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ON THE OPTIMAL CHOICE OF THE CUBE AND STAR REPLICATIONS IN RESTRICTED SECOND-ORDER DESIGNS

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Abstract

Two variations of N-point central composite design that are either orthogonally or rotatably restricted are compared. The basis of variation in this type of design is the common distance of the axial points from the centre of the design. Calculations from expressions obtained based on the concept of Schur's ordering of designs or D-optimality criterion as the case may be, are made and used in the comparison for the duo. The results obtained indicate that replicated cubes plus one star variation is better than one cube plus replicated stars variation.

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1. Introduction

It is sometimes desirable to replicate the points in a design, that is, to run each combination of factor levels in the design more than once. This will allow the experimenter to later estimate the pure error in the experiment. The analysis of such experiments is discussed by many authors: see, for example, Cochran and Cox ([6], chap. 2), Montgomery ([12], chap. 9) and Atkinson and Donev ([1], chap. 8); however, it should be clear that, when replicating the design points, the experimenter can compute the variability of measurements within each unique combination of factor levels. This variability will give an indication of the random error in the measurements 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 the manipulated factors: see, for example, Box and Draper ([4], p.115). When it is not possible or feasible to replicate each unique combination of factor levels, that is, the full design, the experimenter can still gain an estimate of pure error by replicating only some of the runs (points) in the design. In this situation where there will be partial replications, it becomes a problem for the experimenter to choose the points to be replicated and the points not to be replicated in the design.

Many possible experimental designs may be used to obtain data suitable for model fitting. The specific choice of design would depend on the relative importance to the experimenter of various design features. In this work, we are specifically interested in the central composite design (ccd), which is the most practically useful class of second-order designs. A ccd consists of a 2^K factorial or a 2^{K-q} fractional factorial portion, 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 (a situation where the main effects and two-factor interactions are not aliased with any other main effects or two-factor interactions) or higher, plus a set of $2K$ axial points at a distance α from the origin, usually called a star, plus one or more centre points. Typically, the value of α will be chosen to satisfy the property of orthogonality or rotatability: see, for example, Draper and John [8]. The cube and star may be replicated also: see, for example, Draper [7] and Draper and Lin [9]. Natural occurrence of experimental units may bring about partial replications, thereby causing unequal replications of the centre, cube and star points. For instance, consider carrying out an experiment with two independent variables in twenty experimental units. Assuming curvature of the response in each of the two factors, a ccd is employed to estimate the associated full quadratic response surface model. Usually, the 2^2 ccd is made up of nine distinct points: four points from the 2^2 factorial portion $(\pm 1, \pm 1)$, i.e., the cube, another four points at the 2(2) axial points, which are at equal distance, α, from the centre of the design $[(\pm\alpha, 0), (0, \pm\alpha)]$, i.e., the star and a single centre point. Given this situation, the experimenter is bound to have unequal replications of the points in order to exhaust all the experimental units made available. Variations of such unequal replications include one cube plus one star plus twelve centre points (one cube plus one star variation), two cubes plus one star plus eight centre points (replicated cubes plus one star variation), and one cube plus two stars plus eight centre points (one cube plus replicated stars variation). In general, for any N-point ccd there are three rational (in the sense of cost) variations: the one cube plus one star, the replicated cubes plus one star, and the one cube plus replicated stars. The two latter ways are given consideration in this paper because as we shall see later the value of α that forms the basis of variation in a restricted ccd does not depend on the number of centre points but on the numbers of cube and star replications as well as the number of factors and total number of support points involved. Draper [7] examined these three variations of ccd in order to obtain the optimum number of centre points under each of the following criteria:

(1) orthogonality due to Box and Hunter [5];
(2) rotatability also due to Box and Hunter [5],
(3) Variance-plus-bias criterion of Box and Draper [2];
(4) "third-order lack-of-fit detectability" criterion of Box and Draper [2];
(5) the criterion given by the function, $\frac{\nu}{\sigma^2} = \frac{(r - \frac{P^2}{N})}{N}$, provided by Box and Draper [3], where r is the sum of squares of diagonal elements of $X(X'X)^{-1}X'$, P is the number of parameters in the model, and N is the total number of points;
(6) D-efficiency criterion: see Lucas [11]; and
(7) integrated variance criterion due to Draper [7].

In these considerations, the criteria of Box and Hunter [5] called for the number of centre points that seemed to be somewhat too large in the light of practical experience. The other criteria also called for designs with relatively small numbers of centre points for optimality.

Also, in Draper [7], three values of α, the axial distance of the star points were specifically considered for each variation of ccd; namely α equal to one, α equal to the radius of a spherical region and α value that ensures that a design is rotatable. Obviously, Draper [7] was not comparing the three variations of restricted ccd but tried to get the optimum number of centre points for each variation of restricted ccd using specified α values.

Given any two designs, ξ and η, with information matrices, $M(\xi)$ and $M(\eta)$, respectively, and ordered eigenvalues, $\lambda_1(\xi) \leq \lambda_2(\xi) \leq \ldots \leq \lambda_P(\xi)$ and $\lambda_1(\eta) \leq \lambda_2(\eta) \leq \ldots \leq \lambda_P(\eta)$, of the respective information matrices, where if an eigenvalue repeats itself r times it is repeated r times in the corresponding ordering, then ξ is a better design than η if and only if $\sum_{i=1}^{k} \lambda_i(\xi) \geq \sum_{i=1}^{k} \lambda_i(\eta)$; $k = 1, 2, \ldots, P$ and if and only if there is a strict inequality for at least one k: see Pazman ([16], p. 52). This method of comparing designs is known as Schur's ordering of designs. In this article, we shall compare the replicated cubes plus one star and the one cube plus replicated stars variations of restricted ccd using the above inequality. When the inequality $\sum_{i=1}^{k} \lambda_i(\xi) \geq \sum_{i=1}^{k} \lambda_i(\eta)$; $(k = 1, 2, \ldots, P)$ in the definition of Schur's ordering does not hold 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 [14] that the D-optimum concept can be used as the theoretical basis for building and comparing response surface designs in use. Nevertheless, the Schur's ordering is the premium criterion in this paper because if a design is optimal according to this concept, that design is equally optimal according to the A-, D- and E-optimality criteria: see Pazman ([16], p. 120).

