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Characterization of Prediction Variance Properties of Rotatable Central Composite Designs for 3 to 10 Factors

Eugene C. Ukaegbu[1] and Polycarp E. Chigbu[2]

[1]*Department of Statistics, University of Nigeria, Nsukka, Nigeria*
[2]*Department of Statistics, University of Nigeria, Nsukka, Nigeria*

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Abstract: Rotatability is a very important property of the central composite designs (CCD) in predicting responses with stable prediction variance throughout the design region. A central composite design is made rotatable by the choice of α, the axial distance from the centre of the design region. In this work, we evaluate the prediction variance properties of the CCD with rotatable α by replicating the cube and star portions of the CCD. Three design optimality criteria, the *D*-efficiency, *G*-efficiency and *V*-criterion are utilized in evaluating the performances of the designs. The fraction of design space (FDS) plots for the scaled and unscaled prediction variances are employed in studying the performance characteristics of the prediction variance of the designs throughout the design region. The results show that, for k = 3 to 10 factors and with three centre points, the cube-replicated CCDs are *D*-efficient. Replicating the cube or star portions of the CCD improves the prediction capability of the designs. However, none of the design options, cube-replicated and star-replicated, is consistently superior to the others with respect to *G*-efficiency, *V*-criterion and FDS plots for any of the k factors considered. Analytical formulae for obtaining the *G*-efficiency and *V*-criterion when portions of the CCD are replicated are also given.

Keywords: replication, optimality criteria, axial distance, response surface, design efficiency, design space.

1. Introduction

The central composite design (CCD) of [1] is the most common and practically useful class of second-order response surface designs. The CCD is made up of three distinct portions: (i) the 2^{k-q} full $(q=0)$ or fractional $(q>0)$ factorial portion (called the cube) of resolution V or higher, where q is an integer and k is the number of factors. The cube has coordinates of the form, $(x_1, x_2, \ldots, x_k) = (\pm 1, \pm 1, \ldots, \pm 1)$. (ii) the $2k$ axial portion (called the star) with coordinates of the form, $(\pm\alpha, 0, \ldots, 0), (0, \pm\alpha, 0, \ldots, 0), \ldots, (0, 0, \ldots, \pm\alpha)$; and (iii) n_0 number of centre points of the form, $(0, 0, \ldots, 0)$. Therefore, the CCD uses $N = 2^{k-q} + 2k + n_0$ number of design runs to estimate the $p = (k+1)(k+2)/2$ number of model parameters, see, for example, [2], [3], [4], [5] and [6].

Among the numerous criteria listed in [7], [8] and [9] for choosing response surface designs, rotatability is the most desirable. A design that the variance, $V\{\hat{y}(\mathbf{x})\}$, of the predicted response, $\hat{y}(\mathbf{x})$, is constant at any given point, $\mathbf{x}$, in the design space such that equal information is obtained in all directions at equal radius from the centre of the design space is said to be rotatable. This means that for a rotatable design, $V\{\hat{y}(\mathbf{x})\}$ is the same at all points, $\mathbf{x}$, that are the same distance from the centre of the design region. See [10], [11], [12] and [5] for further discussions on rotatability and measures of rotatability.

Rotatability is a reasonable basis for the selection of a response surface design in response surface optimization and it is wise to choose a design that provides equal precision of estimation in all directions. The CCD is made rotatable by the choice of α. If the cube is replicated n_c times and the star, n_s times, then, $\alpha = \{n_c f / n_s\}^{1/4}$ yields a rotatable CCD, where $f = 2^{k-q}$ is the number of factorial points in the design. In this study, we evaluate the prediction capability and stability of the CCD when $\alpha = \{n_c f / n_s\}^{1/4}$ by replicating the cube and star portions of the CCD. The

E-mail: eugene.ukaegbu@unn.edu.ng, polycarp.chigbu@unn.edu.ng

choice of optimality criteria and graphical procedure (that will be discussed in later sections) enhanced this evaluation. Full factorial portion of the CCD is used for k = 3, 4 and 5 factors. With the number of factors moderately increasing, one-half fraction of the factorial portion is considered for k = 6 and 7 factors while one-quarter fraction is considered for k = 8, 9 and 10 factors. Each design option is augmented with $n_0 = 3$ centre points.

2. The Prediction Variance

In fitting the second-order design, the second-order model for describing the relationship between the response, y, and the variables, $x_1, x_2, \ldots, x_k$, is

$$y(\mathbf{x}) = \beta_0 + \mathbf{x}'\boldsymbol{\beta} + \mathbf{x}'\mathbf{B}\mathbf{x} + \mathbf{e} \tag{1}$$

where β_0 is a constant, $\boldsymbol{\beta}$ is the vector of the k parameters of the linear components, $\mathbf{B}$ is a $k \times k$ matrix whose diagonal elements are coefficients of the pure quadratic terms and the off-diagonal elements are the coefficients of the mixed (interaction) terms and, $\mathbf{e}$ is the random error that is normally distributed with mean, zero and variance, σ^2. For a point, $\mathbf{x}$, in the design space, the prediction variance is

$$V\{\hat{y}(\mathbf{x})\} = \sigma^2 \mathbf{x}'^m (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}^m, \tag{2}$$

where $\mathbf{x}^m = \left[x_0, x_1, \ldots, x_k; x_1^2, \ldots, x_k^2; x_1x_2, \ldots, x_{k-1}x_k\right]$ is a point in the design space expanded to model form and $\mathbf{X}$ is the $N \times p$ expanded design matrix derived from the $N \times k$ design matrix. Each row in $\mathbf{X}$ denotes an experimental observation such that the total number of rows in $\mathbf{X}$ represent the total number of design runs, N, while the total number of columns represent the total number of parameters.

