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ON IMPROVED ALGORITHM FOR CYCLING DISCONTINUITY IN A VARIANCE EXCHANGE PROCESS FOR D-OPTIMAL DESIGN

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Abstract

This work seeks to construct a variance exchange algorithm that will disable the influence of cycling, whenever it occurs, in an iterative process. A variance exchange process is one of several iterative techniques employed in the construction of $D-$ optimal Designs. A design is $D-$ optimal if among several other designs, it has the maximum determinant of the information matrices. This happens when the bounded monotone non-decreasing sequence of determinants converge to some limit. A theoretical framework that gives the structure of a variance exchange algorithm was provided and a modification was made to improve on the algorithm by providing a key to breaking cycling. Generated data from two-variable experimental space was analyzed using the improved algorithm, in linear, interactive and quadratic order effects with three different $N-$ point designs. Computations were conducted and the Figures produced in R version 4.1.1 (2021). The results from the study showed that applying the improved algorithm when cycling occurs in an iterative sequence, will discontinue cycling and raise the determinants.

Keywords: Cycling, $D-$ optimality, Variance Exchange, Improved Algorithm, Two-variable Response function.

1. Introduction

Considers, X, a metric space of factor levels

$$X = x_1, x_2, \ldots, x_N, x_{N+1}, \ldots, x_{\tilde{N}}$$

Define $\xi_N^{(1)}$ and $\xi_N^{(1)c}$, the starting and complement designs in a variance exchange process, as

.

$$\xi_N^{(1)} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_N \end{pmatrix}, \ \xi_N^{(1)c} = \begin{pmatrix} \mathbf{x}_{N+1} \\ \mathbf{x}_{N+2} \\ \vdots \\ \mathbf{x}_{\tilde{N}} \end{pmatrix}.$$

The variance exchange process is an iterative improvement process in a search for $D-$ optimal design, which involves exchanging a vector $\mathbf{x}_i$, the point with minimum variance in the design $\xi_N^{(1)}$, with $\mathbf{x}_j$ the point with maximum variance in the complement design $\xi_N^{(1)c}$, often with increase in the determinant of the information matrix. This process continues until a point where the minimum variance in the current design is equal to or greater than the maximum variance in the complement design. When this happens, the iterative process is said to have converged to a $D-$ optimal design (Atkinson, Donev and Tobias (2007)).

However, it is practically almost impossible to achieve a design with this desired optimum in the algorithmic process. This is because at the course of the exchange process, there is a misnomer which leads to either steady or fluctuating determinants resulting to different patterns of convergence. This misnomer is referred to as “cycling” (Ikpan and Nwobi (2021)). This means that certain vector points having obviously low variances are removed from the design at onestage but turn out to have high variances at some other stages, enough to be included back in the design. Such variance points are seen to revolve round a current design at one stage and a complement design at some other stage (Atkinson, et. al. 2007).

In this paper we intend to construct an algorithm to break cycling, when it occurs, in a variance exchange process searching for $D-$ optimum designs.

2. Literature review

Several authors have worked on constructing exact $D-$ optimal design using the variance exchange process. In this paper, we made reference to the works of Wynn (1970), the exchange algorithm (EA) for constructing a converging sequence of discrete (exact) designs; the general EAby Fedorov (1972), for obtaining $D-$ optimal designs; the adjustment of Mitchell and Miller’s (EA) by Van Schalkwyk (1971) by interchanging some of its steps; the DETMAX by Mitchell (1974), generalizing their basic exchange algorithm to permitting excursions; the modification of Fedorov’s EA by Cook and Nachtsheim (1980); the generalization of the Modified Fedorov Exchange Algorithm (MFEA) due to Johnson and Nachtsheim (1983); the KL-EA by Atkinson and Donev (1989), a further modification of the Fedorov’s EA; A Fedorov exchange algorithm for D-optimal design by Miller and Nguyen (1994);the algorithm by Al Labadi (2015), which simultaneously added or exchanged two or more points in a rather new modification of the Fedorov’s EA; and the application of VEA by Ikpan and Nwobi (2021), in addressing the influence of cycling.

