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A HILL-CLIMBING COMBINATORIAL ALGORITHM FOR CONSTRUCTING N-POINT D-OPTIMAL EXACT DESIGNS

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Abstract: A method that makes use of combinatorics for selecting N objects out of $\bar{N}$ distinguishable objects is developed for constructing D-optimal N-point exact designs. The difficulties which are experienced in the variance exchange algorithms for constructing D-optimal exact designs, such as cycling, slow convergence and failure to converge to the desired optimum, are not experienced by this method. The method converges rapidly and absolutely to the desired N-point D-optimal design and is effective for determining optimal designs in block experiments as well as in non-block experiments for finite or infinite number of support points in the space of trials.

Keywords: D-optimality, Exact design, Block experiments, Non-block experiments

1. Introduction

Given the experimental space, $\{\tilde{X}, F_x, \Sigma_x\}$, the problem in this work is to develop an algorithm for constructing an N-point D-optimal exact design measure

$$\xi_N^* = \begin{pmatrix} \underline{x}_1 & w_1 \\ \underline{x}_2 & w_2 \\ \bullet & \bullet \\ \bullet & \bullet \\ \bullet & \bullet \\ \underline{x}_N & w_N \end{pmatrix}$$

$$\underline{x}_i = (x_{1i}, x_{2i}, \ldots, x_{ni}) \in \tilde{X};$$

$$w_i = \frac{1}{N} \text{ for all } i$$

where,

$\tilde{X}$ is an n-dimensional space of trials which is compact, continuous and metric (see Onukogu; 1997). The space of trials, $\tilde{X}$, shall be considered as having a regular or an irregular geometric area and shall consist of support points, $\{x_1, x_2, \ldots, x_{\bar{N}}\}$, where $\bar{N}$ represents the number of support points in a finite space of trials. By regular geometric area we imply a geometric area that has a single simple mathematical formula for computing its area. By irregular geometric area we imply a geometric area that does not have a single simple mathematical formula for computing its area. By finite space of trials we imply a space of trials for which the underlying pointset is finite. That is, a space for which there are only finitely many points.

F_x = { f(x) } is a linear space of finite dimensional continuous function defined on $\tilde{X}$.
$\sum_x$ is a space of random observation error defined on $\tilde{X}$.

Following Kiefer and Wolfowitz (1959), we assume that at each point, $\underline{x} \in \tilde{X}$, a random variable, namely,
$y_{\underline{x}} = \underline{\beta}' f(\underline{x}) + \varepsilon$
is defined and is such that
$E(y_{\underline{x}}) = \underline{\beta}' f(\underline{x})$
where
$\underline{\beta} = (\beta_1, \beta_2, \ldots, \beta_p)'$
is a px1 vector of unknown parameters which are estimated on the basis of N uncorrelated observations;
ε is the random additive error associated with $y_{\underline{x}}$ and is independent and identically distributed with E(ε) = 0 and $E(\varepsilon^2) = \sigma_\varepsilon^2$; a constant. We also assume that Var $(y_{\underline{x}}) = \sigma^2$ (normalized for convenience = 1), Cov $(y_{\underline{x}_1}, y_{\underline{x}_2}) = 0$; $\underline{x}, \underline{x}_1, \underline{x}_2 \in \tilde{X}$ $(\underline{x}_1 \neq \underline{x}_2)$.

In defining experimental designs, it is important to distinguish between exact designs and continuous designs. According to Cook and Nachtsheim (1980), a design ξ_N is an N-point exact design if ξ_N is a probability measure on $\tilde{X}$ 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 $\Xi_{\tilde{X}}^N$. On the other hand, a continuous design is a probability measure ξ on $\tilde{X}$ such that $\int_{\tilde{X}} \xi dx = 1$.

The measure ξ is an element of the space, $\Xi_{\tilde{X}}$, of probability measure on $\tilde{X}$ and Nξ need not be an integer.

The above stated problem is a combinatorial one; a problem of choosing N out of $\overline{N}$ in $\tilde{X}$ such that the determinant of the information matrix of the design is maximized. The information matrix, $M(\xi_N)$, of the design ξ_N is given by

$$M(\xi_N) = \frac{1}{N} X'X$$

where X is an Nxp design matrix of ξ_N, whose i^{th} row is $f(\underline{x}_i)$. According to Karlin and Studden (1966), the determinant value of the information matrix is a simple measure of the magnitude of the information matrix. Thus, if $M(\xi_N^{(1)})$ and $M(\xi_N^{(2)})$ are two pxp non-singular information matrices associated with $\xi_N^{(1)}$ and $\xi_N^{(2)}$, respectively,
$M(\xi_N^{(1)}) \geq M(\xi_N^{(2)}) \Rightarrow |M(\xi_N^{(1)})| \geq |M(\xi_N^{(2)})|$ (see Onukogu (1997), pg. 69). The maximization of the determinant of a real-valued non-singular pxp information matrix, say,

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

is achieved when m_{jj}; j = 1, 2, …, p are maximized and $|m_{jj'}|$; $j \neq j'$ are minimized; Onukogu and Chigbu (2002). A design, ξ_N^* , is said to be a D-optimal exact design if the determinant of the information matrix, M(ξ_N^*), is maximized over all $\xi_N \in \Xi_{\tilde{X}}^N$ (see Cook and Nachtsheim (1980)).

