Optimal Partially Replicated Cube, Star and Center Runs in Face-centered Central Composite Designs

M. P. Iwundu

Correspondence: M. P. Iwundu, Department of Mathematics and Statistics, Faculty of Physical Science and Information Technology, University of Port Harcourt, Nigeria. E-mail: mary_iwundu@yahoo.com

Received: July 30, 2015Accepted: August 17, 2015Online Published: September 23, 2015doi:10.5539/ijsp.v4n4p1URL: http://dx.doi.org/10.5539/ijsp.v4n4p1

Abstract

The variations of the Face-centered Central Composite Design under partial replications of design points are studied. The experimental conditions include replicating the cube points while the star points and center point are held fixed or not replicated, replicating the star points while the cube points and the center point are held fixed or not replicated and replicating the center point while the cube points and the star points are held fixed or not replicated. As a measure of goodness of the designs, D- and G-efficiency criteria are utilized. Results show that for the two- and three-variable 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-optimality criterion as well as G-optimality criterion. When compared with the traditional method of replicating the center point, the two cube portions, one star portion and a center point are point variation was relatively better in terms of design efficiency.

Keywords: Replication, cube points, star points, center point, D-efficiency, G-efficiency

1. Introduction

Unreplicated designs are very widely used in experimental situations. However, fitting full model for unreplicated designs results in zero degrees of freedom for error and hence tests about main and interaction effects of factors cannot be carried out. This constitutes a potential problem in statistical testing (Farrukh, 2014). Two common approaches to this problem require either pooling high-order interactions, assumed to be negligible, to estimate the error or replicating one or more experimental runs. Generally, replication of design points offers an independent and more precise estimate of experimental error.

In model building, designs with factors that are set at two levels implicitly assume that the effect of the factors on the response variable is linear and one would usually anticipate fitting the first-order model. When it is suspected that the relationship between the factors in the design and the response variable is not linear, there is the need to include one or more experimental runs. The first-order models with the presence of interaction terms are capable of representing some curvature in the response function. However, in some cases, the curvature in the response function is not adequately modeled and therefore the need to consider the second-order model for better representation.

Central Composite Designs (CCDs) originally proposed by Box & Wilson (1951) have been the practically used designs for estimating second-order response surfaces. They are so advantageous in Response Surface Methodology (RSM) for building models of the response variables without needing to carry out complete three-level factorial experiments. Applications of Central Composite Designs can be seen in various fields of study including biological, chemical, pharmaceutical fields. The CCD is particularly useful in the determination of optimum values of influential parameters of a response variable (see e.g. Alalayah *et al.* (2010)). A review of some aspects of Central Composite Designs in spherical region is presented in Chigbu *et al.* (2009).

A CCD consists of three distinct sets of experimental runs:

- i. A set of factorial or fractional factorial design (cube portion) in the factors studied and each having two levels;
- ii. A set of axial points (star portion);
- iii. A set of center points.

In augmenting Central Composite Designs, the common practice has been the replication of only the center point

for estimation of the experimental error, improvement of the precision of the experiments and to maintain minimum number of design runs which an experimenter can afford. Two ways of replicating design are the DESIGNREP procedure which involves replicating the entire design and the POINTREP procedure which involves replicating each point in the design. When it is not possible to replicate the full design, the experimenter can obtain an estimate of pure error by replicating only some of the points in the design. One challenge of partial replications of design points is that the experimenter faces the problem of choosing the points to be replicated and the points not to be replicated in the design. Authors including Cochran and Cox (1957), Montgomery (1997) and Atkinson and Donev (1992) have discussed extensively the analysis of such replicated experiments.

Quite recently, many experimenters have focused on the effect of replicating the non-center points as against the usual replication of the center point in exploring response surfaces. Chigbu and Ohaegbulem (2011) considered the preference of replicating factorial runs to axial runs in restricted second-order designs. They observed in general that under orthogonality and rotatability restrictions, the replicated cubes plus one star variation was better than the one cube plus replicated star variation in the sense of D-optimality. The number of experimental runs employed was $N = n_1 2^k + n_2 2k + n_0$ where n_1 is the number of cubes, n_2 is the number of stars and n_0 is the number of center point. Although allowing for partial replication of the cubes and the stars, every point in the cube as well as the star was utilized. Ukaegbu and Chigbu (2014) considered the performance of the partially replicated cube and star portions of orthogonal Central Composite Designs in spherical regions. One particular focus was the performance of the Central Composite Designs with respect to stability, small predictive variance and prediction capability was studied using graphical techniques and single-value optimality criteria. Results indicate that replicating the star portions of the Central Composite Designs considerably reduces the prediction variance and thus improves G-efficiency than replicating the cube portion.

Oyejola and Nwanya (2015) considered the performance of five varieties of Central Composite Design when the axial portions are replicated and the center point increased one and three times. Ahn (2015) devised a new CCD called the CCD-R for experiments not just at the center but also at non-center points. The flexibility of the CCD-R is seen in the existence of a myriad of perfectly orthogonal and nearly rotatable designs. Ahn (2015) considered that when a two-level full or fractional experiment is conducted, a few center runs would be adequate to detect the quadratic effects over the region of exploration. However, in situations where the parameters of quadratic model are to be separately estimated, more runs at some more design points are needed. In addressing this problem, the augmentation of the two-level full or fractional factorial design with a center and 2k axial points was proposed, where k is the number of independent factors in the experiment.

