An Efficient Algorithm for Constructing D-Optimal Designs

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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 $g_1, g_2, ..., g_i$, 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 studying 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:

$$\mathbf{t}_0 = [t_1; t_2; ...; t_r]$$

where, $t_r$ is the initial number of support points taken from group $g_r$, $t_i$ is the initial number of support points taken from group $g_i$, $r_j$ is the initial number of support points taken from group $g_i$, $r_i$ is the initial number of support points taken from group $g_i$, $r_i$ is the initial number of support points taken from group $g_i$.

The group $g_j$ contains the number of support points, $r_j$ held fixed while making increments on the $r_i$ of the other groups. By incremental changes on the $r_i$ the optimal number of support points, namely, $r_1$, $r_2$, ..., $r_n$, taken from the H-groups while holding $r_j$ value fixed are approached. After defining the initial tuple of support points $\mathbf{t}_0 = [t_1, t_2, ..., t_n]$, the determinant value $d_0$ of the best design in the category or combination is evaluated. Holding $r_j$ value fixed, the sequence proceeds to obtain the optimal number of support points from a group, say, $g_j$. This requires effecting an increment on $r_j$ value by 1. Hence, $2\cdot (H-2)$ tuples of support points are defined in step 1. These tuples are:

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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, \(d_{i11}, d_{i12}, \ldots, d_{i10-2}, d_{i11}, d_{i12}, \ldots, d_{i10-2}.\) By comparing the determinant values, the best determinant value in step 1 is \(d_i = \max\{d_{i11}, d_{i12}, \ldots, d_{i10-2}, d_{i11}, d_{i12}, \ldots, d_{i10-2}\}.\) Suppose \(d_i < d_0,\) then the optimal value \(r_i^\bullet\) holding \(r_i\) value fixed has been obtained. Thus, the best determinant value of information matrix when \(r_i\) is held fixed is \(d_i^* = d_i.\) To obtain \(r_i^\bullet\) holding \(r_i\) and \(r_i^\bullet\) fixed, a similar process is carried out by affecting an increment on \(r_i\) value. The process continues similarly for \(r_2, r_3, \ldots, r_h.\) Note however, if at step 1, \(d_i > d_0,\) the algorithm proceeds to affect an increment of 2 on \(r_i,\) Assuming that \(d_i\) is associated with the tuple:

\[ L(l) = [r_1^1; r_2^1; r_3^1; \ldots; r_i^1; \ldots; r_h^1] \]

increments in the decreasing direction is required and we do not need to explore all sub-steps of step 2. Incrementing \(r_i\) by 2 is equivalent to incrementing \(r_i-1\) by 1. Consequently, the required tuples of support points at this iteration are:

\[ L(l) = [r_1^2; r_2^2; r_3^1; \ldots; r_i^2; \ldots; r_h^2] \]

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 \(d_i.\) This value will again be compared with \(d_i\) to check for convergence. If \(d_i > d_i,\) an increment of 3 is effected on \(r_i.\) If otherwise, then \(d_i^* = d_i.\) Continuing the process will yield the tuple of support points \(L(l) = [r_1^1; r_2^1; r_3^1; \ldots; r_i^1; \ldots; r_h^1].\) The remaining task is that of attempting to affect increments on \(r_i\) so as to obtain the optimal number of support points \(r_i^*\) taken from group \(g_i.\) Effecting increments on \(r_i\) value obviously affects the values of \(r_1^*, r_2^*, r_3^*, \ldots, r_h^*.\) Consequently, the tuple that results in the global best determinant value is defined by:

\[ L^* = [r_1^*; r_2^*; r_3^*; \ldots; r_i^*; \ldots; r_h^*] \]

where, \(r_i^*\) is the optimal number of support points taken from the \(i^{th}\) group \(g_i, i = 1, 2, \ldots, H.\) The D-optimal exact design is contained in the immediate tuple and is associated with \(d_i^*.\)