When the experiment is to be performed in b incomplete blocks of sizes $k_1, k_2, \ldots, k_b$ respectively, we seek an N-point D-optimal design

$$\xi_N^* = \begin{pmatrix} \underline{x}_{11} \\ \underline{x}_{21} \\ \bullet \\ \bullet \\ \bullet \\ \underline{x}_{k11} \end{pmatrix} \begin{pmatrix} \underline{x}_{12} \\ \underline{x}_{22} \\ \bullet \\ \bullet \\ \bullet \\ \underline{x}_{k22} \end{pmatrix} \ldots \begin{pmatrix} \underline{x}_{1b} \\ \underline{x}_{2b} \\ \bullet \\ \bullet \\ \bullet \\ \underline{x}_{kbb} \end{pmatrix}$$

$\underline{x}_{ij} = (x_{1ij}, x_{2ij}, \ldots, x_{nij}) \in \tilde{X}$; $i = 1, 2, \ldots, k_j$ $j = 1, 2, \ldots, b$,

$$N = \sum_{j=1}^{b} k_j$$

Defining X_t as an N x p coefficient matrix for treatments and X_B as an N x b indicator matrix for blocks with 0 and 1 elements, N x (p + b) design matrix is

$$\underset{Nx(p+b)}{X} = \left(\underset{Nxp}{X_t} \vdots \underset{Nxb}{X_B} \right)$$

and the information matrix to be maximized is

$$M(\xi_N) = X_t'X_t - X_t'X_B(X_B'X_B)^{-1}(X_B'X_t)$$

2. Literature Review

The exchange algorithms cited above become slow due to the need to follow each. They have been of much usefulness in the construction of D-optimal exact designs. One of the earliest of such algorithms is due to Mitchell-Miller (1970). The algorithm begins with a randomly chosen N-run design and moves in the direction of increasing value of the determinant of information matrix. The procedure involves two stages at each iteration by first adding an $(N + 1)^{st}$ run to the initial design and then subtracting from the resulting design the point that leads to the minimum possible decrease in determinant value of information matrix. The algorithm stops when there is no further improvement in the determinant value or when the same point is deleted and then re-entered. The point added corresponds to point of maximum variance of prediction over $\tilde{X}$ and the point deleted corresponds to the point of minimum variance of prediction. The algorithm of Van Schalkwyk (1971) is similar to that of Mitchell-Miller (1970) but first deletes at each iteration the point in the initial N-point design with minimum variance of prediction. The N-point design is then recovered by adding a point from $\tilde{X}$ that gives a maximum increase in the determinant value of information matrix. The algorithm stops when the same point deleted is afterwards re-entered.

An application of the Van Schalkwyk (1971) algorithm in comparison with the Mitchell-Miller (1970) algorithm on the problem of constructing a 7-point D-optimal exact design over the space, $\tilde{X}$; $-1 \leq \tilde{X} \leq 1$, for a bivariate quadratic surface,

$f(x_1, x_2) = a_{00} + a_{10}x_1 + a_{20}x_2 + a_{12}x_1x_2 + a_{11}x_1^2 + a_{22}x_2^2 + \varepsilon$,

reveals that the number of variance evaluations are reduced by not less than 50%. Although the Van Schalkwyk algorithm in application is more direct. However, both algorithms are computationally demanding due to the need to update the designs and evaluate the determinant at each iteration.

The exchange algorithm of Fedorov (1972), pg. 164 begins with an N-point design and at each iteration evaluates all possible exchanges of the pairs of points, x_k , from the design and x_l from the set of candidate points. The exchange giving the maximum increase in the determinant value of information matrix is considered. The procedure continues as long as an interchange increases the determinant. The Fedorov's exchange algorithm is made slow by the large number of points to be considered at each iteration. As a way of speeding up the Fedorov's algorithm, many modifications have been suggested (see e.g. Cook and Nachtsheim (1980), and Johnson and Nachtsheim (1983), Atkinson and Donev (1992). Each of these modifications aims at reducing the number of points to be considered for exchange. For example the KL algorithm of Atkinson and Donev (1992), pg. 173 exchanges points in the design having relatively low variance of prediction with candidate points for which variances are relatively high. The algorithm begins with an N-point design and moves one step at a time in the direction of increasing value of determinant of information matrix. When there is no longer any exchange that would increase the determinant value, the algorithm terminates. The KL algorithm is followed by an adjustment algorithm which searches away from the candidate list (see Atkinson and Donev (1992), pg. 175-178). They also investigated the properties of optimum designs when there are both qualitative factors (represented by the blocks) and quantitative factors. The modified algorithm (BLKL) provides the opportunity to divide the experimental trials into blocks of specified sizes (see Altkinson and Donev (1989, 1992)).

The DETMAX algorithm of Mitchell (1974) though slightly different from the exchange algorithms described above is a generalized version of the Mitchell-Miller algorithm. It begins with a randomly chosen N-run design and a pre-specified list of candidate set. A chosen number of points is sequentially added to and then deleted from the design (following its excursion scheme) thus improving the starting design. In DETMAX, the requirement that an (N + 1)-point design be returned immediately to an N-point design is relaxed. The algorithm makes use of positive and negative "excursions" during which the size of the design may vary from N to N + K and from N to N – K, respectively, where K is a user-selected integer constant. The DETMAX algorithm is run several times (≥ 10 times) in each case, each time starting with a different randomly selected initial N-run design and the "Best DETMAX design" is that which gives the largest determinant value in the number of tries. When an excursion size reaches K, the algorithm terminates.