In this work, the effect of partially replicating the factorial points and the star points of the Face-centered Central Composite Designs with respect to replicating the center point on response surface designs is investigated. This requires

- i. Constructing partially replicated exact designs for two and three variable quadratic models.
- ii. Assessing the goodness of the designs using two single-value criteria, namely D- and G-efficiency criteria.

For two input variables (i.e. k = 2), the Face-centered Central Composite Design consists of n_c center points, four factorial points and four axial points. For three input variables (i.e. k = 3), the Face-centered Central Composite Design consists of n_c center points, eight factorial points and six axial points. The axial points are parallel to each variable axis on a circle of radius, $\alpha = 1.0$ and origin at the center point. The designated α is the radius which determines the geometry and defines a square for two input variables and a cube for three input variables. According to Montgomery (1997) and Zahran (2002). Face-centered Central Composite Design is the most useful cuboidal region in practice because it requires only three levels of each factor.

Draper and Guttman (1988) observed that the adequacy of an experimental design can be determined from the information matrix. Some criteria that are based on the information matrix include A-, D-, E-, G- and I-optimality criteria. Rady *et al.* (2009) gave a concise survey on the optimality criteria with particular attention on relationships among the several optimality criteria. Following the definitions of Atkinson and Donev (1992), A-optimality criterion seeks to minimize the trace of the variance-covariance matrix. This criterion results in minimizing the average variance of the estimated regression coefficients. D-optimality criterion maximizes the amount of information in an experimental design. As assessed by the information matrix, D-optimality criterion maximizes the determinant of information matrix of the design and equivalently minimizes the determinant of the variance-covariance matrix. Hence for a specified model, a D-optimal design minimizes the variances of parameter estimates as well as the covariances between parameter estimates. On the other hand, G-optimality criterion minimizes the maximium variance of prediction over the design space.

A number of standard measures have been proposed in the literature to summarize the efficiency of a design. Some of these measures can be seen in Atkinson and Donev (1992), Wong (1994) and Chukwu and Yakubu (2012). To assess the goodness of designs, two single-value efficiency criteria, namely, the D- and G-efficiencies are commonly employed. As in the literature on optimal designs, efficiency values lie between zero and one, a design having efficiency value of 1.0 implies that the design is 100% efficient. Hence in comparing designs, a design with a higher efficiency value would be preferred. According to Atkinson and Donev (1992), D-efficiency of an arbitrary design, ξ_N , over an optimal design, ξ_N^* is defined as

$$D_{eff}\!=\!-\frac{M(\xi_N^{})}{M(\xi_N^*)}~.$$

The G-efficiency of an arbitrary design, ξ_N , is defined as

$$G_{eff} = \frac{d(\xi_N^*)}{d(\xi_N)} = \frac{p}{d(\xi_N)} ;$$

Where $d(\xi_N^*)$ is the maximum variance of predicted response associated with ξ_N^* and $d(\xi_N)$ is the maximum variance of predicted response associated with ξ_N .

Here, p is the number of model parameters and N is the number of requested runs. The D-efficiency can be interpreted as the relative number of runs (in percent) that would be required by an orthogonal design to achieve the same value of the determinant $|X^TX|$. In practice, an orthogonal design may not be possible in many cases; hence orthogonality becomes only a theoretical "yard-stick." Therefore, one should use D-efficiency measure rather as a relative indicator of efficiency to compare other designs. D-efficiency measure relates to D-optimality criterion as G-efficiency measure relates to the G-optimality criterion, which concentrates on minimizing the maximum value of the standard error of the predicted response.

2. Method

In this work, the variation of the Central Composite Design (CCD) is studied when

(i) The cube points are replicated while the star points and center point are held fixed or not replicated;

(ii) The star points are replicated while the cube points and the center point are held fixed or not replicated;

(iii) The center point is replicated while the cube points and the star points are held fixed or not replicated.

Efficiencies of the constructed designs are assessed using D- and G- efficiency criteria.

In studying the partial replication of Central Composite Design, the second-order polynomial model in equation (1) is employed.

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \sum_{j>i}^k \beta_{ij} x_i x_j + \sum_{i=1}^k \beta_{ii} x_{ii}^2 + \varepsilon$$
(1)

This model can be rewritten as

$$Y = X\beta + \varepsilon \tag{2}$$

Where

Y is the Nx1 vector of observed values

X is the design matrix

 β is the px1 vector of unknown 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.

To explore the Face-centered Central Composite Design with partial replication of the cube or the factorial points, we observe that the k-variable second-order full model has p model parameters given by

$$p = \frac{(k+1)(k+2)}{2}$$
(3)

The factorial portion of the Central Composite Design comprises of experimental runs of the 2^k factorial design. For k = 2, the experimental runs are

$$V = \begin{pmatrix} 1 & 1 \\ -1 & 1 \\ 1 & -1 \\ -1 & -1 \end{pmatrix}$$

For k = 3, the experimental runs are

$$\mathbf{V} = \begin{pmatrix} -1 & -1 & -1 \\ -1 & -1 & +1 \\ +1 & -1 & -1 \\ -1 & +1 & -1 \\ -1 & +1 & +1 \\ +1 & -1 & +1 \\ +1 & +1 & -1 \\ +1 & +1 & +1 \end{pmatrix}$$

The star portion of the Central Composite Design comprises of the experimental runs

$$S = \begin{pmatrix} \alpha & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ -\alpha & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & \alpha & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & -\alpha & 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \cdots & \alpha \\ 0 & 0 & 0 & 0 & \cdots & \cdots & -\alpha \end{pmatrix}$$

