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IMPOSING D-OPTIMALITY CRITERION ON THE DESIGN REGIONS OF THE CENTRAL COMPOSITE DESIGNS (CCD)

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ABSTRACT

The effect of D-optimality criterion in the construction of N-point exact designs on the design regions of the face-centered central composite design, rotatable (circumscribed) central composite design and inscribed central composite design, respectively, is investigated using a second order response surface model. Each geometric region has a finite number of support points defined by the factorial points, the axial points and the center point of the three central composite design regions. For the six parameter second order polynomial model used, the D-optimal design defined over the rotatable (circumscribed) Central Composite Design (CCD) region has better determinant values than those obtained over the face-centered central composite design region and the inscribed central composite design region. Furthermore, results indicate that D-optimal designs defined over the rotatable CCD region give better parameter estimates as the variances and covariances of the parameters are minimized.

Keywords: D-optimality criterion, face-centered CCD, inscribed CCD, circumscribed CCD

INTRODUCTION

Central Composite Designs (CCDs) play a vital role in the design of experiments. There are basically three types of CCDs, namely, the face-centered CCD, the rotatable CCD and the inscribed CCD. Each CCD consists of the corner points, the axial points and the center points and these components play important roles in the estimation of model parameters. For two variates, the face-centered CCD comprises of the four corner points [(-1,-1),(1,-1),(-1,1),(1,1)],four axial points [(1,0),(-1,0),(0,1),(0,-1)] and n_0 centre points [(0,0), (0, 0), . . . , (0, 0)], where n_0 is the number of centre points chosen. The rotatable CCD comprises of four corner points [(-1,-1),(1,-1),(-1,1),(1,1)],four axial points [(1.414,0),(-1.414,0),(0,1.414),(0,-1.414)] and n_0 centre points [(0,0), (0,0), . . . (0, 0)]. The inscribed CCD comprises of four corner points [(0.7,0.7), (-0.7,0.7), (-0.7,-0.7), (0.7,-0.7)], four star points [(0, 1), (0, -1), (-1, 0), (1, 0)] and n_0 centre points [(0,0), (0,0), . . . , (0, 0)].

In any experimental work it is important to choose the best design in a class of existing designs. The choice is solely dependent of the interest of the experimenter and the adequacy of an experimental design can be determined from the information matrix. Many criteria exist for choosing experimental designs to meet specific purposes, some of these criteria include orthogonality and rotatability. The orthogonality and rotatability criteria have been imposed on the three central composite designs (Box & Hunter (1957), Montgomery (1997)). In this work, we investigate the effect of imposing the D-optimality criterion on each region of the Central Composite Designs.Specifically, we explore each region of the three central composite designs to identify an N-point D-optimal exact design for a six-parameter bivariate quadratic model;

$$f\ (x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \varepsilon. \qquad 1.1$$

METHODOLOGY

As can be seen in Box and Behnken (1960), D-optimality criterion emphasizes the precision of the estimated coefficients of the assumed model. The optimality criterion used in generating D-optimal designs is one of maximizing $|X^{'}X|$, the determinant of the information matrix $X^{'}X$. This optimality criterion results in minimizing the generalized variance of the parameter estimates for a pre-specified model.Donev and Atkinson (1988) have observed that, in practice, D-optimal designs often perform well in relation to designs that are optimal by other optimality criteria.In attempting to investigate the effect of D-optimality on the regions of the Central Composite Designs (CCDs), we rely on the combinatorial algorithm of Iwundu and Chigbu (2012) which is closely related to the algorithm of Onukogu and Iwundu(2007). We however, present the algorithm more explicitly.

We assume that the $\bar{N}$ support points that make up the experimental area have been grouped into $g_1, g_2, . . . , g_H$ groups. From the H groups, we shall attempt to obtain an optimal combination of support points that shall produce D-optimal exact designs. This shall be established for N sized designs, where N ranges from p to 2p, where p is the number of model parameters. The procedure moves sequentially one step at a time in both the increasing and decreasing values of each component, $r_1, r_2, . . , r_f ..., r_H$ of the groups, $g_1, g_2, . . ., g_r, ... , g_H$ in the direction of increasing determinant value of the associated information matrix. The required exact D-optimum is reached and it is associated with the design class $\underline{t}_k* = [r_1*, r_2*, . . ., r_f^*, ..., r_H*]$, where r_i* is the optimal number of support points taken from g_i; i=1, 2, . . ,f, ... , H. Let us suppose that at the k^{th} step the number of support point $r_{1k}, r_{2k}, . . ., r_{fk}, ... , r_{Hk}$ are obtained from $g_1, g_2, . . ., g_r, . . ., g_H$ respectively. If $\underline{t}_k$ is the H-tuple of support points at the k^{th} step, then the H-tuple of support points at $(k+1)^{st}$ step is formed by holding H-2 of the r_{ik} values fixed and altering the values of the just two balls. That is, only two values of the r_{ik} are altered while the remaining H-2 values of r_{ik} are held fixed subject to $\sum r_{ik} = N$; N is the design size.