**MATERIALS AND METHODS**

It was assumed that for given experimental space, \{\(X, F_i, \Sigma_i\}\) where, \(X, F_i\) and \(\Sigma_i\) assume their usual definition as used by Omukogu (1997), the support points in the candidate set have been arranged into \(H\) groups, namely, \(g_1, g_2, \ldots, g_H\) according to their distances \(d_i\) from the centre of \(X\) such that \(d_1 > d_2 > \ldots > d_H.\) The group, \(g_i\) holds \(N_i\) support points, \(g_i\) holds \(N_i\) support points, etc and \(N_1 + N_2 + \ldots + N_H = N.\) For the design class \(C = \{r_1; r_2; \ldots; r_h\}\), it require selecting \(r_i\) support points from \(g_1, g_2, \ldots, g_h\) support points from \(g_1, g_2, \ldots, g_h\) support points from \(g_1, g_2, \ldots, g_h\) points from \(g_1, g_2, \ldots, g_h\) point. 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 \(C = \{r_1; 0; \ldots; 0; 0\}\) be the design class to search for the best design in terms of D-optimality criterion. An \(N\) point design such that \(r_1 = N\) is required. The following steps make up the algorithm:

- Obtain:
  \[ a_i = \left( \begin{array}{c} N \\ r_i \end{array} \right) \]

  sub-designs from \(g_i(N_i)\)

- List the \(a_i\) sub-designs as \(\xi_i = \{a_{i1}\}, \xi_2 = \{a_{i2}\}, \ldots, \xi_{a_i} = \{a_{ia}\}\)

- Compute \(\det i = \det M(\xi_i); i = 1, 2, \ldots, a_i\)

- Set \(d_i^* = \max \{\det 1, \det 2, \ldots, \det a_i\}\)

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

\[ a_1 = \begin{pmatrix} N_1 \\ \xi_1 \end{pmatrix} \]

sub-designs from \( g_i(N_i) \) and:

\[ a_2 = \begin{pmatrix} N_2 \\ \xi_2 \end{pmatrix} \]

sub-designs from \( g_i(N_i) \)

• List the \( a_i \) sub-designs as:

\[ \xi_{i1} = (a_{i1}), \xi_{i2} = (a_{i2}), \ldots, \xi_{in} = (a_{in}) \]

and the \( a_j \) sub-designs as:

\[ \xi_{j1} = (a_{j1}), \xi_{j2} = (a_{j2}), \ldots, \xi_{jn} = (a_{jn}) \]

• Form sets of composite designs from \( a_i \) and \( a_j \) sub-designs as:

  • Set 1:

\[ \xi^{(1)} = \begin{pmatrix} \xi_{i1} \\ \xi_{j1} \end{pmatrix}, \xi^{(2)} = \begin{pmatrix} \xi_{i2} \\ \xi_{j2} \end{pmatrix}, \ldots, \xi^{(n_1)} = \begin{pmatrix} \xi_{in} \\ \xi_{jn} \end{pmatrix} \]

  • Set 2:

\[ \xi^{(1)} = \begin{pmatrix} \xi_{i1} \\ \xi_{j2} \end{pmatrix}, \xi^{(2)} = \begin{pmatrix} \xi_{i2} \\ \xi_{j2} \end{pmatrix}, \ldots, \xi^{(n_1)} = \begin{pmatrix} \xi_{in} \\ \xi_{jn} \end{pmatrix} \]

• Set \( a_i \):

\[ \xi^{(1)} = \begin{pmatrix} \xi_{i1} \\ \xi_{i2} \end{pmatrix}, \xi^{(2)} = \begin{pmatrix} \xi_{i1} \\ \xi_{i2} \end{pmatrix}, \ldots, \xi^{(n_1)} = \begin{pmatrix} \xi_{in} \\ \xi_{jn} \end{pmatrix} \]

This arrangement holds provided \( a_i \geq a_j \). However, if \( a_j > a_i \), the groups within the class, say:

\[ c_i = \{ r_1, r_j \} \]

may be repositioned as \( c_i = \{ r_2, r_i \} \)

• Choose any set \( i \) (i = 1, 2, ..., \( a_i \)) and compute detM (\( \xi^{(1)} \)) = det 1, detM (\( \xi^{(2)} \)) = det 2, ..., detM (\( \xi^{(n_1)} \)) = det \( a_j \)

• Set \( d_i = \max \{ \text{det 1, det 2, ..., det} \}

It was remarked that provided the designs are such that \( \| \sum X_j \|_J = 1 \) is maximized and \( \| \sum X_j \|_J > 0 \) is minimized (where each \( x_j \) is a diagonal element of the information matrix and each \( x_{ij} \) is an off-diagonal element of the information matrix) each set \( i \) contains the best determinant value (\( d_i \)).