Other reference sources are, Foundations of optimal experimental designs byPazman (1986); Optimal experimental designs by Atkinson and Donev (1992); Foundations of Optimal Exploration of Response Surfaces by Onukogu (1997); and Optimum

Experimental Designs, with SAS by Atkinson et al (2007).

3. Theoretical framework

The search strategy is determined by the variance exchange algorithm

(I) From a metric space of factor levels, X, select N support points from the candidate set N, to make up an initial N point design measure, $\xi_N^{(1)}$.

(II) Compute the variances of points in the current and complement design matrices and compare $d\left(\mathbf{x}_w, \xi_N^{(1)c}\right)$ and $d\left(\mathbf{x}_u, \xi_N^{(1)}\right)$, the minimum and maximum variances respectively of the current and complement designs.

$$d\left(\mathbf{x}_u, \xi_N^{(k)}\right) = \underset{\mathbf{x}\in X_N^{(1)}}{\text{Min}}\ \mathbf{x}_i' M^{-1}\left(\xi_N^{(k)}\right)\mathbf{x}_i, \tag{1}$$

$$d\left(\mathbf{x}_w, \xi_N^{(k)}\right) = \underset{\mathbf{x}\in X_N^{(1)c}}{\text{Min}}\ \mathbf{x}_i' M^{-1}\left(\xi_N^{(k)}\right)\mathbf{x}_i, \tag{2}$$

If $d\left(\mathbf{x}_W, \xi_N^{(1)}\right) \le d\left(\mathbf{x}_u, \xi_N^{(1)}\right)$, stop.

If otherwise, exchange the point with minimum variance in $\xi_N^{(1)}$ with the point with maximum variance, from $\xi_N^{(1)c}$, the complement design, and define a new design measure, $\xi_N^{(2)}$.

(III) Repeat step (II) until

$$d\left(\mathbf{x}_W, \xi_N^{(k)c}\right) \le d\left(\mathbf{x}_u, \xi_N^{(k)}\right),$$

The exchange process above, like other algorithms of the exchange type, leads to the greatest increase in the determinant of the information matrix. The algorithm terminates when there is no longer any exchange which would increase the determinant. However, a common challenge of this procedure is that of cycling and therefore does not usually lead to the best exact $D-$ optimum design.When cycling occurs in the sequential process, the value of the determinant of the information matrix stagnates often with the attendant consequence of preventing convergence to $D-$ optimality. To address the effect of cycling and improve on the rate of convergence, an improved algorithm is proposed in the following section.

4. The improved algorithm

The improved algorithm is defined by the following iterative steps

(I) From an experimental space X, a metric space of factor levels, set up a starting design, with measure $\xi_N^{(1)}$, of size $N > p$, where p is the number of parameters of the response function.

$$\mathrm{X} = \mathrm{x}_1, \mathrm{x}_2, \ldots, \mathrm{x}_N, \mathrm{x}_{N+1}, \ldots, \mathrm{x}_{\tilde{N}}$$

.

$$\xi_N^{(1)} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_v \\ \vdots \\ \mathbf{x}_N \end{pmatrix}, \quad \xi_N^{(1)\mathrm{c}} = \begin{pmatrix} \mathbf{x}_{N+1} \\ \mathbf{x}_{N+2} \\ \vdots \\ \mathbf{x}_m \\ \vdots \\ \mathbf{x}_{\widetilde{N}} \end{pmatrix}$$

(II) Calculate the determinant of the resulting Information Matrix, $\det M\left(\xi_N^{(1)}\right)$. Compute also, the variances, $d\left(\mathbf{x}_i, \xi_N^{(1)}\right)$ and $d\left(\mathbf{x}_j, \xi_N^{(1)\mathrm{c}}\right)$ of the $N-$ points in the current design and of the remaining points in the candidate set, the complement design.