For k = 2, this becomes

$$\mathbf{S} = \begin{pmatrix} \alpha & 0\\ -\alpha & 0\\ 0 & \alpha\\ 0 & -\alpha \end{pmatrix}$$

For k = 3,

$$\mathbf{S} = \begin{pmatrix} \alpha & 0 & 0 \\ -\alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & -\alpha & 0 \\ 0 & 0 & \alpha \\ 0 & 0 & -\alpha \end{pmatrix}$$

The center portion of the Central Composite Design comprises of the experimental run

 $C = (0 \ 0 \ \dots \ 0).$

For k = 2, this becomes

 $C = (0 \ 0)$

For k = 3, it becomes

 $C = (0 \ 0 \ 0).$

The information matrix of a CCD shall be expressed in terms of the number of cube points, star points and center point. Thus, the number of experimental runs is given by $N = n_1 2^k + \binom{n_{11}}{r} + n_2 2k + \binom{n_{22}}{r} + n_0$ where n_1 is the number of cube portions, n_2 is the number of star portions, n_0 is the number of center points, n_{11} refers to the number of cube points in the cube portion of the CCD and n_{22} refers to the number of star points in the star portion of the CCD. For the purpose of this work n_1 and n_2 are set at unity, $V + \binom{n_{11}}{r}$ implies taking the cube portion and additional r distinct cube points from the available n_{11} cube points, $S + \binom{n_{22}}{r}$ implies taking the cube star portion and additional r distinct star points from the available n_{22} star points and C+2 implies taking the center point and additional two center points.

For k = 2, the various variations or experimental conditions to study in replicating the vertex points while the star points and center point are held fixed or not replicated are as tabulated in Table 1.

Table 1. Variations	for replicating the ve	ertex points $(k = 2)$
---------------------	------------------------	------------------------

Expe	Design Size N		
Vertex	Star	Center	
$V + {}^4C_4$	S	С	13
$V+{}^{4}C_{3}$	S	С	12
$V+^4C_2$	S	С	11
$V+{}^{4}C_{1}$	S	С	10

In replicating the star points while the vertex points and center point are held fixed or not replicated, the various variations or experimental conditions to study are as tabulated in Table 2.

Table 2. Variations for replicating the star points (k = 2)

Ex	Experimental Condition			
Vertex	Star	Center		
V	$S+^4C_4$ $S+^4C_3$ $S+^4C_2$ $S+^4C_1$	С	13	
V	$S+^4C_3$	С	12	
V	$S+^4C_2$	С	11	
V	$S+^4C_1$	С	10	

In replicating the center point while the vertex points and star points are held fixed or not replicated, the various variations or experimental conditions to study are as tabulated in Table 3

Table 3. Variations for replicating the center point (k = 2)

Ex	Experimental Condition			
Vertex	Star	Center		
V	S	C+4	13	
V	S	C+3	12	
V	S	C+2	11	
V	S	C+1	10	

For k = 3, the various variations or experimental conditions to study in replicating the vertex points while the star points and center point are held fixed or not replicated are as tabulated in Table 4.

Table 4. Variations for replicating the vertex points (k = 3)

Expe	Experimental Condition				
Vertex	Star	Center	_		
$V + {}^{8}C_{8}$	S	С	23		
$V + {}^{8}C_{7}$	S	С	22		
$V + {}^{8}C_{6}$	S	С	21		
$V+{}^{8}C_{5}$	S	С	20		
$V + {}^{8}C_{4}$	S	С	19		
$V + {}^{8}C_{3}$	S	С	18		
$V + {}^{8}C_{2}$	S	С	17		
$V + {}^{8}C_{1}$	S	С	16		

In replicating the star points while the vertex points and center point are held fixed or not replicated, the various variations or experimental conditions to study are as tabulated in Table 5

Exp	Experimental Condition				
Vertex	Star	Center	_		
V	$S + {}^{8}C_{8}$	С	23		
V	$S + {}^{8}C_{7}$	С	22		
V	${ m S+}^8{ m C_6} { m S+}^8{ m C_5}$	С	21		
V		С	20		
V	$S+{}^{8}C_{4}$	С	19		
V	$S+{}^{8}C_{3}$	С	18		
V	$S+{}^{8}C_{2}$	С	17		
V	$S+^{8}C_{1}$	С	16		

Table 5.	Variations	for rep	olicating	the star	points	(k = 3)

In replicating the center point while the vertex points and star points are held fixed or not replicated, the various variations or experimental conditions to study are as tabulated in Table 6

Table 6. Variations for replicating the star points $(k = 3)$	Table 6.	Variations	for rep	olicating	the star	points ((k = 3))
---	----------	------------	---------	-----------	----------	----------	---------	---

Expe	Experimental Condition				
Vertex	Star	Center			
V	S	C+8	23		
V	S	C+7	22		
V	S	C+6	21		
V	S	C+5	20		
V	S	C+4	19		
V	S	C+3	18		
V	S	C+2	17		
V	S	C+1	16		

For each experimental condition, an *N*-point design shall be chosen to maximize the determinant of information matrix. Onukogu and Iwundu (2007), Madukaife and Oladugba (2010) and Iwundu and Albert-Udochukwuka (2014) have provided helpful rules for selecting design points to maximize the determinant of information matrix.