The Algorithm

We present the details of the algorithm in Tables 1 below. The table consists of sixmain columns, namely, step k, sub-step m, ball combination, number of available designs, sub-step m best determinant value and step k best determinant value. Since the algorithm aims at getting the best combination of support points that contains the D-optimal design, we shall attempt to obtain $r_1*, r_2*, ..., r_f^*... , r_H*$, the optimal number of support points taken from $g_1, g_2, . . ., g_r, ... , g_H$. The immediate tables shall illustrate how to obtain r_1*. The process can be generalized for $r_2*, . . . , r_H*$.

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Table 1a:Combinatorics for Choosing D-optimal Exact Design

Step k	Sub-step m	BALL COMBINATION							Number of available designs	Sub-step m best determinant value	Step k best determinant value
		g_1	g_2	g_3	…	g_f	…	g_H			
0	1	r_1	r_2	r_3	…	r_f	…	r_H	a_0	d_0	d_0
1	1	r_1-1	r_2+1	r_3	…	r_f	…	r_H	a^-_{111}	d^-_{111}	d_1
	2	r_1-1	r_2	r_3+1	…	r_f	…	r_H	a^-_{112}	d^-_{112}	
	…	…	…	…	…	…	…	…	…	…	
	H-2	r_1-1	r_2	r_3	…	r_f	…	r_H+1	$a^-_{11(H-2)}$	$d^-_{11(H-2)}$	
	1	r_1+1	r_2-1	r_3	…	r_f	…	r_H	a^+_{111}	d^+_{111}	
	2	r_1+1	r_2	r_3-1	…	r_f	…	r_H	a^+_{112}	d^+_{112}	
	…	…	…	…	…	…	…	…	…	…	
	H-2	r_1+1	r_2	r_3	…	r_f	…	r_H-1	$a^+_{11(H-2)}$	$d^+_{11(H-2)}$	
2	1	r_1-2	r_2+2	r_3	…	r_f	…	r_H	a^-_{211}	d^-_{211}	d_2
	2	r_1-2	r_2+1	r_3+1	…	r_f	…	r_H	a^-_{212}	d^-_{212}	
	…	…	…	…	…	…	…	…	…	…	
	H-2	r_1-2	r_2+1	r_3	…	r_f	…	r_H+1	$a^-_{21(H-2)}$	$d^-_{21(H-2)}$	
	1	r_1-2	r_2-1	r_3+1	…	r_f	…	r_H	a^-_{221}	d^-_{221}	
	2	r_1-2	r_2	r_3+2	…	r_f	…	r_H	a^-_{222}	d^-_{222}	
	…	…	…	…	…	…	…	…	…	…	
	H-2	r_1-2	r_2	r_3+1	…	r_f	…	r_H+1	$a^-_{22(H-2)}$	$d^-_{22(H-2)}$	
	…	…	…	…	…	…	…	…	…	…	
	1	r_1-2	r_2+1	r_3	…	r_f	…	r_H+1	a^-_{2q1}	d^-_{2q1}	
	2	r_1-2	r_2	r_3+1	…	r_f	…	r_H+1	a^-_{2q2}	d^-_{2q2}	
	…	…	…	…	…	…	…	…	…	…	
	H-2	r_1-2	r_2	r_3	…	r_f	…	r_H+2	$a^-_{2q(H-2)}$	$d^-_{2q(H-2)}$	
	1	r_1+2	r_2-2	r_3	…	r_f	…	r_H	a^+_{211}	d^+_{211}	
	2	r_1+2	r_2-1	r_3+1	…	r_f	…	r_H	a^+_{212}	d^+_{212}	
	…	…	…	…	…	…	…	…	…	…	
	H-2	r_1+2	r_2-1	r_3	…	r_f	…	r_H-1	$a^+_{21(H-2)}$	$d^+_{21(H-2)}$	
	1	r_1+2	r_2-1	r_3-1	…	r_f	…	r_H	a^+_{221}	d^+_{221}	
	2	r_1+2	r_2	r_3-2	…	r_f	…	r_H	a^+_{222}	d^+_{222}	
	…	…	…	…	…	…	…	…	…	…	
	H-2	r_1+2	r_2	r_3-1	…	r_f	…	r_H-1	$a^+_{22(H-2)}$	$d^+_{22(H-2)}$	
	…	…	…	…	…	…	…	…	…	…	
	1	r_1+2	r_2-1	r_3	…	r_f	…	r_H-1	a^+_{2q1}	d^+_{2q1}	
	2	r_1+2	r_2	r_3-1	…	r_f	…	r_H-1	a^+_{2q2}	d^+_{2q2}	
	…	…	…	…	…	…	…	…	…	…	
	H-2	r_1+2	r_2	r_3	…	r_f	…	r_H-2	$a^+_{2q(H-2)}$	$d^+_{2q(H-2)}$	
…	…	…	…	…	…	…	…	…	…	…	…