Is $d\left(\mathbf{x}_v, \xi_N^{(1)}\right) > d\left(\mathbf{x}_m, \xi_N^{(1)\mathrm{c}}\right)$?,

(i) Yes, Stop

(ii) No, exchange, $\left(\mathbf{x}_v, \xi_N^{(1)}\right)$, the point having minimum variance in the design $X_N^{(1)}$, with $\left(\mathbf{x}_m, \xi_N^{(1)\mathrm{c}}\right)$, the point maximum having variance in the complement design $X_N^{(1)c}$, and define a new design measure, $\xi_N^{(2)}$.

(iii) Compute the Determinant, $\left|M\left(\xi_N^{(2)}\right)\right|$ and notice that $\left|M\left(\xi_N^{(2)}\right)\right| > \left|M\left(\xi_N^{(1)}\right)\right|$.

(III) Repeat steps (II) and (III) until the k^{th} step.

If $\det M\left(\xi_N^{(k)}\right) > \det M\left(\xi_N^{(k-1)}\right)$? and $d\left(\mathbf{x}_w, \xi_N^{(k)c}\right) \leq d\left(\mathbf{x}_v, \xi_N^{(k)}\right)$?

If Yes, Stop.

The process has converged, and the design $\xi_N^{(k)} = \xi_N^{(*)}$, $D-$ optimum.

If no, then $d\left(\mathbf{x}_m, \xi_N^{(k)c}\right) > d\left(\mathbf{x}_v, \xi_N^{(k-1)}\right)$ and $\det M\left(\xi_N^{(k)}\right) \leq \det M\left(\xi_N^{(k-1)}\right)$

Cycling has set in.

(IV) At the point of cycling, replace $\left(\mathbf{x}_{m^*}, \xi_N^{(k)}\right)$, the point having maximum variance in the design $\xi_N^{(k)}$, with $\left(\mathbf{x}_v, \xi_N^{(k)}\right)$, its point having minimum variance, and define a new design measure $\xi_N^{(k+1)}$. Compute the determinant and notice that.

$$\det M\left(\xi_N^{(k+1)}\right) > \det M\left(\xi_N^{(k)}\right).$$

In this way, cycling is broken.

5. Analysis

In this section, we present the computational and graphical forms of analyses of the variance exchange process involving linear, interactive and quadratic effect components in an experimental space of two – variable response function on three different $N-$ point designs; the $9-$, $10-$ and $11-$point designs.

The statistical models for two-variable response function for each of the linear, interactive and quadratic components, are respectively

$$f(x_1,x_2)=a_0+\sum_{i=1}^{2}a_ix_i+e \quad (3)$$

$$f(x_1,x_2)=a_0+\sum_{i=1}^{2}a_ix_i+\sum_{i<j}a_{ij}x_ix_j+e \quad (4)$$

$$f(x_1,x_2)=a_0+\sum_{i=1}^{2}a_ix_i+\sum_{i=1}^{2}a_{ii}x_i^2+\sum_{i<j}\sum a_{ij}x_ix_j+e \quad (5)$$

The experimental space is given as

$\tilde{X}=\{x_1,x_2;x_1=-2,-1,0,1,2,x_2=-1,-0.5,0.5,1\}$, $\text{Var}(e)=\sigma_e^2$

The experimental set, the set of candidate points, for each of the two-variable models (3) – (5), consists of N = 20 vector points. The vector points $\mathbf{x}_i$, for the linear, interactive and quadratic component designs are given as $\mathbf{x}_i=(1,x_1,x_2)$, $\mathbf{x}_i=(1,x_1,x_2,x_1x_2)$, and $\mathbf{x}_i=(1,x_1,x_2,x_1x_2,x_1^2,x_2^2)$, respectively. Computations are conducted and the Figures produced.in R version 4.1.1 (R Core Team (2021))

