Journal of Applied Sciences

ISSN 1812-5654

science alert

ANSInet
an open access publisher
http://ansinet.com

Journal of Applied Sciences 14 (24): 3547-3554, 2014
ISSN 1812-5654 / DOI: 10.3923/jas.2014.3547.3554

An Efficient Algorithm for Constructing D-Optimal Designs

M.P. Iwundu and E.B. Albert-Udochukwuka
Department of Mathematics and Statistics, Faculty of Physical Science and Information Technology,
University of Port Harcourt, Port Harcourt, Nigeria

Abstract: The main aim of the study was to develop an efficient search algorithm for locating D-optimal exact design. Within a design class, the procedure requires not more than 25% search on the total available designs. Specifically, under some arrangements, there exists a D-optimal exact design within a set of designs constituting about 25% of the total designs. An interesting property of the algorithm is that it eliminates as much as 80% of the total available designs, a lot of which are inferior to the optimal design. Also the new algorithm gives reduction in the number of determinant evaluations. With some rules of selection, the algorithm is certain to locate the required D-optimal exact design. The working of the algorithm has been tested using first order bivariate model defined on a design region that is supported by the points of the Circumscribed Central Composite Design.

Key words: D-optimality, exact designs, first order bivariate models, circumscribed central composite design

INTRODUCTION

Algorithms play very important roles in design construction and have been widely used in the construction of D-optimal designs. Most D-optimal designs were generated by search algorithms such as the DETMAX algorithm of Mitchell (1974). The combinatorial algorithm of Onukogu and Iwundu (2007) 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, serves extensively well in locating D-optimal designs and is applicable under varying experimental conditions as seen in the study of Onukogu (2012). 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, have been suggested in the study of Iwundu (2010). The principles embodied in the combinatorial algorithm were utilized by Iwundu and Otaru (2014), while studing the effects of imposing D-optimality criterion on the design regions of the Central Composite Designs. Although the algorithm is certain to converge to the required optimal design measure, there is the need to reduce the number of determinant evaluations. The essence of this study was to present an algorithm that allows not more than a 25% search in locating the best design within a design class. The fundamental principles used in this study are as in the study of Onukogu and Iwundu (2007) and the elaborated algorithm of Iwundu and Otaru (2014). The sequential steps involved in the elaborated algorithm of Iwundu and Otaru (2014) are briefly outlined.

The algorithm assumes the initial tuple of support points at step 0 as:

$$\underline{t}_0 = [r_1: r_2:...: r_f:...: r_H]$$

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 number of support points, r_f held fixed while making increments on the r s_i.of the other groups. By incremental changes on the r_i, the optimal number of support points, namely, $r_1', r_2',..., r_H'$, taken from the H-groups while holding r_f value fixed are approched. After defining the initial tuple of support points $\underline{t}_0 = [r_1, r_2,... r_f,.., r_H]$, the determinant value d_0 of the best design in the category or combination is evaluated. Holding r_f value fixed, the sequence proceeds 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, 2(H-2) tuples of support points are defined in step 1. These tuples are:

Corresponding Author: M.P. Iwundu, Department of Mathematics and Statistics,
Faculty of Physical Science and Information Technology, University of Port Harcourt, Port Harcourt, Nigeria

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

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

$\vdots$

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

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

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

$\vdots$

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

At each sub-step of step 1, the determinant value of information matrix associated with the best design in the category is evaluated. These determinant values are respectively, $d^-_{111}, d^-_{112},..., d^-_{11(H-2)}$, $d^+_{111}, d^+_{112},..., d^+_{11(H-2)}$. By comparing the determinant values, the best determinant value in step 1 is $d_1 = \max\ [d^-_{111}, d^-_{112},..., d^-_{11(H-2)}, d^+_{111}, d^+_{112},..., d^+_{11(H-2)}]$. Suppose $d_1<d_0$, then the optimal value r_1' holding r_f value fixed has been obtained. Thus, the best determinant value of information matrix when r_f is held fixed is $d_f^* = d_0$. To obtain r_2' holding r_f and r_1' fixed, a similar process is carried out by affecting an increment on r_2 value. The process continues similarly for $r_3, r_4, ..., r_H$ Note however, if at step 1, $d_1>d_0$, the algorithm proceeds to affect an increment of 2 on r_1. Assuming that d_1 is associated with the tuple:

$$\underline{t}_{111} = [r_1\text{-}1: r_2\text{+}1: r_3: r_4:...: r_f:...: r_H]$$

increments in the decreasing direction is required and 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:

