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A COMBINATORIAL PROCEDURE FOR CONSTRUCTING D-OPTIMAL EXACT DESIGNS

I.B. Onukogu, M.P. Iwundu

1. INTRODUCTORY REMARKS

The subject of constructing optimal N-point exact designs for response surfaces is one that has received research attention over the last half century. For some polynomial and trigonometric response functions defined in regular geometric spaces, it is possible to determine optimal designs algebraically; see, e.g. Federov (1972, ch. 3), Pazman (1986; ch. V, VI). In 2^n central composite factorial experiments, optimal designs can be obtained analytically for second order response surfaces; see, Box and Draper (1951), Onukogu (1997; ch. 4).

However, in more general settings, analytical solutions become intractable and iterative methods come into consideration; see the variance – exchange algorithm in Mitchell (1974), Atkinson and Donev (1992, ch. 13), and Pazman (1986). Unfortunately, many iterative methods are not guaranteed to reach the global optimum or they reach it rather slowly.

Under the present procedure the support points that make up the space $\widetilde{X}$ are grouped into H concentric balls,

$$g_1 = \begin{pmatrix} \underline{x}_{11} \\ \underline{x}_{12} \\ \dots \\ \underline{x}_{1n_1} \end{pmatrix}, g_2 = \begin{pmatrix} \underline{x}_{21} \\ \underline{x}_{22} \\ \dots \\ \underline{x}_{2n_2} \end{pmatrix}, \dots, g_H = \begin{pmatrix} \underline{x}_{H1} \\ \underline{x}_{H2} \\ \dots \\ \underline{x}_{Hn_H} \end{pmatrix},$$

such that,

$$\underline{x}_{hk}\text{, } a \text{ constant for all } k=1, 2,\dots, n_h \tag{1}$$

$\underline{x}_{hk}$ is an n-component vector of support points in $\tilde{X}$, h = 1, 2, ..., H; k = 1, 2, ..., n_h and $d_1 > d_2 \dots > d_H$; $\sum_{h=1}^{H} n_h = \tilde{N}$ is the total number of support points in $\tilde{X}$.

At any point *j* in the sequence, a set of design measures ξ_N is specified by an *H*-tuple, $(r_{1j}, r_{2j}, ..., r_{Hj})$; where r_{hj} is the number of support points to be taken from ball *h*;

$$N = \sum_{h=1}^{H} r_{hj}, \quad r_{hj} \geq 0.$$

Therefore, each design measure ξ_N is a composite of the sub-measures from the different balls;

$$\xi_N = \begin{pmatrix} \xi_1 \\ \xi_2 \\ \dots \\ \xi_H \end{pmatrix}.$$

Also, the number of available designs at the jth step is $a_j = a_{1j} \cdot a_{2j} \cdot \dots \cdot a_{Hj}$; where a_{hj} is the number of available designs from the h^{th} ball. These numbers can be easily computed; for example, if selection of support points from the h^{th} all is without replacement,

$$a_{hj} = \begin{pmatrix} n_h \\ r_{hj} \end{pmatrix} = \frac{n_h!}{r_{hj}!(n_h - r_{hj})!}.$$

The combinatorial procedure strives to reach the *D*-optimal design by
1) minimizing the number of determinantal evaluations needed to be made in the set of a_j available designs, and
2) minimizing the number of steps required to convergence.

2. EQUIVALENCE OF DESIGNS

Let $M(\xi_1)$ and $M(\xi_2)$ be two non-singular $p \times p$ information matrices, then:

$$\det(M(\xi_1)) > \det(M(\xi_2)) \Rightarrow \xi_1 \text{ is better than } \xi_2.$$

$$\det(M(\xi_1)) = \det(M(\xi_2)) \Rightarrow \xi_1 \text{ is equivalent to } \xi_2.$$

For more discussions on the equivalence of designs see, for example Pazman (1986), Onukogu (1997).