2. Central Composite Designs

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

2.1. **Orthogonal Restriction.** Consider the response surface, say, $\phi(x_1, x_2, \dots, x_K)$, represented in the experimental area, $[\pm\alpha, \pm1]$, by the quadratic function

$$y_j = \beta_{00} + \sum_{i=1}^{K} \beta_{i0} x_{ij} + \sum_{i=1}^{K-1} \sum_{i'=i+1}^{K} \beta_{ii'} x_{ij} x_{i'j} + \sum_{i=1}^{K} \beta_{ii} x_{ij}^2 + \varepsilon_j \tag{2.1}$$

$$\sum_{j=1}^{N} x_{ij} = 0 \quad \forall \quad i = 1, 2, \dots, K;$$

where y_j and ε_j are respectively the response and the random error of the j^{th} observation; β_{00}, β_{i0}, $\beta_{ii'}$ and β_{ii} are the unknown parameters of the regression model, and $x_1, x_2, \dots, x_K$ are the independent variables. Alternatively, in vector notation, equation 2.1 is given by

$$Y = X\beta + e; \tag{2.2}$$

where Y and e are the respective $(N \times 1)$ response and error column vectors; $\mathrm{E}(e) = 0$, $\mathrm{Var}(e) = \sigma_e^2 I$; X is an $(N \times P)$ matrix of independent variables of rank P; β is the $(P \times 1)$ column vector of the unknown parameters. From equation 2.1, we obtain the average

$$\bar{y} = \beta_{00} + \sum_{i=1}^{K} \beta_{i0} \bar{x}_i + \sum_{i=1}^{K-1} \sum_{i'=i+1}^{K} \beta_{ii'} \bar{x}_i \bar{x}_{i'} + \sum_{i=1}^{K} \beta_{ii} \bar{x}_i^2 + \bar{\varepsilon}. \tag{2.3}$$

By subtracting equation 2.3 from equation 2.1, we obtain

$$y_j - \bar{y} = \sum_{i=1}^{K} \beta_{io}(x_{ij} - \bar{x}_i) + \sum_{i=1}^{K-1} \sum_{i'=i+1}^{K} \beta_{ii'}(x_{ij}x_{i'j} - \bar{x}_i\bar{x}_{i'}) + \sum_{i=1}^{K} \beta_{ii}(x_{ij}^2 - \bar{x}_i^2) + (\varepsilon_j - \bar{\varepsilon}), \tag{2.4}$$

where $\bar{y} = \frac{1}{N}\sum_{j=1}^{N} y_j$ and $\bar{\varepsilon} = \frac{1}{N}\sum_{j=1}^{N} \varepsilon_j$.

Recall from equation 2.1 that

$$\sum_{j=1}^{N} x_{ij} = 0, \quad \text{hence} \quad \bar{x}_i = 0 \quad \forall \quad i \quad \text{and} \quad \bar{x}_i\bar{x}_{i'} = 0 \quad \forall \quad i \quad \text{and} \quad i',$$

then equation 2.2 becomes

$$Y - \underline{\bar{y}} \quad = \quad X\beta + (e - \underline{\bar{e}}) \tag{2.5}$$

after subtracting equation 2.3 from it, where $\underline{\bar{y}} = (\bar{y}, \bar{y}, \ldots, \bar{y})'$ and $\underline{\bar{\varepsilon}} = (\bar{\varepsilon}, \bar{\varepsilon}, \ldots, \bar{\varepsilon})'$.

Hence, for the 2^K factorial orthogonally restricted ccd, the matrix, $\bar{X}$, spanned by the vector

$$(x_1 \quad x_2 \quad \ldots \quad x_K \quad x_i x_{i'} \quad x_1^2 - \bar{x_1^2} \quad x_2^2 - \bar{x_2^2} \quad \ldots \quad x_K^2 - \bar{x_K^2}) \tag{2.6}$$

is the $(N \times (P-1))$ design matrix adjusted for second-order terms; where $N = 2^K n_1 + 2Kn_2 + n_0$, $P = \frac{(K+1)(K+2)}{2}$, n_1 is the number of cube replications, n_2 is the number of star replications and n_0 is the number of centre points. Thus,