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

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

$\vdots$

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

As before, the determinant value of the best designs in each of the combinations or categories are computed. At step 2, the best determinant value is d_2. This value will again be compared with d_1 to check for convergence. If $d_2>d_1$, an increment of 3 is effected on r_1. If otherwise, then $d_f^* = d_1$. Continuing the process will yield the tuple of support points $\underline{t}_f' = [r_1': r_2': r_3': r_4':...: r_f:...: r_H']$. The remaining task is that of attempting to affect increments on r_f so as to obtain the optimal number of support points r_f^* taken from group g_f. Effecting increments on r_f value obviously affects the values of $r_1', r_2', r_3', r_4',.., r_H'$. Consequently, the tuple that results in the global best determinant value is defined by:

$$\underline{t}^* = [r_1^*: r_2^*: r_3^*: r_4^*:...: r_f^*:...:r_H^*]$$

where, r_i^* 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_c^*.

MATERIALS AND METHODS

It was assumed that for given experimental space, $\{\tilde{X}, F_X, \Sigma_X\}$ where, $\tilde{X}$, F_X and Σ_X assume their usual definition as used by Onukogu (1997), the support points in the candidate set have been arranged into H groups, namely, $g_1, g_2,..., g_H$ according to their distances d_i from the centre of $\bar{X}$ 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 $N_1+N_2+...+N_H = \bar{N}$. For the design class $C = \{r_1: r_2:...: r_H\}$, it require selecting r_1 support points from g_1, r_2 support points from $g_2,..., r_H$ support points from g_H. Without loss of generality, the algorithm was presented for H = 1, H = 2 and H = 3 which are, respectively, called H_1, H_2 and H_3 search.

H_1 search: The H_1 search represents the algorithm when all support points are taken from only one group. Let $\underline{C} = \{r_1: 0: 0:...: 0: 0\}$ be the design class to search for the best design in terms of D-optimality criterion. An N point design such that $r_1 = N$ is required. The following steps make up the algorithm:

- Obtain:

$$a_1 = \binom{N_1}{r_1}$$

  sub-designs from $g_1(N_1)$
- List the a_1 sub-designs as $\xi_1 = \{a_{11}\}$, $\xi_2 = \{a_{12}\},..., \xi_{a_1} = \{a_{1a_1}\}$
- Compute det i = det $M(\xi^i)$; i = 1, 2,..., a_1
- Set $d_c^* = \max\ \{\det 1, \det 2,..., \det a_1\}$

H_2 search: The H_2 search represents the algorithm when support points are taken from only two groups. Let $\underline{C} = \{r_1: r_2: 0:...: 0: 0\}$ be the design class to search for the best design in terms of D-optimality criterion. An N point design such that $r_1+r_2 = N$ is required. The following steps make up the algorithm.

- Obtain:

$$a_1 = \binom{N_1}{r_1}$$

sub-designs from $g_1(N_1)$ and:

$$a_2 = \binom{N_2}{r_2}$$

sub-designs from $g_2(N_2)$

- List the a_1 sub-designs as:

$$\xi_{11} = \{a_{11}\}, \xi_{12} = \{a_{12}\}, \ldots, \xi_{1a_1} = \{a_{1n_1}\}$$

and the a_2 sub-designs as:

$$\xi_{21} = \{a_{21}\}, \xi_{22} = \{a_{22}\}, \ldots, \xi_{2a_2} = \{a_{2a_2}\}$$

