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Experiments with Replicate Runs at the Cube and Star Points of Inscribed Central Composite Designs

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Abstract

Replication has been a fundamental aspect in any design of experiment. This study looks at the impact replication have on inscribed central composite design (ICCD) when the cube and star points are replicated. The D-, A-,and G-optimality criteria were applied to find the optimal ICCD for experiments when two and three replicate runs are made at the cube and star points of the design at several levels of factor (k = 2 – 7). Results showed that Inscribed central composite design with replicated cube points (ICCD-R_F) reduces the A-optimal values of the design in all the factors of considered in the study whereas at lower factors of k (k = *2 and 3*), it also reduces the D-optimal values of the design and also increases the G-optimal values for most of the factors considered in the study. Also replication at the star points of Inscribed central composite design (ICCD-R_A) increases the A- and D-optimal values of the design in all the factors considered in the study while for G-optimality criterion, replication at the star points increases the criterion values but not in all the factor levels.

Keywords: Replication, Inscribe Central Composite Design.

1. Introduction

Replication has been one of the ways an experimenter can, through statistical design, manage extreme variability in experimental results. While this technique does not totally remove or reduce the intrinsic test result variability, but its appropriate application can immensely improve the precision of statistics applied in the estimation of factor effects.

In a process where a two-level factorial experiment is piloted, an experimenter may use the present operating condition as the center for the design and also use the square terms in the second-order model to test the linearity of the region of operability. Few runs at the center of design would be adequate to identify the quadratic effects against the hypothesis of linearity over the region of operability. On the other hand, there are moments where the parameters of the square terms are to be estimated separately. In order to do this, a second-order model is required for this estimation. To do this, more runs are required at the center, cube and star points of the design to estimate all the parameters in the second-order model. Augmenting the two level factorial design with center and $2k$ star points will be the effective solution for the problem. [3] Proposed a rotatable central composite design that plays an important role in design of experiment and also determine the axial distance value. In real life situation, an experimenter may encounter situation that need a certain number of replicate runs at the cube or star points for some reasons. To examine complete ranges of experimental variables while not including non-permissible operating conditions at some extremes design region, the inscribed central composite design (ICCD) is employed. ICCD is applied when the region of exploration matches with the region of interest. The cube portion of the inscribed central composite design (ICCD) by [14], are carried into the interior of the design space and then set at a distance from the center point that reserves the proportional distance of the factorial points to the axial points. Replication as one of the main principle of design of experiment, has helped researchers offer improved precision and also obtain an estimate of the experimental error. In response surface methodology (RSM), many experimenters have applied replication in the study of response surface design. [6], studied the effects replication on the factorial and axial points of two variations central composite design (CCD) namely rotatable central composite design and orthogonal central composite design for factors k = 2 - 8. His results show that replication at the axial points of both variations of CCD have a better potential for improved precision of prediction than replication at the factorial points of the design. Variance dispersion graphs (VDG) has been applied to study prediction capability of replicated response surface designs such as central composite design, small composite design, Box-Behnken etc. (see [7]) [4], using the D-optimality criterion, also compared partially replication of the factorial and axial points of two variations of the CCD namely rotatable central composite design and orthogonal central composite design. They concluded that replication at the factorial points enhances the D-optimality performance of both CCD better than the replication at the axial points. [11], used two types of plots namely the fraction of design space (FDS) plot and variance dispersion graphs (VDG) to study the prediction capabilities of partial replication of orthogonal CCD in a spherical region. The outcome showed that replication at the axial points of the orthogonal CCD by large extent, decreases the prediction variance, thereby enhancing the G-efficiency of the design in the spherical region. [12], applied the G- and I-optimality criteria and also included the fraction of design space (FDS) plots to study partial replication of central composite design in the hypercube region. Their results showed that the replication of the axial points produces small *G*- and *I*-optimal values when compared with replication at the cube points with equal number of replications. [8], in their study, selecting the right central composite used the D-, G- and A-optimality criteria to study five variations of the CCD. They revealed that replication of the star points decreases the D- and G-optimal values of the variations central composite design in all the factors that were examined but for A-optimality criterion it was not so. [13], applied quantile plots to study the prediction variance of partial replication of two variation of CCD namely face center cube and rotatable central composite design. They study revealed that the CCD performs better with one factorial and replicated axial points in both designs. [1], proposed a CCD for the experiments with replicate runs at design points called CCD-R. This CCD-R proved to be valuable and flexible, especially when replication are desired in the experiment. [10], also examined the effects of replication on five variations of the CCD when the model characteristics of the design are reduced using the optimality criteria. Their results revealed that replication of the axial points with increase in center points reduces the D-, A- and G-optimality criteria of the CCDs when there is non-inclusion of the square terms of the design variables while it increases the optimality criteria of some of the CCDs when non-inclusion of interaction terms of the design variables. [9], on prediction variance performance of inscribe CCD revealed that replication at the cube points of the design provides a better maximum and average scaled prediction variance at high factor level while non-replicated cube points has a better maximum and average scaled prediction variance at low factor level.