H3 search: The H3 search represents the algorithm when support points are taken from only three groups. Let \( C = \{ r_1, r_2, r_j \} \) be the design class to search for the best design in terms of D-optimality criterion. An N point design such that \( r_i + r_j + r_j = N \) is required. The following steps make up the algorithm:

• Obtain:

\[ a_1 = \begin{pmatrix} N_1 \\ \xi_1 \end{pmatrix} \]

sub-designs from \( g_i(N_i) \):

\[ a_2 = \begin{pmatrix} N_2 \\ \xi_2 \end{pmatrix} \]

sub-designs from \( g_i(N_i) \) and:

\[ a_3 = \begin{pmatrix} N_3 \\ \xi_3 \end{pmatrix} \]

sub-designs from \( g_i(N_i) \)

• List the \( a_i \) sub-designs as:

\[ \xi_{i1} = (a_{i1}), \xi_{i2} = (a_{i2}), \ldots, \xi_{in} = (a_{in}) \]

and the \( a_j \) sub-designs as:

\[ \xi_{j1} = (a_{j1}), \xi_{j2} = (a_{j2}), \ldots, \xi_{jn} = (a_{jn}) \]

• Form sets of composite designs from \( a_i \), \( a_j \) and \( a_j \) sub-designs as:

  • Set 1:

\[ \xi^{(1)} = \begin{pmatrix} \xi_{i1} \\ \xi_{i2} \\ \xi_{j1} \end{pmatrix}, \xi^{(2)} = \begin{pmatrix} \xi_{i1} \\ \xi_{i2} \\ \xi_{j2} \end{pmatrix}, \ldots, \xi^{(n_1)} = \begin{pmatrix} \xi_{in} \\ \xi_{in} \\ \xi_{jn} \end{pmatrix} \]

\[ \xi^{(1)} = \begin{pmatrix} \xi_{i1} \\ \xi_{j1} \\ \xi_{j2} \end{pmatrix}, \xi^{(2)} = \begin{pmatrix} \xi_{i1} \\ \xi_{j1} \\ \xi_{j2} \end{pmatrix}, \ldots, \xi^{(n_1)} = \begin{pmatrix} \xi_{in} \\ \xi_{jn} \end{pmatrix} \]

• Set \( a_i \):

\[ \xi^{(1)} = \begin{pmatrix} \xi_{i1} \\ \xi_{i2} \\ \xi_{j1} \end{pmatrix}, \xi^{(2)} = \begin{pmatrix} \xi_{i1} \\ \xi_{i2} \\ \xi_{j2} \end{pmatrix}, \ldots, \xi^{(n_1)} = \begin{pmatrix} \xi_{in} \\ \xi_{jn} \end{pmatrix} \]

This arrangement holds provided \( a_i \leq a_j \). However, if \( a_i > a_j \), the groups within the class, say:

\[ c_i = \{ r_1, r_j \} \]
• Set 2:

\[
\begin{array}{c}
\xi^{(1)} = \left( \xi_{21}, \xi_{22}, \xi_{23} \right) \\
\xi^{(2)} = \left( \xi_{31}, \xi_{32}, \xi_{33} \right) \\
\vdots \\
\xi^{(2a)} = \left( \xi_{na}, \xi_{na}, \xi_{na} \right)
\end{array}
\]

\[
\begin{array}{c}
\xi^{(3)} = \left( \xi_{21}, \xi_{22}, \xi_{23}, \xi_{24} \right) \\
\xi^{(4)} = \left( \xi_{31}, \xi_{32}, \xi_{33}, \xi_{34} \right) \\
\vdots \\
\xi^{(4a)} = \left( \xi_{na}, \xi_{na}, \xi_{na}, \xi_{na} \right)
\end{array}
\]

