
7	1	8	704	0.0088	21	4.250	616.19	0.0468	19.00	5.75
	2	9	720	0.0072	19.50	3.889	652.60	0.0462	14.63	5.22
	3	10	840	0.0054	19.70	3.600	796.74	0.0368	13.75	4.80
8	1	9	684	0.0098	19.25	4.111	612.17	0.0615	19.69	5.89
	2	10	824.298	0.0081	17.98	3.800	810.10	0.0654	14.38	5.40
	3	11	830.211	0.0061	18.00	3.546	799.40	0.0554	13.07	5.00

4.2 Discussion based on the D-optimality criterion

It was observed that the D-optimality of the non-spherical face centred central composite design increases steadily as the radial points increases for 1 centre point, while that of spherical equiradial design for axial distance of 1.0 decreases for radial point n=6, but increases from n=7 to 8 radial points. The non-spherical face centred CCD is better than the spherical equiradial design for radial points of 5, 6, 7 and 8 with 1 centre point each. Obviously, researches have shown that equiradial design of axial distance 1.0 is better than the inscribed CCD with same axial distance of 1.0. This was also affirmed in Tables 1-3. Though, as the axial distance

increased to 1.414, both the spherical equiradial and spherical circumscribed CCD performed better than the non-spherical face centred CCD.

4.3 Comparisons of non-spherical face centred and spherical designs based on grand mean and optimality criteria

4.3.1 Comparisons based on grand mean

From Tables 5-8, it was observed that for radial point n=5 with centre points 1-10 inclusive, the Grand mean of the non-spherical face centred designs has equal or approximately equal Grand mean with all the spherical designs studied. As the radial point increases from 5 to 6, 7 and 8 with increasing centre points, the non-spherical face centred CCD begins to have inflated Grand mean above the other spherical designs. This could be as a result of the non-spherical nature of the face centred CCD in the presence of spherical designs. It is believed in this study, that the non-spherical face centred CCD is showing inferiority in the presence of spherical designs. The spherical designs with axial distance of 1.414 (equiradial and circumscribed) has better D-optimality, A-optimality and T-optimality than the non-spherical face centred CCD, while, the spherical designs with axial distance of 1.0 (equiradial and inscribed) has inferior D-optimality, A-optimality and T-optimality compared to the non-spherical face centred CCD with axial distance of 1.0.

5 Recommendations

The study recommends the following to researchers, companies, governments and any other authority that deals with optimization process, that;

1. In second order designs, the results of non-spherical designs are inferior and misleading, hence, should not be used for anything serious.
2. If Non-spherical designs must be used for any reason, to analyze a second order system, for comparable results to be obtained, it is advisable to use a second order design with radial point of n=5 with centre point from 1-10 inclusive.
3. Designs with axial distances of 1.0 are better than those with axial distance of 1.414 on the basis of Sum of Square Errors and variance estimation.

6 Conclusion

The study concludes that in comparing spherical and non-spherical second-order designs, the second-order designs with axial distance or radius of 1.0 give minima sum of square errors and variance estimation, while the designs with axial distance or radius of 1.414 had very high values of sum of square errors and variance estimation. The increase in center points increases the sum of square errors, variances and also the grand means of all the designs studied. The spherical designs had better alphabetic optimality than the non-spherical design.

Competing Interests

Authors have declared that no competing interests exist.

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