- Form sets of composite designs from a_1 and a_2 sub-designs as:
  - **Set 1:**

$$\xi^{(11)} = \begin{pmatrix} \xi_{11} \\ \xi_{21} \end{pmatrix}, \xi^{(12)} = \begin{pmatrix} \xi_{11} \\ \xi_{22} \end{pmatrix}, \ldots, \xi^{(1a_2)} = \begin{pmatrix} \xi_{11} \\ \xi_{2a_2} \end{pmatrix}$$

  - **Set 2:**

$$\vdots$$

$$\xi^{(21)} = \begin{pmatrix} \xi_{12} \\ \xi_{21} \end{pmatrix}, \xi^{(22)} = \begin{pmatrix} \xi_{12} \\ \xi_{22} \end{pmatrix}, \ldots, \xi^{(2a_2)} = \begin{pmatrix} \xi_{12} \\ \xi_{2a_2} \end{pmatrix}$$

$$\vdots$$

  - **Set a_1:**

$$\xi^{(a_1 1)} = \begin{pmatrix} \xi_{1a_1} \\ \xi_{21} \end{pmatrix}, \xi^{(a_1 2)} = \begin{pmatrix} \xi_{1a_1} \\ \xi_{22} \end{pmatrix}, \ldots, \xi^{(a_1 a_2)} = \begin{pmatrix} \xi_{1a_1} \\ \xi_{2a_2} \end{pmatrix}$$

This arrangement holds provided $a_1 \le a_2$. However, if $a_1 > a_2$, the groups within the class, say:

$c_2 = \{r_1, r_2\}$ may be repositioned as $c_2 = \{r_2, r_1\}$

- Choose any set i (i = 1,2,..., a_1) and compute detM (ξ^{i1}) = det 1, detM (ξ^{i2}) = det 2,..., detM (ξ^{ia_2}) = det a_2
- Set $d_c^* = \max\{\det 1, \det 2, \ldots, \det a_2\}$

It was remarked that provided the designs are such that $\left\|\sum x_j^2\right\|; j = 1, 2, \ldots, n$ is maximized and $\left\|\sum x_{jj'}\right\|; j \ne j'$ is minimized (where each x_j is a diagonal element of the information matrix and each $x_{jj'}$ is an off-diagonal element of the information matrix) each set i contains the best determinant value (d_c^*).

H_3 search: The H_3 search represents the algorithm when support points are taken from only three groups. Let $\underline{C} = \{r_1: r_2: r_3: 0: \ldots: 0: 0\}$ be the design class to search for the best design in terms of D-optimality criterion. An N point design such that $r_1+r_2+r_3 = N$ is required. The following steps make up the algorithm:

- 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 $g_3(N_3)$

- List the a_1 sub-designs as:

$$\xi_{11} = \{a_{11}\}, \xi_{12} = \{a_{12}\}, \ldots, \xi_{1a_1} = \{a_{1a_1}\}$$

a_2 sub-designs as:

$$\xi_{21} = \{a_{21}\}, \xi_{22} = \{a_{22}\}, \ldots, \xi_{2a_2} = \{a_{2a_2}\}$$

and a_3 sub-designs as:

$$\xi_{31} = \{a_{31}\}, \xi_{32} = \{a_{32}\}, \ldots, \xi_{3a_3} = \{a_{3a_3}\}$$

- Form sets of composite designs from a_1, a_2 and a_3 sub-designs as:
  - **Set 1:**

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

$$\xi^{(121)} = \begin{pmatrix} \xi_{11} \\ \xi_{21} \\ \xi_{31} \end{pmatrix}, \xi^{(122)} = \begin{pmatrix} \xi_{11} \\ \xi_{22} \\ \xi_{32} \end{pmatrix}, \ldots, \xi^{(12a_3)} = \begin{pmatrix} \xi_{11} \\ \xi_{22} \\ \xi_{3a_3} \end{pmatrix}$$

$$\vdots$$

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

- **Set 2:**

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

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

$$\vdots$$

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

$$\vdots$$

- **Set a_1:**

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

$$\xi^{(a_121)} = \begin{pmatrix} \xi_{1a_1} \\ \xi_{22} \\ \xi_{31} \end{pmatrix}, \xi^{(a_122)} = \begin{pmatrix} \xi_{1a_1} \\ \xi_{22} \\ \xi_{32} \end{pmatrix}, \ldots, \xi^{(a_12a_3)} = \begin{pmatrix} \xi_{1a_1} \\ \xi_{22} \\ \xi_{3a_3} \end{pmatrix}$$

$$\vdots$$

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

This arrangement holds provided $a_1 \le a_2 \le a_3$. Where the restriction does not hold, the groups within the class may be repositioned to achieve the restriction.