The exchange algorithms cited above become slow due to the need to follow each successful exchange by updating the design, the information matrix, the variance-covariance matrix, the variances of the predicted values at the design and candidate points and the evaluation of respective determinant values of information matrices. Moreover, these algorithms are based on the variance of the predicted response and hence, have the high probability of getting trapped at a local optimum**.** We present a new method of constructing D-optimal designs. The method is based on the combinatorics of the support points that make up $\tilde{X}$ and is such that for given $\{\tilde{X}, F_x, \Sigma_x\}$, the support points that make up $\tilde{X}$ can be arranged into concentric balls (groups) and an optimal combination of these balls can be obtained so that the corresponding N-point exact design measure is D-optimal. An attractive feature of this method is that by grouping it is easy to identify sets of information matrices with equal diagonal elements, so as to compare the information matrices within a given set on the basis of the off-diagonal elements without necessarily evaluating their determinant values. By some rules for selecting the design points to go into the design, non-promising designs within a given design class are eliminated and by proper use of the algorithm the number of classes to be examined for a particular problem is reduced to only a few. The procedure moves sequentially in the direction of increasing value of determinant of information matrix as the search proceeds from one optimum to another. The required exact D-optimum design is reached when there is no further improvement in the determinant value of information matrix.

3. Methodology

In order to solve the problem defined in section 1.1 above the $\bar{N}$ support points are arranged into H concentric balls, $g_1, g_2, \ldots, g_H$, such that the h^{th} ball, g_h, is defined by

$$g_h = \begin{pmatrix} \underline{x}_{h_1} \\ \underline{x}_{h_2} \\ \vdots \\ \underline{x}_{h_{n_h}} \end{pmatrix} ; \ \underline{x}_{h_i} = (x_{11}, x_{12}, \dots, x_{1n})$$

and consists of n_h support points and $\Sigma n_h = \overline{N}$; h = 1, 2, … , H. Moreover, each support point in g_h is of distance, $r_h = \underline{x}_{h_i}' \underline{x}_{h_i}$; i = 1, 2, … , n_h from the centre of $\tilde{X}$. Besides, $r_1 > r_2 > \dots > r_H$. The purpose of the grouping is to make it easy to identify sets of p x p information matrices with equal diagonal elements, so as to compare the information matrices within a given set (without necessarily evaluating the determinant values) on the basis of the off-diagonal elements.

4. The Algorithm

The Hill-Climbing combinatorial algorithm is embodied in the sequence of steps following. If $\underline{t}_k$ is the H-tuple of support points at the k^{th} step, then the H-tuple of support points at $(k+1)^{st}$ step is formed by holding H-2 of the r_{hk} values fixed and altering the values of just two balls. That is, only two values of the r_{hk} are altered while the remaining H-2 values are held fixed subject to $\Sigma r_{hk} = N$; N is the design size.

Given $\overline{N}$ support points in $\tilde{X}$ which have been partitioned into H groups (balls) as, we suppose that at the k^{th} step of the sequence an H-tuple, $\underline{t}_k = \{r_{1k}, r_{2k}, \dots, r_{Hk}\}$, of support points are selected from the balls.

Then the number of available designs at this k^{th} step is $a_k = \prod_{h=1}^{H} a_{hk}$

where a_{hk} is the number of sub-designs in the h^{th} ball and is computed simply as

$$a_{hk} = \binom{n_h}{r_{hk}} ; \ n_h \geq r_{hk}$$

However, when n_h is less than r_{hk} we shall compute a_{hk} as

$$a_{hk} = \binom{n_h}{f_{hk}}$$

where f_{hk} is a positive integer value defined by

$f_{hk} = r_{hk} - \theta n_h$

and θ is a positive integer value such that $f_{hk} < n_h$.

For convenience, we shall present the details of the algorithm starting with

H = 2, H = 3, etc.

S_2 Search (H=2):

The S_2 search is embodied in the sequence of steps in Table 1 below.

Table 1: Combinatorics for Choosing D-Optimal Design

Step k	Ball combination g_1	g_2	Number of available designs, a_k	Determinant Value, d_{2k}
0	r_1	r_2	a_0	d_{20}
1	r_1+1	r_2-1	a_1	d_{21}
2	r_1+2	r_2-2	a_2	d_{22}
⋮	⋮	⋮	⋮	⋮
m	r_1+m	r_2-m	a_m	d_{2m}
m+1	r_1+m+1	r_2-m-1	a_{m+1}	$d_{2(m+1)}$
m+2	r_1-1	r_2+1	a_{m+2}	$d_{2(m+2)}$
m+3	r_1-2	r_2+2	a_{m+3}	$d_{2(m+3)}$
⋮	⋮	⋮	⋮	⋮
q	r_1-w	r_2+w	a_q	d_{2q}
q+1	r_1-w-1	r_2+w+1	a_{q+1}	$d_{2(q+1)}$

$w = q - m$ 4.1

$$\left.\begin{array}{l} d_{21} < d_{22} < \ldots < d_{2m} > d_{2(m+1)} \\ d_{2(m+2)} < d_{2(m+3)} < \ldots < d_{2q} > d_{2(q+1)} \end{array}\right\} \quad 4.2$$

$$d_{2k} = \max_{a_k} \{\det M(\xi_k^{(i,j)})\}; \; M(\xi_k^{(i,j)}) \in S_k^{pxp}; \; k = 0, 1, 2, \ldots, q+1$$

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

The sequential steps involved in setting up the table are as follows:

