

## STARTING DESIGN FOR USE IN VARIANCE EXCHANGE ALGORITHMS

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### ABSTRACT

*A new method of constructing the initial design for use in variance exchange algorithms is presented. The method chooses support points to go into the design as measures of distances of the support points from the centre of the geometric region and of permutation-invariant sets. The initial design is as close as possible to the optimal design as measured by the determinant values. A Comparison of the performance of the new method is made with the commonly used random selection method and is found to be comparatively efficient.*

**Key Words:** Initial design, support point distance, permutation-invariant sets, variance exchange.

### INTRODUCTION

Optimal designs are a class of experimental designs that are optimal with respect to some statistical criterion. The optimality of a design depends on the statistical model and is assessed with respect to a statistical criterion which is basically related to the variance-covariance matrix. A series of papers on the subject of optimal design of experiments have been published and vast literature dealing with theoretical and numerical results in the subject of optimal design exist. In particular, Fedorov (1972) contributed immensely to the use of variance exchange algorithm to solve optimal design problems. So many works have been done to improve the working of the variance exchange algorithm and these include of works of Mitchell (1974), Cook and Nachtsheim (1980), Johnson and Nachtsheim (1983), Atkinson and Donev (1992) etc.

Basically, the variance exchange algorithms exchange a point in the initial design having minimum variance of prediction with a point in the design region having maximum variance of prediction. The exchange process continues until when it is no longer possible to do any further exchange that would yield an increase in the determinant value of the information matrix of the associated design measure. Most of the variance exchange algorithms in the literature rely on random selection of the support points that make up the initial N-point design measure. When the design region has a large number of candidate set, the design constructed from the randomly selected points may have determinant value of information matrix that is very inferior to that of the optimal design. Moreover, the process may require many iterations to reach the optimal design.

A combinatorial approach to finding D-optimal exact design was introduced in Onukogu and Iwundu (2008). This algorithm utilizes the concept of grouping the design points according to their distances from the centre of the design region. It has been found in Iwundu and Chigbu (2012) as useful for regular or irregular geometric regions and in the presence or absence of blocking principles. The starting combination of groups, though arbitrarily chosen, seems to take more support points from the group having the maximum distance from the centre of the design region. An attempt has been made by Iwundu (2010) to obtain a near optimal starting point for the combinatorial procedure. We present in this work a new method of obtaining the initial design for use in variance exchange algorithms. The design is formed as a measure of distance of support points from the centre of the design region and permutation-invariance. By permutation-invariant sets we mean that the combinations of support points within each set can all be obtained from one another by permuting the support points (Mitchell and Bayne (1978)). An interesting feature of the initial design obtained using the new technique is that the determinant value of its information matrix is as close as possible to that of the optimal design.

## MATERIALS AND METHODS

Given the triple  $\{\tilde{X}, F_x, \Sigma_x\}$  where  $\tilde{X}$ , the space of trials of the experiment,  $F_x$  is the space of finite dimensional continuous functions defined on  $\tilde{X}$  and  $\Sigma_x$  is the space of a random observation errors defined on  $\tilde{X}$ , we seek a 'good' N-point initial design measure,  $\xi_N^0$ , that will lead to an N-point D-optimal exact design measure,  $\xi_N^*$ , in few iterations. The initial design,  $\xi_N^0$ , is such

that  $\det M(\xi_N^0)$  is as close as possible to  $\det M(\xi_N^*)$ , where  $\det M(\xi_N^*) = \max \{ \det M(\xi_N^i) \}$ ;  $M(\xi_N^i), M(\xi_N^j) \in S^{p \times p}$ ,  $i = 0, 1, 2, 3, \dots$  and  $S^{p \times p}$  is the space of non-singular information matrices defined on  $\tilde{X}$ .