Table 1b

Step k	Sub-step m	g_1	g_2	g_3	…	g_f	…	g_H	Number of available designs	Sub-step m best determinant value	Step k best determinant value
0	1	r_1'	r_2'	r_3'	…	r_f	…	r_H'	aa_0	d_f^*	d_f^*
1	1 2 … H-1	$r_1'+1$ r_1' … r_1'	r_2' $r_2'+1$ … r_2'	r_3' r_3' … r_3'	… … … …	r_f-1 r_f-1 … r_f-1	… … … …	r_H' r_H' … $r_H'+1$	aa_{111}^- aa_{112}^- … $aa_{11(H-1)}^-$	dd_{111}^- dd_{112}^- … $dd_{11(H-1)}^-$	dd_1
	1 2 … H-1	$r_1'-1$ r_1' … r_1'	r_2' $r_2'-1$ … r_2'	r_3' r_3' … r_3'	… … … …	r_f+1 r_f+1 … r_f+1	… … … …	r_H' r_H' … $r_H'-1$	aa_{111}^+ aa_{112}^+ … $aa_{11(H-1)}^+$	dd_{111}^+ dd_{112}^+ … $dd_{11(H-1)}^+$	
2	1 2 … H-1	$r_1'+2$ $r_1'+1$ … $r_1'+1$	r_2' $r_2'+1$ … r_2'	r_3' r_3' … r_3'	… … … …	r_f-2 r_f-2 … r_f-2	… … … …	r_H' r_H' … $r_H'+1$	aa_{211}^- aa_{212}^- … $aa_{21(H-1)}^-$	dd_{211}^- dd_{212}^- … $dd_{21(H-1)}^-$	dd_2
	1 2 … H-1	$r_1'+1$ r_1' … r_1'	$r_2'+1$ $r_2'+2$ … $r_2'+1$	r_3' r_3' … r_3'	… … … …	r_f-2 r_f-2 … r_f-2	… … … …	r_H' r_H' … $r_H'+1$	aa_{221}^- aa_{222}^- … $aa_{22(H-1)}^-$	dd_{221}^- dd_{222}^- … $dd_{22(H-1)}^-$	
	…	…	…	…	…	…	…	…	…	…	
	1 2 … H-1	$r_1'+1$ r_1' … r_1'	r_2' $r_2'+1$ … r_2'	r_3' r_3' … r_3'	… … … …	r_f-2 r_f-2 … r_f-2	… … … …	$r_H'+1$ $r_H'+1$ … $r_H'+2$	aa_{2q1}^- aa_{2q2}^- … $aa_{2q(H-1)}^-$	dd_{2q1}^- dd_{2q2}^- … $dd_{2q(H-1)}^-$	
	1 2 … H-1	$r_1'-2$ $r_1'-1$ … $r_1'-1$	r_2' $r_2'-1$ … r_2'	r_3' r_3' … r_3'	… … … …	r_f+2 r_f+2 … r_f+2	… … … …	r_H' r_H' … $r_H'-1$	aa_{211}^+ aa_{212}^+ … $aa_{21(H-1)}^+$	dd_{211}^+ dd_{212}^+ … $dd_{21(H-1)}^+$	
	1 2 … H-1	$r_1'-1$ r_1' … r_1'	$r_2'-1$ $r_2'-2$ … $r_2'-1$	r_3' r_3' … r_3'	… … … …	r_f+2 r_f+2 … r_f+2	… … … …	r_H' r_H' … $r_H'-1$	aa_{221}^+ aa_{222}^+ … $aa_{22(H-1)}^+$	dd_{221}^+ dd_{222}^+ … $dd_{22(H-1)}^+$	
	…	…	…	…	…	…	…	…	…	…	
	1 2 … H-1	$r_1'-1$ r_1' … r_1'	r_2' $r_2'-1$ … r_2'	r_3' r_3' … r_3'	… … … …	r_f+2 r_f+2 … r_f+2	… … … …	$r_H'-1$ $r_H'-1$ … $r_H'-2$	aa_{2q1}^+ aa_{2q2}^+ … $aa_{2q(H-1)}^+$	dd_{2q1}^+ dd_{2q2}^+ … $dd_{2q(H-1)}^+$	
…	…	…	…	…	…	…	…	...	…	…	…

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where, step k = 0, 1, 2, . . . , n, n+1,n+2, . . . , q, q+1

$$\left.\begin{array}{l} d_0 < d_1 < d_2 < \ldots < d_n > d_{(n+1)} \\ d_{(n+2)} < d_{(n+3)} < \ldots < d_q > d_{(q+1)} \end{array}\right\} \quad 2.1.1$$

$d_k^* = \max\{(\det M(\xi_k^{(i,j)})\}; M(\xi_k^{(i,j)}) \in S_k^{pxp}$; k = 0, 1, 2, ... ,q+1

S_k^{pxp} is the space of non-singular pxp information matrices at the k^{th} step.