1) At k = 0, define an initial 2-tuple,
   $\underline{t}_0 = (r_1 \; , \; r_2)$
   of support points such that $r_1 \geq 0$, $r_2 \geq 0$ and $r_1 + r_2 = N$
2) Compute the values of a_{10} and a_{20} designs from ball 1 and ball 2, respectively, and set $a_0 = a_{10}\, a_{20}$; a_0 is the number of all the available designs at step k = 0,
3) Express the a_{10} designs from g_1 and a_{20} designs from g_2, respectively, as follows:
   $\xi_{10}^{(1)}, \xi_{10}^{(2)}, \ldots, \xi_{10}^{(a_{10})}$; $\quad \xi_{20}^{(1)}, \xi_{20}^{(2)}, \ldots, \xi_{20}^{(a_{20})}$,
4) Define the a_0 designs as composite designs; i.e.

$$\xi_0^{(1,1)} = \begin{pmatrix} \xi_{10}^{(1)} \\ \xi_{20}^{(1)} \end{pmatrix}, \ldots, \; \xi_0^{(1,a_{10})} = \begin{pmatrix} \xi_{10}^{(a_{10})} \\ \xi_{20}^{(1)} \end{pmatrix}$$

$$\xi_0^{(2,1)} = \begin{pmatrix} \xi_{10}^{(1)} \\ \xi_{20}^{(2)} \end{pmatrix}, \ldots, \; \xi_0^{(2,a_{10})} = \begin{pmatrix} \xi_{10}^{(a_{10})} \\ \xi_{20}^{(2)} \end{pmatrix}$$

$$\vdots$$

$$\xi_0^{(a_{20},1)} = \begin{pmatrix} \xi_{10}^{(1)} \\ \xi_{20}^{(a_{20})} \end{pmatrix}, \ldots, \; \xi_0^{(a_{20},a_{10})} = \begin{pmatrix} \xi_{10}^{(a_{10})} \\ \xi_{20}^{(a_{20})} \end{pmatrix}$$

Where, $M\left(\xi_0^{(i,j)}\right) \in S_0^{pxp}$; $i = 1, 2, \ldots, a_{20}$; $j = 1, 2, \ldots, a_{10}$

It will be noticed that the a_0 design measures are grouped into a_{20} sets, each set containing a_{10} designs and within each set the diagonal elements of information matrices are exactly the same. For example, consider an experimental area whose support points are grouped into

$$g_1 = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 1 & -1 \\ -1 & -1 \end{pmatrix}; \qquad g_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \\ 0 & -1 \\ 1 & 0 \end{pmatrix}; \qquad g_3 = (0 \;\; 0).$$

Suppose

$\underline{t}_0 = \{3, 3, 0\}$

then $a_{10} = 4$, $a_{20} = 4$, $a_{30} = 1$, $a_0 = 16$

The $a_{10} = 4$ designs from g_1 are

$$\xi_{10}^{(1)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & -1 \end{pmatrix}; \quad \xi_{10}^{(2)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & 1 \end{pmatrix}; \quad \xi_{10}^{(3)} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \\ -1 & 1 \end{pmatrix}; \quad \xi_{10}^{(4)} = \begin{pmatrix} 1 & -1 \\ -1 & -1 \\ -1 & 1 \end{pmatrix}$$

and the $a_{20} = 4$ designs from g_2 are

$$\xi_{20}^{(1)} = \begin{pmatrix} 0 & 1 \\ 0 & -1 \\ -1 & 0 \end{pmatrix}; \quad \xi_{20}^{(2)} = \begin{pmatrix} 0 & 1 \\ 0 & -1 \\ 1 & 0 \end{pmatrix}; \quad \xi_{20}^{(3)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix}; \quad \xi_{20}^{(4)} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix}$$

The four sets of designs are as follows:

Set 1:

$$\xi_{0}^{(1,1)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & 1 \\ 0 & -1 \\ -1 & 0 \end{pmatrix}; \quad \xi_{0}^{(1,2)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & 1 \\ 0 & 1 \\ 0 & -1 \\ -1 & 0 \end{pmatrix}; \quad \xi_{0}^{(1,3)} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \\ -1 & 1 \\ 0 & 1 \\ 0 & -1 \\ -1 & 0 \end{pmatrix}; \quad \xi_{0}^{(1,4)} = \begin{pmatrix} 1 & -1 \\ -1 & -1 \\ -1 & 1 \\ 0 & 1 \\ 0 & -1 \\ -1 & 0 \end{pmatrix}$$

Set 2:

$$\xi_{0}^{(2,1)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \end{pmatrix}; \quad \xi_{0}^{(2,2)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & 1 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \end{pmatrix}; \quad \xi_{0}^{(2,3)} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \\ -1 & 1 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \end{pmatrix}; \quad \xi_{0}^{(2,4)} = \begin{pmatrix} 1 & -1 \\ -1 & -1 \\ -1 & 1 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \end{pmatrix}$$

Set 3:

$$\xi_{0}^{(3,1)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & 1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix}; \quad \xi_{0}^{(3,2)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & 1 \\ 0 & 1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix}; \quad \xi_{0}^{(3,3)} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \\ -1 & 1 \\ 0 & 1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix}; \quad \xi_{0}^{(3,4)} = \begin{pmatrix} 1 & -1 \\ -1 & -1 \\ -1 & 1 \\ 0 & 1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix}$$

Set 4:

$$\xi_{0}^{(4,1)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix}; \quad \xi_{0}^{(4,2)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix}; \quad \xi_{0}^{(4,3)} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \\ -1 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix}; \quad \xi_{0}^{(4,4)} = \begin{pmatrix} 1 & -1 \\ -1 & -1 \\ -1 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix}$$