One of the characteristics of these composite designs is that they can be grouped into sets of equal size such that designs belonging to the same set have equal diagonal elements in their information matrices. This means for instance that if $\xi_{11}, \xi_{12}, ..., \xi_{1p}$ and $\xi_{21}, \xi_{22}, ..., \xi_{2q}$ are the sub-design measures from balls one and two respectively, then the N-points composite designs; namely,

$$\begin{pmatrix}\xi_{11}\\ \xi_{21}\end{pmatrix}\begin{pmatrix}\xi_{12}\\ \xi_{21}\end{pmatrix}\cdots\begin{pmatrix}\xi_{1p}\\ \xi_{21}\end{pmatrix}\begin{pmatrix}\xi_{11}\\ \xi_{22}\end{pmatrix}\cdots\begin{pmatrix}\xi_{1p}\\ \xi_{2q}\end{pmatrix}$$

can be grouped into q sets:

$$\begin{pmatrix}\xi_{11}\\ \xi_{21}\end{pmatrix}\begin{pmatrix}\xi_{12}\\ \xi_{21}\end{pmatrix}\cdots\begin{pmatrix}\xi_{1p}\\ \xi_{21}\end{pmatrix};\ \begin{pmatrix}\xi_{11}\\ \xi_{22}\end{pmatrix}\begin{pmatrix}\xi_{12}\\ \xi_{22}\end{pmatrix}\cdots\begin{pmatrix}\xi_{1p}\\ \xi_{22}\end{pmatrix};\ ...;\ \begin{pmatrix}\xi_{11}\\ \xi_{2q}\end{pmatrix}\begin{pmatrix}\xi_{12}\\ \xi_{2q}\end{pmatrix}\cdots\begin{pmatrix}\xi_{1p}\\ \xi_{2q}\end{pmatrix}.$$

Notice that each set contains p N-point designs and it is shown in theorem 1 that the corresponding diagonal elements of the information matrices of the designs in a set are equal.

Theorem 1.

Let $\xi_N = \begin{pmatrix}\xi_1\\ \xi_2\\ \vdots\\ \xi_H\end{pmatrix}$ be an N-point H-tuple composite design; where ξ_H has a_h available designs, h = 1, 2, ... H. Then, the $a_1 \times a_2 \times ... \times a_H$ available designs can be grouped into $a_2 \times a_3 \times ... \times a_H$ sets, each set containing a_1 designs, such that for any two N-point designs ξ_1 and ξ_2 in a set, the corresponding diagonal elements of their information matrices are equal; *i.e.* $m_{ii}(\xi_1) = m_{ii}(\xi_2),\ i = 1, 2, ..., p$.

Proof. The composition of the designs in each set differs only in the support points selected from ball 1 whereas from each of the other balls the support points remain exactly the same. Hence from equation (1) the theorem follows.

Theorem 2. Let $M(\xi_1) = (m_{ij}(\xi_1))$ and $M(\xi_2) = (m_{ij}(\xi_2))$ be $p \times p$ non singular information matrices such that $m_{ii}(\xi_1) = m_{ii}(\xi_2),\ \forall\ i = 1, 2, ..., p$.
Then, $M(\xi_1) \geq M(\xi_2)$ if

a) $\left\| m_{ij}(\xi_1) \right\| \leq \left\| m_{ij}(\xi_2) \right\|,\ i \neq j$, where $\|.\|$ denotes absolute value.

b) $\sum_{i=1}^{p} u_i^2 \geq \sum_{i=1}^{p} v_i^2$ where $\underline{u}^{/} = (u_1, u_2, ..., u_p)$, $\underline{v}^{/} = (v_1, v_2, ..., v_p)$ are two non-zero vectors, such that $M(\xi_1) = D + \underline{u}\underline{u}^{/}$, $M(\xi_2) = D + \underline{v}\underline{v}^{/}$; $D = diag\{m_{11}, m_{22}, ..., m_{pp}\}$ are the diagonal elements of $M(\xi_1)$ and $M(\xi_2)$.

