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A COMPARATIVE STUDY OF THE PERFORMANCE OF CUBIC AND QUADRATIC MODELS FOR HEPTAGONAL SPHERICAL TWO-FACTOR SECOND-ORDER DESIGNS BASED ON THE SUM OF SQUARE ERRORS

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Abstract

The power of Heptagonal Spherical two-factor second-order designs for a cubic model more than its quadratic counterpart based on the sum of square errors was presented. This study used spherical second-order designs such as; Equiradial designs of the radius or axial distance of 1.0 and 1.414 and Central Composite Designs of Face centred, Inscribed and Circumscribed designs. The Inscribed is a radius of 1.0 and Circumscribed CCD is of a radius of 1.414. These designs were studied with the addition of only one centre point. It was observed that all the designs studied recorded a minimum sum of square errors when the shape is a pentagon, and this occurred only for the quadratic model. The sum of the square error value of Face centred CCD of zero (0) is misleading, since nothing is done humanly that is free of error. The Face centred CCD was found to behave differently from the other designs, this could be because it is not a spherical design. As the shape of these designs increases the sum of square errors increases indiscriminately. The study revealed that all the designs except Face Centered CCD gave the minimum sum of square error for the cubic model, while Face Centered CCD gave a singular matrix for the cubic model in all the shapes. The axial distance affects the sum of square errors for the quadratic model, that is to say, the sum of square errors for an axial distance of 1.0 is minimum, while for an axial distance of 1.414, the sum of square errors is maximized. The study proposed the cubic model as a robust model for second-order designs when the shape is Heptagon (n=7) and the quadratic model as a robust model for second-order designs with a radius or axial distance of 1.0.

Keywords: Spherical Design, Heptagonal Design, Hexagonal Design, Cubic Model. Second-Order Design.

Introduction

A Second-order Design arises when there is a lack of fit in the first-order design initially applied. That is to say, there is an indication that the current region has curvature and is near the optimum. At this point augmentation of the first-order design is carried out. The augmentation is by the addition of axial points and a centre point which yields the Second-order design. There are several types of second-order designs and they include; Equiradial Designs, Central Composite Designs (Circumscribed, Inscribed and Face Centered), 3^K Factorial Designs (Full Factorial and Fractorial Designs), Doehlert Designs, Box Behnken Designs. The Central Composite Design, Doehlert Design and the Box Behnken Design can be modelled as two or three factors Designs, whereas Equiradial Design can only be modelled as a two-factor Design, while 3^{K} Design can be modelled only as a threefactor Design. Central Composite Design can be made to be Spherical according to Iwundu and Onu (2017), by taking the square root of the axial or the star point α such as $\alpha = \sqrt{k}$, where k is equal to the number of predictors in the model. (Chigbu et al., 2009). According to Onu et al. (2022), the Equiradial Design has its points found on a common spherical region, while Myer et al. (1989) said it is a special and interesting design that is always in two factors. Doehlert Design, according to Sergio et al. (2004) is a useful and alternative experimental design for second-order models. It is known as a uniform shell design proposed by Doehlert in 1970. This Design offer advantages relative to central composite and Box-Behnken designs. They need fewer experimental runs, which are more efficient and can move through the experimental domain. The Doehlert design defines a spherical

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experimental field and it talks about uniformity in space filling. Though the matrix of Doehlert Design is neither orthogonal nor rotatable.

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. (Iwundu & Onu, 2017; Iwundu 2016a). 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 Centre. (Khuri & Cornell, 1996; Iwundu 2016b, Iwundu & Onu, 2017). Central Composite Design is a second-order design developed by Box and Wilson in 1951 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 {(±1, 0, . . . , 0), (0, ±1, . . . , 0), . . . , (0, 0, . . . , ±1)} and then the centre point(s) c given as (0, 0, . . . , 0). This process is called the augmentation of 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 2^k design points properly arranged such that two points are selected on each axis of the explanatory variables with an axial distance of α taken from the design centre, (Khuri & Mukhopadhyay, 2010; Sankha, 2021). While fitting quadratic response models, the CCD is a better alternative to the full factorial three-level design because its performance is comparable at a lower cost. (Myer et al., 2009).

