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# D-Optimally-Constructed Exact Designs under the Variation of Non-D-Optimality Criteria for Varying Regression Polynomials

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**Abstract:** The behaviour of *D*-optimal exact designs, constructed using a combinatorial algorithm, is examined under the variations of *A*-, *E*- and *G*-optimality criteria. In particular, the question of whether designs that are optimal with respect to one criterion are also optimal with respect to other criteria is addressed. The Condition Numbers (CN) of the designs as well as the equivalence relations of the criteria are noted. The *D*-optimal designs under consideration are for low-order bivariate polynomial models. By the rules of the algorithm, not more than 25 percent search on the total available designs is required within a design class since a lot of inferior designs, with respect to the search for optimal design are eliminated. The models, which could be with or without intercept, are defined on design regions which are supported by the points of the circumscribed central composite design. The points are classified into three groups with respect to their distances from the centre of the design region. Results show that *D*-optimally-constructed designs need not be *A*-, *E*- or *G*-optimum. For the first order models considered, the global best *D*-optimal exact designs were each, *A*-, *E*- and *G*-optimum. For the bivariate quadratic model considered, the global best *D*-optimal exact design was not necessarily *G*-optimum. However, the design was both *A*- and *E*-optimum. The prediction capabilities of these designs were graphically evaluated.

**Keywords:** *D*-optimality, Variance of Prediction, Trace, Eigenvalue, Condition number

## 1 Introduction

The use of *D*-optimality has gained much popularity as a vast number of literature on optimal designs centres around the *D*-optimality criterion. This is perhaps, due to the assertion that designs which are optimal with respect to the *D*-optimality criterion are invariably at least good in many other respects such as having low variances for the parameters, low correlations among parameters, low maximum variance of prediction over the design region, see [1]. As observed in [2], the importance of using a design that is deemed adequate for several optimality criteria cannot be overemphasized since optimality with respect to a particular optimality criterion usually represents an approximation to some notion of goodness. It is therefore important to examine the designs constructed under an optimality criterion with respect to other optimality criteria. [2] considered numerically, the efficiencies of different types of optimal designs under various model assumptions. In the work, the robust properties of *A*, *D*, *E* and *G*-optimal designs were compared for continuous designs only. Results showed that a design that is deemed adequate under one optimality criterion can perform poorly in terms of another optimality criterion. It was further revealed that a number of properties common to *A*, *D* and *G*-optimal designs were not possessed by *E*-optimal designs. One of such properties was observed for polynomial regression of degree $k$ when the hypothesized model is of degree $j$. It was noted that for *A*-, *D*- and *G*-optimal designs, the associated efficiency functions are non-increasing functions of $k$ whereas for the *E*-optimal designs, the efficiency function remained remarkably stable for $1 \leq j \leq k \leq 8$ and hence *E*-optimal designs do not possess the monotonic property. This result places caution on the use of *E*-optimal designs as slightly mis-specified model can result in severe loss in efficiency of the design. [3] compared the efficiencies of *A*-, *D*- and *G*-optimality for second-order split-plot Central Composite Design under various degrees of correlation. For the second-order reduced split-plot Central Composite Design models

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considered, $D$-, $A$- and $G$-optimality criteria were not robust across reduced models. [4] carried out a comparative study of some varieties of the Central Composite Design using the $A$-, $D$- and $G$-optimality criteria. The varieties of the Central Composite Design considered include Spherical Central Composite Design (SCCD), Rotatable Central Composite Design (RCCD), Orthogonal Central Composite Design (OCCD), Slope Rotatable Central Composite Design (Slope-R) and Face center Cube (FCC).

In studying the behaviour of $D$-optimally constructed exact designs under the variation of non-$D$-optimality criteria, comparisons made are under the assumption that the true model is a polynomial of degree $m$. Although the form of the true underlying relationship between the response variable and the independent variables is usually unknown, [5] has it that the relationship can be approximated by a low-order polynomial such as the first- and second-order response surface models in equations (1) and (2), respectively;

$$y_{ij} = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j>i}^{k} \beta_{ij} x_i x_j + \varepsilon_{ij} \tag{1}$$

and

$$y_{ij} = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j>i}^{k} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \beta_{ii} x_{ii}^2 + \sum_{j>i}^{2} \beta_{jj} x_{jj}^2 + \varepsilon_{ij}, i = 1,2,\dots,k; j > i \tag{2}$$

where $y_{ij}$'s are the observations due to the univariate response variable; $\beta$'s are the parameter coefficients; $x_i$'s and $x_j$'s are the independent variables; $\varepsilon_{ij}$'s are the error terms associated with the $y_{ij}$'s which are normally and independently distributed with zero mean and constant variance.

In this work, the design space is taken to be the spherical region in two variables, supported by the points $(\pm 1, \pm 1)$, $(\pm 1.414, 0)$, $(0, \pm 1.414)$ and centred at the point $(0,0)$. Unlike some works where interest is on continuous designs, only exact designs are considered here. This follows from the remarks of [6] that in practice, all designs are exact. According to[7], a design, $\xi_N$, is an $N$-point exact design if $\xi_N$ is a probability measure on the design region, $\tilde{X}$, which attaches a mass $\frac{1}{N}$ to each point of the design and $N\xi_N$ is a non-negative integer for $\underline{x} \in \tilde{X}$. We shall denote the space of $N$-point exact designs on $\tilde{X}$ by $\Xi_{\tilde{X}}^N$. The information matrix, $M(\xi_N)$, of an exact design, $\xi_N$, is given by $M(\xi_N) = \frac{1}{N} X'X$, where $X$ is an $N \times p$ design matrix of $\xi_N$, whose ith row is $f(\underline{x_i})$. The design, $\xi_N^*$, is a $D$-optimal exact design if the determinant of the information matrix, $M(\xi_N^*)$, is maximized over all $M(\xi_N)$ for $\xi_N \in \Xi_{\tilde{X}}^N$. The $D$-optimality criterion introduced by [8] is basically a parameter estimation criterion and puts emphasis on the quality of the parameter estimates.

