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OPTIMAL PREDICTION VARIANCE CAPABILITIES OF INSCRIBED CENTRAL COMPOSITE DESIGNS

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ABSTRACT: *This study looks at the effects of replication on prediction variance performances of inscribe central composite design especially those without replication on the factorial and axial portion (ICCD1), inscribe central composite design with replicated axial portion (ICCD2) and inscribe central composite design whose factorial portion is replicated (ICCD3). The G-optimal, I-optimal and FDS plots were used to examine these designs. Inscribe central composite design without replicated factorial and axial portion (ICCD1) has a better maximum scaled prediction variance (SPV) at factors k = 2 to 4 while inscribe central composite design with replicated factorial portion (ICCD3) has a better maximum and average SPV at 5 and 6 factor levels. The fraction of design space (FDS) plots show that the inscribe central composite design is superior to ICCD3 and inscribe central composite design with replicated axial portion (ICCD2) from 0.0 to 0.5 of the design space while inscribe central composite design with replicated factorial portion (ICCD3) is superior to ICCD1 and ICCD2 from 0.6 to 1.0 of the design space for factors k = 2 to 4.*

KEY WORDS: Inscribe Central Composite Design, Scaled Prediction Variance, Fraction of Design Space

INTRODUCTION

The inscribed central composite design (ICCD) is a design that enables one to study the full ranges of the experiment variables while excluding non-allowable operating conditions at one or more of the extremes of the design region. It is used when the region of operability coincides with the region of interest. The factorial points of ICCD according to Verseput (2001), are brought into the interior of the design space and set at a distance from the centre point that preserves the proportional distance of the factorial points to the axial points. The prediction variance stability and capability of CCD performance when replication is at the axial and factorial portion has been of interest to many scholars of second order design. Replication being one of the basic principles of design of experiment help researchers to provide increased precision and to obtain an estimate of the experimental error. Replication has been variously applied by many researchers in the study of central composite design. Dykstra Jr (1960), considered the replication of the factorial and axial portion of rotatable central composite and orthogonal central composite designs for factors $k = 2$, 3,…, 8. His results show that replicating the axial portion of both designs have a better potential for improved precision of prediction than replicating the factorial portion. Some second order design prediction capability was studied by Zahran *et al* (2003). They used fraction of design space (FDS). Their plots revealed that the CCD with three center points was superior to other designs. The prediction variance properties by Park *et al* (2005) assessed some second-order designs for cuboidal regions using the G- and I-optimality criteria. They recommended the G-efficient design over any other standard design presented in their work and recommend Face centered cube (FCC) and Hoke designs for small number of design variables. Chigbu, *et al* (2009), in the spherical region, compared prediction variance performance of central composite design, minimum resolution *v* design and small composite design. Their conclusion is that central composite design has a better prediction variance over minimum resolution *v* designs and small composite design. The partially replicated factorial and axial portions of the rotatable central composite and orthogonal central composite designs was evaluated by Chigbu and Ohaegbulem (2011) using the D-optimality criterion. In their conclusion, they pointed out that replicating the factorial portion enhances the D-optimality performance of both central composite designs better than the replicating the axial portion. The fraction of design space and variance dispersion graph were used by Ukaegbu and Chigbu (2014), to study the prediction capabilities of partially replicated orthogonal central composite design in a spherical region. They pointed out that replicating the axial portions of the orthogonal central composite design by far reduces the prediction variance, thus improving the G-efficiency in the spherical region. Also Ukaegbu and Chigbu (2015) considered variations of partially replicated central composite designs in the hypercube using the G- and I-optimality criteria as well as the fraction of design space plots. They concluded that the replicated-star options always give smaller *G*- and *I*-optimal values than the corresponding replicated-cube options with equal number of replications. Umelo-Ibemere and Amuji (2015) used quantile plots to compare the prediction variance of partially replicated face center cube and rotatable central composite design. They concluded that the performance of the factorial with replicated axial points in both design is preferred to the replicated factorial portion with one axial portion. Even where the replicated factorial plus one axial portion perform better than the one factorial plus replicated axial portion, the latter still show a pronounced superiority as one moves towards the design perimeter. Sümeyra *et al* (2016) applied inscribe central composite design for modeling and optimization of marble quality. Fujiwara and Matsuura (2019) studied prediction variance of a central composite design with missing observation, they derived an expression for the inflation amount of the prediction variance. This derived expression showed that rotatable central composite design inflation amount of the prediction variance depends only on the Euclidean norms and the inner product of the two vectors of factor values at which the observation is missing and the response is predicted. Giovannitti-Jensen and Myers (1989), Borkowski (1995), Montgomery (2005), Anderson-Cook et al (2009) have highlighted the benefits of scaled prediction variance in model assessment of second order designs. The G- and I-optimality criteria are prediction variance oriented which are single number criteria. Single number criteria, may not reflect the prediction variance characteristics of a design. Zahran *et al* (2003) fraction of design space plot is an alternative to single-number criteria. The FDS plot shows the characteristics of the prediction variance in the entire design space and the characteristics of scaled prediction variance (SPV) in a multidimensional region of a single two-dimensional graph with a single curve.