Let

$$\xi_N = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1k} \\ x_{21} & x_{22} & \dots & x_{2k} \\ \vdots & \vdots & \vdots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{Nk} \end{pmatrix}$$

be an N-point design measure depending on k-variable quadratic model, having p-parameters. The Nxp design matrix

$$\mathbf{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1k} \\ 1 & x_{21} & x_{22} & \dots & x_{2k} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{N1} & x_{N2} & \dots & x_{Nk} \end{pmatrix}$$

gives the values of independent variables that are used in the statistical models and further contains the column of 1's that represent the intercept term as well as the columns for the products and powers associated with other model terms. The pxp information matrix, M, associated with ξ_N is obtained from X^TX and normalized as $\frac{1}{N}$ X^TX, where the notation, (.)^T represents transpose. The criterion that allows maximization of determinant of

information matix of a design is the D-optimality criterion.

Let ξ_N^1 , ξ_N^2 , ..., ξ_N^m be m design measures defined on the design region of the Face-centered Central Composite Design and having non-singular information matrices $M_1, M_2, ..., M_m$, respectively. The design measure ξ_N^1 is preferred, in terms of D-optimality criterion, to the design measures $\xi_N^2, ..., \xi_N^m$ iff the determinant

Det
$$(M_1) = \max \{ \text{Det } (M_1), \text{Det } (M_2), \dots, \text{Det } (M_m) \}.$$

Also let $\underline{x}_i = (1 \quad x_{i1} \quad x_{i2} \quad \dots \quad x_{ik})$; $i = 1, 2, \dots, N$ be the ith row of the design matrix X, associated with the design point $(x_{i1} \quad x_{i2} \quad \dots \quad x_{ik})$. The variance of prediction, $V\{y(\underline{x}_i)\}$, at the ith design point $\underline{x}_i = (1 \quad x_{i1} \quad x_{i2} \quad \dots \quad x_{ik})$ is

 $V{y(x_i)} = (1 \quad x_{i1} \quad x_{i2} \quad \dots \quad x_{ik}) \quad M^{-1}(1 \quad x_{i1} \quad x_{i2} \quad \dots \quad x_{ik})^{T}$

The criterion that allows minimization of the maximum predictive variance is the G-optimality criterion. Suppose

 $V^1 = V\{y(\underline{x}_1)\}$ is the maximum variance of prediction associated with the design measure ξ_N^1 , $V^2 = V\{y(\underline{x}_2)\}$ is the maximum variance of prediction associated with the design measure ξ_N^2 , \vdots

 $V^m = V\{y(\underline{x}_m)\}$ is the maximum variance of prediction associated with the design measure ξ_N^m .

The design measure ξ_N^1 is preferred in terms of G-optimality criterion to the design measures ξ_N^2, \dots, ξ_N^m iff

$$V{y(\underline{x}_1)} = \min \{ V{y(\underline{x}_2)}, V{y(\underline{x}_2)}, \dots, V{y(\underline{x}_m)}\}.$$

3. Results

Using the second-order polynomial model in equation (1), the partial replications of the factorial points and the star points with respect to replicating the center point are investigated with the following results.

3.1 Two-Factor Partially Replicated Central Composite Design

In exploring the two-factor Face-centered Central Composite Design with partial replication of the cube or factorial points, it is observed that the two-variable second-order full polynomial model has six model parameters. For the Face-centered Central Composite Design in two variables, there are basically nine design points or experimental runs. The cube points otherwise called vertex or factorial points

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

are denoted V.

The axial or star points

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

are denoted S.

The center point, $\begin{pmatrix} 0 & 0 \end{pmatrix}$ is denoted C.

Case I: Replicating the vertex points while the star points and center point are held fixed or not replicated.

Using the experimental conditions in Table 1, partially replicated exact designs of size N = 13, 12, 11, 10 are constructed.

The design measure for N = 13 is

For the six parameter model, the design matrix is

The corresponding information matrix is

$$M = \frac{1}{N}X^{T}X = \begin{pmatrix} 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.7692 & 0.7692 \\ 0.0000 & 0.7692 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.7692 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.7692 & 0.0000 & 0.0000 \\ 0.7692 & 0.0000 & 0.0000 & 0.0000 & 0.7692 & 0.7692 \\ 0.7692 & 0.0000 & 0.0000 & 0.0000 & 0.7692 & 0.7692 \\ 0.7692 & 0.0000 & 0.0000 & 0.0000 & 0.7692 & 0.7692 \\ \end{pmatrix}$$

The determinant value of the information matrix is

Det
$$M = 0.01127$$

The variance of prediction at each design point of ξ_{13} is, respectively

$$V_{1} = 5.7544$$

$$V_{2} = 5.7544$$

$$V_{3} = 5.7544$$

$$V_{4} = 5.7544$$

$$V_{5} = 5.7544$$

$$V_{7} = 5.7544$$

$$V_{8} = 5.7544$$

$$V_{9} = 8.1824$$

$$V_{10} = 6.2706$$

$$V_{11} = 6.2706$$

$$V_{12} = 6.2706$$

$$V_{13} = 6.8824$$

The maximum predictive variance is 8.1824.