Most $D$-optimal designs are generated by search algorithms such as the DETMAX algorithm of [1], the K-L algorithm of [6], etc. [9] introduced the combinatorial algorithm which requires grouping design points in the design region according to their distances from the centre of the design region into $g_1$, $g_2$, ... , $g_H$ groups. This algorithm serves extensively well in locating $D$-Optimal designs and is applicable under varying experimental conditions as seen in [10]. [11] suggested rules for obtaining a starting design that is as close as possible to the optimal design as measured by the determinant value of the information matrix. [12] utilized the principles embodied in the Combinatorial Algorithm while studying the effects of imposing $D$-Optimality criterion on the design regions of the Central Composite Designs. Results showed that the $D$-optimality criterion performed better on the region supported by design points of the Circumscribed Central Composite Design.

Attempts have been made to reduce the determinantal evaluations of the basic combinatorial algorithm to a manageable number. One of such attempts is due to [13] whose efficient algorithm eliminates a large number of inferior designs and allows not more than a 25 percent search in locating the best design within a design class. The essence of this work therefore is to examine the behaviour of $D$-optimally-constructed exact designs, under the variations of $A$-, $E$- and $G$-optimality criteria. In particular, we examine whether these exact designs are optimal with respect to the optimality criteria under consideration. In Design of Experiments, the $D$-optimality criterion has been most frequently encountered (see also, [14]). As a determinant-based criterion, the $D$-optimality criterion has the objective of maximizing the determinant of the information matrix of the design. By maximizing the determinant of the information matrix, the determinant of the variance-covariance matrix of the parameter estimates is also minimized. The implication of this is that the variances of the parameter estimates as well as the covariances among the parameters are minimized.

In assessing the goodness of an already constructed $D$-optimal exact design, we shall employ $A$-, $E$- and $G$-optimality criteria as well as the condition number of the design. The criterion of $A$-optimality, introduced by [15], maximizes the trace of the information matrix of the design and hence minimizes the trace of the variance-covariance matrix, $M^{-1}(\xi)$ thereby minimizing the variances of the parameter estimates. Unlike the $D$-optimality criterion, the $A$-optimality criterion does not take into account the covariances among parameters. The $G$-optimality criterion introduced by [16] seeks to minimize the maximum variance of any predicted response value over the experimental space (design region). The variance of the predicted response at $\underline{x}$ is given by

$$Var(\hat{y}(\underline{x})) = \sigma^2 f'(\underline{x}) M^{-1}(\xi) f(\underline{x}). \quad (3)$$

Without loss of generality, we assume that $\sigma^2$ is a constant, say 1. The criterion of $E$-optimality introduced by [17] seeks to maximize the minimum eigenvalue of the information matrix and hence minimizes the maximum eigenvalue of the variance-covariance matrix. The criterion of $E$-optimality is defined symbolically by

$$max\lambda_{min}(M^{-1}(\xi)) = min\lambda_{max}(M^{-1}(\xi)), \quad (4)$$

where $\lambda_{min}$ is the minimum eigenvalue of $M(\xi)$ and $\lambda_{max}$ is the maximum eigenvalue of $M^{-1}(\xi)$: see, for example, [18] and [6] for further details. The Condition Number (CN) is an evaluation criterion used to rate an already created $D$-optimal design. It evaluates the sphericity and the symmetricism of the $D$-optimal design. Let

$$M = \begin{pmatrix} m_{11} & m_{12} & \ldots & m_{1p} \\ m_{21} & m_{22} & \ldots & m_{2p} \\ . & . & \ldots & . \\ . & . & \ldots & . \\ . & . & \ldots & . \\ m_{p1} & m_{p2} & \ldots & m_{pp} \end{pmatrix}$$

be a $p \times p$ symmetric matrix such that $m_{ij} = m_{ji}$. The condition number of the matrix, $M$ is defined by $Cond(M) = \|M\| \|M-1\|$, where the matrix norm, $\|M\|$, can easily be computed as the maximum absolute column sum (or row sum) given by $\|m\| = max_j \sum_{i=1}^{p} |m_{ij}|$; $\|m\| > 0$ if $m \neq 0$. The matrix norm, $\|M-1\|$, is similarly computed. For any matrix $M$, $Cond(M) \geq 1$. According to [19], a design with a Condition Number of 1 would be orthogonal, while an increasing Condition Number indicates a less orthogonal design.

We shall employ the combinatorial algorithm outlined in Section 2 in the construction of the $D$-optimal designs. The Condition Numbers of the designs as well as the possible equivalence relations of the $A$-, $E$- and $G$-criteria shall be noted. In this study, the $D$-optimal designs constructed are for low-order bivariate polynomial models which could be with or without intercept. The models shall be defined on design region that is supported by the points of the Circumscribed Central Composite Design. The design points of the design region shall be classified into three groups with respect to their distances from the centre of the design region. Although this work considers low-order polynomials and design points of the circumscribed central composite design, the working of the algorithm is not restricted to low-order polynomials nor to design points of the Circumscribed Central Composite Design.

## 2 Methodology

For the algorithm, we assume that the support points that define the design region have been arranged into $H$ groups, namely, $g_1$, $g_2$, ..., $g_H$ according to their distances, $d_i$ , from the centre of the region, $\tilde{X}$, and are such that $d_1 > d_2 > ... > d_H$. The group, $g_1$ holds $N_1$ support points, $g_2$ holds $N_2$ support points, etc and $N_1 + N_2 + ... + N_H = \overline{N}$, where $\overline{N}$ is the total number of distinct support points in the design region. The design class, say, $\underline{C} = \{r_1 : r_2 : ... : r_H\}$, requires selecting $r_1$ support points from $g_1$, $r_2$ support points from $g_2$, ... , $r_H$ support points from $g_H$. There are $a_i$ ways of selecting $r_i$ support points from $g_i$ and hence we obtain $a_i$ sub-designs.

