Faculty of Natural and Applied Sciences Journal of Mathematical and Statistical Computing Print ISSN: 3026-8605 www.fnasjournals.com Volume 1; Issue 2; March 2024; Page No. 60-70.



Statistical Modeling of the Impact of Centre Points Replications on Second-Order Spherical Unit-Radial Points Designs

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Abstract

The study considered statistical modelling of the impact of centre point replications on second-order spherical unitradial point designs. A second-order quadratic model was built with Gross Domestic Products of Nigerian as the response variable with replication of centre points from 1 to 5 inclusive. The second-order designs used in this study were Doehlert Design (DD), Equiradial Design (ED) and Inscribed Central Composite Design (INSD) all having radius of 1.0, hence the name (unit-radial point Designs). Ordinary Least Square method was applied on the model and the model parameters were estimated. The sum of square error was applied for each centre points to obtain better interpretation of the estimated parameters. It was observed that for radial point of n= 6, Inscribed CCD and Doehlert design gave grand means that slightly differs from that of equiradial design for 1 centre point. The sum of square error value of equiradial design is less than that of doehlert design by 0.000222. As the centre point replicates increases to 2, all the designs recorded maximum value of sum of square errors with the error value of doehlert, equiradial and inscribed designs as 1.547889, 1.546521 and 1.938783 respectively. The study recommends among other things that in order to maximize the economy of Nigeria using spherical second-order unit-radial point design(s) one should consider the addition of 4 centre points.

Keywords: Unit-Radial Point Designs, Equiradial Design, Doehlert Design, Inscribed Design, Ordinary Least Square.

Introduction

Second-order design is a design used when there is the presence of curvature in the system. There are several of such designs and they include; the 3^k , the central composite (inscribed, face centred and circumscribed), equiradial (of radius 1.0 and 1.414), Doehlert and Box-behnken designs. These designs are modelled by the second-order models. According to Bezerra et al. (2008), a second order model is a model in which the highest power of the control variable is 2. It is also called a quadratic model. The complete 3^k factorial designs and the central composite designs are used in modeling second-order functions in Response Surface Methodology. Obviously, when there is sign of curvature in the response function, attention is shifted to central composite designs, whose design points include the factorial points, the axial points and the centre point runs. It addresses the curvature experienced in the system. The 3^k is also appropriate in the modeling of the second-order functions, but due to its large number of design points or experimental runs, hence central composite design (Box-Wilson design) became prominent in analyzing the model with curvature. Equiradial designs have also proven to be an alternative in modeling second-order response functions.

Doehlert Design (DD) is an alternative and very useful experimental design for second-order models. It is a uniform shell design proposed by Doehlert in the year 1970 for k=2 factors design. Doehlert designs are easily applied to optimize variables and offer advantages in relation to Central Composite Designs (CCD) and Box-Behnken Designs (BBD), (Anuar et al. 2013). According to Alhaddad et al. (2020), Doehlert designs are regular simplex like geometric figure, formed a k+1 equally spaced point in a k-dimensional space of equilateral triangle to form a hexagonal shape. 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 obtained 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), (-

⁶⁰ Cite this article as:

Richard-Igweh, A.E., Ijomah, M. A., & Onu, O.H. (2024). Statistical modeling of the impact of centre points replications on second-order spherical unit-radial points designs. FNAS Journal of Mathematical and Statistical Computing, 1(2), 60-70

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. It is a spherical design. It has an advantage of fewer number of experimental runs over the Central Composite Designs and the advantage over Equiradial Designs is that it can be modeled in more than two factors. Equiradial Design (ED) is an alternative second-order design in modeling second-order response functions. It is a design that is made up of more than one set of points such that each point in a set has an equal distance from the centre of the design region. It is a k factor design used as an alternative second-order design to the popularly encountered central composite design. In two-dimensions, the equiradial design has five points in a set defined for radius $\rho \ge 1$ from the centre of the design. This design is a spherical design that have equal axial distance from the design centre. It starts with a pentagon of equally spaced points and this design is augmented by the addition of centre points. Every design commences with the initial addition of a centre point (0,0) and the centre point can be increased if the initial one added lack fit, then the design can be augmented to fit the model under study. According to Myers et al. (1989), Onu et al. (2023), Iwundu and Onu (2017) and Suliman, (2017), response Surface Methodology (RSM) is defined as the bringing together of some scientific (Mathematical, and Statistical) ways or skills in building models for experimental purpose. In the design of experiments and model building, the interest of the experimenter is generally aimed at maximizing the outflow (gain) and minimizing the inflow (cost) of running the system under study. The experimenter wishes to increase the gains and reduce the cost of running the entire system, and this is affected by so many variables, known as the independent variables (inflow variables), or the control variables. The response variables (out flow variables) usually depend on the amount of inflow invested in the system. Hence Response Surface Methodology can be employed in wide range of fields, such as Agriculture, Manufacturing, and Multi-National companies, etc., where some information about the independent variables is made available. The unit-radial point designs are known as the designs with a radius of 1.0.