$$\bar{X} \quad = \quad \begin{array}{c} \begin{matrix} x_1 & x_2 & \ldots & x_K & x_i x_{i'} & x_1^2 - \bar{x_1^2} & x_2^2 - \bar{x_2^2} & \ldots & x_K^2 - \bar{x_K^2} \end{matrix} \\ \left[\begin{matrix} \pm 1 & \pm 1 & \ldots & \pm 1 & \pm 1 & 1 - \bar{x_1^2} & 1 - \bar{x_2^2} & \ldots & 1 - \bar{x_K^2} \\ \pm 1 & \pm 1 & \ldots & \pm 1 & \pm 1 & 1 - \bar{x_1^2} & 1 - \bar{x_2^2} & \ldots & 1 - \bar{x_K^2} \\ . & . & \ldots & . & . & . & . & \ldots & . \\ . & . & \ldots & . & . & . & . & \ldots & . \\ \pm 1 & \pm 1 & \ldots & \pm 1 & \pm 1 & 1 - \bar{x_1^2} & 1 - \bar{x_2^2} & \ldots & 1 - \bar{x_K^2} \\ \pm\alpha & 0 & \ldots & 0 & 0 & \alpha^2 - \bar{x_1^2} & -\bar{x_2^2} & \ldots & -\bar{x_K^2} \\ 0 & \pm\alpha & \ldots & 0 & 0 & -\bar{x_1^2} & \alpha^2 - \bar{x_2^2} & \ldots & -\bar{x_K^2} \\ . & . & \ldots & . & . & . & . & \ldots & . \\ . & . & \ldots & . & . & . & . & \ldots & . \\ 0 & 0 & \ldots & \pm\alpha & 0 & -\bar{x_1^2} & -\bar{x_2^2} & \ldots & -\bar{x_K^2} \\ 0 & 0 & \ldots & 0 & 0 & -\bar{x_1^2} & -\bar{x_2^2} & \ldots & -\bar{x_K^2} \end{matrix} \right] \end{array} \tag{2.7}$$

The information matrix of the design is obtained as

$$M \quad = \quad \bar{X}'\bar{X} = \begin{pmatrix} M_1 I_K & 0 & 0 \\ 0 & M_2 I_t & 0 \\ 0 & 0 & M_3 \end{pmatrix}. \tag{2.8}$$

In equation 2.8, M is a $(P-1) \times (P-1)$ matrix, M_1 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_3 is a $(K \times K)$ 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 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, $M_1 = 2^K n_1 + 2n_2\alpha^2$, $M_2 = 2^K n_1$, $M_3 = (p-q)I_K + qJ_K$. Note that, I_K is a $(K \times K)$ identity matrix, I_t is a $(t \times t)$ identity matrix $\left(t = \frac{K(K-1)}{2}\right)$ and $J_K = \underline{1}\underline{1}'$, $\underline{1}$ is a column vector of K components. Using 2.6 and hence equation 2.7, we obtain

$$\begin{aligned} q &= 2^K n_1 (1 - \bar{x^2})^2 - 4n_2(\alpha^2 - \bar{x^2})\bar{x^2} + 2n_2(K-2)\bar{x^2} + n_0\bar{x^2} \\ &= \frac{2^K n_1 (2^K n_1 + 2Kn_2 + n_0) - (2^K n_1 + 2n_2\alpha^2)^2}{N} \end{aligned}$$

$$\begin{aligned} p &= 2^K n_1 (1 - \bar{x^2})^2 + 2n_2(\alpha^2 - \bar{x^2})^2 + 2n_2(K-1)\bar{x^2}^2 \\ &= q + 2\alpha^4 n_2 \end{aligned}$$

where $\bar{x^2} = \frac{(2^K n_1 + 2K n_2 \alpha^2)}{N}$. Having obtained the design matrix, $\bar{X}$, adjusted for second-order terms and consequently the information matrix, $\bar{X}'\bar{X}$, the definition of orthogonally restricted ccd is given below.

Definition 2.1 (Orthogonally restricted ccd)**.** A ccd is orthogonally restricted if $\bar{X}'\bar{X}$ has a diagonal structure, i.e., if and only if $q = 0$ in M_3 of equation 2.8.

2.2. **Rotatable Restriction.** The concept of rotatability was first introduced by Box and Hunter [5] 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: see, for example, Khuri [10]. A succinct characterization of rotatability is given in terms of the elements of $X'X$. These elements are known as design moments although originally, the elements of $\frac{1}{N}(X'X)$, were referred to as design moments: see also, Khuri [10]. On the whole, a design moment for a model such as the one given in equation 2.1 of order $d(d = 2)$ and in K input variables is denoted by $(1^{\delta_1} 2^{\delta_2} \dots K^{\delta_K})$ and is given by

$$(1^{\delta_1} 2^{\delta_2} \dots K^{\delta_K}) \quad = \quad \sum_{j=1}^{N} {x_{1j}}^{\delta_1} {x_{2j}}^{\delta_2} \dots {x_{Kj}}^{\delta_K}, \tag{2.9}$$

where $\delta_1, \delta_2, \dots, \delta_K$ are nonnegative integers. The sum, $\sum_{i=1}^{K} \delta_i$, is called the order of the design moment and is denoted by $\delta(\delta = 0, 1, \dots, 2d)$. For example, $(1^1 \quad 3^1 \quad 5^3)$ is a design moment of order $\delta = 5$ and is equal to $\sum_{j=1}^{N} x_{1j} x_{3j} x_{5j}^3$.

A necessary and sufficient condition for a design for fitting a model such as that of equation 2.1 to be rotatable is that the design moments of $\delta(\delta = 0, 1, \dots, 2d)$ be of the form

$$(1^{\delta_1} 2^{\delta_2} \dots K^{\delta_K}) \quad = \quad \begin{cases} 0, & \text{if any } \delta_i \text{ is odd} \\ \dfrac{\lambda_\delta \prod_{i=1}^{K} \delta_i!}{2^{\frac{\delta}{2}} \prod_{i=1}^{K} \left(\frac{\delta_i}{2}\right)!}, & \text{if all of the } \delta_i\text{'s are even} \end{cases} \tag{2.10}$$

where λ_δ is a quantity that depends on d, δ and N: see Box and Hunter [5] and Myers ([13], chap. 7). According to Myers ([13], p. 145), a second-order design with moments, which have the following conditions:

(1) all moments that have at least one δ_i to be odd are zero;
(2) pure fourth moments denoted by [iiii], which is equal to $\frac{1}{N}\sum_{j=1}^{N} x_{ij}^4$, are three times the mixed fourth moments, i.e.,

$$\sum_{j=1}^{N} x_{ij}^4 \quad = \quad 3 \sum_{j=1}^{N} x_{ij}^2 x_{i'j}^2, \tag{2.11}$$

is rotatable.