The following steps make up the algorithm for constructing the $D$-optimal exact designs:

Step I: Obtain $a_i = \binom{N_i}{r_i}$ sub-designs from $g_iN_i$. The notation, $g_iN_i$, implies that group $g_i$ holds $N_i$ supports points.

Step II: List the $a_i$ sub-designs, $a_1, a_2, ..., a_{ai}$

StepIII: Form sets of composite designs from the $a_i$ sub-designs such that $a_1 < a_2 < ... < a_{ai}$. Where this restriction does not hold, the groups within the class may be repositioned to achieve the restriction.

StepIV: Choose any set, $i$, and compute $detM(\xi^{ijk})$, the determinant of information matrix associated with $\xi^{ijk}$ ; $i=1,2,...,a_i$ ; $j=1,2,...,ai; k=1,2,...,a_i$ .

StepV: Set $d_c^* = max[detM(\xi^{ijk})]$.

Specifically, for $H=3$, we require an $N$-point design such that $r_1+r_2+r_3=N$ with design class, $\underline{C} = r_1 : r_2 : r_3$, following the steps that make up the algorithm.

i. Obtain $a_1 = \binom{N_1}{r_1}$ sub-designs from $g_1(N_1)$, $a_2 = \binom{N_2}{r_2}$ sub-designs from $g_2(N_2)$ and $a_3 = \binom{N_3}{r_3}$ sub-designs from $g_3(N_3)$.

ii. List the $a_1$ sub-designs as $\xi_{11} = \{a_{11}\}$, $\xi_{12} = \{a_{12}\}$, ... , $\xi_{1a_1} = \{a_{1a_1}\}$, $a_2$ sub-designs as $\xi_{21} = \{a_{21}\}$, $\xi_{22} = \{a_{22}\}$, ... , $\xi_{2a_2} = \{a_{2a_2}\}$ and $a_3$ sub-designs as $\xi_{31} = \{a_{31}\}$, $\xi_{32} = \{a_{32}\}$, ... , $\xi_{3a_3} = \{a_{3a_3}\}$.

iii. Form sets of composite designs from $a_1$, $a_2$ and $a_3$ sub-designs as:

Set 1: $\xi^{(111)} = \begin{pmatrix}\xi_{11}\\ \xi_{21}\\ \xi_{31}\end{pmatrix}, \xi^{(112)} = \begin{pmatrix}\xi_{11}\\ \xi_{21}\\ \xi_{32}\end{pmatrix}, ..., \xi^{(11a_3)} = \begin{pmatrix}\xi_{11}\\ \xi_{21}\\ \xi_{3a_3}\end{pmatrix}$

$\xi^{(121)} = \begin{pmatrix}\xi_{11}\\ \xi_{22}\\ \xi_{31}\end{pmatrix}, \xi^{(122)} = \begin{pmatrix}\xi_{11}\\ \xi_{22}\\ \xi_{32}\end{pmatrix}, ..., \xi^{(12a_3)} = \begin{pmatrix}\xi_{11}\\ \xi_{22}\\ \xi_{3a_3}\end{pmatrix}$ .

.
.

$\xi^{(1a_31)} = \begin{pmatrix}\xi_{11}\\ \xi_{2a_2}\\ \xi_{31}\end{pmatrix}, \xi^{(1a_32)} = \begin{pmatrix}\xi_{11}\\ \xi_{2a_2}\\ \xi_{32}\end{pmatrix}, ..., \xi^{(1a_3a_3)} = \begin{pmatrix}\xi_{11}\\ \xi_{2a_2}\\ \xi_{3a_3}\end{pmatrix}$

$Set2:$ $\xi^{(211)} = \begin{pmatrix}\xi_{12}\\ \xi_{21}\\ \xi_{31}\end{pmatrix}, \xi^{(212)} = \begin{pmatrix}\xi_{12}\\ \xi_{21}\\ \xi_{32}\end{pmatrix}, ..., \xi^{(21a_3)} = \begin{pmatrix}\xi_{12}\\ \xi_{21}\\ \xi_{3a_3}\end{pmatrix}$

$\xi^{(221)} = \begin{pmatrix}\xi_{12}\\ \xi_{22}\\ \xi_{31}\end{pmatrix}, \xi^{(222)} = \begin{pmatrix}\xi_{12}\\ \xi_{22}\\ \xi_{32}\end{pmatrix}, ..., \xi^{(22a_3)} = \begin{pmatrix}\xi_{12}\\ \xi_{22}\\ \xi_{3a_3}\end{pmatrix}$

.
.
.

$\xi^{(2a_31)} = \begin{pmatrix}\xi_{12}\\ \xi_{2a_2}\\ \xi_{31}\end{pmatrix}, \xi^{(2a_32)} = \begin{pmatrix}\xi_{12}\\ \xi_{2a_2}\\ \xi_{32}\end{pmatrix}, ..., \xi^{(2a_3a_3)} = \begin{pmatrix}\xi_{12}\\ \xi_{2a_2}\\ \xi_{3a_3}\end{pmatrix}$

.
.
.