- Choose any set i (say i = 2) and compute $\det M(\xi^{ijk})$; i = 2; j = 1, 2,..., a_3; k = 1, 2,..., a_3
- Set $d_c^* = \max \{\det M(\xi^{ijk})\}$; i = 2; j = 1, 2,..., a_3; k = 1, 2,..., a_3.

It is reminded that here the essence of the new algorithum is to reduce the number of designs to be included in the search to the bearest minimum without losing the required optimal design. When selection is from only one group, it was observed that the number of designs to be investigated is reasonably small and a 100% search is tolerable. However, it is possible to do a 25% search or less if the selection rules of Oladugba and Madukaife (2009) are adhered to. Furthermore, S_3 search is equivalent to S_2 search if one of the groups contains only one support point. The difference lies in the inclusion of the one support point in the design. Similarly, S_2 search is equivalent to S_1 search if one of the groups contains only one support point. The difference also lies in the inclusion of the one support point in the design. Where there is only one support point in a group, we say that there is no competing design point in that group.

Selection rules: The following selection rules should be adhered to when considering design points from a design class to go into the design measure in the construction of D-optimal exact N-point designs:

- When selection of design points is only from one group; perform a 100% search. However, with the rules of Oladugba and Madukaife (2009), a 25% search or less is possible
- When selection is from more than one group, perform a 25% search in the direction of maximum set combination to obtain the desired design measure. In performing the 25% search, selection of points to go into the design measure are such that:
  - $\sum_{k=1}^{N} x_{kj}^2$ is maximize
  - $\left\| \sum_{k=1}^{N} x_{kj} x_{kj} \right\|$ is maximize

RESULTS

The algorithm was applied on the problem of locating a 5-point D-Optimal exact design for the no intercept, three parameter first order model $y(x_1, x_2) = a_1x_1+a_2x_2+a_{12}x_1a_2+e$ defined on the geometric region in Fig. 1.

Following the suggestion of Iwundu (2010), the initial tuple of support points is {3: 1: 1}. Since the number of parameters, p, equals 3, the design size, N, need not exceed 7. Pazman (1987) has shown that $N \le 1/2\, p\,(p+1)+1$.

Also, by the algorithm of Onukogu and Iwundu (2007) the design points, {(1,1), (1,-1), (-1,1), (-1,-1), (1.414,0), (-1.414,0), (0,1.414), (0,-1.414), (0,0)}, that make up the design region, are arranged into H=3 groups according to their distances from the center of the design region. The group formation yields the following three groups with the associated design points:

- g_1: {(1, 1), (1, -1), (-1, 1), (-1, -1)}
- g_2: {(1.414, 0), (-1.414, 0), (0, 1.414), (0, -1.414)}
- g_3: {(0, 0)}

With the initial tuple, {3:1:1}, it is required to select 3 support points from g_1, 1 support point from g_2 and 1 support point from g_3. Since, there are four design points in g_1 the following design points are admissible:

- g_{11}: {(1, 1), (1, -1), (-1, 1)}
- g_{12}: {(1, 1), (1, -1), (-1, -1)}
- g_{13}: {(1, -1), (-1, 1), (-1, -1)}
- g_{14}: {(1, 1), (-1, 1), (-1, -1)}