Notice from the portion of a typical design matrix, X, for the general ccd containing the second-order terms, i.e.,

$$\begin{array}{ccccc} x_1^2 & x_2^2 & x_3^2 & \dots & x_K^2 \\ 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & \dots & 1 \\ . & . & . & \dots & . \\ . & . & . & \dots & . \\ 1 & 1 & 1 & 1 & 1 \\ \alpha^2 & 0 & 0 & \dots & 0 \\ \alpha^2 & 0 & 0 & \dots & 0 \\ 0 & \alpha^2 & 0 & \dots & 0 \\ 0 & \alpha^2 & 0 & \dots & 0 \\ . & . & . & \dots & . \\ . & . & . & \dots & . \\ 0 & 0 & 0 & \dots & \alpha^2 \\ 0 & 0 & 0 & \dots & \alpha^2 \\ 0 & 0 & 0 & \dots & 0 \end{array},$$

that

$$\sum_{j=1}^{N} x_{ij}^4 = 2^K n_1 + 2\alpha^4 n_2, \quad \text{and} \tag{2.12}$$

$$\sum_{j=1}^{N} x_{ij}^2 x_{i'j}^2 = 2^K n_1. \tag{2.13}$$

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: see Myers ([13], p. 150). Thus, it only remains to find the value of α for which the second condition holds. From equations 2.12 and 2.13 and by equating $\sum_{j=1}^{N} x_{ij}^4$ to $3\sum_{j=1}^{N} x_{ij}^2 x_{i'j}^2$, we have

$$2^K n_1 + 2\alpha^4 n_2 = 3(2^K n_1). \tag{2.14}$$

Now for the information matrix in equation 2.8,
$M_1 = 2^K n_1 + 2n_2\alpha^2$, $M_2 = 2^K n_1$ and $M_3 = (p-q)I_K + qJ_K$, where $q = 2^K n_1$ and $p = 2^K n_1 + 2n_2\alpha^4$.

Definition 2.2 (Rotatably restricted ccd)**.** A ccd is rotatably restricted if and only if $2^K n_1 + 2\alpha^4 n_2 = 3(2^K n_1)$.

3. Cube Replications versus Star Replications in Restricted CCD

We shall now employ the inequality of Schur's ordering of designs as well as the D-optimality criterion, where necessary, in comparing the replicated cubes plus one star and one cube plus replicated stars variations of the restricted ccd. The first restriction to be illustrated here is that for which the design is orthogonal. Recall from Definition 2.1 that for orthogonality to be ensured in the ccd, the condition $q = 0$ must be satisfied, which implies that $\left(a - \frac{a+2\alpha^2 n_2}{N}\right) = 0$.

Hence $\alpha = \left\{\frac{(aN)^{\frac{1}{2}} - a)}{2n_2}\right\}^{\frac{1}{2}}$ is the value that always gives an orthogonal ccd, where $a = 2^K n_1$. Consequently, the information matrix for the orthogonal ccd, M_O, in equation 2.8 becomes $M_O = \bar{X}'\bar{X} = diagonal\{M_1 I_K, M_2 I_t, p_O I_K\}$, where $p_O = 2\alpha^4 n_2$. Substituting for α in M_1 and p_O, we obtain $M_1 = \{aN\}^{\frac{1}{2}}$ and $p_O = \frac{a^2+aN-2a\{aN\}^{\frac{1}{2}}}{2n_2}$. Obviously, the eigenvalues of M_O are its diagonal elements. For the sake of comparison, denote the replicated cubes plus one star variation of restricted ccd by ξ. Also, denote the corresponding information matrix for this variation by $M(\xi)$, hence, $\lambda_1(\xi) \leq \lambda_2(\xi) \leq \ldots \leq \lambda_{P-1}(\xi)$, are the ordered eigenvalues of this matrix. Similarly, let η denote the one cube plus replicated stars variation of the restricted ccd while $M(\eta)$ denotes the information matrix for the variation, η, and $\lambda_1(\eta) \leq \lambda_2(\eta) \leq \ldots \leq \lambda_{P-1}(\eta)$, denote the ordered eigenvalues of the matrix, $M(\eta)$. Since each variation of the restricted ccd has N as one of the eigenvalues (the eigenvalue arising from the constant term), the consideration in this paper will be limited to only $(P-1)$ eigenvalues.