\[
\begin{array}{c}
\xi^{(5)} = \left( \xi_{21}, \xi_{22}, \xi_{23}, \xi_{24}, \xi_{25} \right) \\
\xi^{(6)} = \left( \xi_{31}, \xi_{32}, \xi_{33}, \xi_{34}, \xi_{35} \right) \\
\vdots \\
\xi^{(5a)} = \left( \xi_{na}, \xi_{na}, \xi_{na}, \xi_{na}, \xi_{na} \right)
\end{array}
\]

\[
\begin{array}{c}
\xi^{(6)} = \left( \xi_{21}, \xi_{22}, \xi_{23}, \xi_{24}, \xi_{25}, \xi_{26} \right) \\
\xi^{(7)} = \left( \xi_{31}, \xi_{32}, \xi_{33}, \xi_{34}, \xi_{35}, \xi_{36} \right) \\
\vdots \\
\xi^{(6a)} = \left( \xi_{na}, \xi_{na}, \xi_{na}, \xi_{na}, \xi_{na}, \xi_{na} \right)
\end{array}
\]

This arrangement holds provided \(a_1 \leq a_2 \leq a_3\). 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 \(\det(\xi^{(2)})\), \(i = 2, j = 1, 2, ..., a_3\).

• Set \(d^*_i = \max \{\det(\xi^{(2)})\}; \ i = 2, j = 1, 2, ..., a_3\).

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 Madukachie (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:

\[
\sum \lambda_i x_i \text{ is maximize}
\]

\[
\sum \lambda_i x_i \text{ is maximize}
\]

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 \(y(x_1, x_2) = a_1x_1 + a_2x_2 + a_3x_1x_2 + e\) 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 \(N\leq (p+1)\).

Also, by the algorithm of Omokong and Iwundu (2007) the design points, \(\{(1,1), (-1,1), (-1,1), (1,1), 0\}\), 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:

• \(g_1: \{(1,1), (-1,1), (-1,1), (-1,1)\}\)

• \(g_2: \{(0,1), (0, -1), (0, 0)\}\)

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:

• \(g_1: \{(1,1), (-1,1), (-1,1)\}\)

• \(g_2: \{(0,1), (0, -1), (0, 0)\}\)

• \(g_3: \{(-1,1), (1,1), (-1,1)\}\)
Fig. 1: Geometric region supported by points of Circumscribed Central Composite Design

Also since there are four design points in g₂, the following designs points are admissible:

- \( g_5: \{(0, 0, 1.414, 0)\} \)
- \( g_6: \{(0, -1, 1.414)\} \)
- \( g_7: \{(-1, 1.414, 0)\} \)
- \( g_8: \{(0, 1.414)\} \)

For \( g_5 \), since there is only one design point, the admissible design point is:

- \( g_5: \{(0, 0)\} \)

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

\[
\begin{align*}
\xi_{51} &= \begin{pmatrix} 1,1 \\ -1, -1 \end{pmatrix}, \quad \xi_{52} = \begin{pmatrix} 1,1 \\ -1, -1 \end{pmatrix}, \quad \xi_{53} = \begin{pmatrix} 1,1 \\ -1, -1 \end{pmatrix}, \quad \xi_{54} = \begin{pmatrix} 1,1 \\ -1, -1 \end{pmatrix} \\
\xi_{51} &= (1.414, 0, 1.414, 0), \quad \xi_{52} = (0, -1.414, 0, 1.414), \\
\xi_{53} &= (1.414, 0, 0, 1.414), \quad \xi_{54} = (0, 0, 0, 0) \\
\xi_{55} &= (0, 0)
\end{align*}
\]

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 \( g_5 \), select 3 support points from \( g_i \), and 1 support point from \( g_2 \). The sub-designs are rearranged as:

\[
\begin{align*}
\xi_{51} &= (0, 0, 0, 0) \\
\xi_{52} &= (1, 1, -1, -1) \\
\xi_{53} &= (1, 1, -1, -1) \\
\xi_{54} &= (1, 1, -1, -1) \\
\xi_{55} &= (1, 1, -1, -1)
\end{align*}
\]

Thus, it has \( a_1 a_2 a_3 = 24 \).