The prediction variance is scaled by multiplying by N and dividing by the process variance, σ^2, so that the scaled prediction variance (SPV) is

$$\frac{NV\{\hat{y}(\mathbf{x})\}}{\sigma^2} = N\mathbf{x}'^m (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}^m. \tag{3}$$

The scaling is used to facilitate comparison among various competing designs and penalizes larger designs. It is believed that scaling will help the experimenter ascertain if there is substantial decrease in prediction variance by additional run considering the cost, represented by N, of additional design run. However, some practitioners prefer the unscaled (standardized) prediction variance (UPV),

$$\frac{V\{\hat{y}(\mathbf{x})\}}{\sigma^2} = \mathbf{x}'^m (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}^m, \tag{4}$$

in design evaluation and comparison. The quality of the design is not considered to be a function of the cost in using UPV as opposed to using SPV. In their works, [13] [14] and [6] discussed in details, the reasons why the UPV should be the ideal choice for design comparison in practical situations. Furthermore, [14] argued that larger designs often lead to smaller prediction variances and provide the experimenter with more useful information than scaling the prediction variance. In this study, we explore the advantages of UPV and SPV throughout the entire design space using FDS plots. The results presented here will help the practitioner to decide which option to adopt, to scale or not to scale.

3. Numerical And Graphical Methods of Evaluation

In this section, we discuss briefly, the concepts of the three optimality criteria and the graphical technique that were used for the comparisons.

A. Optimality Criteria

The D-efficiency, G-efficiency and V-criterion are the three optimality criteria used in evaluating the various design options in this study. The D-efficiency is given by

$$D = 100 \times |\mathbf{X}'\mathbf{X}|^{1/p} / N, \tag{5}$$

where $|\mathbf{X}'\mathbf{X}|$ is the determinant of the information matrix, $\mathbf{X}'\mathbf{X}$, of the design. The G-efficiency is given by

$$G = \frac{100p}{N \max V\{\hat{y}(\mathbf{x})\}/\sigma^2}. \tag{6}$$

The V-criterion minimizes the normalized average integrated prediction variance and is defined as

$$V = \min \frac{N}{\psi} \int_R V\{\hat{y}(\mathbf{x})\} d\mathbf{x}, \tag{7}$$

where $\psi = 2^k$ and R is the region of interest. See [15] and [8] for detailed discussions on the relevance of these optimality criteria in design evaluation and comparison. We shall develop exact G-efficiency and V-criterion for the replicated portions of the CCD.

B. Fraction of Design Space Plots

Single-value criteria, like those defined above, do not completely reflect the characteristics of the prediction variance of the design. Therefore, graphical display of the prediction variance of the design across the design space is more informative. One of such graphical methods is the fraction of design space (FDS) plot. The works of [16] introduced the FDS plot. The FDS plots have been used extensively in robust design studies and evaluations: see, for example, [17], [18], [19], [20] and [21]. According to [19], the graphs allow for comparison of scaled and unscaled prediction variances of competing designs for any fraction of the design space, showing which design is dominant with smaller prediction variance for all fractions of the design space. Small values of SPV or UPV are seen as lines close to the horizontal axis on the FDS plot. The flatter the graph, the stronger the stability and prediction capability of the design. The FDS graphs will be plotted for the scaled and unscaled prediction variances in this study.

C. Exact G- and V-optimality Criteria

[3], [4] and [22] strongly recommend the choice of exact optimality criteria for design evaluation since the exact value is more reliable than the average prediction variance provided by many statistical software packages. [22] argues that statistical software packages merely provide approximate results rather than the exact values, leading to poor design evaluation. In this study, we propose computational formulae for obtaining exact G- and V-optimality criteria when the cube or star or both cube and star portions of the CCD are replicated. [4] have already proposed exact G- and V-optimality criteria that are based on replication of the centre points alone for reduced models in the hypercube. However, the formulae proposed in this study accommodate the appropriate replication of the centre point for the CCD. We now give the exact V- and G-optimality for the three cases under consideration. MATLAB software 2008a was used extensively in doing the necessary matrix algebra that gave rise to the desired results after very tedious algebra.

Case One: Only the star is replicated

When only the star portion of the CCD is replicated n_s times, the V-criterion is

$$V_1 = N_1\left\{\mathbf{\Delta}_{11} + \frac{2k\mathbf{\Delta}_{21}}{3} + \frac{k}{3\left(f+2n_s\alpha^2\right)} + \frac{k}{45 n_s\alpha^4 Q_1}\left[9n_s N_1\alpha^4 + 2(k-1)\rho_1\right] + \frac{k(k-1)}{18f}\right\}, \tag{8}$$

where $N_1 = f + 2n_s k + n_0$, $\mathbf{\Delta_{11}} = \left(kf + 2n_s\alpha^4\right)/Q_1$, $Q_1 = 2n_s N_1\alpha^4 + k\rho_1$, $\rho_1 = N_1 f - \left(f+2\alpha^2\right)^2$, $\mathbf{\Delta_{21}} = -\left(f+2n_s\alpha^2\right)/Q_1$. The G-efficiency is given by

$$G_1 = \frac{100p}{\max V_1\{\hat{y}(\mathbf{x})\}}, \tag{9}$$

where

$$V_1\{\hat{y}(\mathbf{x})\} = N_1\left\{\mathbf{B}_{01} + \mathbf{B}_{11}\sum_{i=1}^{k} x_i^2 + \mathbf{B}_{21}\sum_{i=1}^{k} x_i^4 + \mathbf{B}_{31}\sum_{i<j}^{\binom{k}{2}} x_i^2 x_j^2\right\}, \tag{10}$$