Now, given any variation, the ordered eigenvalues of M_O are

$$\frac{a^2+aN-2a\{aN\}^{\frac{1}{2}}}{2n_2} \leq \cdots \leq \frac{a^2+aN-2a\{aN\}^{\frac{1}{2}}}{2n_2} \leq a \leq \ldots \leq a \leq \{aN\}^{\frac{1}{2}} \leq \ldots \leq \{aN\}^{\frac{1}{2}},$$

where $\frac{a^2+aN-2a\{aN\}^{\frac{1}{2}}}{2n_2}$ and $\{aN\}^{\frac{1}{2}}$ each has K multiplicities in the above ordering while a has $\frac{K(K-1)}{2}$ multiplicities in the same ordering. Using the eigenvalues and their respective multiplicities, expressions that are used in comparing the variations of orthogonally restricted ccd according to Schur's ordering are obtained. For $k = 1, 2, \ldots, K$, the expression is

$$\sum_{i=1}^{k} \lambda_i(.) = \frac{na^2 + naN - 2na(aN)^{\frac{1}{2}}}{2n_2}; \quad n = k. \tag{3.1}$$

For $k+1, k+2, \ldots, K + \binom{K}{2}$, the expression is

$$\sum_{i=1}^{k} \lambda_i(.) = \frac{Ka^2 + KaN - 2Ka(aN)^{\frac{1}{2}} + 2nan_2}{2n_2}; \quad n = k - K. \tag{3.2}$$

For $K + \binom{K}{2} + 1, K + \binom{K}{2} + 2, \ldots, 2K + \binom{K}{2}$, the expression is

$$\sum_{i=1}^{k} \lambda_i(.) = \frac{Ka^2 + KaN - 2Ka(aN)^{\frac{1}{2}} aK(K-1)n_2 + 2nn_2(aN)^{\frac{1}{2}}}{2n_2}; \quad n = k - K + \binom{K}{2}. \tag{3.3}$$

Equations 3.1 through 3.3 altogether are used to obtain the numerical values of $\sum_{i=1}^{k} \lambda_i(\xi)$ and $\sum_{i=1}^{k} \lambda_i(\eta)$ for each variation of orthogonally restricted ccd given in Tables 1, 2 and 3.

Another interesting and important restriction in this article is that of rotatability. A design is rotatable when the variance of the estimated response is a function of only the distance from the centre of the design and not on the direction. Following definition 2.2, a ccd is rotatably restricted if and only if $2^K n_1 + 2\alpha^4 n_2 = 3(2^K n_1)$. Therefore $\alpha^4 = \frac{a}{n_2}$ always gives a rotatable ccd. Thus, $\alpha = \{\frac{a}{n_2}\}^{\frac{1}{4}}$ and the information matrix for the rotatble ccd, M_R, could be written as $M_R = X'X = diagonal\{M_1 I_K + aJ_k\}$. It can easily be seen that the eigenvalues of M_R has a regular pattern, hence the ordered eigenvalues of this matrix are $a \leq \ldots \leq a \leq (a + 2\{an_2\}^{\frac{1}{2}}) \leq \ldots \leq (a + 2\{an_2\}^{\frac{1}{2}}) \leq 2a \leq \ldots \leq 2a \leq (K+2)a$, where a has $\frac{K(K-2)}{2}$ multiplicities, $(a + 2\{an_2\}^{\frac{1}{2}})$ has K multiplicities, $2a$ has $(K-1)$ multiplicities and $(K+2)a$ occurs only once in the ordering. Using the eigenvalues and their respective multiplicities, the expression for comparing the variations of rotatably restricted ccd according to the Schur's ordering are also obtained. For $k = 1, 2, \ldots, \binom{K}{2}$, the expression is

$$\sum_{i=1}^{k} \lambda_i(.) = an; \quad n = k. \tag{3.4}$$

For $k = \binom{K}{2} + 1, \binom{K}{2} + 2, \ldots, \binom{K}{2} + K$, the expression is

$$\sum_{i=1}^{k} \lambda_i(.) = \frac{aK(K-1)}{2} + an + 2n(an_2)^{\frac{1}{2}}; \quad n = k - \binom{K}{2}. \tag{3.5}$$

For $k = \binom{K}{2} + K + 1, \binom{K}{2} + K + 2, \ldots, \binom{K}{2} + 2K - 1$, the expression is

$$\sum_{i=1}^{k} \lambda_i(.) = aK^2 + K^2(an_2)^{\frac{1}{2}} + K(an_2)^{\frac{1}{2}} + 2a(n+1); \quad n = k - \binom{K}{2} + K. \tag{3.6}$$

For $k = \binom{K}{2} + 2k$, the expression is

$$\sum_{i=1}^{k} \lambda_i(.) = 2aK^2 + (K^2 + K)(an_2)^{\frac{1}{2}} + 2a(2K+1). \tag{3.7}$$

Using equations 3.4 through 3.7 accordingly, the numerical values of $\sum_{i=1}^{k} \lambda_i(\xi)$ and $\sum_{i=1}^{k} \lambda_i(\eta)$ for each variation of rotatably restricted ccd given in Tables 5, 6 and 7 are obtained.

4. Discussion of Results

The following variations of the designs have been examined for illustration: one cube ($n_1 = 1$) plus two replicated stars ($n_2 = 2$); one cube ($n_1 = 1$) plus three replicated stars ($n_2 = 3$); one cube ($n_1 = 1$) plus four replicated stars ($n_2 = 4$); two replicated cubes ($n_1 = 2$) plus one star ($n_2 = 1$); three replicated cubes ($n_1 = 3$) plus one star ($n_2 = 1$); and four replicated cubes ($n_1 = 4$) plus one star ($n_2 = 1$). In Tables 1, 2, 3, 4, 5, 6 and 7, the results of the comparison are shown. We have obtained the numerical values of $\sum_{i=1}^{k} \lambda_i(\xi)$ and $\sum_{i=1}^{k} \lambda_i(\eta)$ 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 centre 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 α which differs from each other for the two variations.