Using the quadratic model

$f(x_1, x_2) = a_{00} + a_{10}\, x_1 + a_{20}\, x_2 + a_{12}\, x_1 x_2 + a_{11}\, x_1^2 + a_{22}\, x_2^2 + \varepsilon$,

the information matrices of the four designs in the first set are respectively,

$$M_1 = \begin{pmatrix} 6 & 0 & -1 & 1 & 4 & 5 \\ 0 & 4 & 1 & -1 & 0 & 1 \\ -1 & 1 & 5 & 1 & -1 & -1 \\ 1 & -1 & 1 & 3 & 1 & 1 \\ 4 & 0 & -1 & 1 & 4 & 3 \\ 5 & 1 & -1 & 1 & 3 & 5 \end{pmatrix}; \quad M_2 = \begin{pmatrix} 6 & 0 & 1 & -1 & 4 & 5 \\ 0 & 4 & -1 & 1 & 0 & 1 \\ 1 & -1 & 5 & 1 & 1 & 1 \\ -1 & 1 & 1 & 3 & -1 & -1 \\ 4 & 0 & 1 & -1 & 4 & 3 \\ 5 & 1 & 1 & -1 & 3 & 5 \end{pmatrix}$$

$$M_3 = \begin{pmatrix} 6 & -2 & 1 & 1 & 4 & 5 \\ -2 & 4 & 1 & 1 & -2 & -1 \\ 1 & 1 & 5 & -1 & 1 & 1 \\ 1 & 1 & 1 & 3 & 1 & 1 \\ 4 & -2 & 1 & 1 & 4 & 3 \\ 5 & -1 & 1 & 1 & 3 & 5 \end{pmatrix} \; ; M_4 = \begin{pmatrix} 6 & -2 & -1 & -1 & 4 & 5 \\ -2 & 4 & -1 & -1 & -2 & -1 \\ -1 & -1 & 5 & -1 & -1 & -1 \\ -1 & -1 & -1 & 3 & -1 & -1 \\ 4 & -2 & -1 & -1 & 4 & 3 \\ 5 & -1 & -1 & -1 & 3 & 5 \end{pmatrix}$$

It is clearly seen that the diagonal elements of the information matrices of all design in the first set are exactly the same. This is also true for the other designs in the same sets.

5) By comparing the absolute values of the off-diagonal elements of the information matrices belonging to the same set, identify the best design, $\xi_0^{(i)}$, in the i[th] set, such that
$M\left(\xi_0^{(i)}\right) = \max_j M(\xi_0^{(i,j)})$; i = 1, 2, …, a_{20} ; $M\left(\xi_0^{(i)}\right)$, $M\left(\xi_0^{(i,j)}\right) \in S_0^{pxp}$.

6) Define ξ_0 such that
$\det\{M(\xi_0)\} = \max_i \det\{M(\xi_0^{(i)})\} = d_{20}$; i = 1, 2, … , a_{20}.

7) Set $\underline{t}_k = (r_1+k \;,\; r_2-k)$; k = 1, 2, …, m+1, m+2, …, q+1 and following steps 2 to 5 ,above obtain { d_{2k} }. From equation 4.2, determine d_{2m} and d_{2q}.

8) Set d^c = max {d_{20}, d_{2m}, d_{2q}}. Then ξ_N^c , the corresponding design measure is the required D-optimal exact design.

S_3 Search (H = 3):

As with S_2 search, we assume that the $\overline{N}$ support point in $\tilde{X}$ have been grouped into g_1, g_2 and g_3 balls and we proceed with the following steps;

1) At k = 0, define an initial 3-tuple $\underline{t}_0 = (r_1, r_2, r_3)$ of support points taken from g_1, g_2 and g_3, respectively, such that $r_1 \geq 0$, $r_2 \geq 0$, $r_3 \geq 0$ and
$r_1 + r_2 + r_3 = N$.

2) Holding ball g_1 fixed at r_1, apply the procedures of S_2 search on the remaining two balls and obtain $d_{30}(r_1+0)$ and the corresponding tuple
$\underline{t}_0^* = (r_1, r_2^*, r_3^*)$; r_2^* and r_3^* are the optimal number of support points taken from g_2 and g_3, respectively, when ball g_1 is held fixed at r_1.

3) Set k = 1, 2, …, q+1 and obtain { $d_{3k(r_1+k)}$ } as in steps 1 and 2 above. Hence, determine $d_{3m(r_1+m)}$ and $d_{3q(r_1+q)}$.

4) Set d^c = max { $d_{30(r_1+0)}$, $d_{3m(r_1+m)}$, $d_{3q(r_1+q)}$ }. Then ξ_N^c , the corresponding design measure is the required D-optimal exact design.

S_H Search (for general H) :

For S_H search, the $\overline{N}$ support points in $\tilde{X}$ are arranged into H balls, namely, g_1, g_2, …, g_H following the usual procedure and the search proceeds along the following steps;

1) At k = 0, define an initial H-tuple,
$\underline{t}_0 = (r_1, r_2, \ldots, r_H)$,
of support points taken from g_1, g_2, …, g_H, respectively, such that $r_1 \geq 0$, $r_2 \geq 0$, … , $r_H \geq 0$ and $r_1 + r_2 + \ldots + r_H = N$.