5.1 linear order effect designs

The initial and complement design matrices for the $N-$point linear component designs are as follows:

.

$$\xi_9^{(1)} = \begin{pmatrix} 1 & -2 & -1 \\ 1 & -2 & -0.5 \\ 1 & -1 & -1 \\ 1 & -1 & 0.5 \\ 1 & 0 & -1 \\ 1 & 1 & -0.5 \\ 1 & 1 & 1 \\ 1 & 2 & 0.5 \\ 1 & 2 & 1 \end{pmatrix}, \xi_9^{(1)c} = \begin{pmatrix} 1 & -2 & 0.5 \\ 1 & -2 & 1 \\ 1 & -1 & -0.5 \\ 1 & -1 & 1 \\ 1 & 0 & -0.5 \\ 1 & 0 & 0.5 \\ 1 & 0 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 0.5 \\ 1 & 2 & -1 \\ 1 & 2 & -0.5 \end{pmatrix}, \xi_{10}^{(1)} = \begin{pmatrix} 1 & -2 & -0.5 \\ 1 & -2 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & 0.5 \\ 1 & 0 & -1 \\ 1 & 0 & -0.5 \\ 1 & 1 & 0.5 \\ 1 & 1 & 1 \\ 1 & 2 & -1 \\ 1 & 2 & 1 \end{pmatrix}, \xi_{10}^{(1)c} = \begin{pmatrix} 1 & -2 & -1 \\ 1 & -2 & 0.5 \\ 1 & -1 & -0.5 \\ 1 & -1 & 1 \\ 1 & 0 & 0.5 \\ 1 & 0 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & -0.5 \\ 1 & 2 & -0.5 \\ 1 & 2 & 0.5 \end{pmatrix}$$

$$\xi_{11}^{(1)} = \begin{pmatrix} 1 & -2 & -1 \\ 1 & -2 & -0.5 \\ 1 & -2 & 0.5 \\ 1 & -2 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & -0.5 \\ 1 & -1 & 0.5 \\ 1 & -1 & 1 \\ 1 & 0 & -1 \\ 1 & 0 & -0.5 \\ 1 & 0 & 0.5 \end{pmatrix}, \quad \xi_{11}^{(1)c} = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & -0.5 \\ 1 & 1 & 0.5 \\ 1 & 1 & -1 \\ 1 & 1 & -0.5 \\ 1 & 2 & -1 \\ 1 & 2 & -0.5 \\ 1 & 2 & 0.5 \\ 1 & 2 & 1 \end{pmatrix}$$

The successive determinants of the k^{th} iterative steps of the different $N-$point linear order effect designs are given in Table 1

Table 1: Summary table of k successive determinants of the linear component, two-variable N – point designs.

$\xi_N^{(k)}$	$\left\|M\left(\xi_9^{(k)}\right)\right\|$	$\left\|M\left(\xi_{10}^{(k)}\right)\right\|$	$\left\|M\left(\xi_{11}^{(k)}\right)\right\|$
1	887.75	1090	474
2	1116	1461	1203
3	1392.75	1774.5	1974