The work is aimed at studying the impact of increasing centre points in a second-order spherical unit-radial point designs using statistical modelling approach. This approach will entail the application of ordinary least square method on second-order quadratic model to estimate the parameters of the model and sum of square error will be applied for different centre points. The studied designs were, doehlert design (DD), equiradial design (ED) and inscribed central composite design (INSD). All of these designs have a unit radial point (r=1) in common. The centre point addition starts from 1 to 5 inclusive. Because the doehlert design is a hexagonal design, hence the hexagonal points of the equiradial and the inscribed ccd will only be applied in this study, in order to have unbiased analyses. The response variable in this study will be the Gross Domestic Product of Nigeria. Obviously, the above stated problem is not so visible in the literature. Many researchers have even studied the addition of centre points even above 10, but their actual meaning and proper interpretation have not been given. Also, there could be design(s) that can positively benefit from increasing centre points while some will have their estimation values reduced as the centre points increases. Just recently, Inamete et al. (2022) studied the impact of increasing centre points on three-factor spherical N-point Design using full quadratic model. In their study, full quadratic model was applied on three-factor designs, like the Box-Behnken, Central Composite and the Doehlert Designs for three-factors with varying radial points. In this current research, spherical second-order designs with only radial point of 1.0. That is the meaning of unit-radial point designs. Inamete et al. (2022) observed that the Doehlert Design which produced the smallest determinants across all the studied centre points, produced the largest sum of square errors for all the centre points and the Box-Behnken Design gives the smallest sum of square error for 1 to 3 centre points but for 4 and 5 centre points, the Central Composite Circumscribed Design gave better sum of square error. The sum of square error for Box-Behnken Design for 4 and 5 centre points are approximately equal. This shows that Box-Behnken Design is better than other studied designs for 1 to 3 centre points for full model. Iwundu and Onu (2017), studied the preferences of equiradial designs in relation to the central composite design for centre points from 1 to 10 inclusive. Other researchers that worked on the replication of centre points in a second-order designs were Onu et al. (2021) and Iwundu, (2016a).

Materials and Methods

The parameters for the Equiradial, Doehlert and Inscribed designs for n=6, with c = 1 - 5 centre points. Response Surface Methodology is mathematically defined as $y = \phi(x_1, x_2, \dots, x_n, \beta)$ (1)

This is a general form of a statistical model. The Quadratic model having all the parameters represented will be applied in this study and the Quadratic model in (1) is given generally as seen:

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

which is written in a reduced form to suit the study and it can be presented in matrix form as

$$y = X\beta + \varepsilon \tag{3}$$

where X is an $N \times P$ matrix, y is an $N \times 1$ vector of observed responses, β is the $P \times 1$ vector of unknown parameters and $\varepsilon \sim N(0, \delta^2)$ is the error term that was distributed in a random form. From equation (1) ϕ is unknown and represents the real functional relationship between the response y (GDP of Nigeria) and the explanatory variables x_1, x_2, \ldots, x_n .

It is intended to compare the three designs for a hexagon (n=6) for Doehlert, equiradial and Inscribed designs on the basis of parameter estimates and sum of square errors. The methods followed above for equiradial design and inscribed CCD will also be applied with the Doehlert design. The models in equation (1) will be applied throughout this study in obtaining Design Matrices for both Equiradial Designs for radius ρ =1.0 and Central Composite Designs Inscribed and Doehlert Design for two variables. The parameters of these models will be estimated. The least square equation which will be used in the estimation of the parameters for both models is given as

$$\underline{\hat{\beta}} = (\frac{X'X}{N})^{-1}X'Y \tag{4}$$

where $\underline{\hat{\beta}}$ 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 size (point) for Central Composite Design is determined by the formula as seen in Onu et al. (2023) as

$$2^k + 2k + c \tag{5}$$

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

$$2^k + k + c \tag{6}$$

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

$$N = n + c \tag{7}$$

where n is the number of points in the design and c is the center point. The design sets of points are obtained for Equiradial Design for R=1.0 is given as