Doehlert Design is an alternative and very useful experimental design for second-order models. It is a uniform shell design proposed in the year 1970 for k=2 factors by Doehlert. This design begins from an equilateral triangle of lengths 1. To construct a regular hexagon (six-sided shape) with 1 centre point (0, 0), then N=n+1 centre point, where n= the radial point obtain from the shape of the design, hence, n=6, making N=7 sized design. The design points of a Doehlert design are; (1,0), (0.5,0.866), (0,0), (-0.5,0.866), (-1,0), (-0.5,-0.866) and (0.5,-0.866). The points on the hexagon, which is to say the 6 outer points lie on a circle of radius 1. A better application of the cubic model in scientific works, especially in Statistics has not been clearly stated in the literature. Emphasis has been on the quadratic model

Statement of the Problem

The importance of the shapes of second-order Designs to the estimation of parameters that is judged by the sum of square errors of the Designs has not been popular in the literature. Attention was drawn to this because, it was observed that second-order designs are of various shapes, ranging from Pentagon (n=5), Hexagon (n=6), Heptagon (n=7), Octagon (n=8), Nonagon (n=9) and Decagon (n=10), etc. it is important to understand how these Shapes affect Equiradial Design both of axial distance or radius of 1.0 and 1.414 and Central Composite Designs of Inscribed (1.0) and Circumscribed (1.414). The study will investigate the effects of these differences in shapes using both quadratic and cubic models. It will propose the most appropriate models for some designs. It is also obvious that a better application of the cubic model in scientific works, especially in Statistics has not been clearly stated in the literature. Emphasis has been on the quadratic model, as a result, this work is designed to bring out the importance of the cubic model for particularized second-order design as regards the shape of the designs. Though, some notable Researchers have worked on these second-order designs (Chigbu et al. 2009; Verdooren, 2017; Iwundu, 2016a & b; Onu et al., 2021). Just recently Onu et al. (2022) studied the Estimation of Parameters and Optimality of Second-Order Spherical Designs Using Quadratic Function Relative to Non-Spherical Face centred CCD. This study compared the parameters of Equiradial Designs of the radius of 1.0 and 1.414 and Central Composite Designs Inscribed and Circumscribed as spherical Designs with the Face Centered Central Composite Design as a non-spherical Design based on their model parameters and optimality, but the emphasis was not placed on the effect of the shapes of this designs on the sum of square errors of the studied designs. It was against this backdrop this work was presented.

Materials and Method

The design size is applied as seen

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$$p \le N \le \frac{1}{2}P(P+1) + 1$$

This was expressed in Iwundu and Onu (2017), Iwundu (2016a), Box and Wilson (1951) and Farombi et al. (2018). Where p represents the number of model parameters and N represents the design size. The quadratic model to be employed is given by Onu et al. (2021) and Onu et al. (2022)

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_{12} + \beta_{11} \beta_1^2 + \beta_{22} x_2^2 + \varepsilon$$
(1)

The design points of equiradial design are given as

$$x_1 = \rho COS\left(\theta + \frac{2\Pi U}{n}\right) \text{ and } x_2 = \rho Sin\left(\theta + \frac{2\Pi U}{n}\right); u = 0, 1, 2, \dots n - 1$$
(2)

is used in generating the Equiradial Design points, in which x_1 represents the values in the first row of the design D_5 and the x_2 represents the values in the second row of the design D_5 , as seen in Khuri and Cornel, (1996) and the cubic model is given as seen

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_{12} + \beta_{11} \beta_1^2 + \beta_{22} x_2^2 + \beta_{111} \beta_1^3 + \beta_{222} x_2^3 + \varepsilon$$
(3)

which is a Cubic Model having all the variables represent.

Obtaining the parameters of the second-order designs with c = 1 - 10 centre points for Quadratic and Cubic Models.