In this work, the G- and I-optimality criteria as well as the fraction of design space plots were used to compare partially replicated variation of the inscribe central composite design which are the inscribe central composite design with replicated factorial portion plus one axial portion (ICCD3), the inscribe central composite design with replicated axial portion (ICCD2) and the inscribe central composite without replicated factorial and axial portion (ICCD1).

Model Development

Table 1: Design Matrix of Inscribe Central Composite Design for $K = 2$

$$
X = \begin{array}{l}
\begin{array}{cccccc} x_0 & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{array} \\
\left.\begin{array}{cccccc}
1 & \frac{-1}{\alpha} & \frac{-1}{\alpha} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2} \\
1 & \frac{-1}{\alpha} & \frac{1}{\alpha} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2} & \frac{-1}{\alpha^2} \\
1 & \frac{1}{\alpha} & \frac{-1}{\alpha} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2} & \frac{-1}{\alpha^2} \\
1 & \frac{1}{\alpha} & \frac{1}{\alpha} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2}
\end{array}\right\} n_c f \\
\left.\begin{array}{cccccc}
1 & -1 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 1 & 0 & 0 \\
1 & 0 & -1 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 1 & 0
\end{array}\right\} 2kr \\
\left.\begin{array}{cccccc}
1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0
\end{array}\right\} n_0
\end{array}
$$

The relationship between the response variable y and the design variables $x_1, x_2, \cdots, x_k$, in an N-run experiment is fitted into a second-order model as

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_{ii}^2 + \sum_{j=i+1}^{k} \sum_{i=1}^{k-1} \beta_{ij} x_i x_j + \varepsilon_{ij} \tag{1}$$

Which in a matrix form is given as

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

Where Y is an N x 1 vector of responses, X is an N x p expanded design matrix. β is a vector of unknown coefficients to be estimated by least square methods from experimental data and ε is the random error term which is distributed as NID $(0, \sigma^2)$. The rows of X represent the experimental run, and the column corresponds to the experimental settings of k design variables. In the expanded design matrix X, the number of columns p, is the number of parameters in the model given as

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

However at a point x in the design space, the prediction variance is given as

$$\mathrm{var}[\hat{y}(x)] = \sigma^2 f^T(x) \left(X^T X\right)^{-1} f(x) \tag{4}$$

where $(X^T X)^{-1}$ is the variance-covariance matrix of the design matrix X, $f(x)$ is the vector of co-ordinates of point in the region of interest expanded to model form. That is, $f^T(x) = [1, x_1 \ldots, x_{k,} x_1^2, \ldots, x_k^2, x_1 x_2, \ldots x_{k-1} x_k]$ of Equation (4) is scaled by multiplying by *N*, the total number of runs, and dividing by σ^2 , the process variance. The resulting expression

$$\frac{N \operatorname{var}[\hat{y}(x)]}{\sigma^2} = Nf^T(x)(X^T X)^{-1} f(x) \qquad (5)$$

is the scaled prediction variance (SPV). This SPV gives a good measure of the precision of the estimated response at any point in the design space.

The *G*-optimality criterion minimizes the maximum scaled prediction variance (SPV). That is

$$\min\{\max N \operatorname{var} \hat{y}(x)\} \quad = \min\left\{N \max \ f^T(x)(\mathrm{X}^T \mathrm{X})^{-1} f(x)\right\} \qquad (6)$$

The *I*-optimality criterion minimizes the average SPV. That is

$$\min\{averageN \operatorname{var} \hat{y}(x)\} = \frac{1}{A} \int_R \operatorname{var}[y(x)] dx \qquad (7)$$

where A is the volume of the design space R.

Partial Replication of the Design

Let the factorial portion $f = 2^k$ replicated n_c times, the axial portion 2*k* replicated *r* times and the centre point replicated n_0 times, then the inscribed central composite design use a total of $N = 2^k n_f + 2k\text{r} + n_0$ number of observations or runs for model parameter estimation.

In this study, three versions of the inscribed central composite design (ICCD) are generated by replicating the factorial and axial portions. The first version is where the factorial and axial portion are not replicated. It is denoted as ICCD1. The second version where factorial portion is not replicated and the axial portion is replicated twice and it is denoted as ICCD2. Finally, the third version is where the factorial portion is replicated twice and the axial portion not replicated. It is denoted is as ICCD3. The number of center points used in all the versions of the ICCD in this study is three.