$Set\ a_1:$ $\xi^{(a_111)} = \begin{pmatrix}\xi_{1a_1}\\ \xi_{21}\\ \xi_{31}\end{pmatrix}, \xi^{(a_112)} = \begin{pmatrix}\xi_{1a_1}\\ \xi_{21}\\ \xi_{32}\end{pmatrix}, ..., \xi^{(a_11a_3)} = \begin{pmatrix}\xi_{1a_1}\\ \xi_{21}\\ \xi_{3a_3}\end{pmatrix}$

$\xi^{(a_121)} = \begin{pmatrix}\xi_{1a_1}\\ \xi_{22}\\ \xi_{31}\end{pmatrix}, \xi^{(a_122)} = \begin{pmatrix}\xi_{1a_1}\\ \xi_{22}\\ \xi_{32}\end{pmatrix}, ..., \xi^{\left(a_{12a_3}\right)} = \begin{pmatrix}\xi_{1a_1}\\ \xi_{22}\\ \xi_{3a_3}\end{pmatrix}$

.
.
.

$\xi^{(a_1a_31)} = \begin{pmatrix}\xi_{1a_1}\\ \xi_{2a_2}\\ \xi_{31}\end{pmatrix}, \xi^{(a_1a_32)} = \begin{pmatrix}\xi_{1a_1}\\ \xi_{2a_2}\\ \xi_{32}\end{pmatrix}, ..., \xi^{(a_1a_3a_3)} = \begin{pmatrix}\xi_{1a_1}\\ \xi_{2a_2}\\ \xi_{3a_3}\end{pmatrix}$

**Table 1a Combinatorics at the initial stage of constructing D-optimal design**

| Step $t$ | Sub-step u | $g_1$ | $g_2$ | $g_3$ | Sub-step u best determinant value | Step $t$ best determinant value |
|---|---|---|---|---|---|---|
| 0 | 1 | $r_1$ | $r_2$ | $r_3$ | $d_0$ | $d_0$ |
| 1 | 1 | $r_1$-1 | $r_2$+1 | $r_3$ | $d^-_{11}$ | $d_1$ |
| | 2 | $r_1$+1 | $r_2$-1 | $r_3$ | $d^+_{12}$ | |
| 2 | 1 | $r_1$-2 | $r_2$+2 | $r_3$ | $d^-_{21}$ | $d_2$ |
| | 2 | $r_1$+2 | $r_2$-2 | $r_3$ | $d^+_{22}$ | |
| 3 | 1 | $r_1$-3 | $r_2$+3 | $r_3$ | $d^-_{31}$ | $d_3$ |
| | 2 | $r_1$+3 | $r_2$-3 | $r_3$ | $d^+_{32}$ | |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |

The steps outlined in Table 1a will yield an optimal design class, $\underline{C}$=$\{r_1' : r_2' : r_3\}$, that is conditioned on holding $r_3$ fixed. Let the associated determinant value of information matrix for the best design in the design class be $d_c$. With the design class $\underline{C}$=$\{r_1' : r_2' : r_3\}$, we proceed to obtain the optimal number of design points taken from $g_3$ by following the steps of Table 1b.

**Table 1b Combinatorics at the later stage of constructing D-optimal design**

| Step $t$ | Sub-step u | $g_1$ | $g_2$ | $g_3$ | Sub-step u best determinant value | Step $t$ best determinant value |
|---|---|---|---|---|---|---|
| 0 | 1 | $r_1'$ | $r_2'$ | $r_3$ | $d_f$ | $d_f$ |
| 1 | 1 | $r_1'+1$ | $r_2'$ | $r_3$ - 1 | $dd^-_{111}$ | $dd_1$ |
| | 2 | $r_1'$ | $r_2'+1$ | $r_3$ - 1 | $dd^-_{112}$ | |
| | 1 | $r_1'-1$ | $r_2'$ | $r_3+1$ | $dd^+_{111}$ | |
| | 2 | $r_1'$ | $r_2'-1$ | $r_3+1$ | $dd^+_{112}$ | |
| 2 | 1 | $r_1'+2$ | $r_2'$ | $r_3$ - 2 | $dd^-_{211}$ | $dd_2$ |
| | 2 | $r_1'+1$ | $r_2'+1$ | $r_3$ - 2 | $dd^-_{212}$ | |
| | 1 | $r_1'+1$ | $r_2'+1$ | $r_3$ - 2 | $dd^-_{221}$ | |
| | 2 | $r_1'$ | $r_2'+2$ | $r_3$ - 2 | $dd^-_{222}$ | |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |

For step $t = 0,1,2,..,n,n+1,n+2,..,q,q+1$ in Table 1a, $d_0 < d_1 < d_2 < \ldots < d_n > d_{(n+1)}$. This similarly applies for the steps in Table 1b.

$$d_t^* = max\left\{\left(detM\left(\xi_t^{(i,j)}\right)\right\}; M\left(\xi_t^{(i,j)}\right) \in S_t^{p\times p} \text{ for all } t.$$

where $S_t^{p\times p}$ is the space of non-singular $p\times p$ information matrices at the $t^{th}$ step. For clarity, it is assumed from Table 1a that the initial design class at step 0 is $\underline{C}$=$\{r_1,r_2,r_3\}$ and is such that $d_0$ is the determinant value of the best design in the design class, 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 $g_3$.

It is further assumed that $r_3$ is held fixed while making increments on the $r_i'$'s of the other groups. By incremental changes on the $r_i$ values, we aim to arrive at the optimal number of support points taken from the $H-1=2$ groups namely, $r_1'$ and $r_2'$ while holding $r_3$ value fixed. Here, $r_1'$ shall be referred to as the conditional optimal number of supports points from $g_1$ and $r_2\prime$ shall be referred to as the conditional optimal number of support points from $g_2$. Holding $r_3$ 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. At each sub-step of step 1, we compute the determinant value of the information matrix associated with the best design in the design class. The best determinant value in step 1 is $d_1$. Suppose $d_1 < d_0$, then we have obtained the optimal value, $r_1'$, holding $r_3$ value fixed. Now, we seek to obtain $r_2'$ holding $r_3$ 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 $r_3$. 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 design class $\underline{C} = [r_1 - 1, r_2 + 1, r_3]$, 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.