4.1. **Comments on Tables 1, 2, 3 and 4.**

4.1.1. *Case one: two cubes plus one star versus one cube plus two stars in orthogonal restriction.* Inspection of Table 1 reveals that for two factors, the strict inequality $\sum_{i=1}^{k} \lambda_i(\xi) > \sum_{i=1}^{k} \lambda_i(\eta)$ holds for all values of k (k = 1, 2, 3, 4 and 5); hence the two replicated cubes plus one star variation is better than the one cube plus two replicated stars variation. However, for more than two factors this inequality does not hold for all values of k. Consequently, the variations for more than two factors cannot be compared based on Schur's ordering of designs.

4.1.2. *Case two: three cubes plus one star versus one cube plus three stars in orthogonal restriction.* Table 2 reveals that for two factors, the inequality $\sum_{i=1}^{k} \lambda_i(\xi) > \sum_{i=1}^{k} \lambda_i(\eta)$ holds also for all values of k (k = 1, 2, 3, 4 and 5); hence the three replicated cubes plus one star variation is better than the one cube plus three replicated stars variation. However, again, for more than two factors, this inequality does not hold for all values of k. Hence, the variations for more than two factors cannot be compared according to Schur's ordering of designs.

4.1.3. *Case three: four cubes plus one star versus one cube plus four stars in orthogonal restriction.* From Table 3, we observe that for two factors, the inequality $\sum_{i=1}^{k} \lambda_i(\xi) > \sum_{i=1}^{k} \lambda_i(\eta)$ holds again for all values of k (k = 1, 2, 3, 4 and 5); hence the four replicated cubes plus one star variation is better than the one cube plus four replicated stars variation. But for more than two factors, this inequality does not hold for all values of k. Thus, the competing variations of orthogonally restricted ccd cannot be compared using Schur's ordering of designs.

Based on the fact that our premium criterion failed in the comparison of the variations in the three cases above for more than two factors, the D-optimality criterion is employed to arrest the situation. For the orthogonally restricted ccd; $|M_O(.)| = \left(\frac{a^2+aN-2a(aN)^{\frac{1}{2}}}{2n_2}\right)^K (a)^{\frac{K(K-1)}{2}} (aN)^{\frac{K}{2}}$; therefore, its D-optimality value, D, is $\frac{\left(\frac{a^2+aN-2a(aN)^{\frac{1}{2}}}{2n_2}\right)^K (a)^{\frac{K(K-1)}{2}} (aN)^{\frac{K}{2}}}{N^{P-1}}$. Table 4 summarizes 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 orthogonally restricted ccd is used. Hence, this variation is preferred to one cube plus replicated stars variation of orthogonally restricted ccd. Also, due to the fact that the A-optimality criterion is inherent in the expressions derived based

K	N	k	$\sum_{i=1}^{k} \lambda_i(\xi)$	$\sum_{i=1}^{k} \lambda_i(\eta)$
2	14	1	3.36	3.03
		2	6.67	6.06
		3	14.67	10.07
		4	25.25	17.55
		5	35.84	25.03
3	25	1	8.00	9.43
		2	16.00	18.86
		3	24.00	28.29
		4	40.00	36.29
		5	56.00	44.29
		6	72.00	55.29
		7	92.00	66.40
		8	112.00	80.53
		9	132.00	94.72
4	43	1	12.98	26.16
		2	25.95	52.32
		3	38.93	78.49
		4	51.91	104.64
		5	83.91	120.65
		6	115.91	136.65
		7	147.91	152.65
		8	179.91	168.65
		9	211.91	184.65
		10	243.91	200.65
		11	281.00	226.88
		12	318.10	253.11
		13	355.19	279.34
		14	392.29	305.57
5	77	1	19.22	77.78
		2	38.44	155.56
		3	57.65	233.34
		4	76.87	311.12
		5	96.09	388.90
		6	160.09	420.90
		7	224.09	452.90
		8	280.09	484.90
		9	352.09	516.90
		10	416.09	548.90
		11	480.09	580.90
		12	544.09	612.90
		13	608.09	644.90
		14	672.09	676.90
		15	736.09	708.90
		16	911.38	845.25
		17	1086.67	981.59
		18	1261.96	1117.93
		19	1437.24	1254.27
		20	1612.53	1390.61

TABLE 1. Two Replicated Cubes plus One Star versus One Cube plus Two Replicated Stars in Orthogonal Restriction

on the concept of Schur's ordering, it is not out of place to use this criterion for the same comparison. In fact, equation 3.3 gives A-optimality value where $k = \binom{K}{2} + 2K$ and again in this case maximizing this value is pursued. The A-optimality value is maximized when replicated cubes plus one star is used, as shown in Tables 1, 2 and 3.

K	N	k	$\sum_{i=1}^{k} \lambda_i(\xi)$	$\sum_{i=1}^{k} \lambda_i(\eta)$
2	19	1	4.80	3.71
		2	4.80	7.42
		3	21.61	11.42
		4	36.71	20.42
		5	61.81	28.85
3	33	1	8.58	11.34
		2	17.16	22.68
		3	25.74	34.02
		4	49.74	42.02
		5	73.74	50.02
		6	97.74	58.05
		7	125.88	74.26
		8	154.03	90.51
		9	182.17	106.76
4	59	1	13.61	36.14
		2	27.21	72.27
		3	40.82	108.41
		4	54.42	144.54
		5	102.42	160.54
		6	150.42	176.54
		7	198.42	192.54
		8	246.42	208.54
		9	294.42	224.54
		10	342.42	240.54
		11	395.64	271.27
		12	448.86	301.99
		13	502.07	332.72
		14	555.29	363.44
5	109	1	19.81	122.03
		2	39.61	244.06
		3	59.42	366.10
		4	79.22	488.14
		5	99.03	610.17
		6	195.03	642.12
		7	291.03	674.17
		8	387.03	706.17
		9	483.03	738.17
		10	597.03	770.17
		11	675.03	802.17
		12	771.03	834.17
		13	867.03	866.17
		14	963.03	989.17
		15	1059.03	930.17
		16	1313.59	1090.39
		17	1568.16	1250.61
		18	1822.72	1410.82
		19	2077.28	1571.04
		20	2331.85	1731.26