 $D_5 = \begin{bmatrix} 1 & 0 \\ 0.309 & 0.951 \\ -0.81 & 0.587 \\ -0.808 & -0.589 \\ 0.311 & -0.95 \end{bmatrix}$

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

 $\xi_{6} =$

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1	0
0.309	0.951
-0.81	0.587
-0.808	-0.589
0.311	-0.95
0	0
$\langle $	

The Doehlert Design is given as

 $D_6 =$

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

The Design measure is

$\xi_7 =$	\int	
	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	\mathbf{X}_1	X_2
Cos (0)	Sin (0)	1	0
Cos (^π / ₃)	Sin (^{<i>π</i>} / ₃)	0.5	0.866
$\cos(2\pi/3)$	Sin $(2\pi/3)$	-0.5	0.866
Cos (^{3π} / ₃)	Sin $(^{3\pi}/_{3})$	-1	0
$\cos (4\pi/3)$	Sin $(^{4\pi}/_{3})$	-0.5	-0.866
$\cos(5\pi/3)$	Sin $(5\pi/3)$	0.5	-0.866
0	0	0	0

Table 1: (sets of points of Doehlert Design)

Sum of Square Errors of these designs for increasing centre point (1-5) inclusive

For each of these designs (Doehlert, Equiradial and Inscribed Designs) with each centre point 1, the estimate of the sum of square errors of the quadratic regression equation would be obtained according to Onu et al. (2022), as shown below:

Let the estimate of y be given as \hat{y} then from the quadratic model in equation (1), the error was obtained by making ε the subject in equation (1), gives:

(9)

 $\varepsilon = (y - \hat{y})$, while, for diverse values of y given as y_i and corresponding values of \hat{y} given as \hat{y}_i gives:

$$\varepsilon_i = (y_i - \hat{y}_i) \tag{8}$$

Summing and squaring (8), we obtain the error sum of square for the quadratic model, and it is given as

$$\varepsilon = (\mathbf{y} - \mathbf{y}),$$

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

1. Results and Discussion

Doehlert Design (DD) for 1 to 5 centre points

The design matrix for Doehlert Design for 1 centre point is given as

	1.0000	1.0000	0	0	1.0000	0	
	1.0000	0.5000	0.8660	0.4330	0.2500	0.7500	
X =	1.0000	-0.5000	0.8660	-0.4330	0.2500	0.7500	
	1.0000	-1.0000	0	0	1.0000	0	
	1.0000	-0.5000	-0.8660	0.4330	0.2500	0.7500	
	1.0000	0.5000	-0.8660	-0.4330	0.2500	0.7500	
	1.0000	0	0	0	0	0	

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The transpose of the design matrix is given as

	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	1.0000	0.5000	-0.5000	-1.0000	-0.5000	0.5000	0
X' =	0	0.8660	0.8660	0 0	-0.8660) -0.8660	0
	0	0.4330	-0.4330	0	0.4330	-0.4330	0
	1.0000	0.2500	0.2500	1.0000	0.2500	0.2500	0
	0	0.7500	0.7500	0	0.7500	0.7500	0
	\						

The information matrix of the design is as seen below

,	/					
	7.0000	0	0	0	3.0000	3.0000
	0	3.0000	0	0	0	0
X'X =	0	0	2.9998	0	0	0
	0	0	0	0.7500	0	0
	3.0000	0	0	0	2.2500	0.7500
	3.0000	0	0	0	0.7500	2.2500

The normalized information matrix is given as

	1.0000	0	0	0	0.4286	0.4286	
	0	0.4286	0	0	0	0	
$\frac{X'X}{7} =$	0	0	0.4285	0	0	0	
	0	0	0	0.1071	0	0	
	0.4286	0	0	0	0.3214	0.1071	
	0.4286	0	0	0	0.1071	0.3214	
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The determinant of the normalized information matrix is obtained as

$$\left|\frac{X'X}{7}\right| = 2.5815e-004$$

The trace is given as seen

$$\operatorname{Trace}\left(\frac{X'X}{7}\right) = 2.6071$$

The variance-covariance matrix is obtained as

$$\left(\frac{x'x}{7}\right)^{-1} = 0$$

$$7.0000 0 0 0 -7.0000 -7.0000$$

$$2.3333 0 0 0 0 0$$

$$0 0 2.3335 0 0 0$$

$$0 0 0 9.3339 0 0$$

$$-7.0000 0 0 0 10.5000 5.8333$$

$$-7.0000 0 0 0 5.8333 10.5000$$

The parameters of the least square estimation are obtained as

$$\underline{\beta} = \begin{pmatrix} 0.0778 \\ 0.4236 \\ -0.1379 \\ 0.2438 \\ 1.3880 \\ 1.8586 \end{pmatrix} \times 1.0e + 007$$