According to Khuri and Mukhopadyay (2010), Response Surface Methodology is mathematically defined as

$$y = \phi(x_1, x_2, \dots, x_n, \boldsymbol{\beta}) \tag{4}$$

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 in (3.1) is given as seen in Iwundu (2016a), and Iwundu and Onu (2017) generally as seen

 $y = \beta_0 + \left(\sum_{i=1}^k \beta_i X_i\right) + \left(\sum_{j=1}^k \beta_j X_j\right) + \left(\sum_{i=1}^k \sum_{i<j}^k \beta_{ij} X_i X_j\right) + \left(\sum_{i=1}^k \beta_{ii} X_i^2\right) + \left(\sum_{j=1}^k \beta_{jj} X_i^2\right) + \varepsilon$ (5) and the Cubic Model in general form is given as

$$y = \beta_0 + (\sum_{i=1}^k \beta_i X_i) + (\sum_{j=1}^k \beta_j X_j) + (\sum_{i
(6)$$

which is written in a reduced form to suit the study and it can be presented in matrix form as $y = X\beta + \varepsilon$

(7)

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 (1) ϕ is not known and represents a real functional relationship between the response y and the explanatory variables (x_1, x_2, \ldots, x_n) . (Oyejola & Nwanya (2015).

The models in (1) and (3) 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 these models will be estimated alongside their Alphabetic Optimality Criteria. The least-square equation which will be used in the estimation of the parameters for both models is given (Kutner et al., 2004; Onu et al., 2021; 2022; Verdooren, 2017; Ukaegbu & Chigbu, 2015).

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$$\underline{\hat{\beta}} = (\frac{X'X}{N})^{-1}X'Y \tag{8}$$

Where $\hat{\beta}$ is an N×1 vector, given as $(\beta_0, \beta_1, \beta_2, \beta_{12}, \beta_{11}, \beta_{22})'$ and $(\frac{x'x}{N})^{-1}$ is the inverse of the normalized information matrix and N is the number of Design size.

The total number of design sizes varies from one design to the other, for instance, the total number of design sizes (points) for a Central Composite Design is determined by the formula

$2^{k} + 2k + c$

 $D_{5} =$

 $\xi_6 =$

where k is the number of variables and c is the number of centre points. The total number of design size points for Doehlert Design is given as

(9)

$$2^k + k + c \tag{10}$$

The Design size or point for Equiradial Design is determined by the formula

$$N = n + c \tag{11}$$

Where n is the number of points in the design and c is the centre point. The design sets of points are obtained for Equiradial Design as

(1)	0
0.309	0.951
-0.81	0.587
-0.808	-0.589
0.311	-0.95

This was obtained from (2) as seen in Khuri and Cornel (1996) and Iwundu and Onu (2017). With the addition of one central point, gives the Design measure given as

	_
1	0
0.309	0.951
-0.81	0.587
-0.808	-0.589
0.311	-0.95
0	0

The Doehlert Design is given as D=

1	0 _
0.5	0.866
-0.5	0.866
-1	0
-0.5	-0.866
0.5	-0.866

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The Design measure is $\xi_7 =$

1	0
0.5	0.866
-0.5	0.866
-1	0
-0.5	-0.866
0.5	-0.866
0	0

These points were obtained as follows

x_1	x_2	x_1	x_2
$\cos(0)$	Sin(0)	1	0
$\cos(\frac{\pi}{3})$	$\operatorname{Sin}(\frac{\pi}{3})$	0.5	0.866
$\cos(\frac{2\pi}{3})$	$Sin(\frac{2\pi}{3})$	- 0.5	0.866
$\cos(\pi)$	$Sin(\pi)$	-1	0
$\cos(\frac{4\pi}{3})$	$Sin(\frac{4\pi}{3})$	-0.5	-0.866
$\cos(\frac{5\pi}{3})$	$Sin(\frac{5\pi}{3})$	0.5	-0.866
0	0	0	0

The above are put in matrix form from equations 1 and 3.