This study seeks to use the D-, A- and G-optimality criteria to find the optimal CCD for experiments with replication at cube and axial points of the design at several levels of factor (k = 2 – 7)

2. Model Development

Let a response variable γ with design variables $s_1, s_2, \cdots, s_k$, in an N number of experiment be described by a model written as

$$\gamma = \beta_0 + \sum_{i=1}^{k} \beta_i s_i + \sum_{i=1}^{k} \beta_{ii} s_{ii}^2 + \sum_{j=i+1}^{k} \sum_{i=1}^{k-1} \beta_{ij} s_i s_j + \varepsilon_{ij} \quad \rightarrow \qquad (1)$$

The above equation is a second-order equation which in matrix format is written as

$$\mathrm{Y} = \mathrm{S}\beta + \varepsilon \quad \rightarrow \qquad (2)$$

where Y denotes an N x 1 vector responses , S denotes an N x p design matrix. β denotes vector of unknown coefficients estimated using the least square method and ε is the error term that is normally and identically distributed with mean zero and variance σ^2 .

From Table 1, the rows of design matrix S denotes the number of runs of the experiment while the column denotes the k settings of design variables of the experiment. The number of columns of this k settings of design variables is denoted as p and it is the exact number of parameters in the model. It is written as

$$p = \tfrac{1}{2}(k+1)(k+2) \qquad \rightarrow \qquad (3)$$

Table 1: Coded Design Matrix of an Inscribe CCD for *K* factors

$$S = \begin{array}{c} \begin{matrix} s_0 & s_1 & s_2 & s_1^2 & s_2^2 & s_1 s_2 & \cdots s_{k-1}s_k \end{matrix} \\ \left.\begin{matrix} 1 & \frac{-1}{\alpha} & \frac{-1}{\alpha} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2} & \cdots\frac{1}{\alpha^2} \\ 1 & \frac{-1}{\alpha} & \frac{1}{\alpha} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2} & \frac{-1}{\alpha^2} & \cdots\frac{1}{\alpha^2} \\ 1 & \frac{1}{\alpha} & \frac{-1}{\alpha} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2} & \frac{-1}{\alpha^2} & \cdots\frac{1}{\alpha^2} \\ 1 & \frac{1}{\alpha} & \frac{1}{\alpha} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2} & \frac{1}{\alpha^2} & \cdots\frac{1}{\alpha^2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\ddots & \end{matrix}\right\} rf \\ \left.\begin{matrix} 1 & -1 & 0 & 1 & 0 & 0 & \cdots 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & \cdots 0 \\ 1 & 0 & -1 & 0 & 1 & 0 & \cdots 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & \cdots 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\ddots & \end{matrix}\right\} 2kr \\ \left.\begin{matrix} 1 & 0 & 0 & 0 & 0 & 0 & \cdots 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & \cdots 0 \end{matrix}\right\} n_0 \end{array}$$

