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

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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 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 Ohaegbulum (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 replication of the cube and star portions without replicating the center point in \( k \)-factor experiment. Also, 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 \( \alpha \) 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 Guttmann (1988) observed that the adequacy of an experimental design can be determined from the information matrix. Some criteria 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 maximum 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, \( \xi_N \), over an optimal design, \( \xi_N^* \) is defined as

\[
D_{\text{eff}} = \frac{M(\xi_N)}{M(\xi_N^*)}.
\]

The G-efficiency of an arbitrary design, \( \xi_N \), is defined as

\[
G_{\text{eff}} = \frac{d(\xi_N^*)}{d(\xi_N)} = \frac{p}{d(\xi_N^*)}.
\]

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

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 \( |X^T X| \). 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.

\[
y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \sum_{j>i}^k \beta_{ij} x_i x_j + \sum_{i=1}^k \beta_{ii} x_i^2 + \epsilon
\]

This model can be rewritten as

\[
Y = X\beta + \epsilon
\]

Where

\( Y \) is the \( N \times 1 \) vector of observed values
\( X \) is the design matrix
\( \beta \) is the \( p \times 1 \) vector of unknown parameters which are estimated on the basis of \( N \) uncorrelated observations.
\( \epsilon \) 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

\[
p = \frac{(k+1)(k+2)}{2}
\]

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
\[
V = \begin{pmatrix}
-1 & -1 & -1 \\
-1 & 1 & +1 \\
+1 & -1 & -1 \\
-1 & +1 & -1 \\
+1 & -1 & +1 \\
+1 & +1 & -1 \\
+1 & +1 & +1
\end{pmatrix}
\]

The star portion of the Central Composite Design comprises of the experimental runs
\[
S = \begin{pmatrix}
\alpha & 0 & 0 & \ldots & \ldots & \ldots & 0 \\
-\alpha & 0 & 0 & \ldots & \ldots & \ldots & 0 \\
0 & \alpha & 0 & \ldots & \ldots & \ldots & 0 \\
0 & -\alpha & 0 & \ldots & \ldots & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \ldots & \ldots & -\alpha \\
0 & 0 & 0 & 0 & \ldots & \ldots & -\alpha
\end{pmatrix}
\]

For \( k = 2 \), this becomes
\[
S = \begin{pmatrix}
\alpha & 0 \\
-\alpha & 0 \\
0 & \alpha \\
0 & -\alpha
\end{pmatrix}
\]

For \( k = 3 \),
\[
S = \begin{pmatrix}
\alpha & 0 & 0 \\
-\alpha & 0 & 0 \\
0 & \alpha & 0 \\
0 & -\alpha & 0 \\
0 & 0 & \alpha \\
0 & 0 & -\alpha
\end{pmatrix}
\]

The center portion of the Central Composite Design comprises of the experimental run
\[
C = (0 \ 0 \ \ldots \ 0).
\]

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 \( N = n_12^k + \binom{n_1}{1} + n_22k + \binom{n_2}{2} + n_0 \) 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 \( n_1, n_2 \) and \( n_0 \) are set at unity. \( V+ \binom{n_1}{1} \) implies taking the cube portion and additional \( r \) distinct cube points from the available \( n_{11} \) cube points. \( S+ \binom{n_2}{2} \) implies taking the 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 vertex points (k = 2)

<table>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Design Size N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertex</td>
<td>Star</td>
</tr>
<tr>
<td>V+^4C_4</td>
<td>S</td>
</tr>
<tr>
<td>V+^4C_3</td>
<td>S</td>
</tr>
<tr>
<td>V+^4C_2</td>
<td>S</td>
</tr>
<tr>
<td>V+^4C_1</td>
<td>S</td>
</tr>
</tbody>
</table>

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)

<table>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Design Size N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertex</td>
<td>Star</td>
</tr>
<tr>
<td>V</td>
<td>S+^4C_4</td>
</tr>
<tr>
<td>V</td>
<td>S+^4C_3</td>
</tr>
<tr>
<td>V</td>
<td>S+^4C_2</td>
</tr>
<tr>
<td>V</td>
<td>S+^4C_1</td>
</tr>
</tbody>
</table>

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)

<table>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Design Size N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertex</td>
<td>Star</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
</tbody>
</table>

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)

