On the Preference of Replicating Factorial Runs to Axial Runs in Restricted Second-order Designs

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Abstract: Two variations of N-point Central Composite Designs (CCDs) which are either orthogonally or rotatably restricted are compared. The basis of variation in these designs is the common distance of the axial points from the center of the design. Using the D-optimality criterion, it is concluded that replicated cubes plus one star variation is preferable to the replicated star plus one cube variation under both restrictions.

Key words: Central composite designs, orthogonal restriction, rotatable restriction, D-optimality criterion

INTRODUCTION

It is sometimes desirable to replicate the points in a design. This will allow the experimenter to later estimate the pure error in the experiment. Many authors have discussed the analysis of such experiments (Cochran and Cox, 1957; Montgomery 1991; Atkinson and Donev, 1992). However, it should be clear that, when replicating the design points, the experimenter could compute the variability of measurements within each unique combination of factor levels. This variability will give an indication of the random error in the measurement because the replicated observations are taken under identical conditions. Such an estimate of the pure error can be used to evaluate the size and statistical significance of the variability that can be attributed to manipulated factors (Box and Draper, 1987). It may not be possible to replicate each unique combination of factor levels, that is, the full design, but the experimenter can still gain an estimate of pure error by replicating only some of the runs (points) in the design. In this case of partial replications, the experimenter faces the problem of choosing the points to be replicated and the points not to be replicated in the design.

In this study, specific interest is centered on the Central Composite Designs (CCDs) which are the most practically useful class of second-order designs and one of many experimental designs where partial replication is applicable. Since the best design option is sought, we shall hover around the restricted CCD (which is a CCD with restrictions such as orthogonality, rotatability, etc., imposed on it). It has been shown in Nwobi et al. (2001) that, with designs, restrictions involving orthogonality or rotatability or even both orthogonality and rotatability is better (in the sense of smaller variance) than the unrestricted. A CCD consists of a $2^k$ factorial or a $2^{k-1}$ fractional factorial portion (run), usually called a cube, with points selected from the $2^k$ points $(x_1, x_2, \ldots, x_k) = (\pm 1, \pm 1, \ldots, \pm 1)$ usually of resolution V or higher, plus a set of $2k$ axial points (runs) at a distance $\alpha$ from the origin, usually called a star, plus one or more center points. In general, the cube and star may be replicated also (Draper, 1982; Draper and Lin, 1990). Thus, we have a total of $N = 2^k n_1 + 2k n_2 + n_0$ points where $n_1$ is the number of cubes; $n_2$ is the number of stars and $n_0$ is the number of center points. Typically, the value of $\alpha$ will be chosen to satisfy the property of orthogonality or rotatability (Draper and John, 1998). More so, CCDs are extremely useful for sequential experimentation in which the cube portion is used to allow for estimation of the first-order effects, the later addition of the star points permits second-order terms to be added to the model and estimated. Although cube and star portions are used at different stages and purposes, it is plausible to know the portion of a restricted CCD to be replicated when it is not possible to replicate all points equally, because of the reason mentioned earlier. Box and Hunter (1957) has pointed out that the variance of estimate can be reduced by increasing $N$, the number of experiments (e.g., by replicating the points), see also Box and Draper (1982). An attempt to break this dilemma is made in this study. The two variations of restricted CCD that will arise

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which are replicated cubes plus one star and replicated stars plus one cube are compared. The variations are

distinguished by the value of \( \alpha \) only.

Our approach to this study is to express the information matrix of a restricted CCD in terms of numbers of
cubes and stars and then find out the desired portion, which optimizes the design under consideration. The
D-optimal design criterion, which maximizes the determinant of the information matrix of a design, is
employed for the comparison in this work. This is so because it has been proved by Nalimov et al. (1977) that
the D-optimum concept can be used as the theoretical basis for building and comparing response surface
designs in use.