A  $p \times p$  information matrix,  $M(\xi_N)$ , corresponding to the design measure,  $\xi_N$ , is defined as

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

The matrix X is defined by the usual linear model

$$E(Y) = X\beta$$

where,

Y is the  $N \times 1$  vector of observations independently distributed and each with constant variance,  $\sigma^2$ .

$\beta$  is a  $p \times 1$  vector of parameters to be estimated on the basis of the N uncorrelated observations.

The  $N \times p$  design matrix X, sometimes called the "expanded design matrix" depends on the chosen model and the design measure.

Thus, for the p- parameter model

$$y(x_1, x_2) = a_0 + a_1 x_1 + a_2 x_2 + a_{11} x_1^2 + a_{22} x_2^2 + e_i$$

we seek an initial N-point design with p distinct support points,

where,

$$p \leq N \leq \frac{1}{2} p(p+1) + 1.$$

The method selects an initial design that is relatively close to the D-optimal exact designs as measured by the determinant value of the associated information matrix. It requires grouping the support points in the design region according to their distances from the centre of the design region and into permutation-invariant sets. Following Iwundu (2010), let  $\tilde{N}$  be the number of

support points in  $\tilde{X}$ ,  $g_i$  is the group of support points with distance  $d_i$  from the centre of  $\tilde{X}$  where  $i=1,2,\dots,H$  and is such that  $d_1 > d_2 > \dots > d_H$ .

$n_i$  is the number of support points in  $g_i$  where  $n_1 + n_2 + \dots + n_H = \tilde{N}$ .

$S_i$  is the number of permutation-invariant sets in  $g_i$ .

$S_1 + S_2 + \dots + S_H = S$  is the number of permutation-invariant sets in  $\tilde{X}$ .

$p_1$  is the number of parameter associated with the first-order linear part of the quadratic model.

$N_1$  is the minimum number of support points from  $g_1$  required to estimate the  $p_1$  parameters of the first order linear part of the quadratic model.

$$v = N - N_1$$

$t$  is the number of times support points may be repeated.

$S_r$  is the number of permutation-invariant sets in  $g_1$  from where the support points are taken.  $S_1^r$  is the number of permutation-invariant sets in  $g_1$  from which the support points are not taken.

$$S_1^r = S_1 - S_r$$

$$q = S - S_r$$

We assume that the design region is convex and of regular geometry. We further assume that the response function is a quadratic. It is also important to remark that at each iteration, the exchange procedure continues until when there is no improvement in the determinant value of the information matrix of the design. The new rules for constructing an initial design for use in variance exchange algorithms are as follows;

- (i) Take  $N_1 = p_1$  support points from  $S_r$  permutation-invariant sets in  $g_1$ , enough to estimate the  $p_1$  parameters

of the first order linear part of the quadratic model.

- (ii) Set the initial tuple of support points as  $t_0 = \{n_1^0, n_2^0, n_3^0, \dots, n_H^0\}$ , where the number of support points taken from  $g_1, g_2, \dots, g_H$ , are computed respectively as;

$$n_1^0 = \frac{v}{q} \left[ \times S_1^r + \right] N_1$$

$$n_j^0 = \frac{v}{q} \times S_j \quad ; \quad j = 2, 3, \dots, H$$

- (iii) Denote the initial design measure by  $\xi_N^i$ ;  $i=0$ .

To obtain an  $N$ -point  $D$ -optimal exact design, we continue from step (iv) below

- (iv) Obtain the information matrix  $M(\xi_N^i)$  and compute the associated determinant  $d_i = \det(M(\xi_N^i))$ ;

- (v) Compute the variance of prediction,  $V\{\hat{y}(\underline{x})\} = \underline{x}^T M^{-1}(\xi_N^i) \underline{x}$ , at every support point  $\underline{x} \in \tilde{X}$ .

- (vi) Exchange the support point in the design measure having minimum variance of prediction with a point in the design region having maximum variance of prediction.

- (vii) Set  $i = i+1$  and repeat steps (iv) and (v) above.