The design measure for N = 12 is

$$\xi_{12} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \\ 1 & -1 \\ -1 & -1 \\ -1 & -1 \\ 1 & -1 \\ 1 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 1 \\ 0 & -1 \\ 0 & 0 \end{pmatrix}$$

For the six parameter model, the design matrix is

The associated information matrix is

$$M = \frac{1}{N}X^{T}X = \begin{pmatrix} 1.0000 & -0.083 & -0.083 & -0.083 & 0.7500 & 0.7500 \\ -0.083 & 0.7500 & -0.083 & -0.083 & -0.083 & -0.083 \\ -0.083 & -0.083 & 0.7500 & -0.083 & -0.083 & -0.083 \\ -0.083 & -0.083 & -0.083 & 0.5830 & -0.083 & -0.083 \\ 0.7500 & -0.083 & -0.083 & -0.083 & 0.7500 & 0.5830 \\ 0.7500 & -0.083 & -0.083 & -0.083 & 0.5830 & 0.7500 \end{pmatrix}$$

The determinant value of the information matrix is

Det M = 0.0102

The variance of prediction at each design point is, respectively

$$V_{1}=9.5303$$

$$V_{2}=5.3129$$

$$V_{3}=5.3129$$

$$V_{4}=5.3509$$

$$V_{5}=5.3129$$

$$V_{6}=5.3509$$

$$V_{7}=5.3129$$

$$V_{8}=5.1488$$

$$V_{9}=5.8955$$

$$V_{10}=5.1488$$

$$V_{11}=5.8955$$

$$V_{12}=6.4274$$

The maximum predictive variance is 9.5303.

The design measure for N = 11 is

$$\xi_{11} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \\ 1 & -1 \\ -1 & -1 \\ -1 & 1 \\ 1 & 1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 1 \\ 0 & -1 \\ 0 & 0 \end{pmatrix}$$

For the six parameter model, the design matrix is

The associated information matrix is

$$\mathbf{M} = \begin{pmatrix} 1.0000 & 0.0000 & 0.1818 & 0.0000 & 0.7272 & 0.7272 \\ 0.0000 & 0.7272 & 0.0000 & 0.1818 & 0.0000 & 0.0000 \\ 0.1818 & 0.0000 & 0.7272 & 0.0000 & 0.1818 & 0.1818 \\ 0.0000 & 0.1818 & 0.0000 & 0.5454 & 0.0000 & 0.0000 \\ 0.7272 & 0.0000 & 0.1818 & 0.0000 & 0.7272 & 0.5454 \\ 0.7272 & 0.0000 & 0.1818 & 0.0000 & 0.5454 & 0.7272' \end{pmatrix}$$

The determinant value of the information matrix is

Det M = 0.00954.

The variance of prediction at each design point is, respectively

$$V_1 = 4.9063$$

$$V_2 = 4.9063$$

$$V_3 = 8.7396$$

$$V_4 = 8.7396$$

$$V_5 = 4.9063$$

$$V_7 = 5.5000$$

$$V_8 = 5.9583$$

$$V_9 = 5.7396$$

$$V_{10} = 5.7396$$

$$V_{11} = 5.9583$$

The maximum predictive variance is 8.7396.

For N = 10

$$\xi_{10} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \\ 1 & -1 \\ -1 & -1 \\ -1 & 1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 1 \\ 0 & -1 \\ 0 & 0 \end{pmatrix}$$

For the six parameter model, the design matrix is

The associated information matrix is

	/ 1.0000	-0.100	0.1000	-0.100	0.7000	$\left(\begin{array}{c} 0.7000\\ -0.100\\ 0.1000\\ -0.1000\\ 0.5000\\ 0.7000 \end{array}\right)$
	-0.100	0.7000	-0.100	0.1000	-0.100	-0.100
М –	0.1000	0.1000	0.7000	-0.100	0.1000	0.1000
101 -	-0.100	0.1000	-0.100	0.5000	-0.1000	-0.1000
	0.7000	-0.100	0.1000	-0.100	0.7000	0.5000
	\0.7000	-0.100	0.1000	-0.100	0.5000	0.7000 /

The determinant value of the information matrix is

Det M = 0.00936

The variance of prediction at each design point is, respectively

 $\begin{array}{l} V_1 = 4.4615 \\ V_2 = 8.0513 \\ V_3 = 7.9487 \\ V_4 = 8.0513 \\ V_5 = 4.4615 \\ V_6 = 5.2821 \\ V_7 = 5.4872 \\ V_8 = 5.4872 \\ V_9 = 5.2821 \\ V_{10} = 5.4872 \end{array}$

The maximum predictive variance is 8.0513.

Case II: Replicating the star points while the vertex points and center point are held fixed or not replicated.

Using the experimental conditions in Table 2, partially replicated exact designs of size N = 13, 12, 11, 10 are constructed.

The design measures for the respective *N*-point exact designs are;

$$\xi_{13} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 0 \end{pmatrix}$$
$$\begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$\xi_{12} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\xi_{11} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$\xi_{10} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}$$

For case II, the associated maximum determinant values and maximum variances of prediction are as tabulated in Table 7.

Table 7. Maximum determinant value and maximum predictive variances for Case II, k = 2

Design Size	Maximum determinant value of	Maximum variance of prediction	
Ν	information matrix		
13	0.005940	9.2857	
12	0.006344	9.0405	
11	0.00705	8.67307	
10	0.00806	7.9762	

Case III: Replicating the center point while the vertex points and star points are held fixed or not replicated.

Using the experimental conditions in Table 3, partially replicated exact designs of size N = 13, 12, 11, 10 are constructed.

The design measures for the respective N-point exact designs are;

$$\xi_{13} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 &$$

$$\xi_{11} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$\xi_{10} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

For Case III, the associated maximum determinant values and maximum variances of prediction are as tabulated in Table 8.