Table 1a assumes the initial tuple of support points at step 0 as

$\underline{t}_0 = [r_1, r_2, \ldots r_f, \ldots, r_H]$

where

r_1 is the initial number of support points taken from group g_1

r_2 is the initial number of support points taken from group g_2

r_3 is the initial number of support points taken from group g_3

.
.
.

r_f is the initial number of support points taken from group g_f

.
.
.

r_H is the initial number of support points taken from group g_H.

The group g_f contains the r_f support points we shall hold fixed while making increments on the r_i's of the other groups. By incremental changes on the r_i, we aim at getting the optimal number of support points taken from the H-groups namely, r_1', r_2', . . . ,r_H' while holding r_f value fixed. We shall hereafter refer to as the conditional optimal number of supports points from g_1 as r_1', the optimal number of support points from g_2 as r_2', etc. After defining the initial tuple of support points $\underline{t}_0 = [r_1, r_2, \ldots r_f, \ldots, r_H]$, we shall obtain the determinant value d_0 of the best design in the category or combination. Holding r_f value fixed, we proceed to obtain the optimal number of support points from a group, say, g_1. This requires effecting an increment on $r_1$value by 1. Hence, we define the 2(H-2) tuples of support points in step 1. These tuples are

$\underline{t}_{11} = [r_1-1 \quad r_2+1 \quad r_3 \quad r_4 \ \ldots \ r_f, \ldots \ldots r_H]$.

$\underline{t}_{12} = [r_1-1 \quad r_2 \quad r_3+1 \quad r_4 \ \ldots \ r_f, \ldots \ldots r_H]$.

.
.
.

$\underline{t}_{1(H-2)} = [r_1-1 \quad r_2 \quad r_3 \quad r_4 \ \ldots \ r_f, \ldots \ldots r_H+1]$.

$\underline{t}_{1H} = [r_1+1 \quad r_2-1 \quad r_3 \quad r_4 \ \ldots \ r_f, \ldots \ldots r_H]$.

$\underline{t}_{1(H+1)} = [r_1+1 \quad r_2 \quad r_3-1 \quad r_4 \ \ldots \ r_f, \ldots \ldots r_H]$.

.
.
.

$\underline{t}_{1(2H-4)} = [r_1+1 \quad r_2 \quad r_3 \quad r_4 \ \ldots \ r_f, \ldots \ldots r_H-1]$.

At each sub-step of step 1, we compute the determinant value of information matrix associated with the best design in the category. These determinant values are, respectively, $\mathbf{d}^{-}_{111}$, $\mathbf{d}^{-}_{112}$, ..., $\mathbf{d}^{-}_{11(H-2)}, \mathbf{d}^{+}_{111}, \mathbf{d}^{+}_{112}, \ldots, \mathbf{d}^{+}_{11(H-2)}$. Comparing these determinant values, the best determinant value in step 1 is $d_1 = \max [\mathbf{d}^{-}_{111}, \mathbf{d}^{-}_{112}, \ldots, \mathbf{d}^{-}_{11(H-2)}, \mathbf{d}^{+}_{111}, \mathbf{d}^{+}_{112}, \ldots, \mathbf{d}^{+}_{11(H-2)}]$. Suppose $d_1 < d_0$, then we have obtained the optimal value r_1' holding r_f value fixed. Thus, the best determinant when r_f is held fixed is $d_f^* = d_0$. Now, we seek to obtain r_2' holding r_f and r_1' fixed. This will require carrying out a similar process by effecting an increment on r_2 value. The process continues similarly for $r_3, r_4, \ldots, r_H$. Note however, that if at step 1, $d_1 > d_0$, we proceed to effect an increment on r_1 by 2. Assuming that d_1 is associated with the tuple $\underline{t}_{111} = [r_1-1, r_2+1, r_3, r_4, \ldots r_f, \ldots \ldots r_H]$, increments in the decreasing direction is required. Hence, we do not need to explore all sub-steps of step 2. Incrementing r_1 by 2 is equivalent to incrementing r_1-1 by 1. Consequently, the required tuples of support points at this iteration are

$\underline{t}_{21} = [r_1-2 \quad r_2+2 \quad r_3 \quad r_4 \ldots r_f, \ldots \ldots r_H]$.

$\underline{t}_{22} = [r_1-2 \quad r_2+1 \quad r_3+1 \quad r_4 \ldots r_f, \ldots \ldots r_H]$.

.

.

.

$\underline{t}_{1(H-2)} = [r_1-2 \quad r_2+1 \quad r_3 \quad r_4 \ldots r_f, \ldots \ldots r_H+1]$.