Proof: (a) Applying the Gaussian elimination method on the $\frac{1}{2}p(p-1)$ off-diagonal elements of $M(\xi_1)$ and $M(\xi_2)$ we get upper triangular matrices, with respective diagonal elements $t_{ii}(\xi_1)$ and $t_{ii}(\xi_2)$, $t_{ii}(\xi_1) \geq t_{ii}(\xi_2)$; see, for example Onukogu (1997),

$$\det(M(\xi_1)) = \prod_{i=1}^{p} t_{ii}(\xi_1) \geq \prod_{i=1}^{p} t_{ii}(\xi_2) = \det(M(\xi_2)).$$

(b) $\det(M(\xi_1)) = \prod_{i=1}^{p} m_{ii}(1 + \underline{u}^{/} D^{-1} \underline{u})$, $\det(M(\xi_2)) = \prod_{i=1}^{p} m_{ii}(1 + \underline{v}^{/} D^{-1} \underline{v})$.

Hence, $M(\xi_1) \geq M(\xi_2)$ if $\sum_{i=1}^{p} u_i^2 = \sum_{i=1}^{p} v_i^2$.

These two theorems provide ways for comparing designs and to reduce to a great extent the number of determinants to be computed; see, the numerical example in section 4, where at $j = 0$, the number of determinants to compute was reduced from 16 to just 2. In addition, the condition that $N \geq p$ and $r_{ij} > 0$ for $i = 1, 2, ..., H$ for non-singular designs, have the effect of eliminating several steps in the sequence. In the numerical example, the 3-tuple (5, 1, 0) gives singular designs only and can therefore be skipped in the sequence.

3. A SYSTEMATIC SEARCH TECHNIQUE

The algorithm converges to an N-point design measure ξ_N^* such that, $\det(M(\xi_N^*)) = \max_{\underline{x} \in \tilde{X}} \{\det(M(\xi_N))\}$, $\forall\, M(\xi_N) \in S^{p \times p}$ where $S^{p \times p}$ is the set of all non-singular $p \times p$ information matrices. The sequence of steps is given for different values of H beginning with $H = 2$,

TABLE 3.1

The S_2 Search when H = 2

Step j	H-tuple		Maximum Determinant
	r_{1j}	r_{2j}	d_{Hj}
0	r_{10}	r_{20}	d_{20}
1	$r_{10} + 1$	$r_{20} - 1$	d_{21}
⋮	⋮	⋮	⋮
k	$r_{10} + k$	$r_{20} - k$	d_{2k}
$k + 1$	$r_{10} + k + 1$	$r_{20} - k - 1$	d_{2k+1}
$k + 2$	$r_{10} - 1$	$r_{20} + 1$	$d_{2k} + 2$
⋮	⋮	⋮	⋮
t	$r_{10} - t$	$r_{10} + t$	d_{2t}
$t + 1$	$r_{10} - t - 1$	$r_{20} + t + 1$	d_{2t+1}

The above table is set up as follows:

i. Start at $j = 0$ with guessed values of r_{10} and r_{20}; $r_{10} + r_{20} = N$; $r_{10}, r_{20} \geq 0$.
ii. Arrange the $n_{10}\, n_{20}$ available designs at $j = 0$ into n_{20} sets, each set containing n_{10} designs that satisfy theorem 1.
iii. Apply theorem 2 to compare the designs and so obtain the best determinant value in each set and let these be $d_1, d_2, \ldots, d_{n20}$,
iv. Set $d_{20} = \max\{d_i\}$; $i = 1, 2, \ldots, n_{20}$
v. Repeat (i) – (iv) at $j = 1, 2, \ldots, t+1$ and thus obtain d_{2k} and d_{2t}; $d_{21} < d_{22} < \ldots < d_{2k} > d_{2k+1}$; $d_{2k+2} < d_{2k+3} < \ldots < d_{2t} > d_{2t+1}$.
vi. Set $d_2^* = \max\{d_{20}, d_{2k}, d_{2t}\}$ and the corresponding design ξ_N^* as the D-optimal design.