- (viii) Is  $d_{i+1} < d_i$ ? If YES, go to (ix), if NO, continue from (vi).

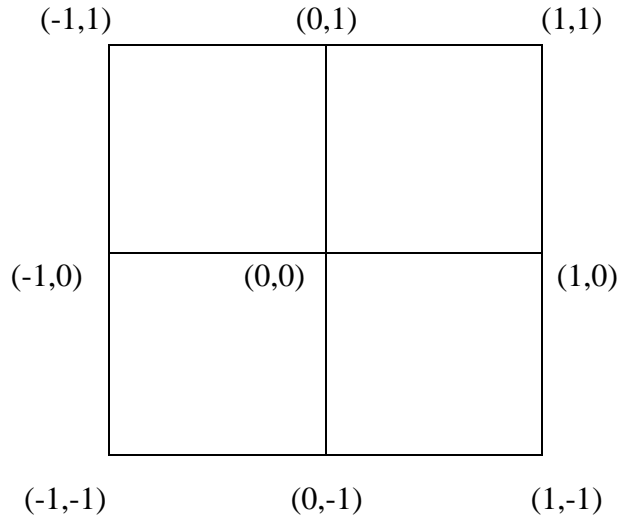
- (ix) Set  $\xi_N^i = \xi_N^{i-1}$  to be the  $N$ -point  $D$ -optimal exact design.

- (x) Stop.

**RESULTS AND DISCUSSION**

Our interest here is to obtain an N-point starting design that is efficient in the construction of an N-point D-optimal exact designs for a bivariate quadratic model

$y(x_1, x_2) = a_0 + a_1x_1 + a_2x_2 + a_{11}x_1^2 + a_{22}x_2^2 + \epsilon_i$  ;  $-1 \leq x_1, x_2 \leq 1$ ; defined on the regular experimental region in the figure below.



**Figure 1: A regular geometric area with support points of  $3^2$  factorial designs.**

Following the method described in section 1.3, we group the support points in the design region as a measure of distance from the centre of  $\hat{X}$  as:

$$g_1 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \end{bmatrix} \quad g_2 = \begin{bmatrix} 1,0 \\ -1,0 \\ 0,1 \\ 0,-1 \end{bmatrix} \quad g_3 = [0,0]$$

We observe that there are three permutation-invariant sets within group  $g_1$ . These permutation-invariant sets are:

$$g_{11} = [1,1] \quad g_{12} = \begin{bmatrix} 1,-1 \\ -1,1 \end{bmatrix} \quad g_{13} = [-1,-1]$$

Similarly, we have two permutation-invariant sets within  $g_2$  namely:

$$g_{21} = \begin{bmatrix} 1,0 \\ 0,1 \end{bmatrix} \quad g_{22} = \begin{bmatrix} -1,0 \\ 0,-1 \end{bmatrix}$$

The permutation-invariant set in  $g_3$  is  $g_{31} = [0,0]$

In other to compute the number of support points taken from  $g_1, g_2$  and  $g_3$  to make up the initial design, we require to evaluate the values of the variables defined in section 1.4. The evaluations yield;

$$S = 6, S_1 = 3, S_2 = 2, S_3 = 1, n_1 = 4, n_2 = 4, n_3 = 1, \tilde{N} = 9, p = 5, p_1 = 3, q = 3, N_1 = 3, S_1^r = 0.$$