As earlier observed, we shall compute the determinant value of the best designs in each of the combinations or categories. At step 2, the best determinant value is d_2. This value will again be compared with d_1 to check for convergence. Again if $d_2 > d_1$, we effect an increment on r_1 by 3. If otherwise, then $d_f^* = d_1$. Continuing the process will yield the tuple of support points

$\underline{t}_f' = [r_1', r_2', r_3', r_4', \ldots, r_f, \ldots r_H']$. The remaining task is that of attempting to effect increments on r_f so as to obtain the optimal number of support points r_f^* taken from group g_f . This will be achieved by defining combination of support points as in table 1b. Again at each step of the table, we shall obtain the determinant value that is associated with the information matrix of the best design. We note however, that effecting increments on r_f value will obviously affect the values of $r_1', r_2', r_3', r_4', \ldots, r_H'$.

Consequently, the tuple that results in the global best determinant value is defined by $\underline{t}^* = [r_1^*, r_2^*, r_3^*, r_4^*, \ldots, r_f^*, \ldots r_H^*]$, where r_j^* is the optimal number of support points taken from the ith group g_i, i=1, 2, . . ., r, . . . , H. The D-optimal exact design is contained in the immediate tuple and is associated with d*. The sequence of steps described in the algorithm presented in this work is used to obtain a D-optimal exact design defined over each of the three regions of the central composite designs. When the determinant values of the resulting D-optimal exact designs are compared, the global D-optimal exact design is that with the best determinant value of information matrix.

Exploration Using Design Region of the Face-Centered Central Composite Design

The nine design points are grouped according to their distance from the center of the design region as follows:

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$$g_1=\begin{bmatrix}(1 \quad 1)\\(1-1)\\(-1 \quad 1)\\(-1-1)\end{bmatrix};\ g_2=\begin{bmatrix}(1 \quad 0)\\(0 \quad 1)\\(-1 \quad 0)\\(0-1)\end{bmatrix};\ g_3=[(0 \quad 0)]$$

Table 2 gives the computations involved in obtaining the required N-point D-optimal exact design defined over the region of the Face-centered CCD.

Table 2: Computations for N-Point D-Optimal Exact Design defined over the region of Face-Centered CCD

Design size N	Required combination			Number of available designs	Best determinant value for the combination	Best determinant value for N-point design
	g_1	g_2	g_3			
6	4	1	1	4	$5.486968437 \times 10^{-3}$	$5.486968437 \times 10^{-3}$
	4	0	2	1	Singular design	
	4	2	0	6	$5.486968437 \times 10^{-3}$	
	3	2	1	24	$1.371742109 \times 10^{-3}$	
	3	1	2	16	Singular design	
	3	3	0	16	$1.371742109 \times 10^{-3}$	
7	4	2	1	6	$8.159865377 \times 10^{-3}$	$8.159865377 \times 10^{-3}$
	4	3	0	4	$6.527892302 \times 10^{-3}$	
	4	1	2	4	$4.351928201 \times 10^{-3}$	
	3	3	1	16	$3.263946151 \times 10^{-3}$	
	3	2	2	24	$2.447959613 \times 10^{-3}$	
	5	2	0	24	$4.351928201 \times 10^{-3}$	
	5	1	1	16	$4.351928201 \times 10^{-3}$	
8	4	3	1	4	8.7890625×10^{-3}	8.7890625×10^{-3}
	4	4	0	1	8.7890625×10^{-3}	
	4	2	2	6	$6.34765625 \times 10^{-3}$	
	3	4	1	4	$3.845214844 \times 10^{-3}$	
	3	3	2	16	$2.685546875 \times 10^{-3}$	
	3	2	3	24	$1.647949219 \times 10^{-3}$	
	5	2	1	24	$7.263183594 \times 10^{-3}$	
	5	3	0	16	$5.615234375 \times 10^{-3}$	
9	4	3	2	4	$7.225637461 \times 10^{-3}$	$9.754610572 \times 10^{-3}$
	4	4	1	1	$9.754610572 \times 10^{-3}$	
	4	5	0	4	$7.225637461 \times 10^{-3}$	
	5	3	1	16	$8.30948308 \times 10^{-3}$	
	5	4	0	4	$7.948201207 \times 10^{-3}$	
	3	5	1	16	$3.432177794 \times 10^{-3}$	
	3	4	2	4	$3.070895921 \times 10^{-3}$	
10	6	3	1	24	8.448×10^{-3}	9.360×10^{-3}
	6	4	0	6	7.680×10^{-3}	
	6	2	2	36	6.528×10^{-3}	
	5	4	1	4	9.360×10^{-3}	
	5	3	2	16	7.360×10^{-3}	
	4	4	2	1	8.064×10^{-3}	
	4	5	1	4	8.064×10^{-3}	
11	6	3	2	24	7.9478×10^{-3}	9.5374×10^{-3}
	6	4	1	6	9.5374×10^{-3}	
	6	5	0	24	$7.153013642 \times 10^{-3}$	
	5	5	1	16	$8.182614091 \times 10^{-3}$	
	5	4	2	4	$8.182614091 \times 10^{-3}$	
	7	3	1	16	$8.70644589 \times 10^{-3}$	
	7	4	0	4	$7.947792936 \times 10^{-3}$	
12	7	3	2	16	8.5305×10^{-3}	1.0154×10^{-2}
	7	4	1	4	1.0154×10^{-2}	
	7	5	0	16	$7.630315482 \times 10^{-3}$	
	6	4	2	6	$8.723422476 \times 10^{-3}$	
	6	5	1	24	$8.610896756 \times 10^{-3}$	
	8	4	0	1	$8.573388182 \times 10^{-3}$	
	8	3	1	4	9.4307001×10^{-3}	