$\mathbf{B}_{01} = \mathbf{\Delta}_{11}$, $\mathbf{B}_{11} = \left[\frac{1}{f+2n_s\alpha^2} - \frac{2\left(f+2n_s\alpha^2\right)}{Q_1}\right]$, $\mathbf{B}_{21} = \frac{1}{2n_s\alpha^4 Q_1}\left[2n_s N_1\alpha^4 + (k-1)\rho_1\right]$ and $\mathbf{B}_{31} = \left[\frac{1}{f} - \frac{\rho_1}{n_s\alpha^4 Q_1}\right]$.

Case Two: Only the cube is replicated

The *V*-criterion when only the cube is replicated n_c times is given by

$$V_2 = N_2\left\{\boldsymbol{\Delta}_{12} + \frac{2k\boldsymbol{\Delta}_{22}}{3} + \frac{k}{3\left(F+2\alpha^2\right)} + \frac{k}{45\alpha^4 Q_2}\left[9N_2\alpha^4 + (k-1)\rho_2\right] + \frac{k(k-1)}{18F}\right\}, \tag{11}$$

where $N_2 = F + 2k + n_0$, $F = n_c f$, $\boldsymbol{\Delta_{12}} = \left(kF + 2\alpha^4\right)/Q_2$, $Q_2 = 2N_2\alpha^4 + k\rho_2$, $\rho_2 = N_2F - \left(F+2\alpha^2\right)^2$, $\boldsymbol{\Delta_{22}} = -\left(F+2\alpha^2\right)/Q_2$. The *G*-efficiency is given by

$$G_2 = \frac{100p}{\max V_2\{\hat{y}(\mathbf{x})\}}, \tag{12}$$

where

$$V_2\{\hat{y}(\mathbf{x})\} = N_2\left\{\mathbf{B}_{02} + \mathbf{B}_{12}\sum_{i=1}^{k} x_i^2 + \mathbf{B}_{22}\sum_{i=1}^{k} x_i^4 + \mathbf{B}_{32}\sum_{i<j}^{\binom{k}{2}} x_i^2 x_j^2\right\}, \tag{13}$$

$$\mathbf{B}_{02} = \boldsymbol{\Delta}_{12},\ \mathbf{B}_{12} = \left[\frac{1}{F+2\alpha^2} - \frac{2\left(F+2\alpha^2\right)}{Q_2}\right],\ \mathbf{B}_{22} = \frac{1}{2\alpha^4 Q_2}\left[2N_2\alpha^4 + (k-1)\rho_2\right] \text{ and } \mathbf{B}_{32} = \left[\frac{1}{F} - \frac{\rho_2}{\alpha^4 Q_2}\right].$$

Case Three: The Cube and Star are replicated

If the cube is replicated n_c times and the star, simultaneously replicated n_s times, then the *V*-criterion is given by

$$V_3 = N_3\left\{\boldsymbol{\Delta}_{13} + \frac{2k\boldsymbol{\Delta}_{23}}{3} + \frac{k}{3\left(F+2n_s\alpha^2\right)} + \frac{k}{45n_s\alpha^4 Q_3}\left[9n_sN_3\alpha^4 + 2(k-1)\rho_3\right] + \frac{k(k-1)}{18F}\right\}, \tag{14}$$

where $\boldsymbol{\Delta_{13}} = \left(kF + 2n_s\alpha^4\right)/Q_3$, $Q_3 = 2n_sN_3\alpha^4 + k\rho_3$, $\rho_3 = N_3F - \left(F+2n_s\alpha^2\right)^2$, $\boldsymbol{\Delta_{23}} = -\left(F+2n_s\alpha^2\right)/Q_3$

The *G*-efficiency is given by

$$G_3 = \frac{100p}{\max V_3\{\hat{y}(\mathbf{x})\}}, \tag{15}$$

where

$$V_3\{\hat{y}(\mathbf{x})\} = N_3\left\{\mathbf{B}_{03} + \mathbf{B}_{13}\sum_{i=1}^{k} x_i^2 + \mathbf{B}_{23}\sum_{i=1}^{k} x_i^4 + \mathbf{B}_{33}\sum_{i<j}^{\binom{k}{2}} x_i^2 x_j^2\right\}, \tag{16}$$

$$\mathbf{B}_{03} = \boldsymbol{\Delta}_{13},\ \mathbf{B}_{13} = \left[\frac{1}{F+2n_s\alpha^2} - \frac{2\left(F+2n_s\alpha^2\right)}{Q_3}\right],\ \mathbf{B}_{23} = \frac{1}{2n_s\alpha^4 Q_3}\left[2n_sN_3\alpha^4 + (k-1)\rho_3\right] \text{ and } \mathbf{B}_{33} = \left[\frac{1}{F} - \frac{\rho_3}{n_s\alpha^4 Q_3}\right].$$

These mathematical expressions can be programmed into any statistical software to obtain the exact *G*- and *V*-optimality criteria .