Results

Variance-Covariance Matrix for Equiradial Design and Central Composite Design Face Centered, Inscribed and Circumscribed for n=5 for Quadratic response function

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

The variance-covariance matrix is as shown;

ne variance-	covariance main	a is as shown,				
$n^{-1} =$						$\overline{}$
	66	-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 n^{-1} obtained from Equiradial Designs with $\rho=1.0$ and c=1 centre point from a Second-Order Model given as

$$y(x_{1}, x_{2}) = \beta_{0} + \beta_{1}x_{1} + \beta_{2}x_{2} + \beta_{12}x_{1}x_{2} + \beta_{11}x_{1}^{2} + \beta_{22}x_{2}^{2} + \varepsilon_{1}$$

We proceed to obtain the estimates of the model parameters, β_0 , β_1 , β_2 , β_{12} , β_{11} , β_{22} respectively using the formula

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

where y is the response or the output variable and X is the Design Matrix generated from the Design points of the Equiradial Designs, the Central Composite Designs or the Doehlert Design the application of equation (1) gives

$y_{6X1} =$

$\left(\right)$	
	20
	50
	40
	80
	30
	70
	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 =

	/						
(1	1	1	1	1	1	20
	1	0.309	-0.81	-0.808	0.311	0	50
	0	0.951	0.587	-0.589	-0.95	0	40
	0	0.294	-0.475	0.476	-0.295	0	80
	1	0.095	0.656	0.653	0.097	0	30
	0	0.904	0.345	0.347	0.903	0	70
1							λ.

C	_
290	
-52.26	
-4.59	
24.93	
104.3	
113.85	_

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=

Applying equation (1) to get the parameters of the second-order model, gives;



 $\hat{y} = 420.024 - 125.618x_1 - 11.124x_2 + 238.824x_1x_2 - 174.288x_1^2 - 137.507 + \varepsilon$ Continuing in this process, for both quadratic and cubic models for 1 centre point, we obtained the summarized results in the table below.

Table 1: Comparison of the Sum of Square Errors and	Variance Estimates for	Quadratic and C	Cubic Models
with 1 Centre point			

Quadrati	c model				Cubic model		
Shapes +1 nc	$\sum \epsilon^2$	Det(M)	VAR	DESIGN	$\sum \epsilon^2$	Det(M)	VAR
5+1	0.0031	0.00026	0.00052	Equi, 1.0	602.32	1.25e-37	100.39
6+1	2011.90	0.00019	287.41	Equi, 1.0	117.48	1.38e-22	19.58
7+1	1959.87	0.00025	244.98	Equi, 1.0	0.0059	1.87e-7	0.00084
8+1	1548.93	0.00024	172.10	Equi, 1.0	1178.77	1.86e-7	130.97
5+1	0.069	0.00012	0.012	Ccd Insc	16191.27	3.93e-38	2698.55
6+1	161.63	0.00014	23.09	Ccd Insc	5165.25	1.52e-22	737.89
7+1	813.19	0.00017	101.65	Ccd Insc	3.8e-11	1.87e-7	4.8e-12
8+1	1894.72	0.00022	210.52	Ccd Insc	2537.95	1.82e-7	281.99
5+1 6+1 7+1 8+1	0 481.67 438 987	0.0055 0.0082 0.0088 0.0098	0 68.81 54.8 109.7	Ccd Fac Ccd Fac Ccd Fac Ccd Fac	Singular Singular Singular singular	Singular Singular Singular Singular	
5+1	2250.79	0.067	375	Equi, 1.414	996.57	-9.07e-33	166.10
6+1	2073.47	0.066	296.21	Equi, 1.414	60.36	1.38e-22	8.62
7+1	1965.95	0.065	245.74	Equi, 1.414	2.37	0.0031	0.30
8 + 1	3541.97	0.062	393.55	Equi, 1.414	2562.99	0.0030	284.78
5+1 6+1	1275.26 4096.63	0.032 0.038	212.54 585.23	Ccd Cir Ccd Cir	1747.18 419.71	2.44e-33 -1.73e-18	291.20 59.96
7+1	1626.44	0.047	203.31	Ccd Cir	0.000058	9.72e-4	0.0000073
8+1	1722.68	0.062	191.41	Ccd Cir	740.87	0.0030	82.32

Discussion of Results

Equiradial Design with axial distance or radius of 1.0. It was observed from the summarized table 1 that for an equiradial design with a pentagon shape, (n=5) with 1 centre point for the quadratic model, the sum of square