4	1608	2100.5	2501
5	1806	2349	2926
6	1806	2352	3204
7		2349	3204

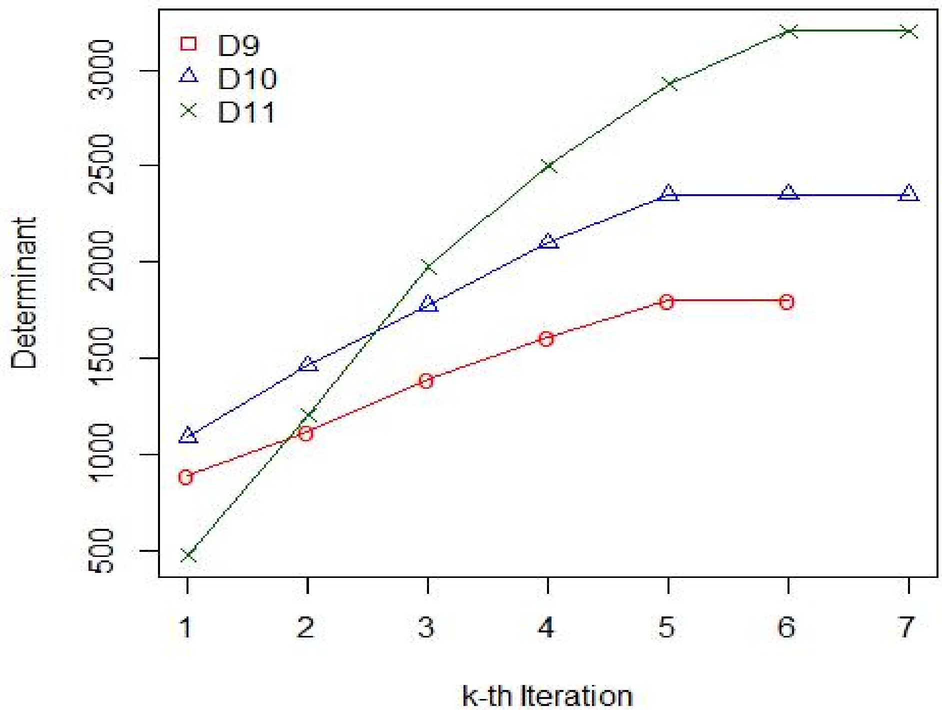

Figure 1:Influence of cycling on the determinant in linear component, N – point designs.

5.2 Interactive order effect designs

The initial and complement design measures for the $N-$point interactive order effect designs are

$$\xi_9^{(1)} = \begin{pmatrix} 1 & -2 & -1 & 2 \\ 1 & -2 & -0.5 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 0.5 & -0.5 \\ 1 & 0 & -1 & 0 \\ 1 & 1 & -0.5 & -0.5 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & 0.5 & 1 \\ 1 & 2 & 1 & 2 \end{pmatrix}, \quad \xi_9^{(1)c} = \begin{pmatrix} 1 & -2 & 0.5 & -1 \\ 1 & -2 & 1 & -2 \\ 1 & -1 & -0.5 & 0.5 \\ 1 & -1 & 1 & -1 \\ 1 & 0 & -0.5 & 0 \\ 1 & 0 & 0.5 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 0.5 & 0.5 \\ 1 & 2 & -1 & -2 \\ 1 & 2 & -0.5 & -1 \end{pmatrix}$$

$$\xi_{11}^{(1)} = \begin{pmatrix} 1 & -2 & -1 & 2 \\ 1 & -2 & -0.5 & 1 \\ 1 & -1 & -0.5 & 0.5 \\ 1 & -1 & 0.5 & -0.5 \\ 1 & -1 & 1 & -1 \\ 1 & 0 & -1 & 0 \\ 1 & 0 & 0.5 & 0 \\ 1 & 1 & -0.5 & -0.5 \\ 1 & 1 & 0.5 & 0.5 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & -1 & -2 \end{pmatrix}, \quad \xi_{11}^{(1)c} = \begin{pmatrix} 1 & -2 & 0.5 & -1 \\ 1 & -2 & 1 & -2 \\ 1 & -1 & -1 & 1 \\ 1 & 0 & -0.5 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & -1 & -1 \\ 1 & 2 & -0.5 & -1 \\ 1 & 2 & 0.5 & 1 \\ 1 & 2 & 1 & 2 \end{pmatrix}$$

$$\xi_{10}^{(1)} = \begin{pmatrix} 1 & -2 & -1 & 2 \\ 1 & -2 & 0.5 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & -0.5 & 0.5 \\ 1 & 0 & -0.5 & 0 \\ 1 & 0 & 0.5 & 0 \\ 1 & 1 & -0.5 & -0.5 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & -1 & -2 \\ 1 & 2 & 0.5 & 1 \end{pmatrix}, \quad \xi_{10}^{(1)c} = \begin{pmatrix} 1 & -2 & -0.5 & 2 \\ 1 & -2 & 1 & -2 \\ 1 & -1 & 0.5 & -0.5 \\ 1 & -1 & 1 & -1 \\ 1 & 0 & -1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 0.5 & 0.5 \\ 1 & 2 & -0.5 & -1 \\ 1 & 2 & 1 & 2 \end{pmatrix}$$