TABLE 2. Three Replicated Cubes plus One Star versus One Cube plus Three Replicated Stars in Orthogonal Restriction

4.2. **Comments on Tables 5, 6 and 7.** Inspection of Tables 5, 6 and 7 shows that for all the three cases in the rotatable restriction, the strict inequality $\sum_{i=1}^{k} \lambda_i(\xi) > \sum_{i=1}^{k} \lambda_i(\eta)$ holds for all values of k ($k = 1, 2, \ldots, (P-1)$) and for any number of factors considered, hence, the

K	N	k	$\sum_{i=1}^{k} \lambda_i(\xi)$	$\sum_{i=1}^{k} \lambda_i(\eta)$
2	23	1	5.07	3.91
		2	10.13	7.82
		3	26.13	11.82
		4	45.32	21.41
		5	64.50	31.00
3	41	1	8.91	12.78
		2	17.82	25.56
		3	26.73	38.34
		4	58.73	46.36
		5	90.73	54.34
		6	122.73	62.34
		7	158.95	80.45
		8	195.18	90.56
		9	231.40	116.67
4	75	1	13.95	43.44
		2	27.90	86.87
		3	41.85	130.31
		4	55.80	173.74
		5	119.80	189.74
		6	183.80	205.74
		7	274.80	221.74
		8	311.80	237.74
		9	375.80	253.74
		10	439.80	269.74
		11	509.08	304.38
		12	578.36	339.03
		13	647.65	373.03
		14	716.93	408.31
5	141	1	20.12	154.63
		2	40.23	309.23
		3	60.35	463.89
		4	80.76	618.51
		5	100.58	773.14
		6	228.58	805.14
		7	356.58	805.14
		8	484.58	869.14
		9	612.58	901.14
		10	740.58	933.14
		11	868.58	965.14
		12	996.58	997.14
		13	1124.58	1029.14
		14	1252.58	1061.14
		15	1380.58	1093.14
		16	1714.01	1268.88
		17	1047.44	1444.62
		18	2380.88	1620.36
		19	2814.31	1796.10
		20	3047.74	1971.84

TABLE 3. Four Replicated Cubes plus One Star versus One Cube plus Four Replicated Stars in Orthogonal Restriction

replicated cubes plus one star variation of rotatably restricted ccd is better than the one cube plus replicated stars variation of the same type of ccd.

In accordance with Schur's ordering of designs, the variations of orthogonally restricted ccd have successfully been compared for two factors only. The D-optimality and A-optimality criteria

K	N	Variation	D
2	14	2 cubes plus a star	1.8640E-02
		2 stars plus a cube	3.8323E-02
	19	3 cubes plus a star	2.5501E-02
		3 stars plus a cube	8.7336E-04
	23	4 cubes plus a star	2.3585E-03
		4 stars plus a cube	8.7336E-04
3	25	2 cubes plus a star	4.3980E-03
		2 stars plus a cube	3.1849E-04
	33	3 cubes plus a star	4.1935E-03
		3 stars plus a cube	6.8978E-05
	41	4 cubes plus a star	3.3653E-03
		4 stars plus a cube	1.9385E-05
4	43	2 cubes plus a star	7.8028E-04
		2 stars plus a cube	5.0352E-05
	59	3 cubes plus a star	5.4282E-04
		3 stars plus a cube	4.1160E-06
	75	4 cubes plus a star	3.3648E-04
		4 stars plus a cube	4.8264E-04
5	77	2 cubes plus a star	9.5991E-05
		2 stars plus a cube	1.7995E-05
	109	3 cubes plus a star	4.0490E-05
		3 stars plus a cube	3.9068E-05
	141	4 cubes plus a star	1.7637E-05
		4 stars plus a cube	1.4109E-08

TABLE 4. Comparison of D-optimality values of the orthogonally restricted variations for selected N-point ccd

were used to compare the variations of orthogonally restricted ccd for $3 \leq K \leq 5$ in this article because the concept of schur's ordering could not help in these values of K. It is imaginably expected that Schur's ordering cannot be used to compare variations of orthogonally restricted ccd for $K \geq 3$. We want to believe that if the number of points in a cube is equal to the number of points in a star ($2^K = 2K$), the Schur's ordering will be applicable for the comparison of these variations of orthogonally restricted ccd for $K \geq 3$. This belief stems from the applicability of the premium criterion in comparing these variations of this type of ccd for two factors, where the number of points in the cube and the number of points in the star are both equal to four. Furthermore, when half-replicate or quarter-replicate of the full factorial design is used, the concept of Schur's ordering becomes applicable and the results remain unchanged. Also, the variations of rotatably restricted ccd were compared successfully according to the Schur's ordering of designs for two, three, four and five factors. We conjecture that this is true for any number of factors.