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error is minimized with the value of 0.0031 and the variance of 0.0052, while for the cubic model for same orientation, the sum of square error was found to be 602.32 with the variance of 100.39. The sum of square error for a quadratic model for equiradial design with hexagonal shape (n=6) with 1 centre point is maximized with the value of 2011.90 and variance of 287.41, while for the cubic model for the same shape, the sum of square error decreased from what was obtained in the pentagonal design with a percentage difference of 80.50. For a heptagonal equiradial design (n=7) for the quadratic model, the sum of square error decreased from what was obtained for the hexagonal design with the difference of 2.59%, while the heptagonal design for the cubic model gave the sum of square error of 0.0059 with the variance of 0.00084.

Inscribed Central Composite Design with axial distance or radius of 1.0. The Inscribed CCD for pentagon has a sum of square error of 0.069 with 1 centre point for the quadratic model, while that of the cubic model was found to be 16191.27. As the shape of this Inscribed CCD for the quadratic model increases for 1 centre point, the sum of square error also increases, likewise their variances. The sum of square error for Inscribed CCD for the cubic model decreases as the shape of the design increases, but it decreases to the minimum value for the heptagonal shape (n=7) with the value of 3.8e-11.

Face Centered Central Composite Design with axial distance or radius of 1.0. The face-centred CCD gave the sum of square error equal to zero (0) for a quadratic model for 1 centre point and the value of the sum of square error increased for a hexagon with 1 centre point, decreased for a heptagon and increased for an octagon (n=8) with 1 centre point, while for the cubic model, all the shapes of the designs gave singular matrix.

Equiradial Design with axial distance or radius of 1.414. The equiradial design for the radius of 1.414 for the quadratic model with a pentagon for 1 centre point had the second highest value of the sum of square error. All the other shapes produced the sum of square errors above 1900, while for the cubic model, the sum of square errors was found to be reasonable values relatively for pentagon and hexagon, while the best sum of square error was recorded for heptagon (n=7) with 1 centre point with the value of 2.37 and the variance of 0.30.

Circumscribed Centered Central Composite Design with axial distance or radius of 1.414. The circumscribed CCD with a radius of 1.414 for the quadratic model had similar behaviour with the equiradial design for a radius of 1.414. Their SSE values were so high, while for the cubic model, the heptagon gave the best sum of square error with a value of 5.8e-5 and a variance of 7.3e-6.

Conclusion

The sum of the square error value of Face-centred CCD of zero (0) is misleading since nothing is done humanly that is free of error. The Face centred CCD was found to behave differently from the other designs, this could be because it is not a spherical design. As the shape of these designs increases the sum of square errors increases indiscriminately. The axial distance affects the sum of square errors for the quadratic model, that is to say, the sum of square errors for an axial distance of 1.0 is minimum, while for an axial distance of 1.414, the sum of square errors is maximized. The study proposed the cubic model as a robust model for second-order designs when the shape is Heptagon (n=7) and the quadratic model for second-order with a radius or axial distance of 1.0.

Recommendations

The following recommendations were made:

- 1. The equiradial design for a pentagonal shape (n=5) for a quadratic model with 1 centre point is better than all the designs studied.
- 2. The equiradial design for a heptagonal shape with the cubic model was found to be slightly less efficient as compared to the equiradial design of a radius of 1.0 for the pentagon with a difference of 47.46%.
- 3. The axial distance or radius of these designs affects the designs. This is because, the designs with an axial distance of 1.0 (equiradial of 1.0 and inscribed CCD of 1.0) had their pentagon (n=5) with 1 centre point produce the minimal sum of square error values for quadratic model, while this was not the case for the designs with an axial distance of 1.414 (equiradial of 1.414 and circumscribed CCD of 1.414).

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The designs with a radius of 1.0 had a better sum of square error than those with a radius of 1.414. This means that they also have high estimating power than the designs with a radius of 1.414.

4. For the cubic model, across all the designs studied, the heptagon gave the consistently smaller sum of square errors for 1 centre point.

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