**CENTRAL COMPOSITE DESIGNS**

The CCD is the \( 2^k \) factorial or a \( 2^{k-p} \) fractional factorial design with the levels of each factor coded
to the usual -1, +1, augmented by the following points: \((\pm \alpha, 0, \ldots, 0), (0, \pm \alpha, \ldots, 0) (0, 0, \ldots, \pm \alpha) \) and \((0, 0, \ldots, 0) \). The experimenter according to some restrictions such as orthogonality or rotatability selects the value of \( \alpha \) in order to show how these restrictions are made in choosing \( \alpha \), attention will be paid to the expanded design matrix, \( X \) and the information matrix, \( XX^T \), for the general CCD.

**Orthogonal restriction:** Consider the response surface, say \( \phi(x_1, x_2, \ldots, x_k) \) represented in the experimental area, \([\pm \alpha, \pm 1]\), by the quadratic function:

\[
y_i = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j=i+1}^{k} \beta_{ij} x_i x_j + \epsilon_i
\]

where, \( y_i \) and \( \epsilon_i \) are, respectively, the response and the random error of the \( i \)th observation, \( \beta_0, \beta_i, \beta_{ij} \) and \( \beta \) are the unknown parameters of the regression model and \( x_1, x_2, \ldots, x_k \) are the independent variables. Alternatively, in vector notation, (1) is given by:

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

where, \( Y \) and \( \epsilon \) are the, respectively \((N \times 1)\) response and error column vectors; \( E(\epsilon) = 0 \), \( Var(\epsilon) = \sigma^2 I \), \( X \) is an \((N \times P)\) matrix of independent variables of rank \( P \); \( \beta \) is the \((P \times 1)\) column vector of the unknown parameters.

From (1), we obtain the average:

\[
y = \bar{y} + \sum_{i=1}^{K} \beta_i \bar{x}_i + \sum_{i=1}^{K} \sum_{j=i+1}^{K} \beta_{ij} \bar{x}_i \bar{x}_j + \bar{\epsilon}
\]

By subtracting Eq. 3 from Eq. 1, we obtain:

\[
y_i - \bar{y} = \sum_{i=1}^{K} \beta_i (x_i - \bar{x}_i) + \sum_{i=1}^{K} \sum_{j=i+1}^{K} \beta_{ij} (x_i x_j - \bar{x}_i \bar{x}_j) + \sum_{i=1}^{K} \beta_i (x_i - \bar{x}_i)^2 + (\epsilon_i - \bar{\epsilon})
\]

where, \( y_i = \frac{1}{N} \sum_{j=1}^{N} y_j \) and \( \bar{\epsilon} = \frac{1}{N} \sum_{i=1}^{N} \epsilon_i \).

Recall from Eq. 1, that:

\[
\sum_{i=1}^{N} x_i = 0 \quad \forall \quad i = 1, 2, \ldots, K
\]

hence, \( \bar{x}_i = 0 \quad \forall \quad i \) and \( \bar{x}_i \). Then, (2) becomes:

\[
Y - \bar{y} = \bar{X} \beta + (\epsilon - \bar{\epsilon})
\]

after subtracting Eq. 3 from it, where \( y = (y, y, \ldots, y)^T, \bar{\epsilon} = (\bar{\epsilon}, \bar{\epsilon}, \ldots, \bar{\epsilon}) \) and:

\[
\bar{X} = \begin{pmatrix}
1 & 1 & 1 & 1 - x_1^2 & 1 - x_2^2 \\
-1 & -1 & 1 & 1 - x_1^2 & 1 - x_2^2 \\
1 & -1 & -1 & 1 - x_1^2 & 1 - x_2^2 \\
-1 & 1 & -1 & 1 - x_1^2 & 1 - x_2^2 \\
\end{pmatrix}
\]

is the \((N \times (P-1))\) design matrix; \( N = 2^k n_1 + 2^2 n_2 + n_0 \)

\[
P = \frac{(K + 1)(K + 2)}{2}
\]

\[
1 = (1, 1, \ldots, 1)^T \text{ is a } 2^k n_1 / 4 \text{ component vector; } \alpha = (\alpha, \alpha, \ldots, \alpha) \text{ is of } n_0 \text{ components; } \alpha^2 = (\alpha^2, \alpha^2, \ldots, \alpha^2) \text{ is of } n_0 \text{ components; } \Omega = (0, 0, \ldots, 0, 0) \text{ of } n_0 \text{ components; } \Omega^2 = (0, 0, \ldots, 0, 0) \text{ is of } (K-2)n_2 \text{ components, } \Omega^3 = (0, 0, \ldots, 0) \text{ is of } n_0 \text{ components. The information matrix of the design is obtained as:}
\]