The estimated model for deohlert design with 1 centre point is given as

 $y = 0.0778 + 0.4236X_1 - 0.1379X_2 + 0.2438X_1X_2 + 1.3880X_1^2 + 1.8586X_2^2 + \varepsilon * 1.0e + 007$ Similarly, we obtained the model estimates for Inscribed and Equiradial designs as seen below.

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Inscribed Central Composite Design (INSD) for n=6, for 1 to 5 centre points

The design matrix with 1 centre point is given as seen below

	1.0000	0.7000	0.7000	0.4900	0.4900	0.4900	
	1.0000	-0.7000	0.7000	-0.4900	0.4900	0.4900	
	1.0000	-0.7000	-0.7000	0.4900	0.4900	0.4900	
X =	1.0000	1.0000	0	0	1.0000	0	
	1.0000	-1.0000	0	0	1.0000	0	
	1.0000	0	-1.0000	0	0	1.0000	
	1.0000	0	0	0	0	0	

The estimated model for Inscribed CCD for 1 centre point is given as

 $y = 0.0713 - 0.2724X_1 + 0.3553 + 0.1225X_1X_2 + 1.2858X_1^2 + 2.0970X_2^2 + \varepsilon * 1.0e + 007$

Equiradial Design of radius 1.0 for n=6, for 1 to 5 centre points

The design matrix for equiradial design with 1 centre point is given as

1.0000 1.0000 0 1.0000 0 0 1.0000 0.5000 0.8660 0.4330 0.2500 0.7500 $1.0000 \quad -0.5000 \quad 0.8660 \quad -0.4330 \quad 0.2500 \quad 0.7500$ 1.0000 -1.0000 -0.0010 0.0010 1.0000 0 1.0000 -0.5000 -0.8670 0.4340 0.2500 0.7520 1.0000 0.5000 -0.8650 -0.4330 0.2500 0.7480 0 0 1.0000 0 0 0

The estimated model for equiradial design for 1 centre point is given as $y = 0.0775 + 0.4251X_1 - 0.1379X_2 + 0.2392X_1X_2 + 1.3880X_1^2 + 1.8590X_2^2 + \varepsilon * 1.0e + 007$

67 Cite this article as:

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Comparison of Doehlert Design, Inscribed CCD and Equiradial Design for n=6 and 1-5 centre points

Table 1: Comparison of Doehlert, Inscribed and Equiradial Designs for n=6, for increasing center points

СР	DESIGNS					
	Parameter estimates $\hat{\theta} \times 1.0e^7$					
	DD	INSD	ED			
1	0.0778	0.0713	0.0775			
	0.4236	-0.2724	0.4251			
	-0.1397	0.3553	-0.1379			
	0.2438	0.1225	0.2392			
	1.3880	1.2858	1.3880			
	1.8586	2.0970	1.8590			
2	0.0996	0.0959	0 000/			
2	0.0770	-0 3112	0.4858			
	-0.1576	0.4058	-0.1575			
	0.2786	0.1398	0.2734			
	1 5756	1 4550	1 5754			
	2.1134	2.3818	2.1137			
3	0.1142	0.1114	0.1141			
	0.5447	-0.3501	0.5465			
	-0.1773	0.4565	-0.1772			
	0.3135	0.1572	0.3076			
	1.7703	1.6334	1.7701			
	2.3754	2.6759	2.3757			
4	0.1249	0.1226	0.1248			
	0.6052	-0.3890	0.6073			
	-0.1970	0.5073	-0.1969			
	0.3483	0.1746	0.3418			
	1.9690	1.8161	1.9688			
	2.6413	2.9745	2.6416			
5	0.1394	0.1374	0.1393			
	0.6657	-0.4279	0.6680			
	-0.2167	0.5580	-0.2166			
	0.3831	0.1921	0.3760			
	2.1639	1.9951	2.1637			
	2.9035	3.2694	2.9038			

Table 2: Sum of Square Error Analysis for replicated centre points

	DD	ED	INSD	Design sizes
nc	SSE	SSE	SSE	
1	0.485911	0.485689	0.538727	7
2	1.547889*	1.546521*	1.938783*	8
3	0.434543	0.432606	0.837509	9
4	0.063172**	0.061344**	0.470575**	10
5	0.434032	0.432445	0.837921	11

Key: * poorest estimate, ** best estimate.