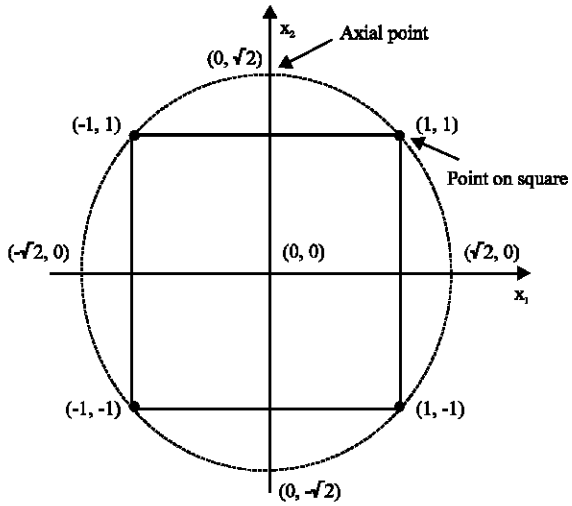

Fig. 1: Geometric region supported by points of Circumscribed Central Composite Design

Also since there are four design points in g_2 the following designs points are admissible:

- g_{21}: {(1.414, 0)}
- g_{22}: {(0, -1.414)}
- g_{23}: {(-1.414, 0)}
- g_{24}: {((0, 1.414)}

For g_3, since there is only one design points, the admissible design point is:

- g_{31}: {(0, 0)}

From the admissible design points the following sets of sub-designs are formed:

$$\xi_{11} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, 1 \end{pmatrix}, \xi_{12} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, -1 \end{pmatrix}, \xi_{13} = \begin{pmatrix} 1, -1 \\ -1, 1 \\ -1, -1 \end{pmatrix}, \xi_{14} = \begin{pmatrix} 1, 1 \\ -1, 1 \\ -1, -1 \end{pmatrix}$$

$$\xi_{21} = (1.414, 0), \xi_{22} = (0, -1.414),$$
$$\xi_{23} = (-1.414, 0), \xi_{24} = (0, 1.414)$$

$$\xi_{31} = (0, 0)$$

where, $a_1 = 4$, $a_2 = 4$ and $a_3 = 1$. Since, the restriction is not satisfied the groups are repositioned within the class of interest as {1: 3: 1}, where we select 1 support point from g_3, select 3 support points from g_1 and 1 support point from g_2. The sub-designs are rearranged as:

$$\xi_{31} = (0, 0)$$

$$\xi_{11} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, 1 \end{pmatrix}, \xi_{12} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, -1 \end{pmatrix}, \xi_{13} = \begin{pmatrix} 1, -1 \\ -1, 1 \\ -1, -1 \end{pmatrix}, \xi_{14} = \begin{pmatrix} 1, 1 \\ -1, 1 \\ -1, -1 \end{pmatrix}$$

$$\xi_{21} = (1.414, 0), \xi_{22} = (0, -1.414),$$
$$\xi_{23} = (-1.414, 0), \xi_{24} = (0, 1.414)$$

Thus, it has $a_3 \le a_1 \le a_2$.

Arranging the sub-designs as composite designs, the following set of designs were formed:

- **Set 1:**

$$\xi^{(11)} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, 1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \xi^{(12)} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, 1 \\ 0, -1.414 \\ 0, 0 \end{pmatrix}, \xi^{(13)} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, 1 \\ -1.414, 0 \\ 0, 0 \end{pmatrix}, \xi^{(14)} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, 1 \\ 0, 1.414 \\ 0, 0 \end{pmatrix}$$

- **Set 2:**

$$\xi^{(21)} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \xi^{(22)} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, -1 \\ 0, -1.414 \\ 0, 0 \end{pmatrix}, \xi^{(23)} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, -1 \\ -1.414, 0 \\ 0, 0 \end{pmatrix}, \xi^{(24)} = \begin{pmatrix} 1, 1 \\ 1, -1 \\ -1, -1 \\ 0, 1.414 \\ 0, 0 \end{pmatrix}$$

- **Set 3:**

$$\xi^{(31)} = \begin{pmatrix} 1, -1 \\ -1, 1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \xi^{(32)} = \begin{pmatrix} 1, -1 \\ -1, 1 \\ -1, -1 \\ 0, -1.414 \\ 0, 0 \end{pmatrix}, \xi^{(33)} = \begin{pmatrix} 1, -1 \\ -1, 1 \\ -1, -1 \\ -1.414, 0 \\ 0, 0 \end{pmatrix}, \xi^{(24)} = \begin{pmatrix} 1, -1 \\ -1, 1 \\ -1, -1 \\ 0, 1.414 \\ 0, 0 \end{pmatrix}$$