S3 Search for H = 3

1. Begin at $j = 0$ with guessed values of a 3-tuple (r_{10}, r_{20}, r_{30}); where r_{10}, r_{20}, r_{30} are respectively the number of support points from balls 1, 2, 3 and $N = r_{10} + r_{20} + r_{30}$; $r_{10}, r_{20}, r_{30} \geq 0$.
2. Holding, for example, r_{10} fixed, perform the S_2 ($H = 2$) search at $j = 0$ between balls 2 and 3 to obtain the maximum determinant value $d_{30(1)}$, showing that this value is obtained at fixed value (r_{10}) of ball 1.
3. Repeat the S_2 search at other values of r_{10}; namely, $r_{10} + 1, r_{10} + 2, \ldots, r_{10} + k + 1, r_{10} - 1, r_{10} - 2, \ldots, r_{10} - t - 1$. Hence, obtain $d_{3k(1)}$ and $d_{3t(1)}$.
4. Define $d_3^* = \max\{d_{30(1)}, d_{3k(1)}, d_{3t(1)}\}$ to be the global value of the determinant of the information matrices and the corresponding ξ_N^* as the D-optimal design.

General case of S_H search

One can infer from the above that the S_H search requires a progressive application of $S_2, S_3, \ldots$.

1. Begin at $j = 0$ with guessed values of the H-tuple, $(r_{10}, r_{20}, ..., r_{H0})$; $N = \sum_{i=1}^{H} r_{i0}, r_{i0} \geq 0$.
2. The first $H-2$ values, *i.e.* $r_{10}, ..., r_{H-2,0}$ are held fixed and an S_2 search is performed on balls $H-1$ and H to obtain $d_{H0(1, 2, ..., H-2)}$.
3. An S_3 search is now performed on the last three balls; namely, $H-2$, $H-1$, and H to obtain $d_{H0(1, 2, ..., H-3)}$.
4. In a similar way an S_4 search, gives a $d_{H0(1, 2, ..., H-4)}$ and so on to S_H that yields d_{H0}.
5. Set $d_{H0} = \max\{d_{H0(1, ..., H-2)}, ..., d_{H0(1)}\}$.
6. Finally, searching at other values of r_{10}; namely at $r_{10}+1$, $r_{10}+2$, ..., $r_{10}+k$, $r_{10}+k+1$, $r_{10}-1$, $r_{10}-2$, ..., $r_{10}-t$, $r_{10}-t-1$,we obtain d_{Hk} and d_{Ht}.
7. Set $d_H^* = \max\{d_{H0}, d_{Hk}, d_{Ht}\}$ and the corresponding ξ_N^* as the D-optimal exact design.

As stated in section 2, theorems 1 and 2 have the effect of reducing the number of determinantal calculations and thus speeding up the rate of convergence of the algorithm. Further increases in the rate of convergence come as a result of the occurrence of singular designs as well as the fact that some r_{ij}*'s* quickly become zero.

Theorem 3. The sequence S_2, S_3, ..., S_H is convergent to the global D-optimal exact design.

Proof: Since the sequence S_3, ..., S_H require progressive repeat of S_2, it is sufficient to prove that S_2 is convergent. The concavity of $\det(M(\xi_N))$; see, *e.g.* Pazman (1986), means that d_{2k} and d_{2t} are respectively the only local maxima in the increasing and decreasing directions of he search. Therefore, d_2^* is a global optimum.

4. A NUMERICAL EXAMPLE

We consider an application of the algorithm to obtain a D-optimal 6-point design for a bivariate quadratic surface defined on the unit cube *i.e.*

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

$$\tilde{X} = \{x_1,\ x_2;\ x_1,\ x_2 = \text{-1, 0, 1}\},\ \sigma_e^2 = 1.$$

The three balls $g_1 = \begin{pmatrix} -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \end{pmatrix}$, $g_2 = \begin{pmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}$, $g_3 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ are of sizes $n_1 = n_2 = 4$, $n_3 = 1$. The combinatorics for this case of $H = 3$ are given in the table hereunder:

TABLE 4.1

An S3 search for 6-point D-optimal design for a quadratic surface defined on a cubic space