Discussion

It was observed that for radial point of n= 6, Inscribed CCD and Doehlert design gave grand means that slightly differs from that of equiradial design for 1 centre point, as the centre point increases, the grand mean of the Inscribed CCD differs more significantly, while the grand mean of the doehlert design begins to close ranks with that of equiradial design. This means that increasing the centre points augments the Doehlert design towards equiradial design. It was

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further revealed that the equiradial design performs better than the doehlert design with a difference of **3.0e-3**, while the doehlert design was found better than the Inscribed CCD based on the D-Optimality criterion. In the other hand, the Doehlert design was slightly better than the equiradial design with a difference of 1.0e-4 based on A-Optimality while the Equiradial design was found better than the Inscribed CCD for 1 centre point. As the centre point increases, the difference between the D-optimality of doehlert design and the equiradial design decreases. The study shows that the strength that was shown by doehlert design over the equiradial design for n=6 and 1 centre point on a constantly from 1-5 centre points with the value of 1.0e-4. This means that if one finds the A-optimality of equiradial design to be say 2.6072, needless of calculating the A-optimality of doehlert design using the normal method that may be seen to be long process. Rather, to obtain the value of A-optimality of the doehlert design, simply subtract this said constant (1.0e-4) from the value of the already known value of A-optimality of the equiradial design (2.6072), also, if you have the A-optimality of doehlert design as 2.6071 and wish to obtain that of equiradial design, just add the constant (1.0e-4) to the already known value of A-optimality of doehlert design (2.6071). The Inscribed CCD in the other hand has shown to be inferior to these two designs. This result is in line to the findings of Iwundu and Onu (2017) that says, that the equiradial design of radial point of 1.414 and circumscribed CCD are better than the equiradial design of radial point of 1.0 and the inscribed CCD on the basis of D-, G-optimality criteria. The results showed that the equiradial design is better than the doehlert design on the basis of D-optimality, while the doehlert design is better than the equiradial design on the basis of A-optimality criterion.

On the sum of square analysis, it was observed that the equiradial design for n=6 with 1 centre point is better than the doehlert design. The sum of square error value of equiradial design is less than that of doehlert design by 0.000222, while the doehlert design was found better than the inscribed design by 0.052816. As the centre point replicates increases to 2, all the designs recorded maximum value of the sum of square errors with the error value of doehlert design as 1.547889, equiradial design error value obtained as 1.546521 and inscribed design error value as 1.938783. This result shows that the addition of 2 centre points spherical second-order unit-radial point design will result in a very poor estimation of the model parameters. This result was in line to the result of Onu et al. (2022). It shows that the difference between the sum of square error of doehlert design with 1 and 2 centre points was 1.060832 and the difference between the sum of square error of doehlert design with 1 and 2 centre points was 0.051978. As the centre point replicates increased further to 3, the sum of square errors of doehlert and equiradial designs decreased and was even found better than what was obtained for I centre point with the difference of about 0.051 and 0.053 respectively, while that of inscribed design decreased as well, but the value obtained for 1 centre point was better than that obtained for 3 centre points. The addition of 4 centre points has proven to be the best for estimation of model parameters for all the studied designs and centre points.

Conclusion

The study of the impact of replication of centre points on spherical second-order unit-point design was done to create clearer awareness what adding more centre points other than 1 can do in a second-order design. Spherical second-order designs with radius of 1.0 (known as unit-radial point design) were considered. They include, Doehlert Design, Equiradial Design and Inscribed central composite Design. Replication of centre points from 1 to 5 inclusive were considered with a quadratic model known as the second-order model. The parameters of this model were estimated for each centre point and sum of square error was used to interpret the estimated parameters.

Recommendations

The study recommends to students and researchers in the field of Design and analysis of experiment, Managers in various companies and others in the optimization processes that,

- 1. To maximize the economy of Nigeria using spherical second-order unit-radial point design(s) one should consider the addition of 4 centre points.
- 2. Equiradial design as the best spherical second-order unit-radial point design in estimation of parameters and sum of square errors.
- 3. Doehlert Design as a better replacement for Equiradial design.

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70