2) Holding ball g_1 fixed at r_1, apply the procedures of S_{H-1} search on the remaining H-1 balls and obtain $d_{H0}(r_1+0)$ and the corresponding tuple,
$\underline{t}_1^* = (r_1, r_2^*, r_3^*, \ldots, r_H^*)$; r_2^*, r_3^* …, r_H^* are the optimal number of support points taken from balls, g_2, g_3, …, g_H, respectively, when ball g_1 is held fixed at r_1.

3) Set k = 1, 2, …, q+1 and obtain { $d_{Hk(r_1+k)}$ } as in steps 1 and 2 above. Hence, determine $d_{Hm(r_1+m)}$ and $d_{Hq(r_1+q)}$.

4) Set d^c = max { $d_{H0(r_1+0)}$, $d_{Hm(r_1+m)}$, $d_{Hq(r_1+q)}$ }. Then ξ_N^c, the corresponding design measure is the required D-optimal exact design.

5. Properties of S_H Search

Every sequential technique can generally be characterized by how to begin the search, in what direction to continue, at what step length and how to end the search. The S_H search is governed by certain properties which for simplicity in presentation are outlined below for H = 2.

1) **Starting point:**
The S_2 search commences at an arbitrary 2-tuple of support points
$\underline{t}_0 = (r_1 , r_2) ; r_1 \geq 0,\ r_2 \geq 0 ; r_1 + r_2 = N$

2) **Direction of search:**
The search moves in the direction of increasing values of determinant, d_{2k}, as in equation 4.2. The direction is determined after examining all the available designs at the preceding step. It should be noted that although a 100% search is required at each step, by the application of Theorem 2 and the properties of the search, the number of determinant evaluations at each step reduces to no more than a_{2k}.

3) **Step length:**
The search moves one step at a time in both the increasing and the decreasing values of (r_1, r_2). That is, at step k, we have the tuple,
$\underline{t}_k = (r_1 + k , r_2 - k)$ or $\underline{t}_k = (r_1 - k , r_2 + k)$; k = 0, 1, …

4) **Stopping point:**
The search terminates at k = q+1, as in equation 4.2.

5) The set of steps given by
$\{ \underline{t}_k \} = \{ (r_1 \pm k,\ r_2 \pm k) \}$
defines a path or direction of search that is in accordance with property 2 above. The set is completely exhaustive of all possible paths. In other words, for any other starting point, say,

$$\underline{t}_\upsilon = (s_1^*, s_2^*);\ s_1^*, s_2^* \geq 0;\ s_1^* + s_2^* = N$$

where

$$s_1^* = s_1 \pm k ;\ s_1 \neq r_1$$

$$s_2^* = s_2 \pm k ;\ s_2 \neq r_2,$$

the path defined by { $\underline{t}_k$ } and { $\underline{t}_v$ } will coincide somewhere along the search. The proof of property 5 is simple since any of the components in $\underline{t}_k = (r_1, r_2)$ takes any integer value from 0 to N and each number pair is such that the components sum upto N. It is obvious that the combinations exhaust all pairs whose components sum upto N. Consequently, { $\underline{t}_k$ } is exhaustive of all possible paths.

We show in Theorem 1 that d^c is the global D-optimum. It is sufficient to establish this for H=2.

Theorem 1

Let $d^* = \det M(\xi_N^*) = \max_{x \in \underset{\sim}{X}} \{\det M(\xi_N)\} \quad \forall\ M(\xi_N) \in S^{pxp}$

be the global value of determinant of all pxp information matrices for all non-singular designs. Then det $M(\xi_N^c) = \det M(\xi_N^*)$,

where

$\det M(\xi_N^c) = \max_k \{\det M(\xi_k)\}$; k = 0, 1, …, m, m+1, m+2, …, q, q+1,

$= d^c$

Proof (By Contradiction)

Suppose { $\underset{\sim}{t}_k$ } converges to the value $d^c \neq d^*$, let it be possible to start a fresh sequence at another point, say, $\underset{\sim}{t}_\upsilon = (s_1^*, s_2^*)$; $s_1^*, s_2^* \geq 0$; $s_1^* + s_2^* = N$

which converges to the value d^g such that $d^g = d^*$. Then with respect to property 5 of the S_2 search, { $\underset{\sim}{t}_v$ } must coincide with { $\underset{\sim}{t}_k$ } somewhere along the search. Then $d^c = d^*$ and ξ_N^c, the corresponding design measure, is the D-optimal exact design. Q.E.D.

5. Numerical Illustrations

We present some illustrations to demonstrate the working of the algorithm developed in section 4. The demonstrations are based on first and second order models. The essence of demonstrating with first order models is to show that this new approach performs credibly well even for first order models, and then extend it to second order models. However, this does not preclude the working of the algorithm for higher order models.

Illustration 1

Given a first order model,

$f(x_1, x_2) = a_0 + a_1x_1 + a_2x_2 + a_{12}x_1x_2 + \varepsilon$,

defined on a regular geometric area having a finite number of support points as in figure I, we seek to construct an N-point D-optimal exact design measure, ξ_N^* ; N = p, p+1, …, 2p

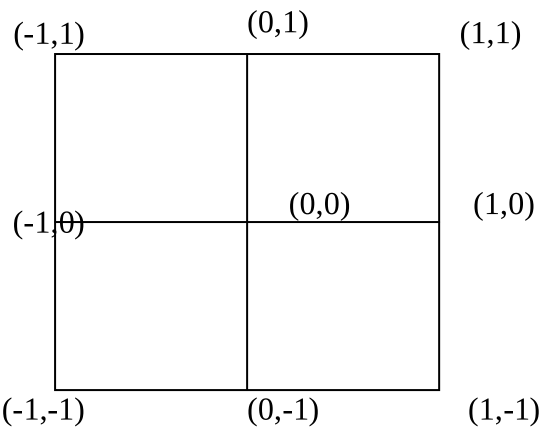

Figure 1: A regular geometric experimental region at specified values.

