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Alternative Second-Order N-Point Spherical Response Surface Methodology Designs and Their Efficiencies

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Abstract

The equiradial designs are studied as alternative second-order N-point spherical Response Surface Methodology designs in two variables, for design radius ρ = 1.0. These designs are seen comparable with the standard second-order response surface methodology designs, namely the Central Composite Designs. The D-efficiencies of the equiradial designs are evaluated with respect to the spherical Central Composite Designs. Furthermore, D-efficiencies of the equiradial designs are evaluated with respect to the D-optimal exact 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 reveal 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 all cases studied. Also, D-efficiency values reveal that the alternative second-order N-point spherical equiradial designs are better than the N-point D-optimal exact designs defined on the design region supported by the design points of the Inscribed Central Composite Design. However, the N-point spherical equiradial designs are inferior to the N-point D-optimal exact designs defined on the design region supported by the design points of the Circumscribed Central Composite Design and those of the Face-centered Central Composite Design, with worse cases with respect to the design region of the Circumscribed Central Composite Design.

Keyword: Equiradial designs, Second-Order Response Surface Methodology Designs, Central Composite Designs, D-efficiency

1. Introduction

Central Composite Designs (CCDs) play a vital role in modelling second-order response functions in the presence of curvature. They are particularly useful at the second phase of process optimization. However, some spherical designs exist and can serve reasonably well when the standard Central Composite Designs are unavailable and/or cannot be employed. One such class of spherical designs is the class of equiradial designs, which according to Myer *etal.* (2009) are some special and interesting two-factor designs for modelling second-order response functions. As the name implies, equiradial designs are designs on a common sphere and are rotatable. The class of equiradial designs begins with a pentagon of equally spaced points on the sphere with design matrix expressed as

$$\begin{matrix} x_1 & x_2 \\ \{\ \rho\, Cos\,(\theta + 2\pi u/n_1) & \rho\, Sin\,(\theta + 2\pi u/n_1)\}; \end{matrix}\ u = 0, 1, 2, \ldots\ , n_1 - 1$$

where x_1 and x_2 represent the two controllable variables, ρ is the radius of the design and n_1 represents the number of points on the sphere. In addition to the n_1 radial points of the design, n_c center points shall be added to the design. As indicated in Myer *etal.* (2009), the value of θ is assumed equal to zero since θ has no effect on the information matrix, $X^T X$, of the design. Thus the equiradial designs are such that the information matrix is invariant to design rotation.

Many works have been done using second-order response surface models and designs. They include the construction of efficient and optimal experimental designs for second-order response surface models (see for example Onukogu and Iwundu (2007)). Concerns about optimality of designs have been investigated for second-order models (see for example Dette and Grigoriev (2014)). Optimal choices of design points have been addressed by a number of researchers including Chigbu and Nduka (2006) and Iwundu (2015). Lucas (1976) compared the performances of several types of second-order response surface designs in symmetric regions on the basis of D- and G-optimality criteria. Graphical methods have been employed in studying the response variance property of second-order response surface designs as seen in Myer *etal.*(1992), Giovannitti-Jensen and Myers (1989), Zahran *etal* (2003). Chigbu *etal.* (2009) compared the prediction variances of some Central Composite Designs in spherical regions with radius $\alpha = \sqrt{k}$ where k is the number of model controllable 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 and Otaru (2014) 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 and Chigbu (2015) 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 (2015) 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. 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. Oyejola and Nwanya (2015) 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 *etal.*(2009).

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. Atkinson and Donev (1992) gave various properties of the D-optimality and D-efficiency of designs under varying design conditions. It is worth noting that second-order models serve importantly 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. The second-order response surface model in two controllable variables, x_1 and x_2, is given as

$$y(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \epsilon \qquad 1.1$$

and written in matrix notation as

$$Y = X\beta + \epsilon \qquad 1.2$$

where

Y is the Nx1 vector of observed values.

X is the Nxp design matrix

β is the px1 vector of unknown model parameters which are estimated on the basis of N uncorrelated observations.

ϵ is the random additive error associated with Y and is independently and identically distributed with zero mean and constant variance.