The successive determinants of the k^{th} iterative steps of the different $N-$ point interactive order effect designs are given in Table 2

Table 2: Summary table of k successive determinants of the interactive component, two-variable N – point designs

$\xi_N^{(k)}$	$\left\|M\left(\xi_9^{(k)}\right)\right\|$	$\left\|M\left(\xi_{10}^{(k)}\right)\right\|$	$\left\|M\left(\xi_{11}^{(k)}\right)\right\|$
1	4258.50	10471.00	10435.50
2	11976.50	23228.25	22698.00
3	27102.87	37962.00	42623.13
4	32814.00	44381.25	49428.00

5	36000.00	50544.00	57011.62
6	36972.00	50400.00	63063.00
7	36972.00		68688.00
8			68688.00

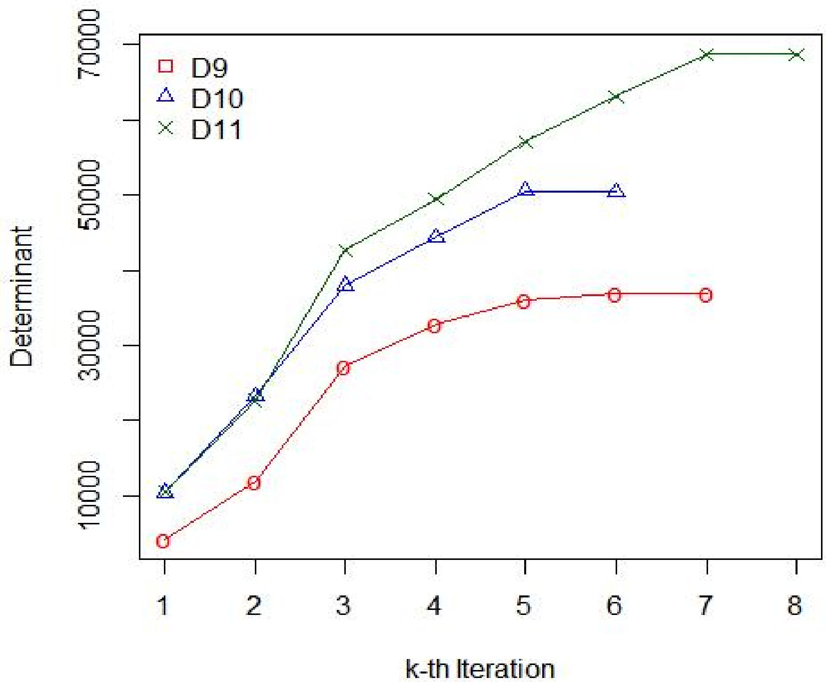

Figure 2: Influence of cycling on determinants in interactive component, N – point designs.

5.3 Quadratic order effects designs

The initial and complement design matrices for the $N-$point quadratic order effect designs are as follows.