4. Design Evaluations And Comparison

In this section, we compare the results obtained by evaluating the replicated options of the CCD using the three alphabetic optimality criteria and fraction of design space plots. The comparisons of designs proceed as follows: in section 5.1, we define the pattern of replication adopted for the evaluation, in section 5.2, comparisons of the various replicated options of the CCD are made using the optimality criteria while in section 5.3, graphical evaluations and comparisons are made.

A. Replication of the CCD

The first replicated option of the CCD is where the cube is replicated twice and the star not replicated. This design option is denoted by C_2S_1. The second design option is where the star is replicated twice and the cube is not replicated, denoted by C_1S_2. Other replicated options are C_3S_1, C_1S_3, C_4S_1 and C_1S_4. These designs are compared together with the traditional version, C_1S_1, where only the centre point is replicated. These seven options of the CCD are all augmented with $n_0 = 3$ centre points and compared using the optimality criteria and FDS plots.

B. Comparison Using Optimality Criteria

The results of the alphabetic optimality criteria for the seven options of the CCD are summarized in Table 1. The results show that, for all the *k* variables under consideration, higher replication of the cube increases the *D*-efficiency of the CCD. Replicating the cube increases α, making it possible for the designs to be evaluated at points closer to the

Table 1: Summary of Design Optimality Criteria

K	*p*	Design	*N*	α	*D*-eff	*G*-eff	*V*-criteion
3	10	C_2S_1	25	2.0000	83.53	136.00	5.6125
		C_1S_2	23	1.4142	53.63	165.22	5.3314
		C_3S_1	33	2.2134	91.86	134.62	5.6628
		C_1S_3	29	1.2779	45.35	180.77	5.4623
		C_4S_1	41	2.3784	97.26	142.04	5.4779
		C_1S_4	35	1.1892	39.66	200.67	5.6714
		C_1S_1	17	1.6818	41.30	177.16	5.4971
4	15	C_2S_1	43	2.3784	90.78	136.57	8.0865
		C_1S_2	35	1.6818	62.13	167.79	7.3539
		C_3S_1	59	2.6322	97.94	148.94	7.6586
		C_1S_3	43	1.5197	53.20	204.35	7.0765
		C_4S_1	75	2.8284	100.00	166.67	7.1250
		C_1S_4	51	1.4142	46.78	245.10	7.0890
		C_1S_1	27	2.0000	76.44	166.79	7.2000
5	21	C_2S_1	77	2.8284	97.69	151.95	8.9429
		C_1S_2	55	2.0000	72.27	136.36	9.0521
		C_3S_1	109	3.1302	103.27	184.52	7.8184
		C_1S_3	65	1.8072	63.55	180.19	7.3464
		C_4S_1	141	3.3636	106.46	214.31	7.0576
		C_1S_4	75	1.6818	56.92	234.90	6.3065
		C_1S_1	45	2.3784	85.64	145.75	8.9682
6	28	C_2S_1	79	2.8284	93.83	141.77	14.0153
		C_1S_2	59	2.0000	67.49	237.29	10.9457
		C_3S_1	111	3.1302	99.71	166.64	12.6258
		C_1S_3	71	2.1491	58.07	339.40	10.2708
		C_4S_1	143	3.3636	103.18	196.96	11.3608
		C_1S_4	83	1.6818	51.04	435.59	10.4258
		C_1S_1	47	2.3784	81.41	180.48	12.1112
7	36	C_2S_1	145	3.3636	100.33	177.15	15.3302
		C_1S_2	95	2.3784	78.82	144.07	17.4405
		C_3S_1	209	3.7224	104.51	231.62	12.9993
		C_1S_3	109	2.1491	70.59	223.93	13.9689
		C_4S_1	273	4.0000	106.79	276.92	11.7361
		C_1S_4	123	2.0000	63.97	321.95	12.5407
		C_1S_1	81	2.8284	90.61	143.21	17.5616
8	45	C_2S_1	147	3.3636	97.86	159.07	20.2443
		C_1S_2	99	2.3784	75.64	236.19	16.5216
		C_3S_1	211	3.7224	102.29	210.27	16.9609
		C_1S_3	115	2.1491	66.72	385.81	14.2918
		C_4S_1	275	4.0000	104.75	285.55	15.0127
		C_1S_4	131	2.0000	59.67	542.75	13.9614
		C_1S_1	83	2.8284	87.87	162.65	19.9353

9	55	C_2S_1	277	4.0000	102.95	236.46	19.0762
		C_1S_2	167	2.8284	85.97	110.78	31.0234
		C_3S_1	405	4.4267	105.78	317.96	16.1704
		C_1S_3	185	2.5558	79.07	187.96	22.2146
		C_4S_1	533	4.7568	107.27	379.37	14.7884
		C_1S_4	203	2.3784	73.23	301.51	18.0602
		C_1S_1	149	3.3636	95.70	146.67	25.7885
10	66	C_2S_1	535	4.7568	105.96	364.85	17.8845
		C_1S_2	299	3.3636	93.88	78.92	48.3387
		C_3S_1	791	5.2643	107.61	461.34	16.0220
		C_1S_3	319	3.0393	88.33	68.08	53.6483
		C_4S_1	1047	5.6569	108.46	527.41	15.1358
		C_1S_4	339	2.8284	81.66	110.32	36.2374
		C_1S_1	279	3.1623	86.97	212.90	52.2161

extremes of the design space than to the centre of the design space. This, consequently, results in increase in the *D*-efficiency as designs are evaluated close to the extremes of the design region.