2. Methodology

For the importance of second-order Response Surface Methodology designs, we consider in this work the equiradial designs which are alternative second-order spherical Response Surface Methodology designs in two variables. The interest here is in comparing the efficiency of the equiradial designs with respect to the standard spherical Central Composite Designs. In particular interest is in how the equiradial designs compare with the Circumscribed and Inscribed Central Composite designs, which are both spherical and rotatable. We shall further consider the efficiencies of equiradial designs with respect to the D-optimal exact designs of Iwundu and Otaru (2014) which were defined on the design regions supported by design points of the Circumscribed Central Composite Design, the Inscribed Central Composite Design and the Face-centered Central Composite Design. The efficiency of a design provides a measure of the optimality of the design. In comparing two designs, the relative efficiency is seen as the ratio of their separate efficiencies.

We shall employ the D-efficiency criterion as the test criterion. This criterion has been extensively used as a single numerical measure of the efficiency of designs. The D-efficiency criterion aims at minimizing the variance-covariance matrix associated with the parameter estimates of the model used. By definition, the D-efficiency of a design $\xi^{(1)}$ is given as

$$D_{eff} = 100\, x\, \left(\det M\left(\xi^{(1)}\right)\right)^{\frac{1}{p}} \qquad 2.1$$

and the D-efficiency of a design $\xi^{(1)}$ relative to the design $\xi^{(2)}$ is given as

$$D_{eff} = \left(\frac{\det M\left(\xi^{(1)}\right)}{\det M\left(\xi^{(2)}\right)}\right)^{\frac{1}{p}} \qquad 2.2$$

where $M(.)$ is the information matrix of the design and p is the number of model parameters. For an N-point design, say ξ_N , the information matrix of the design ξ_N is $X^T X$ and normalized as $\frac{X^T X}{N}$ to remove the effect of changing design sizes. The (Nxp) matrix, X, is the design matrix whose columns are built from the model and the design ξ_N and $(.)^T$ represents transpose. Among other things, D-efficiency values depend on the number of points in the design and the number of controllable variables in the model. In comparing designs, the best design is one with the largest D-efficiency value. In terms of relative efficiency, the ratio in equation 2.2 exceeds unity if the design $\xi^{(1)}$ is better than the design $\xi^{(2)}$.

In comparing the N-point equiradial designs with the Circumscribed Central Composite designs, the 9-point Circumscribed Central Composite design comprising of the factorial points { (1,1), (1,-1), (-1,1), (-1,-1)}, the axial points {(1.414,0), (-1.414,0), (0,1.414), (0,-1.414)} and the center point {(0,0)} shall be employed. Similarly, in comparing the N-point equiradial designs with the Inscribed Central Composite Designs, the 9-point Inscribed Central Composite design comprising of the factorial points { (0.7,0.7), (0.7,-0.7), (-0.7,0.7), (-0.7,-0.7)}, the axial points {(1,0), (-1,0), (0,1), (0,-1)} and the center point {(0,0)} shall be employed. For comparisons with the D-optimal exact designs, the N-point designs generated by Iwundu and Otaru (2014) shall be employed correspondingly with the N-point equiradial designs.

3. Results

The design measures associated with the N-point equiradial designs for ρ = 1, n_1= 5, 6, ⋯ , 11 and n_c = 1 are as follows;

$$\xi_6 = \begin{pmatrix} 1 & 0 \\ 0.31 & 0.95 \\ -0.81 & 0.59 \\ -0.81 & -0.59 \\ 0.31 & -0.95 \\ 0 & 0 \end{pmatrix}$$

$$\xi_7 = \begin{pmatrix} 1 & 0 \\ 0.5 & 0.87 \\ -0.5 & 0.87 \\ -1 & 0 \\ -0.5 & -0.87 \\ 0.5 & -0.87 \\ 0 & 0 \end{pmatrix}$$

$$\xi_8 = \begin{pmatrix} 1 & 0 \\ 0.62 & 0.78 \\ -0.22 & 0.97 \\ -0.90 & 0.43 \\ -0.90 & -0.43 \\ -0.22 & -0.97 \\ 0.62 & -0.78 \\ 0 & 0 \end{pmatrix}$$