Exploration Using the Design Regions of the Circumscribed Central Composite Design

The nine design points are grouped according to their distance from the center of the design region as follows:

$$g_1 = \begin{bmatrix} (-1 & -1) \\ (1 & -1) \\ (-1 & 1) \\ (1 & 1) \end{bmatrix} \qquad g_2 = \begin{bmatrix} (-1.414 & 0) \\ (1.414 & 0) \\ (0 & -1.414) \\ (0 & 1.414) \end{bmatrix} \qquad g_3 = [(0 \quad 0)]$$

Table 3 gives the computations involved in obtaining the required N-point D-optimal exact design defined over the region of the Circumscribed CCD.

Table 3: Computations for N-Point D-Optimal Exact Design defined over the region of Circumscribed CCD

Design size N	Required combination			Number of available designs	Best determinant value for the combination	Best determinant value for N-point design
	g_1	g_2	g_3			
6	4	1	1	4	2.1935×10^{-2}	3.1947×10^{-2}
	4	0	2	1	Singular design	
	4	2	0	6	$8.002097395 \times 10^{-9}$	
	3	2	1	24	3.1947×10^{-2}	
	3	1	2	16	$1.917904894 \times 10^{-16}$	
	2	3	1	24	3.1936×10^{-2}	
	2	2	2	36	Singular design	
	5	0	1	4	Singular design	
	5	1	0	16	Singular design	
7	4	2	1	6	$3.478652316 \times 10^{-2}$	3.8374×10^{-2}
	4	3	0	4	$1.269164043 \times 10^{-8}$	
	3	3	1	16	3.8374×10^{-2}	
	3	2	2	24	$2.533875249 \times 10^{-2}$	
	5	1	1	16	$1.739720013 \times 10^{-2}$	
	5	2	0	24	$6.3467766949 \times 10^{-9}$	
8	4	3	1	4	4.6828×10^{-2}	4.6828×10^{-2}
	4	4	0	1	2.2780×10^{-8}	
	4	2	2	6	3.1226×10^{-2}	
	5	2	1	24	3.1057×10^{-2}	
	5	3	0	16	2.5969×10^{-2}	
	3	4	1	16	3.9613×10^{-2}	
	3	3	2	16	3.4444×10^{-2}	
9	4	3	2	4	4.6198×10^{-2}	6.1584×10^{-2}
	4	4	1	1	6.1584×10^{-2}	
	4	5	0	4	1.9664×10^{-2}	
	3	5	1	16	4.3127×10^{-2}	
	3	4	2	4	$4.617894753 \times 10^{-2}$	
	5	4	0	4	4.6179×10^{-2}	
	5	3	1	16	4.3146×10^{-2}	
10	6	3	1	24	4.2659×10^{-2}	$6.545687882 \times 10^{-2}$
	6	2	2	36	3.1542×10^{-2}	
	6	4	0	6	1.8289×10^{-2}	
	7	2	1	24	$3.051961074 \times 10^{-2}$	
	7	3	0	16	$9.705868151 \times 10^{-2}$	
	5	4	1	4	$5.318619101 \times 10^{-2}$	
	5	3	2	16	$4.585877357 \times 10^{-2}$	
	4	5	1	4	$5.318124827 \times 10^{-2}$	
	4	4	2	1	$6.545687882 \times 10^{-2}$	
	3	5	2	16	$2.845220095 \times 10^{-2}$	
	3	4	3	4	$3.681207836 \times 10^{-2}$	

Scientia Africana, Vol. 13 (No.1), June 2014. Pp109-119
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11	6	3	2	24	4.81595308 $x10^{-2}$	6.004443063 $x10^{-2}$
	6	4	1	6	4.849988508 $x10^{-2}$	
	6	2	3	36	2.67072703 $x10^{-2}$	
	6	5	0	16	1.769754112 $x10^{-8}$	
	7	3	1	16	3.883169145 $x10^{-2}$	
	7	4	0	4	1.76943802 $x10^{-8}$	
	5	5	1	16	4.873431177 $x10^{-2}$	
	5	4	2	4	6.004443063 $x10^{-2}$	
	4	5	2	4	6.003885053 $x10^{-2}$	
	4	4	3	1	5.542305077 $x10^{-2}$	
12	7	3	2	16	4.607707551 $x10^{-2}$	5.782736734 $x10^{-2}$
	7	2	3	24	3.066286558 $x10^{-2}$	
	7	4	1	4	4.62472377 $x10^{-2}$	
	7	5	0	16	1.775025317 $x10^{-8}$	
	8	3	1	4	3.700474095 $x10^{-2}$	
	8	4	0	1	1.800109831 $x10^{-8}$	
	6	5	1	24	4.665371273 $x10^{-2}$	
	6	4	2	6	5.754920024 $x10^{-2}$	
	5	5	2	16	5.782736734 $x10^{-2}$	
	5	4	3	4	5.343583614 $x10^{-2}$	
	4	6	2	6	5.753823369 $x10^{-2}$	
	4	5	3	4	5.34308702 $x10^{-2}$	

Exploration Using the Design Regions of the Inscribed Central Composite Design (CCD).