<table>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Design Size N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertex</td>
<td>Star</td>
</tr>
<tr>
<td>V+^8C_8</td>
<td>S</td>
</tr>
<tr>
<td>V+^8C_7</td>
<td>S</td>
</tr>
<tr>
<td>V+^8C_6</td>
<td>S</td>
</tr>
<tr>
<td>V+^8C_5</td>
<td>S</td>
</tr>
<tr>
<td>V+^8C_4</td>
<td>S</td>
</tr>
<tr>
<td>V+^8C_3</td>
<td>S</td>
</tr>
<tr>
<td>V+^8C_2</td>
<td>S</td>
</tr>
<tr>
<td>V+^8C_1</td>
<td>S</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Design Size N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertex</td>
<td>Star</td>
</tr>
<tr>
<td>V</td>
<td>$S^3C_8$</td>
</tr>
<tr>
<td>V</td>
<td>$S^3C_7$</td>
</tr>
<tr>
<td>V</td>
<td>$S^3C_6$</td>
</tr>
<tr>
<td>V</td>
<td>$S^3C_5$</td>
</tr>
<tr>
<td>V</td>
<td>$S^3C_4$</td>
</tr>
<tr>
<td>V</td>
<td>$S^3C_3$</td>
</tr>
<tr>
<td>V</td>
<td>$S^3C_2$</td>
</tr>
<tr>
<td>V</td>
<td>$S^3C_1$</td>
</tr>
</tbody>
</table>

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>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Design Size N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertex</td>
<td>Star</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
<tr>
<td>V</td>
<td>S</td>
</tr>
</tbody>
</table>

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

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

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

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

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 $p \times p$ information matrix, $M$, associated with $\xi_N$ is obtained from $X^TX$ and normalized as $\frac{1}{N}X^TX$, where the notation, $(\cdot)^T$ represents transpose. The criterion that allows maximization of determinant of information matrix of a design is the D-optimality criterion.

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

$$
\text{Det} (M_1) = \max \{ \text{Det} (M_1), \text{Det} (M_2), \ldots, \text{Det} (M_m) \}.
$$
Also let \( \bar{x}_i = (1 \ x_{i1} \ x_{i2} \ ... \ x_{ik}) \); \( i = 1, 2, \ldots, N \) be the \( i \)th row of the design matrix \( X \), associated with the design point \( (x_{i1} \ x_{i2} \ ... \ x_{ik}) \). The variance of prediction, \( V(y(\bar{x}_i)) \), at the \( i \)th design point \( \bar{x}_i = (1 \ x_{i1} \ x_{i2} \ ... \ x_{ik}) \) is

\[
V(y(\bar{x}_i)) = (1 \ x_{i1} \ x_{i2} \ ... \ x_{ik}) \ M^{-1} (1 \ x_{i1} \ x_{i2} \ ... \ x_{ik})^T
\]

The criterion that allows minimization of the maximum predictive variance is the \( G \)-optimality criterion.

Suppose \( V^1 = V(y(\bar{x}_1)) \) is the maximum variance of prediction associated with the design measure \( \xi_1 \), \( V^2 = V(y(\bar{x}_2)) \) is the maximum variance of prediction associated with the design measure \( \xi_2 \), etc., \( V^m = V(y(\bar{x}_m)) \) is the maximum variance of prediction associated with the design measure \( \xi_m \).

The design measure \( \xi_1 \) is preferred in terms of \( G \)-optimality criterion to the design measures \( \xi_2, \ldots, \xi_m \) iff

\[
V(y(\bar{x}_1)) = \min \{ V(y(\bar{x}_2)), V(y(\bar{x}_3)), \ldots, V(y(\bar{x}_m)) \}.
\]

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

\[
\left( \begin{array}{ccc}
1 & 1 \\
1 & -1 \\
-1 & 1 \\
-1 & -1
\end{array} \right)
\]

are denoted V.

The axial or star points

\[
\left( \begin{array}{ccc}
1 & 0 \\
-1 & 0 \\
0 & 1 \\
0 & -1
\end{array} \right)
\]

are denoted S.