$$\xi_9 = \begin{pmatrix} 1 & 0 \\ 0.71 & 0.71 \\ 0 & 1 \\ -0.71 & 0.71 \\ -1 & 0 \\ -0.71 & -0.71 \\ 0 & -1 \\ 0.71 & -0.71 \\ 0 & 0 \end{pmatrix}$$

$$\xi_{10} = \begin{pmatrix} 1 & 0 \\ 0.77 & 0.64 \\ 0.17 & 0.98 \\ -0.5 & 0.87 \\ -0.94 & 0.34 \\ -0.94 & -0.34 \\ -0.5 & -0.87 \\ 0.17 & -0.98 \\ 0.77 & -0.64 \\ 0 & 0 \end{pmatrix}$$

$$\xi_{11} = \begin{pmatrix} 1 & 0 \\ 0.81 & 0.59 \\ 0.31 & 0.95 \\ -0.31 & 0.95 \\ -0.81 & 0.59 \\ -1 & 0 \\ -0.81 & -0.59 \\ -0.31 & -0.95 \\ 0.31 & -0.95 \\ 0.81 & -0.59 \\ 0 & 0 \end{pmatrix}$$

$$\xi_{12} = \begin{pmatrix} 1 & 0 \\ 0.84 & 0.54 \\ 0.41 & 0.91 \\ -0.14 & 0.99 \\ -0.65 & 0.76 \\ -0.96 & 0.28 \\ -0.96 & -0.28 \\ -0.65 & -0.76 \\ -0.14 & -0.99 \\ 0.41 & -0.91 \\ 0.84 & -0.54 \\ 0 & 0 \end{pmatrix}$$

For the bivariate quadratic model in equation 1.1, the normalized information matrices and the associated determinant values corresponding to the equiradial designs are, respectively, as follows;

$$M(\xi_6) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0.4174 & 0.4168 \\ 0 & 0.4174 & 0 & 0 & -0.0005 & -0.0007 \\ 0 & 0 & 0.4168 & -0.0007 & 0 & 0 \\ 0 & 0 & -0.0007 & 0.105 & 0 & 0 \\ 0.4174 & -0.0005 & 0 & 0 & 0.3132 & 0.105 \\ 0.4168 & -0.0007 & 0 & 0 & 0.105 & 0.3118 \end{bmatrix}$$

$\det M(\xi_6) = 2.639818966\text{x}10^{-4}$

$$M(\xi_7) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0.4285 & 0.4325 \\ 0 & 0.4285 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.4285 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.1081 & 0 & 0 \\ 0.4285 & 0 & 0 & 0 & 0.3214 & 0.1081 \\ 0.4325 & 0 & 0 & 0 & 0.1081 & 0.3273 \end{bmatrix}$$

$\det M(\xi_7) = 2.67816305\text{x}10^{-4}$

$$M(\xi_8) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0.4357 & 0.4357 \\ 0 & 0.4357 & 0 & 0 & -0.0003 & 0.00095 \\ 0 & 0 & 0.4335 & 0.00095 & 0 & 0 \\ 0 & 0 & 0.00095 & 0.1072 & 0 & 0 \\ 0.4357 & -0.0003 & 0 & 0 & 0.3265 & 0.1072 \\ 0.4335 & 0.00095 & 0 & 0 & 0.1072 & 0.3224 \end{bmatrix}$$

$\det M(\xi_8) = 2.37557395\text{x}10^{-4}$

$$M(\xi_9) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0.4462 & 0.4462 \\ 0 & 0.4462 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.4462 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.1129 & 0 & 0 \\ 0.4462 & 0 & 0 & 0 & 0.3351 & 0.1129 \\ 0.4462 & 0 & 0 & 0 & 0.1129 & 0.3351 \end{bmatrix}$$

$\det M(\xi_9) = 2.4889799568\text{x}10^{-4}$

$$M(\xi_{10}) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0.451 & 0.4485 \\ 0 & 0.451 & 0 & 0 & 0.0011 & -0.001 \\ 0 & 0 & 0.4485 & -0.001 & 0 & 0 \\ 0 & 0 & -0.001 & 0.1123 & 0 & 0 \\ 0.451 & 0.0011 & 0 & 0 & 0.3391 & 0.1123 \\ 0.4485 & -0.001 & 0 & 0 & 0.1123 & 0.3352 \end{bmatrix}$$