\[
M = \bar{X} \bar{X} = \begin{pmatrix}
M_{11} & 0 & 0 \\
0 & M_{22} & 0 \\
0 & 0 & M_0
\end{pmatrix}
\]
where, \( M_i \) is the sum of squares of the elements in the vectors associated with the first-order terms while \( M_2 \) is the sum of squares of the elements in the vectors associated with the two-way cross-product terms. However, \( M_i \) is a (K+K) matrix whose diagonal elements (denoted by \( p \)) are the sums of squares of the elements in the vectors associated with the adjusted second-order terms and also, whose off-diagonal elements (denoted by \( q \)) are the sums of cross-products of the elements in the vectors associated with the adjusted second-order terms. Using notations accordingly, \( M_i = 2^m n_j + 2n_j \alpha^j \), \( M_2 = K n_i \), and \( M_3 = (p-q)I_K + q \bar{I}_K \). Note that, \( I_K \) is an (K+K) identity matrix, \( I_i \) is an (t×t) identity matrix; where:

\[
I_i = \begin{pmatrix} 1 & \cdots & 1 \\ \\ 1 & \cdots & 1 \\ \end{pmatrix}
\]

and \( I_K \) is a column vector of K components. Using Eq. 6, we obtain:

\[
q = 2^m n_j (t - \bar{x}_j)^2 - 4n_j \bar{x}_j (\bar{x}_j^2 - \bar{x}_j^3) + n_j (K-2) \bar{x}_j^2 + n_j \bar{x}_j^2
\]

\[
= 2^m n_j (2^m + 2K n_j + 2n_j - (2^m + 2n_j)) \bar{x}_j^2
\]

\[
p = 2^m n_j (t - \bar{x}_j)^2 + 2n_j (\bar{x}_j^2 - \bar{x}_j^3) + n_j (K-1) \bar{x}_j^2 = q + 2 \alpha \bar{x}_j
\]

where:

\[
\bar{x}_j = \frac{2^m n_j + 2K n_j \alpha^j}{N}
\]

Having obtained \( \bar{X} \) and \( \bar{X}^2 \), the definition of orthogonally-restricted CCD is given below.

**Orthogonally-Restricted CCD:** A CCD is orthogonally-restricted if \( \bar{X} \) has a diagonal structure, that is, if and only if \( q = 0 \) in \( M_3 \) of Eq. 7.

**Rotatable restriction:** The concept of rotatability was first introduced by Box and Hunter (1957) and has since become an important design criterion. The important feature of rotatability is that the quality of variance of prediction of the response denoted by \( V[\hat{y}(X)] \) is invariant to any rotation of the coordinate axes in the space of the input variables (Khuri, 1988). A succinct characterization of rotatability is given in terms of the elements of \( \bar{X}^T \bar{X} \). These elements are known as design moments although, originally, the elements of:

\[
\frac{1}{N} \bar{X}^T \bar{X}
\]

are referred to as design moments (Khuri, 1988). One the whole, a design moment for a model such as the one given in Eq. 1 of order \( d \) (d equals 2) and \( K \) input variables is denoted by \( (1^d 2^d \cdots K^d) \) and is given by:

\[
0^d 2^d \cdots K^d = \sum_{ijk} x_{ij} x_{ij} x_{ij}
\]

where, \( \delta_0, \delta_1, \cdots, \delta_k \) are nonnegative integers. The sum:

\[
\sum_{i} \delta_i
\]

is called the order of the design moment and is denoted by \( \hat{d} \) (\( \hat{d} = 0, 1, \cdots, 2d \)). For example, \( (1^1 3^1 5^1) \) is a design moment of order \( \hat{d} = 5 \Delta \) and is equal to:

\[
\sum_{ijk} x_{ijk}^2
\]