For k = 3, 100% *D*-efficiency is not achieved at C_4S_1, though the *D*-efficiency at this point is 97.26%, which is close to 100%. However, 100% *D*-efficiency is achieved at C_4S_1 for k = 4, at C_3S_1 for k = 5, and at C_2S_1 for k = 7. This indicates that the higher the number of variables, the easier it becomes to achieve *D*-efficiency with minimal replication of the cube. It could be observed that higher replications of the cube, for moderately large number of factors, yield *D*-efficiencies greater than 100%, what may be referred to as super *D*-efficiency. However, this is achieved at the cost of very high number of design runs. Again, these super *D*-efficiencies are achieved at very high α values that may appear impractical for some experiments. For instance, for k = 9, C_3S_1 has *D*-efficiency value of 105.78% at α = 4.4267. Considering the remaining points of the design, which are between -1 and +1 for any factor, it is obvious that this α value may not be feasible in many experiments. The design option, C_1S_1, tend to moderate the value of α but this does not achieve the desirable *D*-efficiency except for k = 9 where C_1S_1 is 95.70 *D*-efficient.

On the other hand, none of the star-replicated options is *D*-efficient. In fact, the higher the replication of the star portion, the smaller the *D*-efficiency. This is due to the fact that higher replication of the star results in decrease in the value of α, leading to evaluation of the designs at points closer to the centre of the design space. The smaller the α value, the smaller the *D*-efficiency. In general, replicating the star portion reduces the *D*-efficiency of the CCD.

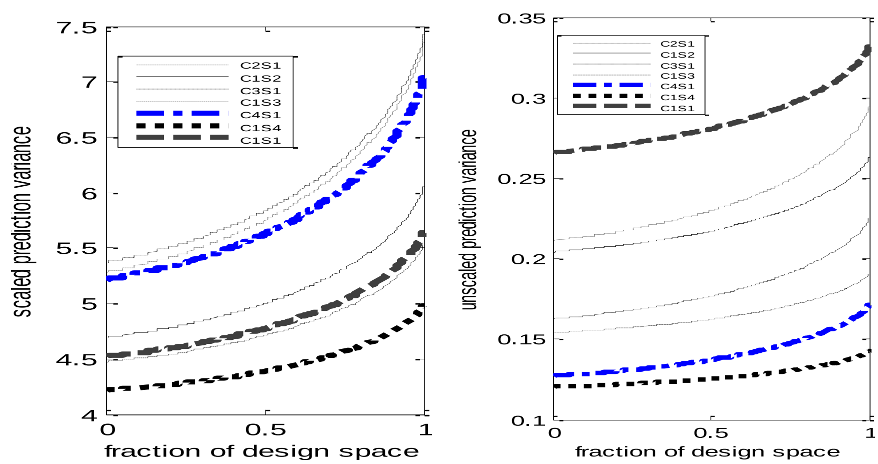
Table 1 has also shown that replicating either the cube or star portions improves the *G*-efficiency of the CCD. However, the *G*-efficiency values of the star-replicated CCD are better than those of the cube-replicated options for k = 3 to 8 factors. These results are reflected in the FDS plots for the scaled prediction variances in Figures 1 to 6 where the higher star-replicated options, C_1S_3 and C_1S_4, have better stable minimum scaled prediction variance than the cube-replicated options and C_1S_1. These results are achieved as the α values get closer to the centre of the design region as replication of the star increases. Contrarily, the *G*-efficiency of the replicated-cube options for k = 9 and 10 are superior to those of the star options for the same number of factors. This could be observed in Figures 7 and 8 where the FDS plots for k = 9 and 10 factors have the smallest and stable SPV that are distributed throughout the entire design space for C_3S_1 and C_4S_1.

The results in Table 1 further reveal that no design option is consistently superior in terms of the *V*-criterion. The design with the smallest average prediction variance is considered the best among the competing designs. For k = 3, the design option, C_1S_2, with the smallest *V*-criterion value is the better design than the others under this criterion. For k = 4 and 6, C_1S_3 has the best *V*-values that are very close to those of C_1S_4. The design option, C_1S_4, has the best values and considered the best design option for k = 5 and 8 factors in terms of the *V*-criterion. Relating this result to the plots in Figures 3 and 5, it could be observed that C_1S_4 maintained the smallest SPV for the entire design region. The cube-replicated option, C_4S_1, provides the best *V*-criterion values for k = 7, 9 and 10. This is obvious in Figures 7 and 8 for k = 9 and 10 factors, respectively, where this design option displays the lowest and smallest SPV throughout the design region.