As earlier observed, we shall compute the determinant value of the best designs in each of the design classes. At step 2, the best determinant value is $d_2$. This value will be compared with $d_1$ to check for convergence. If $d_2 > d_1$ , we effect an increment on $r_1$ by 3. If otherwise, then we have obtained the optimal value $r_{1'}$ holding $r_3$ value fixed. Continuing the process will yield the design class $\underline{C} = [r_1', r_2', r_3]$. The remaining task is that of attempting to effect increments on $r_3$ so as to obtain the optimal number of support points, $r_3^*$, taken from group $g_3$ . 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 $r_3$ value will obviously affect the values of $r_1'$ and $r_2'$. The design class that results in the global best determinant value is defined by $\underline{C}^* = [r_1^*, r_2^*, r_3^*]$ where $r_i^*$ is the optimal number of support points taken from the $i^{th}$ group. The $D$-optimal exact design is contained in the immediate past tuple and is associated with $d^*$, the best determinant value of information matrix.

## 3 Illustrations

We apply the algorithm on the problem of constructing $N$-point $D$-Optimal exact designs for the bivariate polynomial models,

$$i. \qquad y(x_1, x_2) = \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon \tag{5}$$

$$ii. \qquad y(x_1, x_2) = \beta + 0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon \tag{6}$$

$$iii. \qquad y(x_1, x_2) = \beta + 0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \varepsilon \tag{7}$$

defined on the geomtric region in Figure 1.

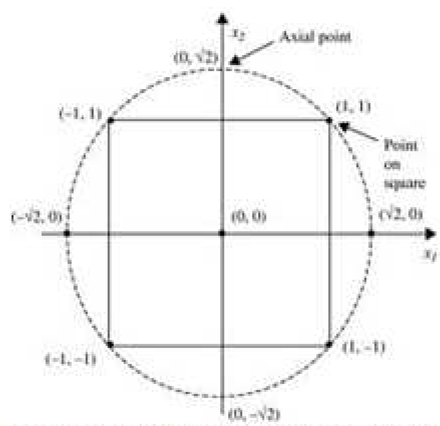



*Figure 1: Spherical Geometric Region with Axial Distance, α=1.414*

We demonstrate constructing a 6-point $D$-optimal exact design for the six-parameter bivariate polynomial model of equation (7).

The needed computations are tabulated in Table 2. Column 1 is the required $t$ steps for constructing the 6-point $D$-optimal exact design, column 2 is the required $u$ sub-steps at each design class, column 3 is the desired design size, column 4 is the design class components where $r_1$ is the number of support points taken from group $g_1$, $r_2$ is the number of support points taken from group $g_2$ and $r_3$ is the number of support points taken from group $g_3$. Column 5 gives the best determinant value of information matrix for the N-point $D$-optimal exact design within the design class. Column 6 gives the best determinant value of information matrix for the required $N$-point $D$-optimal exact design. In listing of the optimal design points, the notations $1,2,3,4,5,6,7,8,9$ shall represent the design points $(1,1)$, $(-1,1)$, $(1,-1)$, $(-1,-1)$, $(1.414,0)$, $(-1.414,0)$, $(0,1.414)$, $(0,-1.414)$ and $(0,0)$, respectively. The results of the search for $N$-point $D$-optimal exact designs for the three models considered are summarized in Table 3 for the no-intercept first order model, Table 4 for the full bivariate first order model and Table 5 for the full bivariate quadratic model.

**Table 2 Combinatorics for constructing 6-point D-optimal exact design**

| Step t | Sub-step u | Design size N | Design class component $r_1$ | $r_2$ | $r_3$ | Det $M(\xi^t)$ | Det $M(\xi^*)$ |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 6 | 4 | 1 | 1 | $2.193461929 \times 10^{-2}$ | |
| 2 | 1 | | 4 | 0 | 2 | Singular design | |
| | 2 | | 4 | 2 | 0 | $8.002099747 \times 10^{-9}$ | |
| 3 | 1 | | 3 | 2 | 1 | $3.19474332 \times 10^{-2}$ | $3.19474332 \times 10^{-2}$ |
| | 2 | | 3 | 1 | 2 | Singular design | |
| 4 | 1 | | 2 | 3 | 1 | $3.193613001 \times 10^{-2}$ | |
| | 2 | | 2 | 2 | 2 | Singular design | |
| 5 | 1 | | 5 | 0 | 1 | Singular design | |
| | 2 | | 5 | 1 | 0 | Singular design | |

**Table 3 Summary statistics for the no-intercept first order model**

| Design size N | Optimal design class component $r_1^*$ | $r_2^*$ | $r_3^*$ | Design points | Best determinant value of information matrix of the design | Best maximum variance of Prediction | Best trace of varaince-covariance matrix | Best minimum eigen value of information matrix of the design | Best condition number of the design |
|---|---|---|---|---|---|---|---|---|---|
| 3 | 3 | 0 | 0 | 1,2,3 | 0.5926 | 3.0000 | 4.5000 | 0.3337 | 4.9998 |
| 4 | 4 | 0 | 0 | 1,2,3,4 | 1.0000 | 3.0000 | 3.0000 | 1.0000 | 1.0000 |
| 5 | 5 | 0 | 0 | 1,2,3,4,1 | 0.8960 | 3.5714 | 3.2142 | 0.8000 | 1.9984 |
| 6 | 6 | 0 | 0 | 1,2,3,4,1,2 | 0.8888 | 4.0000 | 3.2500 | 0.6667 | 2.0000 |
| 7 | 7 | 0 | 0 | 1,2,3,4,1,2,3 | 0.9329 | 4.2000 | 3.1500 | 0.7149 | 1.7987 |
| 8 | 8 | 0 | 0 | 1,2,3,4,1,2,3,4 | 1.0000 | 3.0000 | 3.0000 | 1.0000 | 1.0000 |
| 9 | 9 | 0 | 0 | 1,2,3,4,1,2,3,4,1 | 0.9657 | 3.2727 | 3.0681 | 0.8889 | 1.3871 |
| 10 | 10 | 0 | 0 | 1,2,3,4,1,2,3,4,1,2 | 0.9600 | 3.5000 | 3.0832 | 0.8000 | 1.4995 |
| 11 | 11 | 0 | 0 | 1,2,3,4,1,2,3,4,1,2,3 | 0.9737 | 3.6666 | 3.0555 | 0.6521 | 1.3359 |
| 12 | 12 | 0 | 0 | 1,2,3,4,1,2,3,4,1,2,3,4 | 1.0000 | 3.0000 | 3.0000 | 1.0000 | 1.0000 |