For the construction of a 5-point design,

$$v = 2$$

$$n_1^0 = \left( \frac{v}{q} \times S_1^r \right) + N_1 = \left( \frac{2}{3} \times 0 \right) + 3 = 3$$

$$n_2^0 = \frac{v}{q} \times S_2 = \frac{2}{3} \times 2 = 1.333 \cong 1$$

$$n_3^0 = \frac{v}{q} \times S_3 = \frac{2}{3} \times 1 = 0.6666 \cong 1$$

$$\underline{t}_0 = \{ 3 : 1 : 1 \}$$

For the construction of a 6-point design,

$$v = 3$$

$$n_1^0 = \left[ \frac{v}{q} \times S_1^r \right] + N_1 \left[ \frac{3}{3} \times 0 \right] + 3 = 3$$

$$n_2^0 = \frac{v}{q} \times S_2 = \frac{3}{3} \times 2 = 2$$

$$n_3^0 = \frac{v}{q} \times S_3 = \frac{3}{3} \times 1 = 1$$

$$\underline{t}_0 = \{ 3 : 2 : 1 \}$$

For the construction of a 7-point design,

$$v = 4$$

$$n_1^0 = \left[ \frac{v}{q} \times S_1^r \right] + N_1 \left[ \frac{4}{3} \times 0 \right] + 3 = 3$$

$$n_2^0 = \frac{v}{q} \times S_2 = \frac{4}{3} \times 2 = 2.66 \cong 3$$

$$n_3^0 = \frac{v}{q} \times S_3 = \frac{4}{3} \times 1 = 1.33 \cong 1$$

$$\underline{t}_0 = \{ 3 : 3 : 1 \}$$

For the construction of an 8-point design,

$$v = 5$$

$$n_1^0 = \left[ \frac{v}{q} \times S_1^r \right] + N_1 \left[ \frac{5}{3} \times 0 \right] + 3 = 3$$

$$n_2^0 = \frac{v}{q} \times S_2 = \frac{5}{3} \times 2 = 3.33 \cong 3$$

$$n_3^0 = \frac{v}{q} \times S_3 = \frac{5}{3} \times 1 = 1.66 \cong 2$$

$$\underline{t}_0 = \{ 3 : 3 : 2 \}$$

For the construction of a 5-point design,

$$v = 6$$

$$n_1^0 = \left[ \frac{v}{q} \times S_1^r \right] + N_1 \left[ \frac{6}{3} \times 0 \right] + 3 = 3$$

$$n_2^0 = \frac{v}{q} \times S_2 = \frac{6}{3} \times 2 = 4$$

$$n_3^0 = \frac{v}{q} \times S_3 = \frac{6}{3} \times 1 = 2$$

$$\underline{t}_0 = \{ 3 : 4 : 2 \}$$

For  $\bar{N} < N < 2\bar{N}$  each support point in  $\bar{X}$  may be repeated twice. We shall thus treat the permutation-invariant sets within a given group  $g_h$  as multiples of two sets. Hence, the number of permutation-invariant sets in  $g_h$  is assumed equal to  $2S_h$ ;  $h = 1, 2, \dots, H$ .

Setting  $N = 10, 11, \dots, 16$ ,

$$S = 12, S_1 = 6, S_2 = 4, S_3 = 2, S_1^r = 3, S_r = 3, v = N - N_1 \text{ and } q = S - S_r = 9.$$

We compute the initial support points from  $g_{11}, g_{12}$  and  $g_{13}$  respectively as:

For the construction of a 10-point design,

$$v = 7$$

$$n_1^0 = \left[ \frac{v}{q} \times S \right] + N_1 \left[ \frac{7}{9} \times 3 \right] + 3 = 5.3 \cong 5$$

$$n_2^0 = \frac{v}{q} \times S_2 = \frac{7}{9} \times 4 = 3.11 \cong 3$$

$$n_3^0 = \frac{v}{q} \times S_3 = \frac{7}{9} \times 2 = 1.5 \cong 2$$

$$\underline{t}_0 = \{ 5 : 3 : 2 \}$$

For the construction of an 11-point design,

$$v = 8$$

$$n_1^0 = \left[ \frac{v}{q} \times S \right] + N_1 \left[ \frac{8}{9} \times 3 \right] + 3 = 5.66$$