A necessary and sufficient condition for a design for fitting a model such as that of (1) to be rotatable is that the design moments of \( \hat{d} \) (\( \Delta = 0, 1, \cdots, 2d \)) be of the form:

\[
0^d 2^d \cdots K^d \Rightarrow \begin{cases} 
0, & \text{if any } \delta_i \text{ is odd} \\
\lambda \prod_{i=1}^d \delta_i!, & \text{if all of the } \delta_i \text{s are even}
\end{cases}
\]

where, \( \nu_2 \) is a quantity that depends on \( d \), \( \hat{d} \) and \( N \) (Box and Hunter, 1957). According to Myers (1991), a second-order design with moments, which have the following conditions:

- All moments that have at least one \( \delta_i \) to be odd are zero
- Pure fourth moments, which is equal to \( \frac{1}{N} \sum_{i=1}^N x_{ij}^4 \), are three times the mixed fourth moments, that is:

\[
\sum_{ij} x_{ij}^4 = 3 \sum_{i=1}^N x_{ij}^4
\]

is rotatable. Notice from the portion of a typical design matrix, \( X \) for general CCD containing the second-order terms that:

\[
\sum_{ij} x_{ij}^4 = 2^m n_j + 2 \alpha n_i
\]
\[
\sum_{j=1}^{n} x_j^2 = 2^n n_1
\]  
(14)

Of the two conditions given, which must be met in order that a second-order design is rotatable, the first is automatically met by mere inspection of \( X \) for the CCD (Myers, 1991). Thus, it only remains to find the value of \( \alpha \) for which the second condition holds. Using Eq. 12-14 accordingly, we obtain:

\[
2^n n_1 + 2n_2 \alpha_n = 3(2^n n_1)
\]  
(15)

Now for the information matrix in Eq. 7:

\[
M_1 = 2^n n_1 + 2n_2 \alpha_n^2, M_2 = 2^n n_2, \text{and } M_3 = (p-q)J + q J_k
\]

where, \( q = 2^n n_1 \) and \( p = 2^n n_1 + 2n_2 \alpha_n^2 \)

Rotatably-restricted CCD: A CCD is rotatably-restricted if and only if \( 2^n n_1 + 2n_2 \alpha_n = 3(2^n n_1) \).

CUBE REPLICATIONS VERSUS STAR REPLICATIONS IN RESTRICTED CCD

For the sake of the comparison, denote the replicated cubes plus one star variation of restricted CCD by \( \xi \). Also, denote the corresponding information matrix for this variation by \( M(\xi) \). Similarly, let \( \eta \) denote the one cube plus replicated stars variation of restricted CCD while \( M(\eta) \) denotes its information matrix. The criterion for comparison employed in this papers is the D-optimal design criteria, which is defined thus: given any two designs, \( \xi \) and \( \eta \), with information matrices, \( M(\xi) \) and \( M(\eta) \), respectively, then \( \xi \) is preferred to \( \eta \) if the difference, \( M(\xi) - M(\eta) \), is positive definite, that is:

\[
M(\xi) - M(\eta) \geq 0
\]  
(16)

where, \( \phi \) is the D-optimality criterion function which maximizes the determinant of the information matrix; for instance (Pazman, 1986; Federov, 1972; Onukogu, 1997):

\[
\phi[M(\xi)] = \max M(\xi)
\]  
(17)

The first restriction to be illustrated here is that for which the design is orthogonal. Recall that for orthogonality to be ensured in the CCD, the condition \( q = 0 \) must be satisfied, which implies that:

\[
\left( a - \frac{(a + 2n \alpha_n)^2}{N} \right) = 0
\]

Hence,

\[
\alpha = \left( \frac{(a N)^2 - a}{2n_2} \right)^{\frac{1}{2}}
\]

is the value that always gives an orthogonal CCD, where \( a = 2^n n_1 \). Consequently, the information matrix in Eq. 7 becomes \( m_0 = XX^t = \text{diagonal } (M_1, M_2, M_3, p_0, p_k) \) for: orthogonally-restricted CCD, where, \( p_0 = 2n_2 \alpha_n^2 \). Putting

\[
p_0 = \frac{a^2 + aN - 2a(aN)^{1/2}}{2n_2}
\]

in \( M_1 \) and \( p_0 \) we obtain:

\[
M_1 = (aN)^{1/2}
\]

and

\[
p_0 = \frac{a^2 + aN - 2a(aN)^{1/2}}{2n_2}
\]