Table 1 has shown that replicating the cube portion of the CCD improves the *V*-criterion for all the factors under consideration. This indicates that the *V*-criterion for the replicated-cube options get better as the axial distance gets closer to the extremes of the design space. However, the *V*-criterion for the replicated-star options gets better as the number of factors increases. This explains why, for the star-replicated options, C_1S_2 is the best for k = 3, C_1S_3 is the best for k = 4 and C_1S_4 is the best for k = 5, 6, 7, 8, 9 and 10 factors.

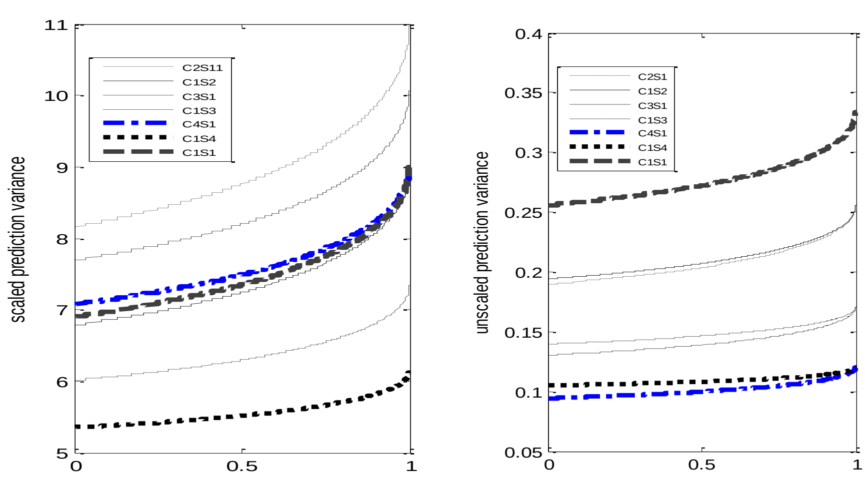
C. Comparison Using Graphs

The FDS plots are displayed in Figures 1-8 for both the scaled and unscaled prediction variances and for all the k number of factors under consideration. Generally, the graphs show that the prediction variances of the designs get better with replication as the higher replicated options displayed the smallest prediction variance (scaled or unscaled). The replicated-star option, C_1S_4, displayed the smallest and most stable SPV for k = 3, 4, 5, 6, 7 and 8 in Figures 1(a), 2(a), 3(a), 4(a) 5(a) and 6(a), respectively. This indicates that replicating the star tends to improve the scaled prediction variance of the rotatable CCD for the stated k number of factors. However, for Figures 7(a) and 8(a), the replicated-cube option, C_4S_1, display the smallest and most stable SPV throughout the entire design space, making the C_4S_1 the best choice in predicting responses for k = 9 and 10 factors.



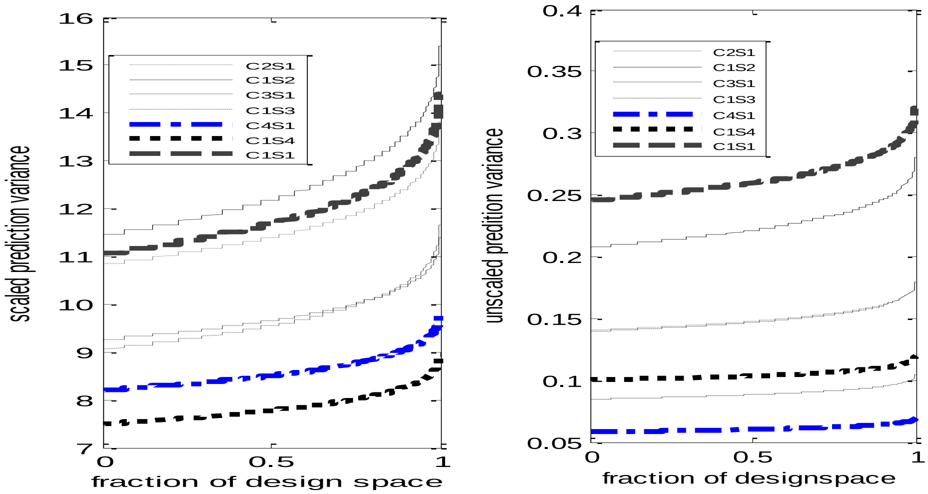
(a) (b)

Figure 1: (a) SPV and (b) UPV for Three-Factor Rotatable CCD.



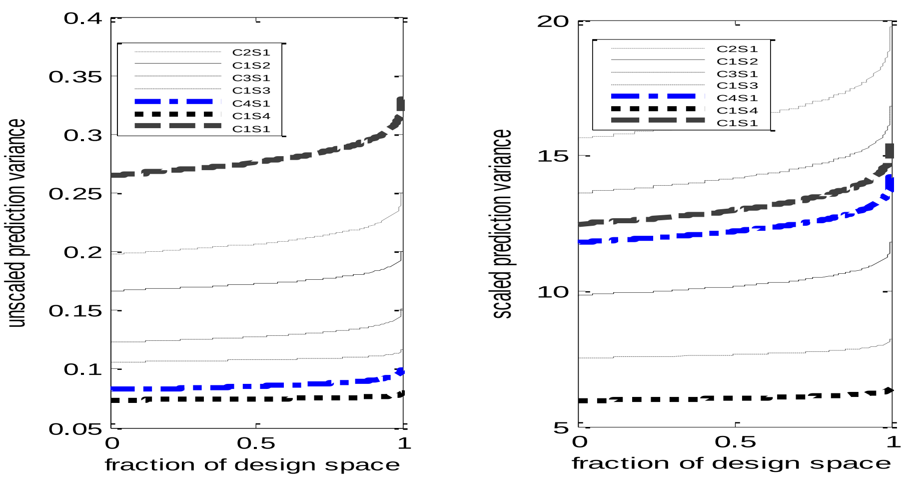
(a) (b)

Figure 2: (a) SPV and (b) UPV for Four-Factor Rotatable CCD.