$$n_2^0 = \frac{v}{q} \times S_2 = \frac{8}{9} \times 4 = 3.55$$

$$n_3^0 = \frac{v}{q} \times S_3 = \frac{8}{9} \times 2 = 1.77$$

By approximating 5.66, 3.55 and 1.77 to the nearest whole numbers

$\sum_{i=1}^h n_i^o$  exceeds  $N=11$ . In order to preserve the design size  $N=11$ , we shall

approximate any two of the  $n_{i's}^o$  to the nearest whole number and further consider the integer part of the remaining  $n_i^o$ . Hence, the initial tuple of support points shall be taken to be any of

$$\underline{t}_o = \{ 6 : 3 : 2 \}, \underline{t}_o = \{ 6 : 4 : 1 \} \text{ or } \underline{t}_o = \{ 5 : 4 : 2 \}$$

For the construction of a 12-point design,  
 $v = 9$

$$n_1^o = \left[ \frac{v}{q} \times S_1^r \right] + N_1 \left[ \left( \frac{9}{9} \times 3 \right) \right] + 3 = 6$$

$$n_2^o = \frac{v}{q} \times S_2 = \frac{9}{9} \times 4 = 4$$

$$n_3^o = \frac{v}{q} \times S_3 = \frac{9}{9} \times 2 = 2$$

$$\underline{t}_o = \{ 6 : 4 : 2 \}$$

For the construction of a 13-point design,  
 $v = 10$

$$n_1^o = \left[ \frac{v}{q} \times S_1^r \right] + N_1 \left[ \left( \frac{10}{9} \times 3 \right) \right] + 3 = 6.33$$

$$n_2^o = \frac{v}{q} \times S_2 = \frac{10}{9} \times 4 = 4.44$$

$$n_3^o = \frac{v}{q} \times S_3 = \frac{10}{9} \times 2 = 2.22$$

By approximating 6.33, 4.44 and 2.22 to the nearest whole numbers,  $\sum_{i=1}^n n_i^o = N$  is less than  $N=13$ . We shall however approximate 6.33 to 6, 2.22 to 2 and treat 4.44 as 5 to preserve the design size. Thus, this yields the initial tuple  
 $\underline{t}_o = \{ 6 : 5 : 2 \}$ .

For  $N = 14, v = 11$

$$n_1^o = \left[ \frac{v}{q} \times S_1^r \right] + N_1 \left[ \left( \frac{11}{9} \times 3 \right) \right] + 3 = 6.66 \cong 7$$

$$n_2^o = \frac{v}{q} \times S_2 = \frac{11}{9} \times 4 = 4.88 \cong 5$$

$$n_3^o = \frac{v}{q} \times S_3 = \frac{11}{9} \times 2 = 2.44 \cong 2$$

$$\underline{t}_o = \{ 7 : 5 : 2 \}$$

For the construction of a 15-point design,  
 $v = 12$

$$n_1^o = \left[ \frac{v}{q} \times S_1^r \right] + N_1 \left[ \left( \frac{12}{9} \times 3 \right) \right] + 3 = 7$$

$$n_2^o = \frac{v}{q} \times S_2 = \frac{12}{9} \times 4 = 5.33 \cong 5$$

$$n_3^o = \frac{v}{q} \times S_3 = \frac{12}{9} \times 2 = 2.66 \cong 3$$

$$\underline{t}_o = \{ 7 : 5 : 3 \}$$

For the construction of a 16-point design,  
 $v = 13$

$$n_1^o = \left[ \frac{v}{q} \times S_1^r \right] + N_1 \left[ \left( \frac{13}{9} \times 3 \right) \right] + 3 = 7.33 \cong 7$$