The center point, \( (0 \ 0) \) 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

\[
\bar{\xi}_{13} = \left( \begin{array}{cccc}
1 & 1 \\
-1 & 1 \\
1 & -1 \\
-1 & -1 \\
-1 & 1 \\
1 & 1 \\
-1 & 1 \\
1 & -1 \\
-1 & -1 \\
1 & 0 \\
-1 & 0 \\
0 & 1 \\
0 & -1 \\
0 & 0
\end{array} \right)
\]
For the six parameter model, the design matrix is

\[ X = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & 1 \\
1 & 1 & 0 & 0 & 1 & 0 \\
1 & -1 & 0 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 0 & 1 \\
1 & 0 & -1 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 
\end{pmatrix} \]

The corresponding information matrix is

\[ M = \frac{1}{N}X^TX = \begin{pmatrix}
1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.7692 & 0.7692 \\
0.0000 & 0.7692 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.7692 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 0.7692 & 0.0000 & 0.0000 \\
0.7692 & 0.0000 & 0.0000 & 0.0000 & 0.7692 & 0.7692 \\
0.7692 & 0.0000 & 0.0000 & 0.0000 & 0.7692 & 0.7692 
\end{pmatrix} \]

The determinant value of the information matrix is

\[ \text{Det } M = 0.01127 \]

The variance of prediction at each design point of \( \xi_{13} \) is, respectively

\[ V_1 = 5.7544 \]
\[ V_2 = 5.7544 \]
\[ V_3 = 5.7544 \]
\[ V_4 = 5.7544 \]
\[ V_5 = 5.7544 \]
\[ V_6 = 5.7544 \]
\[ V_7 = 5.7544 \]
\[ V_8 = 8.1824 \]
\[ V_9 = 6.2706 \]
\[ V_{10} = 6.2706 \]
\[ V_{11} = 6.2706 \]
\[ V_{12} = 6.8824 \]

The maximum predictive variance is 8.1824.

The design measure for \( N = 12 \) is

\[ \xi_{12} = \begin{pmatrix}
1 & 1 \\
-1 & 1 \\
1 & -1 \\
-1 & -1 \\
-1 & 1 \\
1 & -1 \\
1 & 0 \\
-1 & 0 \\
0 & 1 \\
0 & -1 \\
0 & 0 
\end{pmatrix} \]
For the six parameter model, the design matrix is

\[
X = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 & 1 \\
1 & 1 & 0 & 0 & 1 & 0 \\
1 & -1 & 0 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 0 & 1 \\
1 & 0 & -1 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

The associated information matrix is

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

The determinant value of the information matrix is

\[
\text{Det } M = 0.0102
\]

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
\[ X = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 \\
1 & 1 & -1 & -1 & 1 \\
1 & -1 & -1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 \\
1 & 1 & 0 & 0 & 1 \\
1 & -1 & 0 & 0 & 1 \\
1 & 0 & 1 & 0 & 0 \\
1 & 0 & -1 & 0 & 0 \\
1 & 0 & 0 & 0 & 0
\end{pmatrix} \]

The associated information matrix is

\[ M = \begin{pmatrix}
1.0000 & 0.0000 & 0.1818 & 0.0000 & 0.7272 & 0.7272 \\
0.0000 & 0.7272 & 0.0000 & 0.1818 & 0.0000 & 0.0000 \\
0.1818 & 0.0000 & 0.7272 & 0.0000 & 0.1818 & 0.1818 \\
0.0000 & 0.1818 & 0.0000 & 0.5454 & 0.0000 & 0.0000 \\
0.7272 & 0.0000 & 0.1818 & 0.0000 & 0.7272 & 0.5454 \\
0.7272 & 0.0000 & 0.1818 & 0.0000 & 0.5454 & 0.7272
\end{pmatrix} \]

The determinant value of the information matrix is

\[ \text{Det } M = 0.00954. \]

The variance of prediction at each design point is, respectively

\[ V_1 = 4.9063 \]
\[ V_2 = 4.9063 \]
\[ V_3 = 8.7396 \]
\[ V_4 = 8.7396 \]
\[ V_5 = 4.9063 \]
\[ V_6 = 4.9063 \]
\[ V_7 = 5.5000 \]
\[ V_8 = 5.9583 \]
\[ V_9 = 5.7396 \]
\[ V_{10} = 5.7396 \]
\[ V_{11} = 5.9583 \]

The maximum predictive variance is 8.7396.