The information matrix $S^T S$ of an inscribe central composite design is obtain by multiplication of the design matrix *S* in Table 1 and the result as shown by [2], is

$$S^T S = \begin{bmatrix} N & 0 & (rf + 2kr\alpha^2).J_k' & 0 \\ 0 & diag(d_i) & 0 & 0 \\ (rf + 2kr\alpha^2).J_k & 0 & 2kr\alpha^4.I_k + rf.J_k J_k' & 0 \\ 0 & 0 & 0 & rf\, J_k J_k' \end{bmatrix} \qquad \rightarrow \qquad (4)$$

The J_k is a column vector of k x 1 and I_k is a matrix of *k* dimension, 0 matrices of appropriate sizes, and $diag(d_i)$ are diagonal matrices such that

$$\begin{aligned} d_i &= rf + 2kr\alpha^2 \quad \text{for} \quad 1 \le i \le k \\ &= rf \qquad \text{for } k+1 \le i \le k + \binom{k}{2} \end{aligned} \qquad \rightarrow \qquad (5)$$

The block matrix form of $\left(S^T S\right)^{-1}$ for an ICCD is

$$\left(S^T S\right)^{-1} = \begin{bmatrix} \alpha_{11} & 0 & \alpha_{13}J_k' & 0 \\ 0 & \mathrm{diag}(1/d_i) & 0 & 0 \\ \alpha_{13}J_k & 0 & \frac{1}{2r\alpha^4}\left[I_k - \alpha_{33}J_kJ_k'\right] & 0 \\ 0 & 0 & 0 & \frac{1}{f}J_kJ_k' \end{bmatrix} \rightarrow \quad (6)$$

where $\alpha_{11} = \frac{krf + 2r\alpha^4}{T}$, $\alpha_{13} = -\left(\frac{rf + 2r\alpha^2}{T}\right)$, $\alpha_{33} = \frac{Nrf - \left(rf + 2r\alpha^2\right)^2}{T}$ and

$T = 2Nr\alpha^4 + Nkrf - k\left(rf + 2r\alpha^2\right)^2$

To focus on the model parameter estimation, D-optimality criterion is employed. It is the criterion where the determinant of the moment matrix is maximized over all the design. It is given as

$$\omega = \frac{\left(S^T S\right)}{N} \quad \rightarrow \quad (7)$$

Also, among the optimality criteria that tries to minimize the trace of the inverse of the information matrix of the design is the A-optimality. It is stated as

$$\left\{\min\left[trace\left(S^T S\right)^{-1}\right]\right\} \quad \rightarrow \quad (8)$$

The outcome of this criterion always decrease the mean variance of the estimates of the regression coefficients. Contrast to D-optimality criterion, the covariance between the coefficients is not use by the A-optimality criterion.

The criterion that make sure the maximum scaled prediction variance (SPV) in the region of the design is not too large is the G-optimality. That is it seeks to reduce the maximum SPV and is defined as

$$\min\left\{\max N \operatorname{var} \hat{y}(s)\right\} = \min\left\{N \max \pi^T(s)\left(S^T S\right)^{-1}\pi(s)\right\} \quad \rightarrow \quad (9)$$

where $(S^T S)^{-1}$ is the inverse of the information matrix of the design matrix *S*, $\pi(s)$ the vector co-ordinates in the model. That is

$$\pi^T(s) = \left[1, s_1 \ldots, s_{k,} s_1^2, \ldots, s_k^2, s_1 s_2, \ldots s_{k-1}s_k\right] \quad \rightarrow \quad (10)$$

3. Partial Replication Of The Design

The inscribed central composite design runs for model parameter estimation is given as

$$N = rf + 2kr + n_0 \quad \rightarrow \quad (11)$$

where $f = 2^k$ is the cube or factorial portion replicated r times, $2k$ is the star or axial points replicated r times and n_0 the center point.

In this study, the inscribed central composite design (ICCD) whose factorial portions are replicated is denoted as ICCD-R_F while the inscribed central composite design (ICCD) whose star portions are replicated is denoted as ICCD-R_A. The replication of the cube and star points in both designs (ICCD-R_F and ICCD-R_A) were done two and three times with three center points. The design performance of the experiment were examined for this number of factors $k = 2 – 7$ applying the A-, D-, and G-optimality criteria

4. Comparison of the Design

Table 2 show that the replication of cube portion reduces the A-optimality criterion values of the inscribed CCD in all the factors k considered while the replication of star portion improves the design by increasing the A-optimality criterion values of the inscribed central composite design in every factor k that was considered. Replication of the star points of inscribed central composite design performs better under A-optimality criterion when compared with replication of the cube portion of the design.