- **Set 4:**

$$\xi^{(41)} = \begin{pmatrix} 1, 1 \\ -1, 1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \xi^{(42)} = \begin{pmatrix} 1, 1 \\ -1, 1 \\ -1, -1 \\ 0, -1.414 \\ 0, 0 \end{pmatrix}, \xi^{(43)} = \begin{pmatrix} 1, 1 \\ -1, 1 \\ -1, -1 \\ -1.414, 0 \\ 0, 0 \end{pmatrix}, \xi^{(44)} = \begin{pmatrix} 1, 1 \\ -1, 1 \\ -1, -1 \\ 0, 1.414 \\ 0, 0 \end{pmatrix}$$

Determinant evaluations of the information matrices of the designs in set 1 yield respectively:

- $M\{\xi^{(11)}\} = 0.3415$
- $M\{\xi^{(12)}\} = 0.3415$
- $M\{\xi^{(13)}\} = 0.5224$
- $M\{\xi^{(14)}\} = 0.5224$

Table 1: Combinatorics for a 3, 4, 5, 6 and 7-point D-optimal exact design

Steps	g_1	g_2	g_3	No. of available designs	Best determinant value	Max number of designs to investigate
3-point D-optimal exact design						
0	3	0	0	4	0.5926	4
1	2	1	0	24	0.2962	6
2	2	0	1	6	0.0000	6
Total				34		16
4-point D-optimal exact design						
0	3	1	0	16	0.4999	4
1	3	0	1	4	0.2500	1
2	4	0	0	1	1.0000	1
Total				21		6
5-point D-optimal exact design						
0	3	1	1	16	0.2560	4
1	3	2	0	24	0.4799	6
2	3	0	2	4	0.1280	1
3	4	1	0	4	0.7680	1
4	5	0	0	4	0.8960	4
5	2	3	0	24	0.3199	6
6	2	2	1	36	0.1919	6
Total				112		28
6-point D-optimal exact design						
0	3	2	1	24	0.4799	6
1	3	3	0	16	0.4073	4
2	3	1	2	16	0.1481	4
3	4	1	1	4	0.4444	1
4	4	2	0	6	0.6665	6
5	5	1	0	16	0.7407	4
6	6	0	0	6	0.8889	6
7	2	3	1	24	0.1851	6
8	2	4	0	6	0.2962	6
Total				118		43
7-point D-optimal exact design						
0	3	3	1	16	0.2565	4
1	3	4	0	4	0.3730	1
2	3	2	2	24	0.1749	6
3	4	3	0	4	0.5596	1
4	5	2	0	24	0.6646	6
5	6	1	0	24	0.7696	6
6	7	0	0	4	0.9329	4
7	2	5	0	24	0.2564	6
8	2	4	1	6	0.1867	6
Total				130		40

Determinant evaluations of the information matrices of the designs in set 2 yield respectively:

- $M\{\xi^{(21)}\} = 0.5224$
- $M\{\xi^{(22)}\} = 0.5224$
- $M\{\xi^{(23)}\} = 0.3415$
- $M\{\xi^{(24)}\} = 0.3415$

Determinant evaluations of the information matrices of the designs in set 3 yield respectively:

- $M\{\xi^{(31)}\} = 0.3415$
- $M\{\xi^{(32)}\} = 0.5224$
- $M\{\xi^{(33)}\} = 0.3415$
- $M\{\xi^{(34)}\} = 0.5224$

Determinant evaluations of the information matrices of the designs in set 4 yield respectively:

- $M\{\xi^{(41)}\} = 0.5224$
- $M\{\xi^{(42)}\} = 0.3415$
- $M\{\xi^{(43)}\} = 0.5224$
- $M\{\xi^{(44)}\} = 0.3415$

It is remarked that the determinant values need not to be identical for designs in the set. However, notice that in each ith set (i = 1, 2, 3, 4), there is an N-point equivalent design with same maximum determinant value. Irrespective of the set chosen, we are certain to locate the best design. By assessing any ith set, we successfully do a 25% search at the combination {3:1:1}. The rest of the task is as elaborated by Iwundu and Otaru (2014).