For \( N = 10 \)

\[ \xi_{10} = \begin{pmatrix}
1 \\
-1 \\
1 \\
-1 \\
-1 \\
1 \\
-1 \\
1 \\
0 \\
0
\end{pmatrix} \]

For the six parameter model, the design matrix is

\[ X = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 \\
1 & 1 & -1 & -1 & 1 \\
1 & -1 & -1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 \\
1 & 1 & 0 & 0 & 1 \\
1 & -1 & 0 & 0 & 1 \\
1 & 0 & 1 & 0 & 0 \\
1 & 0 & -1 & 0 & 0 \\
1 & 0 & 0 & 0 & 0
\end{pmatrix} \]
The associated information matrix is
\[
M = \begin{pmatrix}
1.0000 & -0.100 & 0.1000 & -0.100 & 0.7000 & 0.7000 \\
-0.100 & 0.7000 & -0.100 & 0.1000 & -0.100 & -0.100 \\
0.1000 & 0.1000 & 0.7000 & -0.100 & 0.1000 & 0.1000 \\
-0.100 & 0.1000 & -0.100 & 0.5000 & -0.100 & -0.1000 \\
0.7000 & -0.100 & 0.1000 & -0.100 & 0.7000 & 0.5000 \\
0.7000 & -0.100 & 0.1000 & -0.100 & 0.5000 & 0.7000 \\
\end{pmatrix}
\]

The determinant value of the information matrix is
\[
\text{Det } M = 0.00936
\]

The variance of prediction at each design point is, respectively
\[
V_1 = 4.4615 \\
V_2 = 8.0513 \\
V_3 = 7.9487 \\
V_4 = 8.0513 \\
V_5 = 4.4615 \\
V_6 = 5.2821 \\
V_7 = 5.4872 \\
V_8 = 5.4872 \\
V_9 = 5.2821 \\
V_{10} = 5.4872
\]

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:

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

\[
\xi_{12} = \begin{pmatrix}
-1 & 1 \\
1 & 1 \\
1 & -1 \\
-1 & -1 \\
0 & 1 \\
0 & -1 \\
1 & 0 \\
-1 & 0 \\
0 & 1 \\
0 & -1 \\
1 & 0 \\
0 & 0
\end{pmatrix}
\]
\[ \xi_{11} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 1 & -1 \\ -1 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{pmatrix} \]

and

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

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**

<table>
<thead>
<tr>
<th>Design Size</th>
<th>Maximum determinant value of information matrix</th>
<th>Maximum variance of prediction</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>0.005940</td>
<td>9.2857</td>
</tr>
<tr>
<td>12</td>
<td>0.006344</td>
<td>9.0405</td>
</tr>
<tr>
<td>11</td>
<td>0.00705</td>
<td>8.67307</td>
</tr>
<tr>
<td>10</td>
<td>0.00806</td>
<td>7.9762</td>
</tr>
</tbody>
</table>

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:

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

\[ \xi_{12} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & 1 \\ 0 & -1 \\ -1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \]
\[ \xi_{11} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ -1 & -1 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \]

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

<table>
<thead>
<tr>
<th>Design Size</th>
<th>Maximum determinant value of information matrix</th>
<th>Maximum variance of prediction</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>0.00346</td>
<td>10.2730</td>
</tr>
<tr>
<td>12</td>
<td>0.00634</td>
<td>9.5000</td>
</tr>
<tr>
<td>11</td>
<td>0.00618</td>
<td>8.7325</td>
</tr>
<tr>
<td>10</td>
<td>0.00806</td>
<td>7.9762</td>
</tr>
</tbody>
</table>

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

\[ \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & -1 \\ -1 & -1 & -1 \end{pmatrix} \]

are denoted V.