Obviously, the eigenvalues of \( M_1 \) are its diagonal elements. Hence, the ordered eigenvalues of \( M_1 \) are:

\[
s_1^2 + aN - 2a(aN)^{1/2} \leq \cdots \leq s_k^2 + aN - 2a(aN)^{1/2} \leq \cdots \leq aN^{1/2} \leq \cdots \leq (aN)^{1/2}
\]

where:

\[
\frac{a^2 + aN - 2a(aN)^{1/2}}{2n_2}
\]

and \( (aN)^{1/2} \) each has \( K \) multiplicities in the above ordering while \( \alpha \) has:

\[
\frac{K(K-1)}{2}
\]

multiplicities in the same ordering. We then have for the orthogonally-restricted CCD that the determinant of the information matrix is given by:

\[
| M(\xi) | = \left( \frac{a^2 + aN - 2a(aN)^{1/2}}{2n_2} \right)^K \left( a \right)^{\frac{K(K-1)}{2}} (aN)^{K/2}
\]  
(18)

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Another interesting and important restriction in this article is that of readability. A design is rotatable when the variance of the estimated response is a function of only the distance from the center of the design and not on the direction. Recall a CCD is rotatably restricted if and only if \( 2^{n_p+2a}n_p = 3(2^{n_p}) \). Therefore:

\[
\alpha = \frac{a}{n_p}
\]

always gives a rotatable CCD. Putting

\[
\alpha = \left( \frac{a}{n_p} \right)^{\frac{1}{2}}
\]

in \( M_1 \) and \( M_1 \) of (7), we obtain \( M_{1a} + 2(\Delta a)^{\frac{1}{2}} \) and \( M_{1b} = 2a_{1b} + aJ_y \). Thus, the information matrix, \( M_{1a} \) for the rotatable CCD could be written as \( M_{1a} = \lambda X = \text{diagonal}(M_{1a} + a_{1b}) \). It can easily be seen that the eigenvalues of \( M_{1a} \) has a regular pattern, hence, the ordered eigenvalues of this matrix are:

\[
a \leq \cdots \leq a \leq (a + 2(\Delta a)^{\frac{1}{2}}) \leq \cdots \leq (a + 2(\Delta a)^{\frac{1}{2}}) \leq 2a \leq \cdots \leq 2a \leq (K + 2)a
\]

where, \( a \) has:

\[
\frac{K(K - 2)}{2}
\]

multiplicities, \((a + 2(\Delta a)^{\frac{1}{2}})^2\) has \( K \) multiplicities, \( 2a \) has \((K - 1)\) multiplicities, and \((K + 2)a\) occurs only once in the ordering. We therefore have for the rotatably-restricted CCD that the determinant of the information matrix is given by:

\[
M_{1a}(\xi) = (a + 2(\Delta a)^{\frac{1}{2}})^K \left( a + 2(\Delta a)^{\frac{1}{2}} \right)^{K - 1} (K + 2)a
\]

Therefore, its D-optimality value becomes:

\[
\phi[M_{1a}(\xi)] = \max |M_{1a}(\xi)| = \frac{\left( a + 2(\Delta a)^{\frac{1}{2}} \right)^K \left( a + 2(\Delta a)^{\frac{1}{2}} \right)^{K - 1} (K + 2)a}{N^{K+1}}
\]

Using Eq. 21, the numerical values of \( \phi[M_{1a}(\xi)] \) and \( \phi[M_{1b}(\eta)] \) for each variation of rotatably-restricted CCD given in Table 2 are obtained.