$$n_2^o = \frac{v}{q} \times S_2 = \frac{13}{9} \times 4 = 5.77 \cong 6$$

$$n_3^o = \frac{v}{q} \times S_3 = \frac{13}{9} \times 2 = 2.88 \cong 3$$

$$\underline{t}_o = \{ 7 : 6 : 3 \}$$

The initial design measures for  $N = 5, 6, \dots, 16$  are, respectively,

$$\xi_5^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,-1 \\ 0,1 \\ 0,0 \end{bmatrix}; \xi_6^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,0 \\ 0,-1 \\ 0,0 \end{bmatrix}; \xi_7^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,0 \\ 1,0 \\ 0,1 \\ 0,0 \end{bmatrix}; \xi_8^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,0 \\ 1,0 \\ 0,1 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_9^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,-1 \\ -1,0 \\ 1,0 \\ 0,1 \\ 0,-1 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_{10}^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ 1,1 \\ -1,0 \\ 1,0 \\ 0,-1 \\ 0,0 \\ 0,0 \end{bmatrix}$$

$$= \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ 1,1 \\ -1,0 \\ 1,0 \\ 0,1 \\ -1,0 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_{12}^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ 1,1 \\ -1,-1 \\ -1,0 \\ 1,0 \\ 0,-1 \\ 0,1 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_{13}^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ 1,1 \\ -1,-1 \\ -1,0 \\ 1,0 \\ 0,-1 \\ 0,1 \\ 1,0 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_{14}^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ 1,1 \\ -1,-1 \\ 1,-1 \\ -1,0 \\ 1,0 \\ -1,0 \\ 0,-1 \\ 0,1 \\ 1,0 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_{15}^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ 1,1 \\ -1,-1 \\ 1,-1 \\ 1,0 \\ 1,0 \\ -1,0 \\ 0,-1 \\ 0,1 \\ 0,0 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_{16}^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ 1,1 \\ -1,-1 \\ 1,1 \\ -1,0 \\ 1,0 \\ -1,0 \\ 0,-1 \\ 0,1 \\ 0,0 \\ 0,0 \\ 0,0 \end{bmatrix}$$

With each initial tuple of support points, we commence search for the N-point D-optimal exact design measure,  $\xi_N^*$ . For the purpose of illustration, we consider a case of N=5. The design matrix associated with  $\xi_5^0$  is given as

$$X = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The normalized information matrix is

$$M_0 = \frac{1}{N} X'X = \begin{pmatrix} 1.0 & 0.2 & 0.0 & 0.6 & 0.8 \\ 0.2 & 0.6 & 0.2 & 0.2 & 0.2 \\ 0.0 & 0.2 & 0.8 & -0.2 & 0.0 \end{pmatrix}$$

$$\begin{matrix} 0.6 & 0.2 & -0.2 & 0.6 & 0.6 \\ 0.8 & 0.2 & 0.0 & 0.6 & 0.8 \end{matrix}$$

The associated determinant value is 0.00512. In order to do an exchange of a support point in the design measure with a support point in the candidate set, we require to compute the variance of prediction at each support point in the candidate set as

$$V\{\hat{y}(x_1, x_2)\} = \underline{x}' M^{-1}(\xi_N^i) \underline{x}$$

The variances are;

$$\begin{matrix} V\{\hat{y}(1,1)\} = 5 \\ V\{\hat{y}(0,0)\} = 5 \\ V\{\hat{y}(-1,-1)\} = 5 \\ V\{\hat{y}(-1,1)\} = 15 \\ V\{\hat{y}(1,-1)\} = 5 \end{matrix}$$

$$\begin{aligned} V\{\hat{y}(0, 1)\} &= 5 \\ V\{\hat{y}(1, 0)\} &= 15 \\ V\{\hat{y}(0, -1)\} &= 15 \\ V\{\hat{y}(-1, 0)\} &= 25. \end{aligned}$$

The support points in the design measure  $\xi_5^0$  having the minimum variance of prediction is exchanged with the support point in  $\tilde{X}$  having the maximum variance of prediction. Where there are ties (that is when two or more support points exhibit the characteristic of having the minimum variance of prediction or the maximum variance of prediction), the exchange of the

pair of support points resulting in the maximum determinant of information matrix is used in the exchange algorithm. Since the variance of prediction of every support point in  $\xi_5^0$  is tied at 5, and the support point in  $\tilde{X}$  having maximum variance of prediction is (-1, 0), an exchange that would yield the maximum determinant value of information matrix is made.