$\det M(\xi_{10}) = 2.298611217\text{x}10^{-4}$

$$M(\xi_{11}) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0.4553 & 0.4547 \\ 0 & 0.4553 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.4547 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.1145 & 0 & 0 \\ 0.4553 & 0 & 0 & 0 & 0.3417 & 0.1145 \\ 0.4547 & 0 & 0 & 0 & 0.1145 & 0.3402 \end{bmatrix}$$

det $M(\xi_{11})$ = 2.224863024x10^{-4}

$$M(\xi_{12}) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0.4594 & 0.4761 \\ 0 & 0.4562 & 0 & 0 & -0.003 & -0.016 \\ 0 & 0 & 0.4593 & -0.0005 & 0.00089 & 0.0047 \\ 0 & 0 & -0.0005 & 0.1134 & -0.0008 & -0.004 \\ 0.4594 & -0.003 & 0.00089 & -0.0008 & 0.3484 & 0.1297 \\ 0.4761 & -0.016 & 0.0047 & -0.004 & 0.1297 & 0.3512 \end{bmatrix}$$

det $M(\xi_{12})$ = 2.149505806x10^{-4}.

These designs are compared with the Circumscribed Central Composite design and the Inscribed Central Composite design whose design points have been listed in Section 2. The respective normalized information matrices M_1 and M_2 together with the determinant values are as listed below, where M_1 represents the normalized information matrix associated with the Circumscribed Central Composite design and M_2 represents the normalized information matrix associated with the Inscribed Central Composite design.

$$M_1 = \begin{bmatrix} 0.9999 & 0 & 0 & 0 & 0.8887 & 0.8887 \\ 0 & 0.8887 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.8887 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.4444 & 0 & 0 \\ 0.8887 & 0 & 0 & 0 & 1.3327 & 0.4444 \\ 0.8887 & 0 & 0 & 0 & 0.4444 & 1.3327 \end{bmatrix}$$

det M_1 = 6.158433838x10^{-4}

$$M_2 = \begin{bmatrix} 0.9999 & 0 & 0 & 0 & 0.44 & 0.44 \\ 0 & 0.44 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.44 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.1067 & 0 & 0 \\ 0.44 & 0 & 0 & 0 & 0.3289 & 0.1067 \\ 0.44 & 0 & 0 & 0 & 0.1067 & 0.3289 \end{bmatrix}$$

det M_2 = 2.224059802x10^{-4}.

The D-efficiency values of the N-point equiradial designs relative to the Circumscribed Central Composite design and the Inscribed Central Composite design are as in Table 1.

Table 1. D-Efficiency values of equiradial designs relative to the Circumscribed and the Inscribed Central Composite designs

Design size N	D-Efficiency values of equiradial designs relative to the Circumscribed Central Composite design	D-Efficiency values of equiradial designs relative to the Inscribed Central Composite design
6	0.4030426836	1.028974504
7	0.4040125476	1.031450583
8	0.3960196875	1.011044681
9	0.3991096601	1.018933432
10	0.3938518937	1.005510269
11	0.3917171302	1.001832841
12	0.3984739855	0.994333398

The equiradial designs are further compared with D-optimal exact designs whose design points are as in Iwundu and Otaru (2014). The D-efficiency values of the N-point equiradial designs relative to the N-point D-optimal exact designs defined on the design regions supported by design points of the Circumscribed Central Composite design, the Inscribed Central Composite design and the Face-centered Central Composite design are as in Tables 2-4. Each table comprises the design size N, the determinant values of the normalized information matrices associated with the equiradial designs, the determinant values of the normalized information matrices associated with the D-optimal exact designs as well as the D-efficiency values.