Under the D-optimality criterion, the replication of cube portion reduces the D-optimality criterion values of the inscribed central composite design for factors $k = 2$ and 3 of the experiment while for factors $k = 4 – 7$, it increases the D-optimality criterion values of the design.

Also, replication of the star points reduces the D-optimality criterion values of the inscribed CCD in every factor that was considered.

Under the G-optimality criterion, replicating both the cube and star points of the inscribed CCD showed an increase in the G-optimality criterion values of the design for factors $k = 2 – 5$, while as the factor level increases ($k = 6$ and 7), replication of star points, decreases the G-optimality criterion values of the inscribed central composite design.

Table 2: Summary Statistics for versions of ICCD

Design	N	r_f	r_a	n_0	A	D	G	Factors k
ICCD	11	1	1	3	13.068	0.1472	6.875	2
ICCD-R_F	15	2	1	3	11.595	0.0855	8.925	
ICCD-R_F	19	3	1	3	10.887	0.0606	11.229	
ICCD-R_A	15	1	2	3	17.43	0.1358	8.925	
ICCD-R_A	19	1	3	3	20.805	0.1261	11.229	
ICCD	17	1	1	3	20.281	0.0870	11.390	3
ICCD-R_F	25	2	1	3	19.025	0.0479	14.450	
ICCD-R_F	33	3	1	3	17.886	0.033	19.041	
ICCD-R_A	23	1	2	3	25.346	0.0810	14.904	
ICCD-R_A	29	1	3	3	28.942	0.0760	18.560	
ICCD	27	1	1	3	28.70	0.0178	15.75	4
ICCD-R_F	43	2	1	3	27.50	0.2337	24.37	
ICCD-R_F	59	3	1	3	25.17	0.7306	33.59	
ICCD-R_A	35	1	2	3	33.73	0.000795	19.88	
ICCD-R_A	43	1	3	3	36.55	0.000078	24.12	
ICCD	45	1	1	3	39.37	0.0387	25.90	**5**
ICCD-R_F	77	2	1	3	35.45	0.6102	43.24	
ICCD-R_F	109	3	1	3	31.57	1.9621	61.30	
ICCD-R_A	55	1	2	3	45.55	0.0011	24.22	
ICCD-R_A	65	1	3	3	45.71	0.0000731	28.33	
ICCD	79	1	1	3	50.34	0.1672	43.70	6
ICCD-R_F	143	2	1	3	41.44	2.4083	79.58	
ICCD-R_F	207	3	1	3	37.27	6.6946	114.5	
ICCD-R_A	91	1	2	3	66.22	0.0039	29.75	
ICCD-R_A	103	1	3	3	62.82	0.000251	32.22	
ICCD	145	1	1	3	56.84	0.00688	80.04	**7**
ICCD-R_F	273	2	1	3	46.683	0.00343	149.604	
ICCD-R_F	401	3	1	3	43.308	0.00228	217.342	
ICCD-R_A	159	1	2	3	89.358	0.00693	46.11	
ICCD-R_A	173	1	3	3	102.935	0.00689	55.014	

5. Conclusion

Replication of any part of the inscribed CCD affect the optimal performance of the design as seen by the study. Inscribed central composite design with replicated factorial (ICCD-R_F) increases the number of runs of the experiment rapidly, it reduces the A-optimality criterion values of the design of every factor of k considered in the study but at lower factors of k (k = 2 and 3), it also reduces the D-optimality criterion values of the design while it increases the G-optimality criterion for most of the factors considered in the study.

Replicating the axial points of the inscribed central composite design (ICCD-R_A) increases the A- and D-optimality criteria values of the design in all the factors considered in the work while for G-optimality criterion, replication increases the criterion values but not in all the factor levels.

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