Comparison of the Design

The results in Table 2 show that the inscribed central composite design without replicated factorial and axial portion (ICCD1) has a better maximum scaled prediction variance (SPV) at factors *k* = 2 to 4. Also the inscribe central composite design with replicated factorial portion (ICCD3) has a better maximum SPV at 5 and 6 factor levels when half replicate of the factorial portion were used while ICCD2 has a better maximum SPV when full replicate of the factorial were used..

The average SPV of ICCD1, ICCD2 and ICCD3 are relatively the same at factors *k* = 2, 3 and 4. The ICCD3 has a better average SPV at factors *k* = 5 and 6 when half replicate of the factorial portion were used while at full replicate, all the versions of the ICCD1 are relatively the same.

The fraction of design space (FDS) plots (Figures 1 to 3) show that the inscribe central composite design (ICCD1) is superior to ICCD3 and ICCD2 from 0.0 to 0.5 of the design space while inscribe

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central composite design with replicated factorial portion (ICCD3) is superior to ICCD1 and ICCD2 from 0.6 to 1.0 of the design space for factors k = 2 to 4. The ICCD2 is superior to ICCD1 and ICCD3 at factor k = 6 (See Figure 5)

Design	***N***	**Max SPV**	**Ave. SPV**	***k***
ICCD1	11	**6.875**	5.995	2
ICCD 2	15	8.925	6.000	
ICCD 3	15	8.925	6.000	
ICCD1	17	**11.39**	9.996	3
ICCD 2	23	14.90	10.005	
ICCD 3	25	14.45	10.000	
ICCD1	27	**15.741**	15.066	4
ICCD 2	35	19.88	15.015	
ICCD 3	43	24.381	15.007	
ICCD1	45	25.290	21.015	5 (full)
ICCD 2	55	**24.200**	21.010	
ICCD 3	77	43.274	21.021	
ICCD1	29	25.520	16.037	5 (half replicate)
ICCD2	39	33.579	20.202	
ICCD 3	45	**20.295**	**14.040**	
ICCD1	79	43.687	27.966	6 (full)
ICCD 2	91	**29.757**	28.028	
ICCD 3	143	79.508	28.028	
ICCD1	47	29.657	20.21	6 (half replicate)
ICCD 2	59	36.58	23.836	
ICCD3	79	**25.438**	**18.486**	

Table 2: Summary Statistics for versions of ICCD

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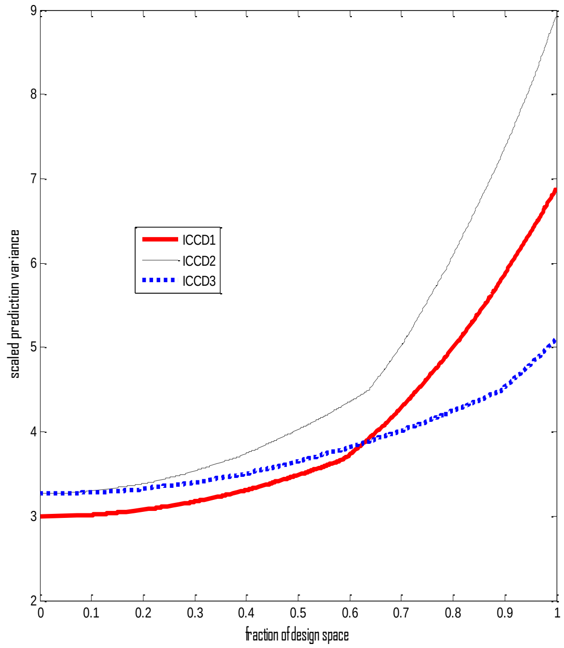