The nine design points are grouped according to their distance from the center of the design region as follows:

$$g_1 = \begin{bmatrix} 0 & -1 \\ -1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \quad g_2 = \begin{matrix} -0.7 & -0.7 \\ 0.7 & 0.7 \\ 0.7 & -0.7 \\ -0.7 & 0.7 \end{matrix} \quad \left(\text{and } g_3 = [0 \quad 0] \right)$$

Table 4 gives the computations involved in obtaining the required N-point D-optimal exact design defined over the region of the Face-centered CCD.

Table 4: Computations for N-Point D-Optimal Exact Design defined over the region of Inscribed CCD

Design size N	Required combination			Number of available designs	Best determinant value for the combination	Best determinant value for N-point design
	g_1	g_2	g_3			
6	4	1	1	4	8.23388201 $x10^{-5}$	1.166000031 $x10^{-4}$
	4	2	0	6	1.317421122 $x10^{-7}$	
	4	0	2	1	Singular design	
	3	0	1	4	Singular design	
	3	1	0	16	Singular design	
	2	2	1	24	1.166000031 $x10^{-4}$	
	2	1	2	16	Singular design	
	5	3	1	24	1.138726121 $x10^{-4}$	
	5	2	2	36	Singular design	
7	4	2	1	6	1.293061227 $x10^{-4}$	1.384704002 $x10^{-4}$
	4	3	0	4	2.068897963 $x10^{-7}$	
	4	1	2	4	6.530612257 $x10^{-5}$	
	3	3	1	16	1.384704002 $x10^{-4}$	
	3	2	2	24	9.248000017 $x10^{-5}$	
	2	4	1	6	1.223792642 $x10^{-4}$	
	2	3	2	24	9.031680016 $x10^{-5}$	
	5	2	0	24	1.044897961 $x10^{-7}$	

	5	1	1	16	$6.530612257 \times 10^{-5}$	
8	4	3	1	4	$1.713104121 \times 10^{-4}$	$1.713104121 \times 10^{-4}$
	4	2	2	6	$1.160639648 \times 10^{-4}$	
	4	4	0	1	$3.676906406 \times 10^{-7}$	
	3	4	1	4	$2.872290039 \times 10^{-5}$	
	3	3	2	16	$1.242783454 \times 10^{-4}$	
	5	3	0	16	$1.742131836 \times 10^{-7}$	
	5	2	1	32	$1.148901361 \times 10^{-4}$	
9	4	3	2	4	$1.689588363 \times 10^{-4}$	$2.224059802 \times 10^{-4}$
	4	4	1	1	$2.224059802 \times 10^{-4}$	
	4	5	0	4	$3.169409453 \times 10^{-7}$	
	4	2	3	6	$8.587633994 \times 10^{-5}$	
	5	4	0	4	$3.178569596 \times 10^{-7}$	
	5	3	1	16	$1.579874833 \times 10^{-4}$	
	3	5	1	16	$1.534964942 \times 10^{-4}$	
	3	4	2	4	$1.644687632 \times 10^{-4}$	
10	6	3	1	24	$1.563596968 \times 10^{-4}$	$2.362949253 \times 10^{-4}$
	6	4	0	6	$2.960404572 \times 10^{-7}$	
	6	2	2	36	$1.167569805 \times 10^{-4}$	
	5	4	1	4	$1.926766644 \times 10^{-4}$	
	5	3	2	16	$1.678763834 \times 10^{-4}$	
	4	5	1	16	$1.914833165 \times 10^{-4}$	
	4	4	2	1	$2.362949253 \times 10^{-4}$	
	3	4	3	4	$1.310962693 \times 10^{-4}$	
	3	5	2	16	$1.631039655 \times 10^{-4}$	
11	6	3	2	24	$1.764737875 \times 10^{-4}$	$2.174265558 \times 10^{-4}$
	6	4	1	6	$1.762975304 \times 10^{-4}$	
	6	2	3	36	$9.885246831 \times 10^{-5}$	
	5	4	2	4	$2.174265558 \times 10^{-4}$	
	5	3	3	16	$1.421298734 \times 10^{-4}$	
	4	5	2	4	$2.160796031 \times 10^{-4}$	
	4	4	3	1	$2.000462835 \times 10^{-4}$	
12	7	3	2	16	$1.694161158 \times 10^{-4}$	$2.090927535 \times 10^{-4}$
	7	4	1	4	$1.686792358 \times 10^{-4}$	
	7	2	3	24	$1.135900047 \times 10^{-4}$	
	6	4	2	6	$2.090927535 \times 10^{-4}$	
	6	3	3	24	$1.570364948 \times 10^{-4}$	
	5	5	2	16	$2.087634435 \times 10^{-4}$	
	5	4	3	4	$1.934679313 \times 10^{-4}$	
	8	2	2	6	$1.22684842 \times 10^{-4}$	
	8	3	1	4	$1.36597303 \times 10^{-4}$	