### RESULTS AND DISCUSSION

The following variations of the designs have been examined for illustration: one cube \( (n_p = 1) \) plus two

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### Table 1: Comparison of D-optimality Values of the Orthogonally-Restricted Variations for Selected N-point CCD

<table>
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<th>K</th>
<th>N</th>
<th>Variation</th>
<th>D</th>
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</thead>
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<tr>
<td>2</td>
<td>14</td>
<td>2 cubes plus one star</td>
<td>1.8545E-02</td>
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<td></td>
<td>19</td>
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<td>3 stars plus one cube</td>
<td>1.6895E-03</td>
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<tr>
<td></td>
<td>41</td>
<td>4 cubes plus one star</td>
<td>2.3448E-02</td>
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<td>43</td>
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### Table 2: Comparison of D-optimality Values of the Rotatably-Restricted Variations for Selected N-point CCD

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<th>Variation</th>
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<td>2.5141E-03</td>
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<tr>
<td></td>
<td>59</td>
<td>2 stars plus one cube</td>
<td>1.5530E-06</td>
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<tr>
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<td>75</td>
<td>3 cubes plus one star</td>
<td>3.1937E-03</td>
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<td>3 stars plus one cube</td>
<td>2.6450E-08</td>
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<td>109</td>
<td>4 cubes plus one star</td>
<td>3.5959E-03</td>
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<td>4 stars plus one cube</td>
<td>1.2315E-02</td>
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<tr>
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<td>2 cubes plus one star</td>
<td>2.5828E-04</td>
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<td>2 stars plus one cube</td>
<td>3.4672E-09</td>
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<td>3 cubes plus one star</td>
<td>2.7672E-04</td>
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<td></td>
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<td>3 stars plus one cube</td>
<td>4.7634E-12</td>
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<tr>
<td>6</td>
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<td>4 cubes plus one star</td>
<td>1.9701E-04</td>
</tr>
<tr>
<td></td>
<td>217</td>
<td>4 stars plus one cube</td>
<td>3.6835E-14</td>
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</table>
replicated stars \((n_i = 2)\); one cube \((n_i = 1)\) plus three replicated stars \((n_i = 3)\); one cube \((n_i = 1)\) plus four replicated stars \((n_i = 4)\); two replicated cubes \((n_i = 2)\) plus one star \((n_i = 1)\); three replicated cubes \((n_i = 3)\) plus one star \((n_i = 1)\) and four replicated cubes \((n_i = 4)\) plus one star \((n_i = 1)\). In Table 1 and 2, the results of the comparison are shown. We have obtained the numerical values of \(\phi[M_{th}(\xi)]\) and \(\phi[M_{th}(\eta)]\) for two, three, four and five factors. For each of these factors, three cases have been considered namely, Case one: two cubes plus one star versus one cube plus two stars; Case two: three cubes plus one star versus one cube plus three stars and Case three: four cubes plus one star versus one cube plus four stars. For each variation of N-point restricted CCD, at least two points are taken from the center in order to make up the required N points and also, to get a minimum of three degrees of freedom for pure error. Observe that the basis of variation in each case is the value of \(\alpha\) which differs from each other for the two variations.

Table 1 and 2 summarize the comparison using the D-optimality values. We can note from the table that in all the three cases and for all the values of K considered, maximum D-optimality values were obtained when replicated cubes plus one star variation of both orthogonally-restricted CCD and rotatably-restricted CCD was used. That is, for the two conditions of restrictions, the strict inequality \(\phi[M_{th}(\xi)] > \phi[M_{th}(\eta)]\) holds. A t-Test: Paired Two Sample for Means conducted afterwards between the D-optimality values of \(M(\xi)\) and \(M(\eta)\) revealed p-values of 0.02 and 0.04, respectively, for one-tailed and two-tailed tests for both orthogonal and rotatable restrictions of the CCD (indicating significant difference). Hence, this variation is preferred to one cube plus replicated stars variation of restricted CCD. We conjecture that this is true for any number of factors.

In general, the one cube plus replicated stars variation does not do well in this comparison.

**CONCLUSION**

The computational results in the tables show that the replicated cubes plus one star variation is better than the one cube plus replicated stars variation when any of the two restrictions considered in this work is imposed on a CCD. Since, in general, the D-optimality values of \(M(\xi)\) are significantly greater than those of \(M(\eta)\), we conclude that the replicated cubes plus one star variation is better than the one cube plus replicated stars variation in the sense of D-optimality criterion.

**REFERENCES**