Table 8. Maximum determinant value and maximum predictive variances for Case III, k = 2

Design Size	Maximum determinant value of	Maximum variance of
Ν	information matrix	prediction
13	0.00346	10.2730
12	0.00634	9.5000
11	0.00618	8.7325
10	0.00806	7.9762

3.2 Three-Factor Partially Replicated Central Composite Design

In exploring the three-factor partially replicated Central Composite Design, it is observed that the three-variable second-order full polynomial model has ten model parameters. For the Face-centered Central Composite Design in three variables, the eight factorial points

The six axial or star points

 $\begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \end{pmatrix}$ are denoted S.

The center point $(0 \ 0 \ 0)$ is denoted C.

Case I: Replicating the vertex points while the star points and center points are held fixed or not replicated.

Using the experimental conditions in Table 4, we construct partially-replicated exact designs of size N = 23, 22, ..., 16.

The design measure for N = 23 is

For the ten parameter model, the design matrix is

The associated information matrix is

	(¹	0	0	0	0	0	0	0.7826	0.7826	0.7826	١
	0	0.7826	0	0	0	0	0	0	0	0	
	0	0	0.7826	0	0	0	0	0	0	0	
	0	0	0	0.7826	0	0	0	0	0	0	
M =	0	0	0	0	0.6956	0	0	0	0	0	
	0	0	0	0	0	0.6956	0	0	0	0	
	0	0	0	0	0	0	0.6956	0	0	0	
	0.7826	0	0	0	0	0	0	0.7826	0.6956	0.6956	
	0.7826	0	0	0	0	0	0	0.6956	0.7826	0.6956	
	0.7826	0	0	0	0	0	0	0.6956	0.6956	0.7826	J

The determinant of information matrix is

Det M = 0.0004106

The variance of prediction at each design point is, respectively

 $V_1 = 9.5672$ $V_2 = 9.5672$ $V_3 = 9.5672$ $V_4 = 9.5672$ $V_5 = 9.5672$ $V_6 = 9.5672$ $V_7 = 9.5672$ $V_8 = 9.5672$ $V_9 = 9.5672$ $V_{10} = 9.5672$ $V_{11} = 9.5672$ $V_{12} = 9.5672$ $V_{13} = 9.5672$ $V_{14} = 9.5672$ $V_{15} = 9.5672$ $V_{16} = 9.5672$ V₁₇= 11.7441 $V_{18} = 11.7441$ V₁₉= 11.7441 $V_{20} = 11.7441$ $V_{21} = 11.7441$ $V_{22} = 11.7441$ $V_{23} = 6.4607$

The maximum variance of prediction is 11.7441

The results for N = 22, 21, ..., 16 are as tabulated in Table 9.

Design Size N	Maximum determinant value of information matrix	Maximum variance of prediction
23	0.00041	11.7441
22	0.00037	15.6689
21	0.00034	15.2767
20	0.00032	14.8206
19	0.00031	14.2856
18	0.00029	14.0184
17	0.00029	13.3526
16	0.00031	12.6714

Case II: Replicating the star points while the vertex points and center point are held fixed or not replicated.

Using the experimental conditions in Table 5, partially replicated exact designs of size N = 21, 20, ..., 16 are constructed. As with Case I, the best *N*-point exact design is obtained and the process continues. The required computations yield the results for N = 21, 20, ..., 16 as tabulated in Table 10.

Design Size N	Maximum determinant value of information matrix	Maximum variance of prediction
21	0.0001187	15.9089
20	0.0001465	15.1729
19	0.0001662	14.6312
18	0.0001938	14.0591
17	0.0002211	13.2672
16	0.0002608	12.6742

Table 10. Maximum determinant values and maximum predictive variances for Case II, k = 3

Case III: Replicating the center point while the vertex points and star points are held fixed or not replicated.

Using the experimental conditions in Table 6, partially replicated exact designs of size N = 23, 22, ..., 16 are constructed. As with Cases I and II, the best *N*-point exact design is obtained and the process continues. The required computations yield the results for N = 23, 22, ..., 16 as tabulated in Table 11.

Design Size N	Maximum determinant value of information matrix	Maximum variance of prediction
23	0.0000147	18.2263
22	0.0000209	17.4382
21	0.0000302	16.6506
20	0.0000440	15.8636
19	0.0000648	15.0776
18	0.0000964	14.2929
17	0.0000144	13.5102
16	0.0000216	12.7310

Table 11. Maximum determinant values and maximum predictive variances for Case III, k = 3

In assessing the goodness of the constructed optimal exact designs we compute the D-efficiency and G-efficiency values as tabulated in Tables 12 and 13 for k = 2 and k = 3, respectively.

Table 12. Optimal values and D- and G-efficiency values (k = 2)

Experi	imental Co	ndition	Design Size N	Determinant of Information	Maximum variance	D-efficiency	G-efficiency
Vertex point	Star point	Center point		matrix	of prediction		
$V+{}^{4}C_{4}$	S	С	13	0.0113	6.8824	1.0000	1.0000
$V+^4C_3$	S	С	12	0.0102	9.5303	0.9831	0.7222
$V+^4C_2$	S	С	11	0.0095	8.7396	0.9715	0.7875
$V+^4C_1$	S	С	10	0.0094	8.0513	0.9698	0.8548
V	$S+^4C_4$	С	13	0.0059	9.2857	0.8974	0.7412
V	$S+{}^4C_3$	С	12	0.0063	9.0405	0.9072	0.6637
V	$S+{}^{4}C_{2}$	С	11	0.0071	8.6731	0.9255	0.7935
V	$S+^4C_1$	С	10	0.0081	7.9762	0.9460	0.8629
V	S	C+4	13	0.0035	10.2730	0.8226	0.6700
V	S	C+3	12	0.0046	9.5000	0.8609	0.7245
V	S	C+2	11	0.0062	8.7325	0.9048	0.7881
V	S	C+1	10	0.0081	7.9762	0.9460	0.8629