Coincidentally, every possible exchange made yields the determinant value 0.00512. Hence, any pair of support points  $\{(1,1), (-1,0)\}$ ,  $\{(0,0), (-1,0)\}$ ,  $\{(0,1), (-1,0)\}$ ,  $\{(1,-1), (-1,0)\}$  and  $\{(-1,-1),(-1,0)\}$  could be used in the exchange.

Using, for instance,  $\{(1,1), (-1,0)\}$  in the exchange results in the new design measure

$$\xi_5^1 = \begin{pmatrix} -1 & 0 \\ 0 & 0 \\ 0 & 1 \\ 1 & -1 \\ -1 & -1 \end{pmatrix}$$

whose determinant values of information matrix is 0.00512. Notice that the exchange made does not improve the determinant value. This implies that the system has converged and the best D-optimal exact design has been reached. At this juncture, we report the D-optimal exact design as:

$$\xi_5^* = \begin{pmatrix} -1 & 0 \\ 1 & 1 \\ 1 & -1 \\ 0 & 1 \\ -1 & 0 \end{pmatrix} \text{ or } \xi_5^* = \begin{pmatrix} -1 & 0 \\ 1 & 1 \\ 1 & -1 \\ -1 & 0 \\ 0 & 0 \end{pmatrix} \text{ or } \xi_5^* = \begin{pmatrix} -1 & 0 \\ 1 & 1 \\ 0 & 1 \\ -1 & 0 \\ 0 & 0 \end{pmatrix}$$

For N= 6,7, ..., 16, the process follows similarly and the system converges only when there is no improvement in the

determinant value of information matrix at the next iteration.

The summary of the search is presented in Table 2 below for N= 5, 6, ..., 16.



**Table 1: Summary of search using Combinatorial Method for selecting the initial design**

Design Size N	Step k	g <sub>1</sub> g <sub>2</sub> g <sub>3</sub>	Determinant Value	Step length
5	0	3 1 1	$5.1200 \times 10^{-3}$	D-optimum reached at step k=0
6	0	3 2 1	$1.2300 \times 10^{-2}$	D-optimum reached at step k=0
7	0	3 3 1	$1.1420 \times 10^{-2}$	D-optimum reached at step k=1
	1	3 3 1	$1.1428 \times 10^{-2}$	
8	0	3 3 2	$9.8000 \times 10^{-3}$	D-optimum reached at step k=1
	1	4 3 1	$1.7558 \times 10^{-2}$	
9	0	3 4 2	$1.5400 \times 10^{-2}$	D-optimum reached at step k=1
	1	4 4 1	$2.1948 \times 10^{-2}$	
10	0	5 3 2	$1.6000 \times 10^{-2}$	D-optimum reached at step k=1
	1	5 4 1	$2.0160 \times 10^{-2}$	
11	0	5 4 2	$1.9370 \times 10^{-2}$	D-optimum reached at step k=0
12	0	6 4 2	$1.9290 \times 10^{-2}$	D-optimum reached at step k=0
13	0	6 5 3	$1.9176 \times 10^{-2}$	D-optimum reached at step k=0
14	0	7 5 2	$1.9516 \times 10^{-2}$	D-optimum reached at step k=0
15	0	7 5 3	$1.8436 \times 10^{-2}$	D-optimum reached at step k=1
	1	7 6 2	$2.0227 \times 10^{-2}$	
16	0	7 6 3	$1.1755 \times 10^{-2}$	D-optimum reached at step k=2
	1	7 6 2	$1.9070 \times 10^{-2}$	
	2	8 6 2	$2.0510 \times 10^{-2}$	