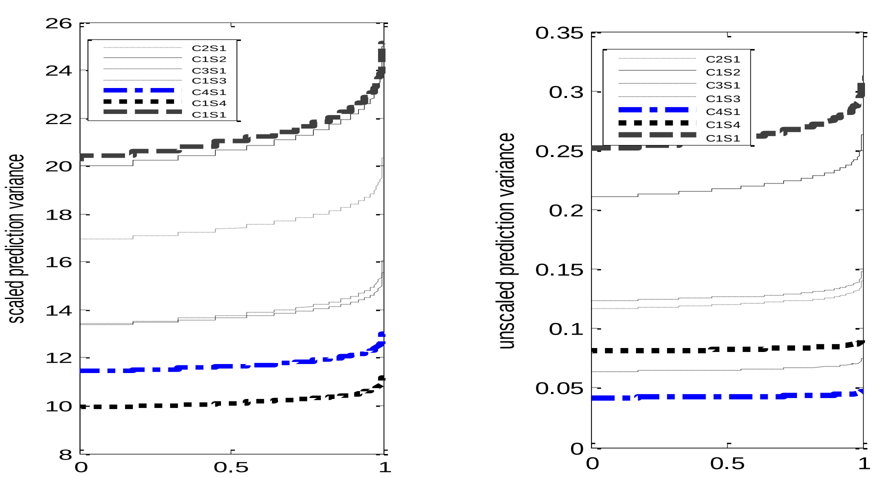
(a) (b)

Figure 3: (a) SPV and (b) UPV for Five-Factor Rotatable CCD



(a) (b)

Figure 4: (a) SPV and (b) UPV for Six-Factor Rotatable CCD



(a) (b)