Experimental Condition			Design Size N	Determinant of Information	Maximum variance of	D-efficiency	G- efficiency
Vertex	Star	Center		matrix	prediction		
point	point	point					
$V + {}^{8}C_{8}$	S	С	23	0.0004106	11.7441	1.0000	1.0000
$V+{}^{8}C_{7}$	S	С	22	0.0003740	15.6689	0.9907	0.7495
$V + {}^{8}C_{6}$	S	С	21	0.0003447	15.2767	0.9827	0.7688
$V + {}^{8}C_{5}$	S	С	20	0.0003225	14.8206	0.9761	0.7924
$V + {}^{8}C_{4}$	S	С	19	0.0003075	14.2856	0.9715	0.8221
$V + {}^{8}C_{3}$	S	С	18	0.0002968	14.0184	0.9681	0.8378
$V + {}^{8}C_{2}$	S	С	17	0.0002945	13.3526	0.9673	0.8795
$V + {}^{8}C_{1}$	S	С	16	0.0003013	12.6714	0.9695	0.9268
v	$S + {}^{6}C_{6}$	С	21	0.0001187	15.9089	0.8833	0.7382
V	$S+{}^{6}C_{5}$	С	20	0.0001465	15.1729	0.9021	0.7740
V	$S+{}^{6}C_{4}$	C	19	0.0001662	14.6312	0.9135	0.8027
V	$S+{}^{6}C_{3}$	C	18	0.0001938	14.0591	0.9277	0.8353
V	$S+{}^{6}C_{2}$	C	17	0.0002211	13.3375	0.9400	0.8805
V	$S+{}^{6}C_{1}$	Ċ	16	0.0002608	12.6742	0.9556	0.9266
V	S	C+8	23	0.0000147	18.2263	0.7168	0.6443
V	S	C+7	22	0.0000209	17.4382	0.7425	0.6735
V	S	C+6	21	0.0000302	16.6506	0.7703	0.7053
V	S	C+5	20	0.0000440	15.8636	0.7998	0.7403
V	S	C+4	19	0.0000648	15.0776	0.8314	0.7789
V	S	C+3	18	0.0000964	14.2929	0.8651	0.8217
V	S	C+2	17	0.0000144	13.5102	0.9005	0.8693
V	S	C+1	16	0.0000216	12.7310	0.9378	0.9225

Table 13. Optimal values and D- and G-efficiency values (k = 3)

4. Discussion

In addressing the problem of partially replicated cube, star and center runs for estimation of error degrees of freedom in Response Surface Methodology, emphasis should not be on the replication of only center point as the replication of non-center points performs credibly well. Design optimality plays a major role in the choice of experimental designs. As observed in the study on the effects of partially replicating the factorial points and the star points of the Face-centered Central Composite Designs with respect to replicating the center points, replicating the cube points offered better designs as measured by the D- and G-efficiency values than replicating the center points.

Specifically, for two-variable quadratic model, the D-optimal exact design was observed under the experimental condition $(V+{}^{4}C_{4})+S+C$, which implies the replication of cube points. This design also had the minimum maximum variance of prediction over all designs considered. In comparison with designs under the varying experimental conditions, the design comprising of two cube portions, one star portion and one center point was more efficient in terms of D- and G-efficiencies. The implication is that replicating cube points allows more precise estimate of model parameters as the variances of the model parameters are minimized and the covariances between the model parameters are minimized. Furthermore, replicating cube points allows minimization of the maximum variance of prediction over the design space.

For three-variable quadratic model, the design comprising of two cube portions, one star portion and a center point performed better than other combinations in terms of D-optimality criterion as well as G-optimality criterion. The D- and G-optimal exact designs were observed using the design comprising of two cube portions, one star portion and a center point. This again implies the preference of replicating the cube points. The design comprising of two cube portions, one star portion and a center point had the maximum determinant value of information matrix as well as the minimum maximum variance of prediction over all designs considered. Again, replicating cube points allowed a more precise estimate of model parameters as the variances of the model parameters are minimized and the covariances between the model parameters are minimized. As with the two-variable model, replicating cube points allowed minimization of the maximum variance of prediction over the design space.

For cases under study, the best D-efficiency value was associated with replicating the cube points and the best D-efficiency value was associated with replicating the cube points was still better than the highest D-efficiency value associated with replicating the cube points was still better than the highest D-efficiency value associated with replicating the cube point. This was generally true for G-efficiency. For each quadratic model considered, the efficiencies of the designs were computed relative to the best design within a class of designs. Specifically, the best D-optimal design for two-variable quadratic model was obtained and the D-efficiencies of other designs were computed relative to this best D-optimal design. Similarly, the best G-optimal design for two-variable quadratic model, the efficiencies of the designs for the three-variable quadratic model was obtained and the D-efficiencies of the best D-optimal design for three-variable quadratic model, the efficiencies of the designs for the three-variable quadratic model was obtained and the D-efficiencies of the designs were computed relative to the best design within a class of designs. Hence, the best D-optimal design for three-variable quadratic model, the efficiencies of the designs for the three-variable quadratic model was obtained and the D-efficiencies of the other designs were computed relative to this best D-optimal design. Similarly, the best G-optimal design for three-variable quadratic model was obtained and the D-efficiencies of the other designs were computed relative to this best D-optimal design. Similarly, the best G-optimal design for three-variable quadratic model was obtained and the D-efficiencies of the other designs were computed relative to this best D-optimal design. Similarly, the best G-optimal design for three-variable quadratic model was obtained and the G-efficiencies of the design for three-variable quadratic model was obtained and the G-efficiencies of the design for three-variable quadratic model was obtained and the