Table 2. D-Efficiency values of equiradial designs relative to the D-optimal exact designs defined on the design regions supported by points of the Circumscribed Central Composite Design

Design size N	Determinant value (equiradial design)	Determinant value (D-optimal exact design)	D-Efficiency value
6	$2.639818966\text{x}10^{-4}$	$3.1947\text{x}10^{-2}$	0.4496321364
7	$2.67816305\text{x}10^{-4}$	$3.837429233\text{x}10^{-2}$	0.4371523047
8	$2.37557395\text{x}10^{-4}$	$4.6828\text{x}10^{-2}$	0.4145184104
9	$2.488979568\text{x}10^{-4}$	$6.1584\text{x}10^{-2}$	0.3991096601
10	$2.298611217\text{x}10^{-4}$	$6.545687882\text{x}10^{-2}$	0.3898687014
11	$2.224863024\text{x}10^{-4}$	$6.004443063\text{x}10^{-2}$	0.3933734922
12	$2.149505806\text{x}10^{-4}$	$5.782736734\text{x}10^{-2}$	0.3935810684

Table 3. D-Efficiency values of equiradial designs relative to the D-optimal exact designs defined on the design regions supported by points of the Inscribed Central Composite Design

Design size N	Determinant value (equiradial design)	Determinant value (D-optimal exact design)	D-Efficiency value
6	$2.639818966\text{x}10^{-4}$	$1.166000031\text{x}10^{-4}$	1.145897918
7	$2.67816305\text{x}10^{-4}$	$1.384704002\text{x}10^{-4}$	1.116211976
8	$2.37557395\text{x}10^{-4}$	$2.224059802\text{x}10^{-4}$	1.018933432
9	$2.488979568\text{x}10^{-4}$	$1.713104121\text{x}10^{-4}$	1.056000521
10	$2.298611217\text{x}10^{-4}$	$2.362949253\text{x}10^{-4}$	0.9954096679
11	$2.224863024\text{x}10^{-4}$	$2.174265558\text{x}10^{-4}$	1.003841429
12	$2.149505806\text{x}10^{-4}$	$2.090927535\text{x}10^{-4}$	1.004615652

Table 4. D-Efficiency values of equiradial designs relative to the D-optimal exact designs defined on the design region supported by points of the Face-centered Central Composite Design

Design size N	Determinant value (equiradial design)	Determinant value (D-optimal exact design)	D-Efficiency value
6	$2.639818966x10^{-4}$	$5.486968437x10^{-3}$	0.6030781776
7	$2.67816305x10^{-4}$	$8.159865377x10^{-3}$	0.5658382953
8	$2.37557395x10^{-4}$	$8.7890625x10^{-3}$	0.5478197267
9	$2.488979568x10^{-4}$	$9.754610572x10^{-3}$	0.5425859777
10	$2.298611217x10^{-4}$	$9.360x10^{-3}$	0.5391359338
11	$2.224863024x10^{-4}$	$9.5374x10^{-3}$	0.5345383641
12	$2.149505806x10^{-4}$	$1.0154x10^{-2}$	0.5259570053

3. Discussion of Results

The equiradial designs have been examined as alternative spherical designs to the rotatable Central Composite Designs (CCDs) and the D-optimal exact designs in modelling second-order response functions. These designs are seen comparable with the standard second-order Response Surface Methodology designs. The equiradial designs which are simple to construct seem to show some appealing optimality properties. A careful look at the D-efficiency values makes it interesting to note that equiradial designs are not generally inferior designs. In fact, they appear more optimal than some frequently used second-order Response Surface Methodology designs. In particular, the study revealed that equiradial designs perform generally better than the Inscribed Central Composite designs and the D-optimal exact designs defined on the design region supported by the design points of the Inscribed Central Composite design for the design sizes considered. Besides N = 12, the equiradial designs were better than the Inscribed Central Composite design under the D-efficiency criterion. Additionally, each N-point equiradial design was better than the corresponding N-Point D-optimal exact design defined on the design region supported by the design points of the Inscribed Central Composite design, except for N=10 which gave relative efficiency value of 0.9954096679. However, it is clear from the relative efficiency value that the 10-point equiradial design is as good the 10-point D-optimal exact design.

It is further observed that the equiradial designs are not as credible as the Circumscribed Central Composite design in terms of D-efficiency. This was seen in the relative efficiency values being less than 50% in all cases considered. The observation is not different for N-Point D-optimal exact designs defined on the design region supported by the design points of the Circumscribed Central Composite design. However, when compared with the D-optimal exact designs defined on the design region supported by the design points of the Face-centered Central Composite design, the equiradial designs were not too inferior as the relative efficiency values exceeded 50% in all cases considered.

Although the equiradial designs could serve as alternatives to the standard Response Surface Methodology designs, they should be used with caution especially when design optimality is paramount.

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