**Table 4 Summary statistics for the full bivariate first order model**

| Design size N | Optimal design class component $r_1^*$ | $r_2^*$ | $r_3^*$ | Design points | Best determinant value of the design | Best maximum variance of Prediction | Best trace of varaince-covariance matrix | Best minimum eigen value of information matrix of the design | Best condition number of the design |
|---|---|---|---|---|---|---|---|---|---|
| 4 | 4 | 0 | 0 | 1,2,3,4 | 1.0000 | 4 | 4 | 1.0000 | 1.00 |
| 5 | 5 | 0 | 0 | 1,2,3,4,1 | 0.8192 | 5.00 | 4.3748 | 0.8000 | 2.50 |
| 6 | 6 | 0 | 0 | 1,2,3,4,1,2 | 0.7901 | 6.00 | 4.5 | 0.6667 | 2.00 |
| 7 | 7 | 0 | 0 | 1,2,3,4,1,2,3 | 0.8530 | 7.00 | 4.3748 | 0.5724 | 2.50 |
| 8 | 8 | 0 | 0 | 1,2,3,4,1,2,3,4 | 1.0000 | 4 | 4 | 1.0000 | 1.00 |
| 9 | 9 | 0 | 0 | 1,2,3,4,1,2,3,4,1 | 0.9364 | 4.50 | 4.1248 | 0.0787 | 1.75 |
| 10 | 10 | 0 | 0 | 1,2,3,4,1,2,3,4,1,2 | 0.9216 | 5.00 | 4.1664 | 0.8000 | 1.50 |
| 11 | 11 | 0 | 0 | 1,2,3,4,1,2,3,4,1,2,3 | 0.9442 | 5.50 | 4.1248 | 0.7282 | 1.75 |
| 12 | 12 | 0 | 0 | 1,2,3,4,1,2,3,4,1,2,3,4 | 1.0000 | 4 | 4 | 1.0000 | 1.00 |

Table 5 Summary statistics for the full bivariate quadratic model

| Design size N | Optimal design class component $r_1^*$ | $r_2^*$ | $r_3^*$ | Design points | Best determinant value for N-point design | Best maximum variance of Prediction | Best trace of varaince covariance matrix | Best minimum eigen value of information matrix | Best condition number |
|---|---|---|---|---|---|---|---|---|---|
| 6 | 3 | 2 | 1 | 1,2,3,6,8,9 | $3.1947433200\times10^{-2}$ | 6 | 17.7268 | 0.1084 | 43.59697290 |
| 7 | 3 | 3 | 1 | 1,2,4,5,6,8,9 | $3.837429226\times10^{-2}$ | 7 | 18.6598 | 0.0930 | 47.99048907 |
| 8 | 4 | 3 | 1 | 1,2,3,4,5,6,7,9 | $4.6828783707\times10^{-2}$ | 8 | 19.0017 | 0.0817 | 47.98398049 |
| 9 | 4 | 4 | 1 | 1,2,3,4,5,6,7,8,9 | $6.158433842\times10^{-2}$ | 9 | 19.6897 | 0.0730 | 49.99292226 |
| 10 | 4 | 4 | 2 | 1,2,3,4,5,6,7,8,9,9 | $6.545687882\times10^{-2}$ | 6.2508 | 14.3767 | 0.1296 | 25.99574004 |
| 11 | 5 | 4 | 2 | 1,1,2,3,4,5,6,7,8,9,9 | $6.004443063\times10^{-2}$ | 6.8560 | 15.1268 | 0.1180 | 31.99612467 |
| 12 | 5 | 5 | 2 | 1,1,2,3,4,5,6,6,7,8,9,9 | $5.782736734\times10^{-2}$ | 7.3626 | 16.9880 | 0.1067 | 39.88088840 |

## 4 Graphical Evaluations

In this section, we closely assess the prediction capabilities of the designs under the three models. The variance dispersion graph (VDG), introduced by [20], was the graphical tool used to display and review the prediction capabilities of the various designs under the different models. The need for graphical considerations is based on the fact that single value criteria, like the $A-$ and $D$-criteria, do not completely describe the performance of a design throughout the region under consideration. Again, condensing the properties of a design to single value may lead to loss of much information as regards the design's potential performance (see, for example, [21], [22],and [23]).

The variance dispersion graph displays the prediction variance of the design at every point radius in the design region. The points of strength and weaknesses of the design in the design region are easily assessed from the VDGs. The VDG procedure in [20] for first-order models was used for models (i) and (ii). For model (iii), the VDG procedure for the second-order central composite designs proposed by [21] was used. The graphs for the designs in the models are displayed in Figures 2, 3 and 4.