By arranging the support points as described in 4, we form the following groups

$g_1 = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 1 & -1 \\ -1 & -1 \end{pmatrix}$; $g_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \\ 0 & -1 \\ 1 & 0 \end{pmatrix}$; $g_3 = (0 \;\; 0)$.

The problem of constructing D-optimal designs for the model is greatly simplified by the fact that to achieve D-optimality, each $\underset{\sim}{x}_i$ must be a vertex point. A proof of this has been given by Box and Draper (1971) for the case when N=p (i.e., when the design size is the same as the number of parameters in the model) and also by Mitchell (1974) for the case when N>p. Since the D-optimal design must consist entirely of corner points (vertex points) we restrict ourselves to the vertex points. In this example the vertex points refer to supports points in ball g_1. The design points of the D-optimal measure, ξ_N^* ; N = 4, 5, 6, 7, 8, are summarized in Table 2 below.

Table 2: Design Points for D-optimal Exact Design for a first order model defined on Figure 1

Design Size, N	**Ball combination** g_1	g_2	g_3	Design Points	**Determinant Value**
4	4	0	0	-11, 11, 1-1, -1-1	1.0000
5	5	0	0	-11, 11, 1-1, -1-1, 11	0.8192
6	6	0	0	-11, 11, 1-1, -1-1, 11, -1-1	0.7901
7	7	0	0	-11, 11, 1-1, -1-1, 11, -1-1, 1-1	0.8530
8	8	0	0	-11, 11, 1-1, -1-1,11,-1-1,1-1,-11	1.0000

These results indicate that for first order models defined on a space of trials as in Figure 1, and for a given N-point D-optimal exact design measure, ξ_N^* , the N+1 point D-optimal exact design measure, ξ^*_{N+1}, is obtained by adding a vertex point (in accordance with the rules for maximizing information matrix) to ξ_N^* .

Illustration 2

Given the first order model, defined on an irregular space of trials as in Figure 2 below, we seek to construct N-point D-optimal exact design measure, ξ_N^* .

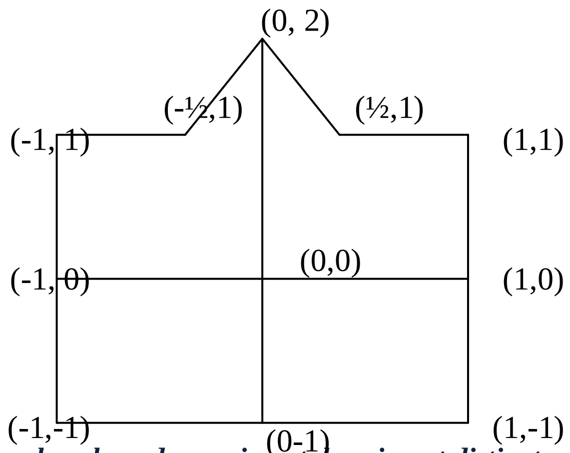

Figure 2: An irregular-shaped experimental region at distinct points

By grouping the vertex points according to their distances from the center of $\tilde{X}$, the following groups are formed;

$g_1 = \begin{pmatrix} -1 & -1 \\ 1 & -1 \end{pmatrix}$ $g_2 = \begin{pmatrix} 0 & 2 \end{pmatrix}$ $g_3 = \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}$ $g_4 = \begin{pmatrix} -½ & 1 \\ ½ & 1 \end{pmatrix}$

The operations that lead to a 4-point D-optimal design are as tabulated in Table 3 below.

Table 3 Combinatorics for obtaining a 4-point D-optimal exact Design on the Irregular Geometric area in Figure 2

Step k	Ball combination g_1	g_2	g_3	g_4	Number of available designs, a_k	Best Determinant Value, d_k
0	2	1	1	0	2	0.56
1	2	2	0	0	1	SINGULAR
2	2	0	2	0	1	1.0000
3	2	0	1	1	2	0.5625
4	3	0	1	0	4	SINGULAR
5	4	0	0	0	1	SINGULAR
6	1	1	2	0	2	0.0625
7	1	0	3	0	4	SINGULAR
8	1	0	2	1	2	4.0625×10^{-16}

$d^* = 1.0000$

The corresponding D-optimal exact design measure is

$$\xi_4^* = \begin{pmatrix} 1 & 1 & ¼ \\ 1 & -1 & ¼ \\ -1 & 1 & ¼ \\ -1 & -1 & ¼ \end{pmatrix}$$

The design points that make up the D-optimal N-point exact design measure (N = 5, 6, 7, 8) are summarized in Table 4 below.