Although there was no consideration on A-efficiency criterion, designs that were D- and G-efficient also maximized the trace of the information matrix thereby minimizing the trace of the variance-covariance matrix. This shows that by replicating the cube points, the average variance of parameter estimates are minimized. For two- and three-variable quadratic models considered, the design comprising of two cube portions, one star portion and a center point, that maximized the determinant of information matrix as well as minimizing the maximum variance of prediction also maximized the trace of the information matrix with trace value of 4.6922 for the two-variable model and trace value of 7.7824 for the three-variable model. In partial replication of design points, complete replication of cube portion offered better designs as measured by the efficiency values than replicating some design points of the cube portion.

5. Conclusion

The effects of partially replicating the non-center points, with respect to replicating the center point of the Face-centered Central Composite Designs were considered using two- and three-variable quadratic models. As a measure of goodness of the designs, D- and G-efficiency single-value criteria were utilized. In all cases considered, the experimental designs associated with replicating only the center point were not as efficient as replicating the cube points in terms of D- and G-efficiency. We recommend that emphasis should shift away from replication of only center points when using response surface designs in optimizing response variables, as non-center points perform credibly well. However, the concepts of rotatability and orthogonality of the designs should be imposed.

References

- Ahn, H. (2015). Central Composite Design for the experiments with replicate runs at factorial and axial points. Department of Industrial Engineering, Scokyeong University, Seoul, Korea 136-704. Link:springer.com/chapter10/10.1007%2F978-3-662-47200-2_101. http://dx.doi.org/10.1007/978-3-662-47200-2_101
- Alalayah, W. M., Kalil, M. S., Kadhum, A. A. H., Jahim, J., Zaharim, A., Alauj, N. M., & Elshafie, A. (2010). Applications of the Box-Wilson design model for Bio-hydrogen production using Clostridium Saccharoperbutylacetonicum N1-4 (ATCC 13564). *Pakistan Journal of Biological Sciences, 13*, 674-682. http://dx.doi.org/10.3923/pjbs.2010.674.682 URL:http://scialert.net/abstract/?doi=pjbs.2010.674.682
- Atkinson, A. C., & Donev, A. N. (1992). On Optimum Experimental Designs. Oxford statistical science series, clarendon press.
- Box, G. E. P., & Wilson, K. B. (1951). On the Experimental Attainment of Optimum conditions. *Journal of the Royal Statistical society. Series B*(1), 1-45.
- Chigbu, P. E., & Ohaegbulem, E. U. (2011). On the Preference of Replicating Factorial Runs to Axial Runs in Restricted Second Order Design. *Journal of Applied Sciences*, 11(22), 3732-3737.
- Chigbu, P. E, Ukaegbu, E. C. and Nwanya, J. C. (2009). On comparing the prediction variances of some Central Composite Designs in spherical region: A review. Statistica, anno, LXIX(4), 285-298.
- Chukwu, A. U., & Yakubu, Y. (2012). Comparison of optimality criteria of reduced models for response surface designs with restricted randomization. *Progress in Applied Mathematics*, 4(2), 110-126.
- Cochran, W. G., & Cox, G. M. (1957). Experimental designs, Second Edition, John Wiley & Sons, New York.
- Draper, N. R., & Gutman, I. (1988). An index of rotatability, Technometrics, 30, pp. 105-111.

- Farrukh, J. (2014). Searching for Optimum: 2^k Factorial Design with Added Central Points, Central Composite Designs, and Response Surface Methods. www.maths.lth.se>kurser>fms072_vt14
- Montgomery, D. C. (1997). Design and analysis of Experiments, (4thed.) John Wiley & Sons, New York.
- Oyejola, B. A., & Nwanya, J. C. (2015). Selecting the right Central Composite Design. *International Journal of Statistics and Applications*, 5(1), 21-30.
- Rady, E. A., Abd El-Monsef, M. M. E., & Seyam, M. M. (2009). Relationship among several optimality criteria, interstat.statjournals.net>YEAR>articles.
- Ukaegbu, E. C., & Chigbu, P. E. (2014). Graphical evaluation of the prediction capabilities of partially replicated orthogonal Central Composite Design. *Quality and Reliability Engineering*, 31(4). http://dx.doi.org/10.1002/qre.1630
- Wong, W. K. (1994). Comparing robust properties of A, D, E and G-optimal designs. *Computational Statistics & Data Analysis, 18*, 441-448.
- Zahran, A. R. (2002). On the efficiency of designs for linear models in non-linear regions and the use of standard designs for generalized linear models. Dissertation, Department of Statistics, Virginia Polytechnic Institute and State University.

Copyrights

Copyright for this article is retained by the author(s), with first publication rights granted to the journal.

This is an open-access article distributed under the terms and conditions of the Creative Commons Attribution license (http://creativecommons.org/licenses/by/3.0/).