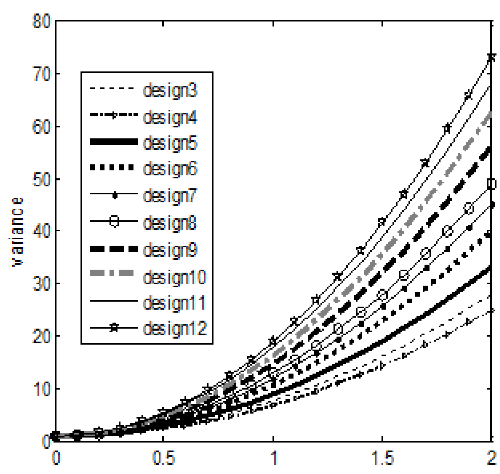


Figure 2: VDG's for the Designs Under the no-Intercept Bivariate First-Order Model

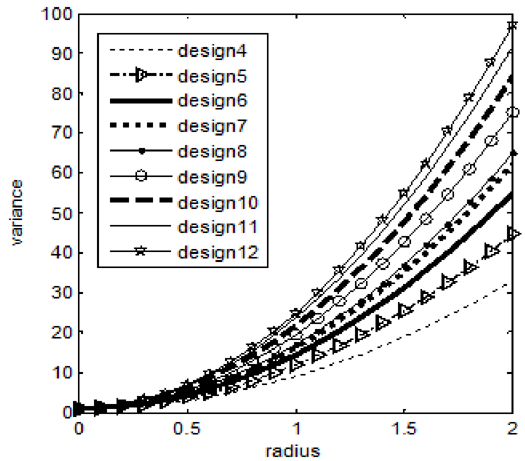


Figure 3: VDG's for the Full Bivariate First-Order Model

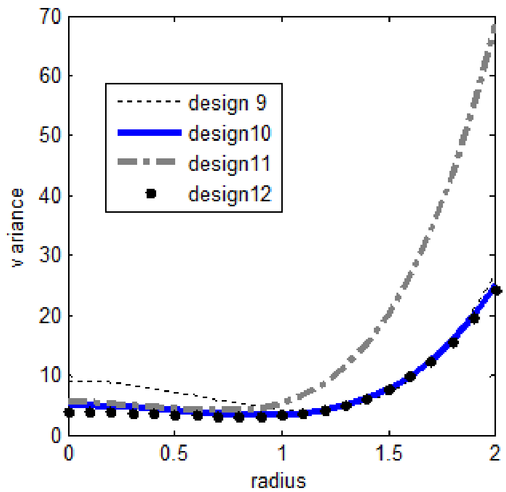


Figure 4: VDG's for the Full Bivariate Second-Order Model

According to the graphs in Figure 2, design4, with design points, $(1,1)$, $(-1,1)$, $(1,-1)$ and $(-1,-1)$, is the best since the design has the smallest prediction variance throughout the entire design region. This is followed by design 3, with design points, $(1,1)$, $(-1,1)$ and $(1,-1)$. The prediction variance of the designs deteriorates as the design size increases such that the design with the worst prediction capability is the design with the largest size of 12 runs. Also, the prediction variances of all the designs get worse close to the extremes of the design region. The graphs show that only the design (design 4) with full factorial component, $(1,1)$, $(-1,1)$, $(1,-1)$ and $(-1,-1)$, has the best prediction variance spread throughout the design region. The other designs, like design three with incomplete factorial component, or the other designs where some or all the factorial points are replicated performed poorly because of the spread of high prediction variances throughout the entire design region except at points close to the centre of the region. These attributes are also obtainable with the designs associated with the full bivariate first-order model as could be seen in Figure 3. The designs' prediction capabilities deteriorate as the design sizes increase and parts or full factorial points are replicated.
For the designs associated with the full bivariate second-order model, the behaviour are different from those of the first-order models discussed above. Designs 6, 8 and 9 display extremely high prediction variances and were therefore removed and not plotted in Figure 4. The graphs displayed in Figure 4 show that designs 10 and 12 display the best prediction variances and compete equally throughout the entire design region except at radius,$0 \leq r \leq 0.5$ , where design 12 is slightly better than design 10 with smaller prediction variance. Design 9 displayed the worst prediction capability at radius, $0 \leq r \leq 1.0$, but competes favourably with designs 10 and 12 towards the extremes of the design region.

## 5 Discussion of results

In addressing the question on whether *D*-optimal exact designs could also be optimal with respect to non-*D*-optimality criteria, the following observations are made for the models and design region under study:

i. *D*-optimally-constructed designs need not be *A*-, *E*- or *G*-optimum.

ii. For the first-order model with intercept term, the global best *D*-optimal exact designs were each, $A-$, $G-$ and *E*-optimum. This is sequel to the fact that the design that maximized the determinant of information matrix also minimized the maximun variance of prediction over the design region as well as minimizing the trace of the variance-covariance matrix. Furthermore, the designs also maximized the minimun eigen value of information matrix over the exact designs considered. The condition number of 1 indicates that the designs are perfectly orthogonal. The equivalence of $D-$ and *G*-optimality criteria was noted for the global best *D*-optimal exact designs since the minimum of the maximum variance of prediction equals the number of model parameters.

iii. For the first-order model without intercept term, the designs that maximized the determinant of information matrix also minimized the maximun variance of prediction over the design region as well as minimizing the trace of the variance-covariance matrix. Furthermore, the designs also maximized the minimun eigen value of information matrix over the exact designs considered. Hence, the global best *D*-optimal exact designs were each, *A*-optimum, *G*-optimun as well as *E*-optimum. The condition number of 1 indicates that the designs are perfectly orthogonal. The equivalence of $D-$ and *G*-optimality criteria was established for the global best *D*-optimal exact designs since the minimum of the maximum variance of prediction equals the number of model parameters.