K	N	k	$\sum_{i=1}^{k} \lambda_i(\xi)$	$\sum_{i=1}^{k} \lambda_i(\eta)$
2	14	1	8.00	4.00
		2	21.66	13.66
		3	35.31	23.31
		4	51.31	31.31
		5	83.31	47.31
3	25	1	16.00	8.00
		2	32.00	16.00
		3	48.00	24.00
		4	72.00	40.00
		5	96.00	56.00
		6	120.00	72.00
		7	152.00	88.00
		8	184.00	104.00
		9	248.00	136.00
4	43	1	32.00	16.00
		2	64.00	32.00
		3	96.00	48.00
		4	128.00	64.00
		5	160.00	80.00
		6	192.00	96.00
		7	235.31	123.31
		8	278.63	150.63
		9	321.92	177.94
		10	265.25	205.25
		11	429.25	237.25
		12	493.25	369.25
		13	557.25	301.25
		14	685.25	365.25
5	77	1	64.00	32.00
		2	128.00	64.00
		3	192.00	96.00
		4	256.00	128.00
		5	320.00	160.00
		6	384.00	192.00
		7	448.00	224.00
		8	512.00	256.00
		9	576.00	288.00
		10	640.00	320.00
		11	720.00	368.00
		12	800.00	416.00
		13	880.00	464.00
		14	960.00	512.00
		15	1040.00	560.00
		16	1168.00	624.00
		17	1296.00	688.00
		18	1424.00	752.00
		19	1552.00	816.00
		20	1808.00	944.00

TABLE 5. Two Replicated Cubes plus One Star versus One Cube plus Two Replicated Stars in Rotatable Restriction

In general, the replicated cubes plus one star variation of restricted ccd is better than the one cube plus replicated stars variation in the sense of Schur's ordering or D-optimality or A-optimality as the case may be. More so, our calculations, when used to compare orthogonal and rotatable designs confirm that rotatable designs are better than orthogonal designs in the sense

K	N	k	$\sum_{i=1}^{k} \lambda_i(\xi)$	$\sum_{i=1}^{k} \lambda_i(\eta)$
2	19	1	12.00	4.00
		2	30.93	14.93
		3	49.86	25.86
		4	73.86	33.86
		5	121.86	49.86
3	33	1	24.00	8.00
		2	48.00	16.00
		3	72.00	24.00
		4	105.80	41.80
		5	139.60	59.60
		6	173.39	77.39
		7	221.39	93.39
		8	369.39	109.39
		9	365.39	141.39
4	59	1	48.00	16.00
		2	96.00	32.00
		3	144.00	48.00
		4	192.00	64.00
		5	240.00	80.00
		6	288.00	96.00
		7	349.86	125.86
		8	411.71	155.71
		9	473.57	185.57
		10	535.43	215.43
		11	631.43	247.43
		12	727.43	279.43
		13	824.43	311.43
		14	1015.43	375.43
5	109	1	96.00	32.00
		2	192.00	64.00
		3	288.00	96.00
		4	384.00	128.00
		5	480.00	160.00
		6	576.00	192.00
		7	672.00	224.00
		8	768.00	256.00
		9	864.00	288.00
		10	960.00	320.00
		11	1075.60	371.60
		12	1191.19	423.19
		13	1306.79	474.79
		14	1422.38	526.38
		15	1537.98	577.98
		16	1729.98	641.98
		17	1921.98	705.98
		18	2113.98	769.98
		19	2305.98	833.98
		20	3689.98	961.98

Table 6. Three Replicated Cubes plus One Star versus One Cube plus Three Replicated Stars in Rotatable Restriction

of smaller variance, just as Nwobi et al [15] concluded. For each of the three cases examined, the sums of the first k ordered eigenvalues for the variations of rotatably restricted ccd are greater than those of orthogonally restricted ccd; hence, rotatable designs are better than orthogonal designs in terms of Schur's ordering of designs and even the D-optimality or A-optimality criteria.

K	N	k	$\sum_{i=1}^{k} \lambda_i(\xi)$	$\sum_{i=1}^{k} \lambda_i(\eta)$
2	23	1	16.00	4.00
		2	40.00	16.00
		3	64.00	28.00
		4	63.00	36.00
		5	160.00	52.00
3	41	1	32.00	8.00
		2	64.00	16.00
		3	96.00	24.00
		4	139.31	43.31
		5	182.63	62.63
		6	225.94	81.94
		7	289.94	97.94
		8	353.94	113.94
		9	481.94	145.94
4	75	1	64.00	16.00
		2	128.00	32.00
		3	192.00	48.00
		4	256.00	64.00
		5	320.00	80.00
		6	384.00	96.00
		7	464.00	128.00
		8	544.00	160.00
		9	624.00	192.00
		10	704.00	224.00
		11	832.00	256.00
		12	960.00	288.00
		13	1088.00	320.00
		14	1344.00	384.00
5	141	1	128.00	32.00
		2	256.00	64.00
		3	384.00	96.00
		4	512.00	128.00
		5	640.00	160.00
		6	768.00	192.00
		7	896.00	224.00
		8	1024.00	256.00
		9	1152.00	288.00
		10	1280.00	320.00
		11	1430.63	374.63
		12	1581.26	429.25
		13	1731.88	483.88
		14	1882.51	538.51
		15	2055.14	593.14
		16	2289.14	657.14
		17	2545.14	721.14
		18	2801.14	785.14
		19	3057.14	849.14
		20	3569.14	977.14

TABLE 7. Four Replicated Cubes plus One Star versus One Cube plus Four Replicated Stars in Rotatable Restriction

5. 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 sum of the first k ordered eigenvalues of $M(\xi)$ are 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 Schur's ordering of designs. Also, we have seen that when Schur's ordering of designs is not applicable, any of D-optimality and A-optimality criteria was used and the result remained the same.

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