For this model, we shall constuct N-point D-optimal exact design; N = 3, 4,..., 7.

For N = 3, the initial tuple of support points is [3: 0: 0]. With this, we commence the search for the D-optimal exact design. The sequential steps are presented in Table 1.

Table 2: Some distinguishing features of the algorithm for the illustrations

Design size (N)	Maximum No. of determinant evaluations required	Relative percentage of maximum No. of determinant evaluations required	Minimum percentage of No. of designs eliminated	Optimal design combination	D-optimum
3	16	17.20	82.80	3:0:0	0.5926
4	6	3.68	96.32	4:0:0	1.0000
5	28	12.33	87.67	5:0:0	0.8960
6	43	14.43	85.57	6:0:0	0.8889
7	40	9.73	90.27	7:0:0	0.9329

The maximum determinant value is det* = 5.926×10^{-1} and it is associated with design class [3:0:0] having the design points [(-11, 1-1, 11) or (-11, 11, -1-1) or (-11, 1-1, -1-1) or (1-1, 11, -1-1)]. Within the class [3:0:0], the number of D-optimal exact designs is 4.

For N = 4, the initial tuple of support points is [3:1:0]. With this, we commence the search for the D-optimal exact design. The sequential steps are presented in Table 1.

The maximum determinant value is det* = 1.000 and it is associated with design class [4:0:0] having the design points [(-11, 1-1, 11,-1-1)]. Within the class [3:1:0], the number of D-optimal exact designs is 1.

For N = 5, the initial tuple of support points is [3:1:1]. With this, we commence the search for the D-optimal exact design. The sequential steps are presented in Table 1. The maximum determinant value is det* = 8.960×10^{-1} and it is associated with design class [5:0:0] having the design points [(-11, 1-1, 11,-1-1, -11) or (-11, 1-1, 11, -1-1, 1-1) or (-11, 1-1, 11, -1-1, 11) or (-11, 1-1, 11, -1-1,-1-),]. Within the class [3:1:1], the number of D-optimal exact designs is 4.

For N = 6, the initial tuple of support points is [3:2: 1]. With this, we commence the search for the D-optimal exact design. The sequential steps are presented in Table 1.

The maximum determinant value is det* = 8.889×10^{-1} and it is associated with design class [6:0: 0] having the design points [(-11, 1-1, 11, -1-1, -11, 1-1) or (-11, 1-1, 11, -1-1, -11, 11) or (-11, 1-1, 11, -1-1, -11, -1-1) or (-11, 1-1, 11, 1-1, 11) or (-11, 1-1, -11-1-1, 1-1, -1-1) or (-11, 1-1, 11, -1-1, 11, -1-1)].

Within the class [3:2:1], the number of D-optimal exact designs is 4.

For N = 7, the initial tuple of support points is [3:3: 1]. With this, we commence the search for the D-optimal exact design. The sequential steps are presented in Table 1.

The maximum determinant value is det* = 9.329×10^{-1} and it is associated with design class [7 0 0] having the design points [(-11, 1-1, 11, -1-1, -11, 1-1, 11) or (-11, 1-1, 11, -1-1, -11, 11, -1-1) or (-11, 1-1, 11, -1-1, -11, 1-1, -1-1) or (-11, 1-1, 11, -1-1, 1-1, 11, 11, -1-1)].

Within the class [3:3:1], the number of D-optimal exact designs is 4.