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 \( N = 23, 22, \ldots, 16. \)

The design measure for \( N = 23 \) is

\[
\xi_{23} = \begin{pmatrix}
-1 & -1 & -1 \\
-1 & -1 & 1 \\
-1 & 1 & -1 \\
1 & -1 & -1 \\
1 & 1 & -1 \\
1 & -1 & 1 \\
-1 & 1 & 1 \\
-1 & -1 & 1 \\
-1 & -1 & -1 \\
1 & 1 & -1 \\
1 & 1 & 1 \\
-1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1 \\
-1 & 0 & 0 \\
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
0 & 0 & -1 \\
0 & 0 & 0
\end{pmatrix}
\]

For the ten parameter model, the design matrix is

\[
X = \begin{pmatrix}
1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\
1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 \\
1 & 1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 \\
1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\
1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 \\
1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]
The associated information matrix is

\[ M = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0.7826 & 0.7826 & 0.7826 \\
0 & 0.7826 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.7826 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.7826 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.6956 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.6956 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0.6956 & 0 & 0 & 0 \\
0.7826 & 0 & 0 & 0 & 0 & 0 & 0 & 0.7826 & 0.6956 & 0.6956 \\
0.7826 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6956 & 0.7826 & 0.6956 \\
0.7826 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6956 & 0.6956 & 0.7826 \\
\end{pmatrix} \]

The determinant of information matrix is

\[ \text{Det } M = 0.0004106 \]

The variance of prediction at each design point is, respectively

\[ V_1 = 9.5672 \]
\[ V_2 = 9.5672 \]
\[ V_3 = 9.5672 \]
\[ V_4 = 9.5672 \]
\[ V_5 = 9.5672 \]
\[ V_6 = 9.5672 \]
\[ V_7 = 9.5672 \]
\[ V_8 = 9.5672 \]
\[ V_9 = 9.5672 \]
\[ V_{10} = 9.5672 \]
\[ V_{11} = 9.5672 \]
\[ V_{12} = 9.5672 \]
\[ V_{13} = 9.5672 \]
\[ V_{14} = 9.5672 \]
\[ V_{15} = 9.5672 \]
\[ V_{16} = 9.5672 \]
\[ V_{17} = 11.7441 \]
\[ V_{18} = 11.7441 \]
\[ V_{19} = 11.7441 \]
\[ V_{20} = 11.7441 \]
\[ V_{21} = 11.7441 \]
\[ V_{22} = 11.7441 \]
\[ V_{23} = 6.4607 \]

The maximum variance of prediction is 11.7441

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

Table 9. Maximum determinant values and maximum predictive variances for Case I, \( k = 3 \)

<table>
<thead>
<tr>
<th>Design Size ( N )</th>
<th>Maximum determinant value of information matrix</th>
<th>Maximum variance of prediction</th>
</tr>
</thead>
<tbody>
<tr>
<td>23</td>
<td>0.00041</td>
<td>11.7441</td>
</tr>
<tr>
<td>22</td>
<td>0.00037</td>
<td>15.6689</td>
</tr>
<tr>
<td>21</td>
<td>0.00034</td>
<td>15.2767</td>
</tr>
<tr>
<td>20</td>
<td>0.00032</td>
<td>14.8206</td>
</tr>
<tr>
<td>19</td>
<td>0.00031</td>
<td>14.2856</td>
</tr>
<tr>
<td>18</td>
<td>0.00029</td>
<td>14.0184</td>
</tr>
<tr>
<td>17</td>
<td>0.00029</td>
<td>13.3526</td>
</tr>
<tr>
<td>16</td>
<td>0.00031</td>
<td>12.6714</td>
</tr>
</tbody>
</table>
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 $N = 21, 20, \ldots, 16$ 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 $N = 21, 20, \ldots, 16$ as tabulated in Table 10.

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

<table>
<thead>
<tr>
<th>Design Size $N$</th>
<th>Maximum determinant value of information matrix</th>
<th>Maximum variance of prediction</th>
</tr>
</thead>
<tbody>
<tr>
<td>21</td>
<td>0.0001187</td>
<td>15.9089</td>
</tr>
<tr>
<td>20</td>
<td>0.0001465</td>
<td>15.1729</td>
</tr>
<tr>
<td>19</td>
<td>0.0001662</td>
<td>14.6312</td>
</tr>
<tr>
<td>18</td>
<td>0.0001938</td>
<td>14.0591</td>
</tr>
<tr>
<td>17</td>
<td>0.0002211</td>
<td>13.2672</td>
</tr>
<tr>
<td>16</td>
<td>0.0002608</td>
<td>12.6742</td>
</tr>
</tbody>
</table>

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 $N = 23, 22, \ldots, 16$ 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 $N = 23, 22, \ldots, 16$ as tabulated in Table 11.