Figure 1: FDS Plot of Designs for k = 2

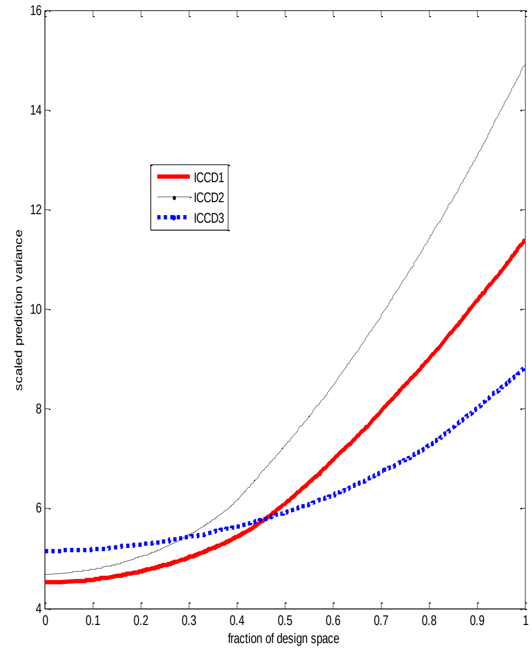

Figure 2: FDS Plot of Designs for k = 3

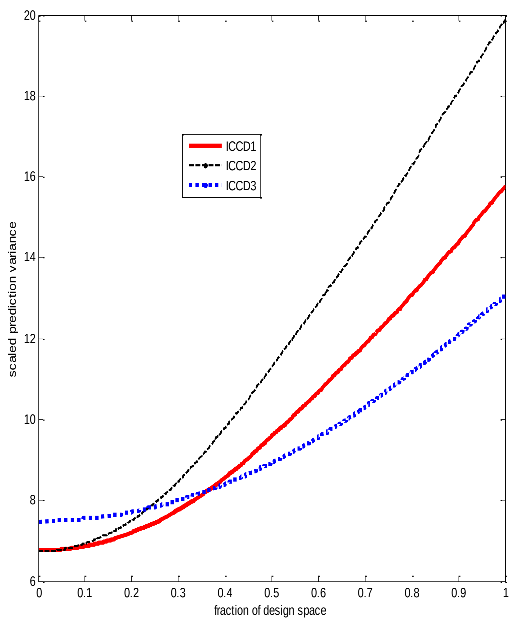

Figure 3: FDS Plot of Designs for k = 4

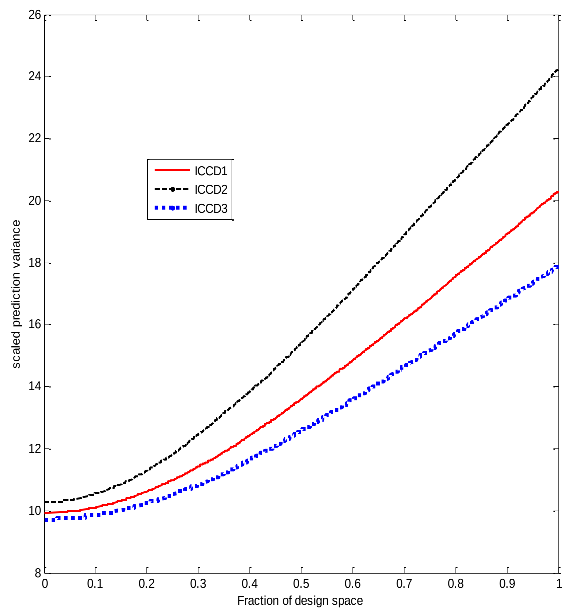

Figure 4: FDS Plot of Designs for k = 5

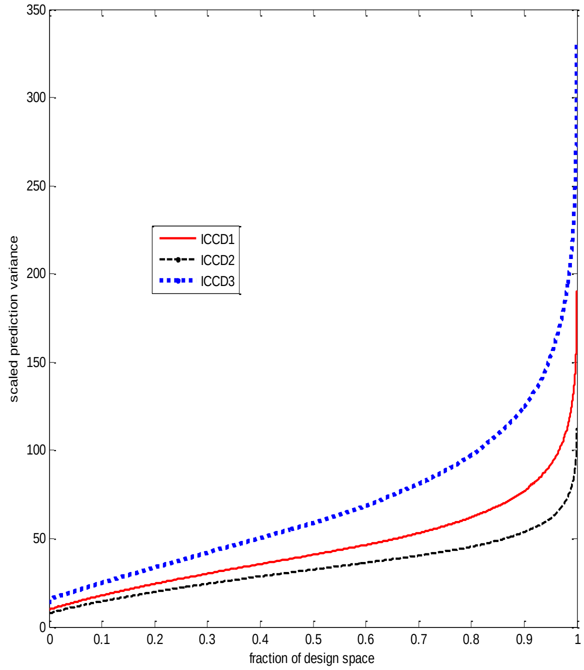

Figure 5: FDS Plot of Designs for k = 6

CONCLUSION

This work has shown how replication of any part of the inscribed central composite design affect prediction variance performance. Inscribed central composite design without replicated factorial and axial portion (ICCD1) has a better maximum scaled prediction variance (SPV) at low factor levels ($k = 2 - 4$), while inscribe central composite design with replicated factorial portion (ICCD3) has better maximum and average SPV at 5 and 6 factor levels. Also the fraction of design space (FDS) plots show that the inscribe central composite design without replicated factorial and axial portion (ICCD1) is superior to ICCD 3 and ICCD 2 from 0.0 to 0.5 of the design space while inscribe central composite design with replicated factorial portion (ICCD3) is superior to ICCD1 and ICCD2 from 0.6 to 1.0 of the design space for factors k = 2 to 4.

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