Figure 5: (a) SPV and (b) UPV for Seven-Factor Rotatable CCD

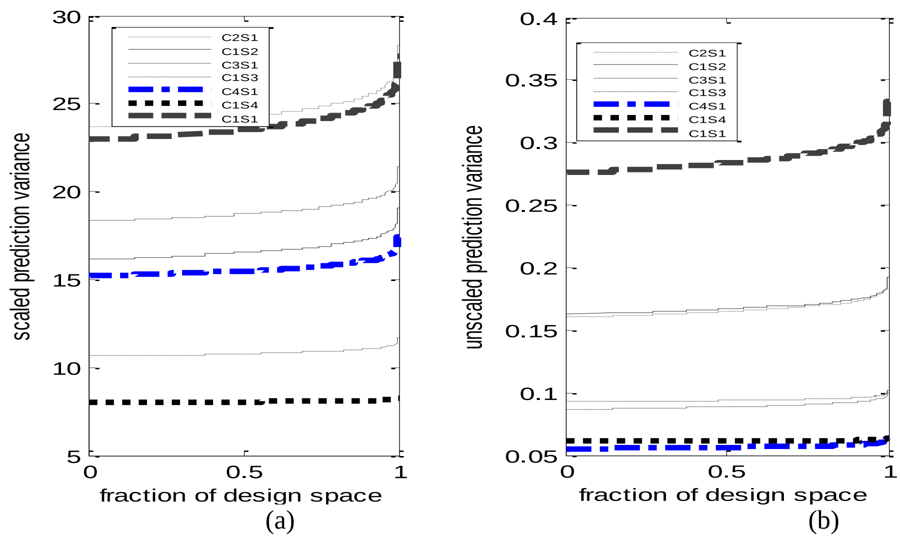


Figure 6: (a) SPV and (b) UPV for Eight-Factor Rotatable CCD

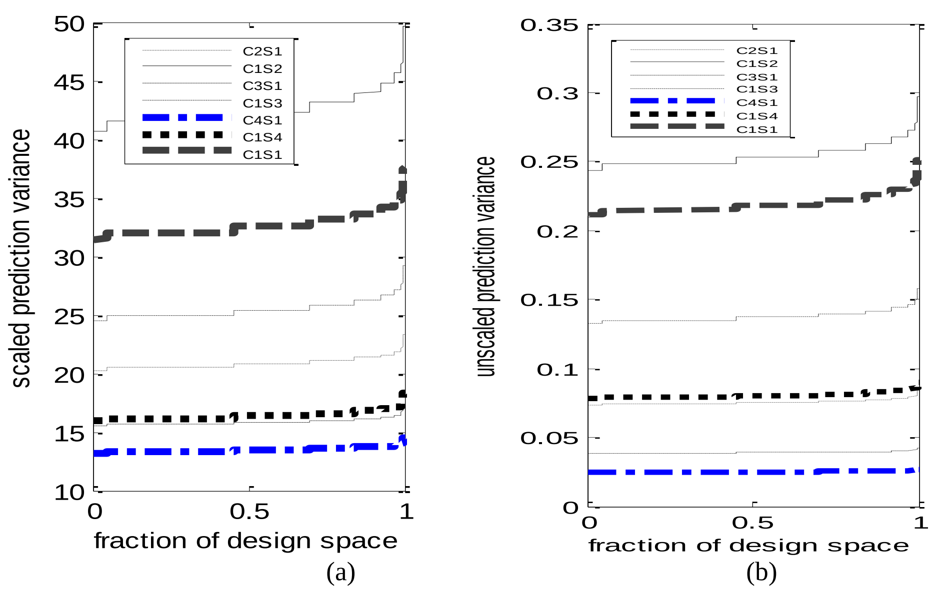


Figure 7: (a) SPV and (b) UPV for Nine-Factor Rotatable CCD

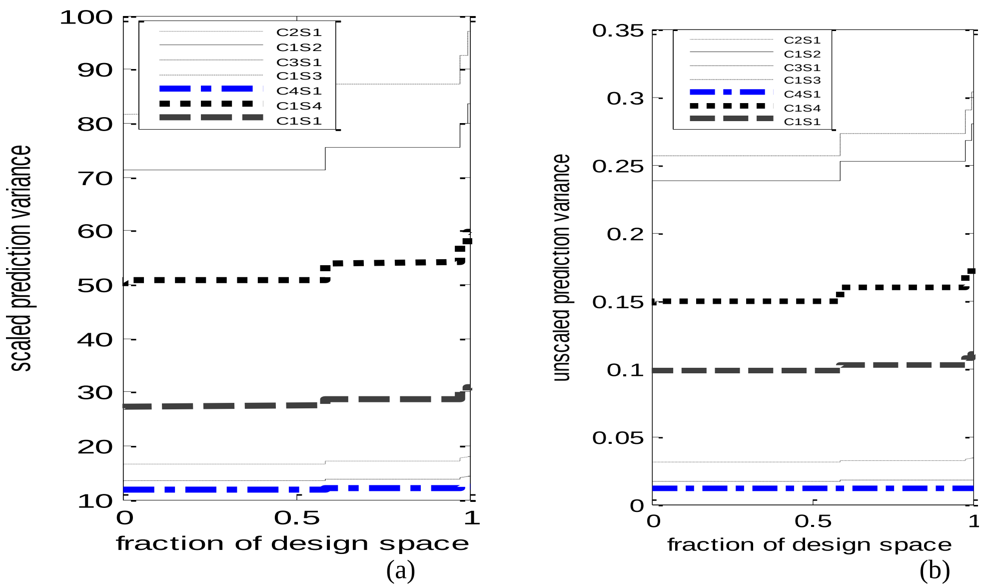


Figure 8: (a) SPV and (b) UPV for Ten-Factor Rotatable CCD

Figures 1(b) and 4(b) show that C_1S_4 has the smallest UPV spread across the entire design region for *k* = 3 and 6 factors than the other replicated options. However, C_4S_1 has the best spread of small UPV for *k* = 4, 5, 7, 8, 9 and 10 factors as shown in Figures 2(b), 3(b), 5(b), 6(b), 7(b) and 8(b). The cost of experimentation, represented by the number of runs, *N*, really influenced the performances of these design options for some of the factors. Figures 2(b), 3(b), 5(b) and 6(b) portray the fact that if the cost of experimentation is not considered, C_4S_1 performs better than the other replicated options in terms of stability and minimum prediction variance.

The choice of plotting the SPV or UPV is very important since comparisons are being made among designs of various sizes. If the experimenter is interested in obtaining efficient designs while considering the cost of adding extra run to increase precision of prediction by reducing the prediction variance, plotting the SPV is preferable. In this case, C_1S_4 is recommended for *k* = 3, 4, 5, 6, 7 and 8 factors for the rotatable CCD while C_4S_1 is recommended for *k* = 9 and 10 factors. Plotting the UPV is a better alternative if the experimenter is not restricted by cost but desires design with high precision for prediction irrespective of the design sample size. The various plots show that larger design runs yield smaller prediction variance since C_4S_1 and C_1S_4, the higher replicated cube and star options with high number of runs, respectively, continuously yield small prediction variances. For the choice of plotting UPV, C_1S_4 is recommended for *k* = 3 and 6 factors while C_4S_1 is recommended for *k* = 4, 5, 7 8, 9 and 10 factors for the rotatable CCD.

5. CONCLUSIONS

Replicating the cube and star portions of the CCD has offered the opportunity to assess the characteristics of the prediction variance of the CCD for predicting responses when the choice of α gives the advantage of having equal variance of prediction round the design at any given point. The results have shown that if the practitioner is interested in *D*-efficient designs, replicating the cube is recommended since all the replicated-cube options are *D*-efficient. Since cost of experimentation could be a discouraging factor, then C_2S_1 may be desirable. However, where the user could afford extra design runs, C_3S_1 and C_4S_1 are ideal. The user is also advised on the use of C_3S_1 and C_4S_1 for larger number of factors as the *D*-efficiency of these design options are estimated at relatively impractical α levels.

None of the seven design options considered in this study has shown any consistent superiority over the others when assessed using the *G*-efficiency, *V*-criterion and FDS plots. For some factors, replicating the star is more advantageous while for other factors, replicating the cube is more advantageous. The choice of plotting the scaled or unscaled prediction variance for proper design evaluation is left for the practitioner based on the priorities as regards cost and desire for minimum variance for prediction.

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