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

<table>
<thead>
<tr>
<th>Design Size $N$</th>
<th>Maximum determinant value of information matrix</th>
<th>Maximum variance of prediction</th>
</tr>
</thead>
<tbody>
<tr>
<td>23</td>
<td>0.0000147</td>
<td>18.2263</td>
</tr>
<tr>
<td>22</td>
<td>0.0000209</td>
<td>17.4382</td>
</tr>
<tr>
<td>21</td>
<td>0.0000302</td>
<td>16.6506</td>
</tr>
<tr>
<td>20</td>
<td>0.0000440</td>
<td>15.8636</td>
</tr>
<tr>
<td>19</td>
<td>0.0000648</td>
<td>15.0776</td>
</tr>
<tr>
<td>18</td>
<td>0.0000964</td>
<td>14.2929</td>
</tr>
<tr>
<td>17</td>
<td>0.0001444</td>
<td>13.5102</td>
</tr>
<tr>
<td>16</td>
<td>0.000216</td>
<td>12.7310</td>
</tr>
</tbody>
</table>

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 ($k = 2$)

<table>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Design Size $N$</th>
<th>Determinant of Information matrix</th>
<th>Maximum variance of prediction</th>
<th>D-efficiency</th>
<th>G-efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V^*C_4$</td>
<td>13</td>
<td>0.0113</td>
<td>6.8824</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>$V^*C_3$</td>
<td>12</td>
<td>0.0102</td>
<td>9.5303</td>
<td>0.9831</td>
<td>0.7222</td>
</tr>
<tr>
<td>$V^*C_2$</td>
<td>11</td>
<td>0.0095</td>
<td>8.7396</td>
<td>0.9715</td>
<td>0.7875</td>
</tr>
<tr>
<td>$V^*C_1$</td>
<td>10</td>
<td>0.0094</td>
<td>8.0513</td>
<td>0.9698</td>
<td>0.8548</td>
</tr>
<tr>
<td>$V$</td>
<td>13</td>
<td>0.0059</td>
<td>9.2857</td>
<td>0.8974</td>
<td>0.7412</td>
</tr>
<tr>
<td>$V$</td>
<td>12</td>
<td>0.0063</td>
<td>9.0405</td>
<td>0.9072</td>
<td>0.6637</td>
</tr>
<tr>
<td>$V$</td>
<td>11</td>
<td>0.0071</td>
<td>8.6731</td>
<td>0.9255</td>
<td>0.7935</td>
</tr>
<tr>
<td>$V$</td>
<td>10</td>
<td>0.0081</td>
<td>7.9762</td>
<td>0.9460</td>
<td>0.8629</td>
</tr>
<tr>
<td>$V$</td>
<td>13</td>
<td>0.0035</td>
<td>10.2730</td>
<td>0.8226</td>
<td>0.6700</td>
</tr>
<tr>
<td>$V$</td>
<td>12</td>
<td>0.0046</td>
<td>9.5000</td>
<td>0.8609</td>
<td>0.7245</td>
</tr>
<tr>
<td>$V$</td>
<td>11</td>
<td>0.0062</td>
<td>8.7325</td>
<td>0.9048</td>
<td>0.7881</td>
</tr>
<tr>
<td>$V$</td>
<td>10</td>
<td>0.0081</td>
<td>7.9762</td>
<td>0.9460</td>
<td>0.8629</td>
</tr>
</tbody>
</table>
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 point. This signifies the preference of replicating non-center points, particularly the cube 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.

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

<table>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Design Size N</th>
<th>Determinant of Information matrix</th>
<th>Maximum variance of prediction</th>
<th>D-efficiency</th>
<th>G-efficiency</th>
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<tbody>
<tr>
<td>V^+C_8</td>
<td>S</td>
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<td>23</td>
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<td>V^+C_1</td>
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<tr>
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<td>12.7310</td>
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</table>

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 point. This signifies the preference of replicating non-center points, particularly the cube points.

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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. In fact, the lowest D-efficiency value associated with replicating the cube points was still better than the highest D-efficiency value associated with replicating the center 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 was obtained and the G-efficiencies of other designs were computed relative to this best G-optimal design. As with the two-variable quadratic model, the efficiencies of the designs for the three-variable quadratic model were computed relative to the best design within a class of designs. Hence, the best D-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 were computed relative to this best G-optimal design. 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


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