Step j	3-tuple			Maximum determinant d_{Hj}	Number of designs at step j	Number of *D*-optimal designs
	n_{1j}	n_{2j}	n_{3j}			
0	3	3	0	1.3717×10^{-3}	16	
1	4	2	0	5.4870×10^{-3}	6	4
2	5	1	0	singular	16	
3	2	4	0	1.3717×10^{-3}	6	
4	1	5	0	singular	16	
5	3	2	1	3.0864×10^{-3}	24	
6	4	1	1	5.4870×10^{-3}	4	all 4
7	5	0	1	singular	4	
8	2	3	1	3.4214×10^{-4}	24	
9	1	4	1	3.4214×10^{-4}	4	

At $j = 0$, for example, the sixteen designs are:

$$\xi_6^{(1)} = \begin{matrix} - & - \\ + & - \\ - & + \\ - & 0 \\ 0 & - \\ + & - \end{matrix}, \quad \xi_6^{(2)} = \begin{matrix} - & - \\ - & + \\ + & + \\ - & 0 \\ 0 & - \\ + & - \end{matrix}, \; \ldots, \; \xi_6^{(4)} = \begin{matrix} + & - \\ - & + \\ + & + \\ - & 0 \\ 0 & - \\ + & 0 \end{matrix}; \quad \xi_6^{(5)} = \begin{matrix} - & - \\ + & - \\ - & + \\ - & 0 \\ 0 & - \\ 0 & + \end{matrix}, \; \ldots, \; \xi_6^{(16)} = \begin{matrix} - & + \\ + & - \\ + & + \\ 0 & - \\ + & 0 \\ 0 & + \end{matrix}$$

The first set of four designs have the corresponding diagonal elements of their information matrices equal, then the next set of four, etc. Now applying theorem 2 on the off-diagonal elements for designs within a set, one can establish the following equalities (inequalities): $(M_3 = M_1) < (M_2 = M_4)$; $(M_7 = M_5) < (M_6 = M_8)$; $(M_{11} = M_{12}) < (M_9 = M_{10})$; $(M_{15} = M_{16}) < (M_{13} = M_{14})$. Comparing between sets, we see that $M_2 = M_9$ and $M_6 = M_{14}$.

Therefore, only two determinant values need be computed. Incidentally, for 3-tuple (3, 2, 1), only one determinant value need be computed because

$$M(\xi_6^{(4)}) = M(\xi_6^{(11)}) = M(\xi_6^{(14)}) = M(\xi_6^{(21)}) = \begin{pmatrix} 6 & 0 & 0 & -1 & 4 & 4 \\ 0 & 4 & -1 & 1 & 0 & 1 \\ 0 & -1 & 4 & 1 & 1 & 0 \\ -1 & 1 & 1 & 3 & -1 & -1 \\ 4 & 0 & 1 & -1 & 4 & 3 \\ 4 & 1 & 0 & -1 & 3 & 4 \end{pmatrix}.$$

The rest are either inferior designs, based on theorem 2, or they are singular designs.

On combinatorial and variance exchange methods

Using the combinatorial technique, it is easy to determine all the designs that are concurrently *D*-optimal. The experimenter can therefore choose one of these designs on the basis of convenience and minimality of cost.

The variance exchange method works well for approximate designs; i.e. when the equivalence between the *G*- and *D*-optimality applies. But for exact designs the method can fail because the equivalence of the *G*- and *D*-optimality criteria no longer applies. On the other hand, the combinatorial technique can be applied to both exact and approximate designs.

The phenomenon of cycling which often occurs in a variance exchange technique; see, Atkinson and Donev (1992), cannot occur in the method of combinatorics.

Department of Statistics IKE BASIL ONUKOGU
University of Nigeria, Nsukka
Enugu State, Nigeria

Department of Mathematics/Statistics MARY PASCAL IWUNDU
University of Port-Harcourt
Rivers State, Nigeria

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SUMMARY

A combinatorial procedure for constructing D-optimal exact designs

The basic problem considered in this paper may be stated as follows: find an *N*-point exact design measure ξ_N which maximizes the determinant of the information matrix of a given response function $f(\underset{\sim}{x})$, where $\underset{\sim}{x}$ is an *n*-component vector of non-stochastic variables defined in a space of trial $\tilde{X}$.

The combinatorial algorithm introduced in the paper reaches the global *D*-optimal design quite rapidly and a comparison against the variance exchange algorithm is indicated.