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

- **Set 1:**

\[
\xi^{(0)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(1)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(2)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(3)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}
\]

- **Set 2:**

\[
\xi^{(0)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(1)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(2)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(3)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}
\]

- **Set 3:**

\[
\xi^{(0)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(1)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(2)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(3)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}
\]

- **Set 4:**

\[
\xi^{(0)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(1)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(2)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}, \quad \xi^{(3)} = \begin{pmatrix} 1,1 \\ -1, -1 \\ 1.414, 0 \\ 0, 0 \end{pmatrix}
\]

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

- \( M \{\xi^{(1)}\} = 0.3415 \)
- \( M \{\xi^{(2)}\} = 0.3415 \)
- \( M \{\xi^{(3)}\} = 0.5224 \)
- \( M \{\xi^{(4)}\} = 0.5224 \)
Table 1: Combinatorics for a 3, 4, 5, 6 and 7-point D-optimal exact design

<table>
<thead>
<tr>
<th>Steps</th>
<th>$r_1$</th>
<th>$r_2$</th>
<th>$r_3$</th>
<th>No. of available designs</th>
<th>Best determinant value</th>
<th>Max number of designs to investigate</th>
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<tbody>
<tr>
<td>3-point D-optimal exact design</td>
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<td>0</td>
<td>0</td>
<td>0.5926</td>
<td>4</td>
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<td>1</td>
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<td>0.2692</td>
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<td>2</td>
<td>0</td>
<td>1</td>
<td>0.0000</td>
<td>6</td>
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<td>Total</td>
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<td>16</td>
</tr>
<tr>
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<td>Total</td>
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<td></td>
<td>21</td>
<td></td>
<td>6</td>
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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:

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

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

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 \( \det^* = 8.960 \times 10^{-4} \) and it is associated with design class [5:0:0] having the design points [(11, 1-1, 1, 1-1, 11) or (-11, 1-1, 1, -1-1, 11) or (11, 1-1, 1, 1-1, 11) or (11, 1-1, 1, 1-1, -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 \( \det^* = 8.889 \times 10^{-1} \) and it is associated with design class [6:0:0] having the design points [(11, 1-1, 1, -1-1, 11, 1-1) or (11, 1-1, 1, 1-1, 11, 1-1) or (-11, 1-1, 1, 1-1, 11, -1-1) or (-11, 1-1, 1, -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 \( \det^* = 9.329 \times 10^{-1} \) and it is associated with design class [7:0:0] having the design points [(11, 1-1, 1, -1-1, 11, 1-1, 11) or (11, 1-1, 1, -1-1, 11, 1-1, 11) or (-11, 1-1, 1, 1-1, -1-1)] within the class [3:3:1], the number of D-optimal exact designs is 4.

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 \( p \times p \) information matrices \( M(\xi_i) = (m_{ij}(\xi_i)) \) and \( M(\xi_j) = (m_{ij}(\xi_j)) \) where, \( m_{ij}(\xi_i) = m_{ij}(\xi_j) \), \( M(\xi) \geq M(\xi_j) \) if \( ||m_{ij}(\xi)|| \leq ||m_{ij}(\xi_j)|| \), \( i,j \), 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, \( M(\xi_i) \) may fall necessarily less than or equal to the corresponding off-diagonal elements of, say, \( M(\xi_j) \). 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 95 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 maximum number of

\[ \text{Table 2: Some distinguishing features of the algorithm for the illustrations} \]

<table>
<thead>
<tr>
<th>Design size (N)</th>
<th>Maximum No. of determinant evaluations required</th>
<th>Relative percentage of maximum No. of determinant evaluations required</th>
<th>Minimum percentage of No. of designs eliminated</th>
<th>Optimal design combination</th>
<th>D-optimum</th>
</tr>
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<tbody>
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<td>87.67</td>
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<td>9.73</td>
<td>90.27</td>
<td>7:0:0</td>
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</table>
designs for which determinant evaluations are required, the relative percentage of maximum 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