SUMMARY

We present in tables 5 and 6 the summary of the D-optima for the three design regions and the design points of D-optimality, respectively. For easy presentation of the design points of D-optimality, we label the candidate points for the region of Face-centered CCD as follows;

1: (1,1), 2: (1.-1), 3: (-1,1), 4: (-1,-1), 5: (1,0), 6: (-1,0), 7: (0,1), 8: (0,-1), 9: (0,0).

For the region of Circumscribed CCD we have;

1: (1,1), 2: (1.-1), 3: (-1,1), 4: (-1,-1), 5: (1.414,0), 6: (-1.414,0), 7: (0,1.414), 8: (0,-1.414), 9: (0,0)

For the region of Inscribed CCD we have;

1: (0.7,0.7), 2: (-0.7,0.7), 3: (-0.7.-0.7), 4: (0.7,-0.7), 5: (1,0), 6: (-1,0), 7: (0,1), 8: (0,-1), 9: (0,0)

It is worth noting that for some N, there are equivalent designs that yield the same determinant value of imformation matrix.

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Table 5: D-optima using the regions of the three central composite designs

Design Size N	Faced-CenteredCCD	CircumscribedCCD	Inscribed CCD
6	$5.486968437x10^{-3}$	$3.1947\ x10^{-2}$	$1.166000031\ x10^{-4}$
7	$8.159865377\ x10^{-3}$	$3.837429233x10^{-2}$	$1.384704002\ x10^{-4}$
8	$8.7890625\ x10^{-3}$	$4.6828\ x10^{-2}$	$1.713104121x10^{-4}$
9	$9.754610572\ x10^{-3}$	$6.1584\ x10^{-2}$	$2.224059802\ x10^{-4}$
10	$9.360\ x10^{-3}$	$6.545687882\ x10^{-2}$	$2.362949253\ x10^{-4}$
11	$9.5374\ x10^{-3}$	$6.004443063\ x10^{-2}$	$2.174265558\ x10^{-4}$
12	$1.0154\ x10^{-2}$	$5.782736734x10^{-2}$	$2.090927535\ x10^{-4}$

Table 6: Some Design points of D-optimality over the regions of the three central composite designs

Design Size N	Faced-Centered CCD		CircumscribedCCD		Inscribed CCD	
	$g_1:g_2:g_3$	Design points	$g_1:g_2:g_3$	Design points	$g_1:g_2:g_3$	Design points
6	4 1 1	1,2,3,4,5,9	3 2 1	1,2,3,6,8,9	3 2 1	1,2,5,6,8,9
7	4 2 1	1,2,3,4,5,8,9	3 3 1	1,2,3,5,6,8,9	3 3 1	1,2,3,5,6,8,9
8	4 3 1	1,2,3,4,5,6,7,9	4 3 1	1,2,3,4,5,6,7,9	4 3 1	1,2,3,4,5,6,8,9
9	4 4 1	1,2,3,4,5,6,7,8,9	4 4 1	1,2,3,4,5,6,7,8,9	4 4 1	1,2,3,4,5,6,7,8,9
10	5 4 1	1,2,3,4,5,6,7,8,9,1	4 4 2	1,2,3,4,5,6,7,8,9,9	4 4 2	1,2,3,4,5,6,7,8,9,9
11	6 4 1	1,2,3,4,5,6,7,8,9,1,2	4 5 2	1,2,3,4,5,6,7,8,9,8,9	5 4 2	1,2,3,4,5,6,7,8,9,9,1
12	7 4 1	1,2,3,4,5,6,7,8,9,1,2,3	5 5 2	1,2,3,4,5,6,7,8,9,9,1,6	6 4 2	1,2,3,4,5,6,7,8,9,9,6,7

By imposing D-optimality criterion on the design regions of the three central composite designs we have obtained an N-point D-optimal exact design for a full bivariate quadratic model. In all cases, D-optimal designs obtained under the Rotatable (Circumscribed) Central Composite Design region had the best determinant values. Hence in estimating the parameters of the bivariate polynomial model, designs defined over the rotatable (circumscribed) central composite design region would give a more precise estimate of model parameters than those defined over the face-centred or inscribed central composite design regions. Also when trying to decide which CCD to use, if the experimenter's interest is in obtaining precision in parameter,then thecircumscribedCCD is recommended.

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