iv. For the first-order model without intercept term, there is a strong aggreement between $D-$ and *A*-optimality criteria. As the determinant value of information matrix increases for changing design size, the trace of the variance-covariance matrix decreases simultaneously. However, the strong aggreement is not observed for $D-$ and the *G*-optimality criteria nor for $D-$ and the *E*-optimality criteria. In comparing the *D*-optimality criterion with the condition number, as the determinant value of information matrix increases for changing design size the condition number simulteneously decreases.

v. The observations for the first-order model without intercept term are generally true for the first order model with intercept term.

vi. For the design size considered using the bivariate quadratic model, the global best *D*-optimal design was not necessarily *G*-optimum. However, the design was $A-$ and *E*-optimum. On the contrary for $N = 6$, the best *D*-optimal exact design was also *G*-optimal and the equivalence of $D-$ and *G*-criteria was noted since the maximum variance of prediction equals the number of model parameters. For changing design size, the relationships among $A-$, $D-$ and *G*-criteria as well as the condition number do not generally apply. Infact, for the bivariate quadratic model, the condition number need not be used as an assessment criterion as the optimal designs are far from being orthogonal. There exists a *G*-optimum design that is far from being $D-$, $A-$ and *E*-optimum. The associated condition number shows much less orthogonality.

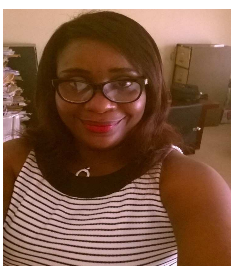
## 6 Conclusion

From the foregoing, *D*-optimally-constructed exact designs for the bivariate first-order polynomial models with or without the intercept term are optimal with respect to the $A-$, $E-$ and *G*-optimality criteria. These designs are also orthogonal. On the other hand, for the full bivariate second-order model, the *D*-optimally-constructed exact designs are not uniformly $A-$, $E-$ and *G*-optimal; neither are they orthogonal. In general, *D*-optimally-constructed exact designs for bivariate first- and second-order polynomial models need not be $A-$, $E-$ and *G*-optimal.

## References

[1] T. J. Mitchell, An Algorithm for the Construction of D-optimal Experimental Designs. Technometrics, **16**, 203-210 (1974).
[2] k. W. Wong, Comparing robust properties of A, D, E and G-optimal designs, Computational Statistics & Data Analysis, **18**, 441-448 (1993).
[3] A. C. Chukwu and Y. Yakubu, Comparison of optimality criteria of reduced models for response surface designs with restricted randomization, Progress in Applied Mathematics, **4**(2), 110-126 (2012).
[4] B. A. Oyejola and J. C. Nwanya, Selecting the right central composite design, Journal of Statistics and Applications, **5**(1), 21-30 (2015).
[5] D. C. Montgomery, Design and Analysis of Experiments, 8th Edition, John Wiley and Sons, New York, (2013).
[6] A. C. Atkinson and A. N. Donev, Optimum Experimental Designs, Oxford University Press, Oxford (1992).

[7] R. D. Cook and C. J. Nachtsheim, A Comparison of Algorithms for Constructing Exact D-Optimum Designs, Technometrics, **22**, 315-324, (1980).
[8] A. Wald, On the Power Function of the Analysis of Variance Test, Ann. Math. Statist., **13**, 434-439, (1942).
[9] , I. B. Onukogu, On Construction of Odd-fractional Factorial Designs, J. Stat. Appl. Pro. **1**(1), 21-27, (2012).
[10] I.B. Onukogu and M.P. Iwundu, A Combinatorial Procedure for Constructing D-Optimal Designs, Statistica, **67**(4), 415-423, (2007).
[11] M.P. Iwundu, On the choice of initial tuple of support points for quadratic response surface designs, African Journal of Physical Sciences, **3**(2), 1-10, (2010).
[12] M.P. Iwundu and O.A.P. Otaru, Imposing D-optimality criterion on the design regions of the Central Composite Designs (CCD). SCIENTIA AFRICANA, **13**(1), 109-119, (2014).
[13] M.P. Iwundu and E.B. Albert-Udochukwuka, An efficient algorithm for D-optimal designs. Journal of Applied Sciences, **14**, 3547-3554, (2014).
[14] H. Dette , Designing Experiments with Respect to Standardized optimality Criteria. Journal of Royal Statistical Society: Series B, **59**(1), 98-110, (1997).
[15] H. Chernoff, Locally Optimum Designs for Estimating Parameters, Ann. Math. Stat; **24**, 586-602, (1953).
[16] K. Smith, On the Standard Deviations of Adjusted and Interpolated Values of an Observed Polynomial Function and its Constants and the Guidance they give Towards A Proper Choice of the Distributions of Observations, Biometrika, **12**, 1-85, (1918.
[17] S. Ehrenfeld, On the Efficiency of Experimental Designs, Ann. Math. Statist, **26**, 247-255, (1955).
[18] V.V. Fedorov, Theory of Optimal Experiments, New York. Academic Press, (1972).
[19] L. Eriksson, E. Johansson, N. Kettaneh-Wold, C. Wikstrom, and S. Wold, Design of experiments: Principles and Applications, Learnways AB, Umea, (2000).
[20] A. Giovannitti-Jensen and R.H. Myers, Graphical Assessment of the Prediction Capability of Response Surface Designs, Technometrics, **31**(2), 159-171, (1989).
[21] J.J. Borkowski, Spherical Prediction Properties of Central Composite and Box-Behnken Designs, Technometrics, **37**(4), 399-410, (1995).
[22] A. Zahran, C.M. Anderson-Cook and R.H. Myers, Fraction of Design Space to Assess the Prediction Capability of Response Surface Designs, Journal of Quality Technology, **35**, 377-386, (2003).
[23] E.C. Ukaegbu and P.E. Chigbu, Graphical Evaluation of the Prediction Capabilities of Partially Replicated Orthogonal Central Composite Designs, Quality and Reliability Engineering International, **31**, 707-717, (2015).



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