By the usual random selection method for choosing the initial design measure, the following initial designs emerged;

$$\begin{aligned}
 \xi_5^D &= \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,0 \\ 0,1 \\ 0,0 \end{bmatrix}; \xi_6^D = \begin{bmatrix} 1,1 \\ 1,-1 \\ 1,0 \\ -1,0 \\ 0,1 \\ 0,0 \end{bmatrix}; \xi_7^D = \begin{bmatrix} 1,1 \\ -1,-1 \\ -1,1 \\ -1,0 \\ 1,0 \\ 0,1 \\ 0,0 \end{bmatrix}; \xi_8^D = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,0 \\ 1,0 \\ 0,1 \\ 0,-1 \\ 0,0 \end{bmatrix}; \xi_9^D = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,-1 \\ -1,1 \\ 1,0 \\ 0,1 \\ 0,-1 \\ -1,0 \\ 0,0 \end{bmatrix}; \xi_{10}^D = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ 1,-1 \\ -1,0 \\ 1,0 \\ 0,-1 \\ 0,1 \\ 0,0 \end{bmatrix}
 \end{aligned}$$

$$\begin{aligned}
 \xi_{11}^0 &= \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ 1,-1 \\ -1,-1 \\ -1,0 \\ 0,-1 \\ -1,0 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_{12}^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ 1,-1 \\ 1,1 \\ 0,1 \\ 1,0 \\ 1,0 \\ 0,-1 \\ 0,-1 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_{13}^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ 1,0 \\ 0,-1 \\ 1,0 \\ 0,-1 \\ -1,0 \\ 0,1 \\ -1,0 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_{14}^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ -1,-1 \\ 1,0 \\ -1,0 \\ -1,0 \\ 0,-1 \\ 0,0 \\ 0,1 \\ 0,-1 \\ 0,1 \\ 0,1 \\ 0,-1 \\ 0,1 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_{15}^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,1 \\ 1,1 \\ 0,-1 \\ 0,-1 \\ 1,0 \\ 1,0 \\ 0,1 \\ 0,1 \\ -1,0 \\ -1,0 \\ 0,0 \\ 0,0 \\ 0,0 \end{bmatrix}; \xi_{16}^0 = \begin{bmatrix} 1,1 \\ 1,-1 \\ -1,1 \\ -1,-1 \\ 1,1 \\ -1,-1 \\ 1,-1 \\ -1,0 \\ 1,0 \\ -1,0 \\ 0,-1 \\ 0,1 \\ 0,1 \\ 0,-1 \\ 0,-1 \\ 0,1 \\ 0,0 \\ 0,1 \\ -1,-1 \end{bmatrix}
 \end{aligned}$$

The best determinant value was reached at step  $k = 0$  for  $N = 5, 8, 9$  and  $10$ . Similarly at  $k = 1$  for  $N = 6, 7, 13$  and  $14$ . Also at  $k = 2$  for  $N = 11$  and  $12$ .

For  $N = 14$ , the best determinant value was reached at step  $k = 1$

For  $N = 15$ , the best determinant value was reached at step  $k = 3$

For  $N = 16$ , the best determinant value was reached at step  $k = 1$

A new method of selecting the initial design for use in variance exchange algorithm has been presented. The method relied on choosing the initial design as a measure of both the distance of support points from the centre of  $\bar{X}$  and permutation-invariant sets. The number of iterations required to arrive at the D-optimal exact design was reduced to only a few.

It was important to ensure that when choosing the number of support points from the various groups,  $\sum_{i=1}^n n_i^0 = N$ . Where the  $n_{i/s}^0$  were not integer values, approximations to the nearest integer values were suggested. A problem was encountered at  $N=11$  and  $N=13$ . It was necessary to allow such approximations that preserved the design sizes. All possible combinations were explored and the best combination as measured by the determinant value reported as the optimal tuple of support points. Numerical illustrations indicated effectiveness in the performance of the algorithm when compared with the commonly used random selection method.

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