Table 4: Design points of D-optimal exact design for a first order model defined on figure 2

Design size N	Ball combination g_1	g_2	g_3	g_4	Design Points	Determinant Value
5	2	1	2	0	-1-1, 1-1, 0 2, -1 1, 1 1	0.9216
6	3	1	2	0	-1-1, -1-1, 1-1, 0 2, -1 1, 1 1	0.8765
7	4	1	2	0	-1-1,-1-1,1-1, 1-1, 0 2, -1 1,1 1	0.9329
8	4	0	4	0	-1-1,-1-1,1-1, 1-1,-1 1,-1 1, 1 1, 1 1	1.0000

Illustration 3

In this illustration, we demonstrate the effectiveness in the performance of the algorithm for constructing D-optimal exact designs in blocks of unequal sizes. For the purpose of illustration, we consider constructing a 7-point D-optimal design measure in two blocks of sizes $k_1 = 4$ and $k_2 = 3$, for the bivariate quadratic surface,

$$f(x_1, x_2) = a_{00} + a_{10}x_1 + a_{20}x_2 + a_{12}x_1x_2 + a_{11}x_1^2 + a_{22}x_2^2 + \varepsilon,$$

defined on a regular and continuous experimental area such as in Figure 1 but with 25 grid points. The points are arranged in the following groups;

$$g_1 = \begin{pmatrix} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \end{pmatrix} \quad g_2 = \begin{pmatrix} -½ & 1 \\ ½ & 1 \\ -½ & -1 \\ ½ & -1 \\ 1 & ½ \\ 1 & -½ \\ -1 & ½ \\ -1 & -½ \end{pmatrix} \quad g_3 = \begin{pmatrix} 0 & -1 \\ 0 & 1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix} \quad g_4 = \begin{pmatrix} -½ & ½ \\ ½ & ½ \\ -½ & -½ \\ ½ & -½ \end{pmatrix} \quad g_5 = \begin{pmatrix} -½ & 0 \\ 0 & ½ \\ ½ & 0 \\ 0 & -½ \end{pmatrix} \quad g_6 = (0 \;\; 0)$$

The sequential procedures for constructing the 7-point D-optimal design are laid out in Table 5 below.

Table 5: Combinatorics for obtaining a 7-point D-optimal exact design in 2 blocks of sizes $k_1 = 4$ and $k_2 = 3$

Step k	Ball Combination g_1	g_2	g_3	g_4	g_5	g_6	No of Available Designs a_k	Best Determinant Value d_k
0	4	0	3	0	0	0	4	1.5737×10^{-3}
1	4	1	2	0	0	0	48	3.8079×10^{-3}
2	4	0	2	1	0	0	24	2.9144×10^{-3}
3	4	0	2	0	1	0	24	4.9736×10^{-3}
4	4	0	2	0	0	1	6	4.9736×10^{-3}
5	4	1	1	0	1	0	128	4.2269×10^{-3}
6	4	0	1	1	1	0	64	1.1016×10^{-3}
7	4	0	1	0	2	0	24	5.3549×10^{-4}
8	4	0	1	0	1	0	16	1.8663×10^{-3}
9	4	1	1	0	0	1	32	7.7713×10^{-5}
10	4	0	1	1	0	1	16	1.2434×10^{-3}
11	4	0	1	0	1	1	16	1.2823×10^{-3}
12	4	0	1	0	0	2	4	1.2434×10^{-3}
13	5	0	2	0	0	0	24	1.2434×10^{-3}
14	5	0	1	0	1	0	64	1.2434×10^{-3}
15	5	0	1	0	0	1	16	1.2434×10^{-3}
16	6	0	1	0	0	0	24	SINGULAR
17	6	0	0	0	1	0	24	SINGULAR
18	6	0	0	0	0	1	6	SINGULAR
19	3	1	3	0	0	0	128	1.0928×10^{-3}
20	3	0	4	0	0	0	4	1.2434×10^{-3}
21	3	0	3	1	0	0	64	9.5250×10^{-4}
22	3	0	3	0	1	0	64	1.4037×10^{-3}
23	3	0	3	0	0	1	16	1.2434×10^{-3}
24	3	1	2	0	1	0	768	1.7076×10^{-3}
25	3	0	2	1	1	0	384	1.7550×10^{-5}
26	3	0	2	0	2	0	144	7.5892×10^{-6}
27	3	0	2	0	1	1	96	5.9499×10^{-5}
28	3	1	2	0	0	1	192	1.0928×10^{-5}
29	3	0	2	1	0	1	96	4.9735×10^{-6}
30	3	0	2	0	0	2	24	SINGULAR
31	2	2	2	0	1	0	4032	1.2568×10^{-4}
32	2	1	3	0	1	0	768	2.5183×10^{-5}
33	2	1	2	1	1	0	4608	2.0384×10^{-5}
34	2	1	2	0	2	0	1728	6.0452×10^{-4}
35	2	1	2	0	1	1	1152	2.6850×10^{-4}

$d^* = 4.9736 \times 10^{-3}$

The corresponding D-optimal design measure is

$$\xi_7^* = \begin{pmatrix} 1 & 1 \\ -1 & 1 \\ 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} -1 & -1 \\ 1 & -1 \\ 0 & 1 \end{pmatrix} \quad \text{or}$$

$$\xi_7^* = \begin{pmatrix} 1 & 1 \\ -1 & 1 \\ 0 & -1 \\ \tfrac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} -1 & -1 \\ 1 & -1 \\ 0 & 1 \end{pmatrix} \quad \text{or}$$

$$\begin{pmatrix} 1 & 1 \\ & \\ & \\ & \end{pmatrix} \begin{pmatrix} -1 & -1 \\ & \\ & \end{pmatrix}$$

$\xi_7^* =$

-1 1	1 -1
0 -1	0 1
0 0	

7. Conclusion

This work has successfully produced a new approach known as the Hill-Climbing Combinatorial procedure, for constructing D-optimal exact designs. Results obtained show that the algorithm compares favourably well with known algorithms.

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