DISCUSSION

One of the fundamental theorems of Onukogu and Iwundu (2007) in constructing D-optimal exact designs is based on the assertion that for the p×p information matrices M (ξ_1) = $(m_{ij}\xi_1)$ and M (ξ_2) = $(m_{ij}\xi_2)$ where, $m_{ii}(\xi_1) = m_{ii}(\xi_2)$, M $(\xi_1)\geq$M (ξ_2) if $\|m_{ij}(\xi_1)\| \leq \|m_{ij}(\xi_2)\|$; I≠j., where, $\|\cdot\|$ denotes the absolute value and m_{ij} denotes the $(ij)^{th}$ element of the information matrix. This condition is not met in many problems as the absolute value of each off-diagonal element of, say, M (ξ_1) may all not necessarily be less than or equal to the corresponding off-diagonal elements of, say, M (ξ_2). Hence, the application of this condition becomes ineffective in some problems.

Furthermore, the combinatorial algorithm of Onukogu and Iwundu (2007) uses arbitrary starting designs which in some cases are very far from the required optimal design as measured by the determinant value of information matrices. Neither the algorithm of Onukogu and Iwundu (2007) nor that of Iwundu and Chigbu (2012) provided information on the possible percentage reduction in the number of determinant evaluations.

The efficiency of the new algorithm is seen in its ability to significantly reduce the number of determinant evaluations. For instance, in constructing a 3-point D-optimal design for the 3-parameter bivariate model, a 100% search requires 93 determinant evaluations. However, using the new algorithm reduces the determinant evaluations to a maximum of 16. Similarly, for N = 4, 5, 6 and 7, the number of available designs for a 100% search are, respectively, 163, 227, 298 and 411. The number of determinant evaluations is drastically reduced to a maximum of 6, 28, 43 and 40, respectively, using the new algorithm. Thus the new algorithm provides computational ease as the number of determinant evaluations needed to reach the required optimal design is significantly reduced.

For the 3-parameter bivariate model, Table 2 summarizes the number of designs within the design classes to be investigated, the maximun number of

designs for which determinant evaluations are required, the relative percentage of maximun number of designs for which determinant evaluations are required, the minimum percentage of designs to be eliminated, the optimal design combination and the D-optimum.

CONCLUSION

The use of optimal designs allows model parameters to be estimated without bias and with minimum variance. These designs are suitable for models with qualitative as well as quantitative factors and require few experimental runs to estimate the parameters. The D-optimal designs are often used when classical designs, such as factorial and fractional factorials are not adequate and are also suitable even for irregular design regions. The construction of D-optimal designs is often iterative and requires a number of determinant evaluations. The algorithm presented in this study converges very rapidly to the desired N-Point D-optimal exact design. The procedure requires not more than 25% search on the total available designs within a design class.

In searching for D-optimal exact design, the algorithm eliminates not less than 80% of the total available designs some of which are very inferior to the optimal design. Once a direction of increasing determinant has emerged, the algorithm continues in that direction and a quick convergence of the procedure to the require optimum is certain.

REFERENCES

Iwundu, M.P., 2010. On the choice of initial tuple of support points for quadratic response surface designs. Afr. J. Phys. Sci., 3: 21-41.

Iwundu, M. and P. Chigbu, 2012. A hill-climbing combinatorial algorithm for constructing n-point d-optimal exact designs. J. Stat. Appl. Pro., 1: 133-146.

Iwundu, M.P. and O.A.P. Otaru, 2014. Imposing D-optimality criterion on the design region of the central composite designs. Scientia Africana, 13: 109-119.

Mitchell, T.J., 1974. An algorithm for the construction of D-optimal experimental designs. Technometrics, 16: 203-210.

Oladugba, A.V. and M.S. Madukaife, 2009. D-optimality and DL-Optimality criteria for incomplete block designs. Global J. Math. Sci., 8: 107-115.

Onukogu, I.B., 1997. Foundations of Optimal Exploration of Response Surfaces. Ephrala Press, Nsukka, Nigeria.

Onukogu, I.B., 2012. On construction of odd-fractional factorial designs. J. Stat. Applic. Prob., 1: 21-27.

Onukogu, I.B. and M.P. Iwundu, 2007. A combinatorial procedure for constructing D-Optimal exact designs. Statistica, 67: 415-423.

Pazman, A., 1987. Foundations of Optimum Experimental Design. D-Reidal Publishing Co., Boston, USA.