.

$$\xi_9^{(1)} = \begin{pmatrix} 1 & -2 & -1 & 2 & 4 & 1 \\ 1 & -2 & -0.5 & 1 & 4 & 0.25 \\ 1 & -2 & -1 & 1 & 1 & 1 \\ 1 & 0 & -0.5 & 0 & 0 & 0.25 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & -0.5 & -0.5 & 1 & 0.25 \\ 1 & 1 & 0.5 & 0.5 & 1 & 0.25 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 1 & 2 & 4 & 1 \end{pmatrix}, \quad \xi_9^{(1)c} = \begin{pmatrix} 1 & -2 & 0.5 & -1 & 4 & 0.25 \\ 1 & -2 & 1 & -2 & 4 & 1 \\ 1 & -1 & -0.5 & 0.5 & 1 & 0.25 \\ 1 & -1 & 0.5 & -0.5 & 1 & 0.25 \\ 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 0 & -1 & 0 & 0 & 1 \\ 1 & 0 & 0.5 & 0 & 0 & 0.25 \\ 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 2 & -1 & -2 & 4 & 1 \\ 1 & 2 & -0.5 & -1 & 4 & 0.25 \\ 1 & 2 & 0.5 & 1 & 4 & 0.25 \end{pmatrix}$$

$$\xi_{10}^{(1)} = \begin{pmatrix} 1 & -2 & -1 & 2 & 4 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -0.5 & 0.5 & 1 & 0.25 \\ 1 & 0 & -1 & 0 & 0 & 1 \\ 1 & 0 & -0.5 & 0 & 0 & 0.25 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & -0.5 & -0.5 & 1 & 0.25 \\ 1 & 1 & 0.5 & 0.5 & 1 & 0.25 \\ 1 & 2 & -1 & -2 & 4 & 1 \\ 1 & 2 & 0.5 & 1 & 4 & 0.25 \end{pmatrix}, \quad \xi_{10}^{(1)c} = \begin{pmatrix} 1 & -2 & -0.5 & 2 & 4 & 0.25 \\ 1 & -2 & 0.5 & -1 & 4 & 0.25 \\ 1 & -2 & 1 & -2 & 4 & 1 \\ 1 & -1 & 0.5 & 0.5 & 1 & 0.25 \\ 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 0 & 0.5 & 0 & 0 & 0.25 \\ 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & -0.5 & -1 & 1 & 0.25 \\ 1 & 2 & 1 & 2 & 4 & 1 \end{pmatrix}$$

$$\xi_{11}^{(1)} = \begin{pmatrix} 1 & -2 & -1 & 2 & 4 & 1 \\ 1 & -2 & -0.5 & 1 & 4 & 0.25 \\ 1 & -1 & -0.5 & 0.5 & 1 & 0.25 \\ 1 & -1 & 0.5 & -0.5 & 1 & 0.25 \\ 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 0 & -1 & 0 & 0 & 1 \\ 1 & 0 & 0.5 & 0 & 0 & 0.25 \\ 1 & 1 & -0.5 & -0.5 & 1 & 0.25 \\ 1 & 1 & 0.5 & 0.5 & 1 & 0.25 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & -1 & -2 & 4 & 1 \end{pmatrix} \quad \xi_{11}^{(1)c} = \begin{pmatrix} 1 & -2 & 0.5 & -1 & 4 & 0.25 \\ 1 & -2 & 1 & -2 & 4 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 0 & -0.5 & 0 & 0 & 0.25 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 2 & -0.5 & -1 & 4 & 0.25 \\ 1 & 2 & 0.5 & 1 & 4 & 0.25 \\ 1 & 2 & 1 & 2 & 4 & 0.25 \end{pmatrix}$$

The successive determinants of the k^{th} iterative steps of the different $N-$point quadratic order effect designs are given in Table 3

Table 3: Summary Table of k successive determinants of the quadratic component, two-variable N – point designs

$\xi_N^{(k)}$	$\left\|M\left(\xi_9^{(k)}\right)\right\|$	$\left\|M\left(\xi_{10}^{(k)}\right)\right\|$	$\left\|M\left(\xi_{11}^{(k)}\right)\right\|$
1	119749.5	53230.5	254229.8
2	380515.5	441414.6	643248.0
3	755712.0	910818.0	1472981.0
4	823680.0	1329552.0	1827636.0
5	787392.0	1521792.0	2033151.0
6		1475712.0	1992587.0

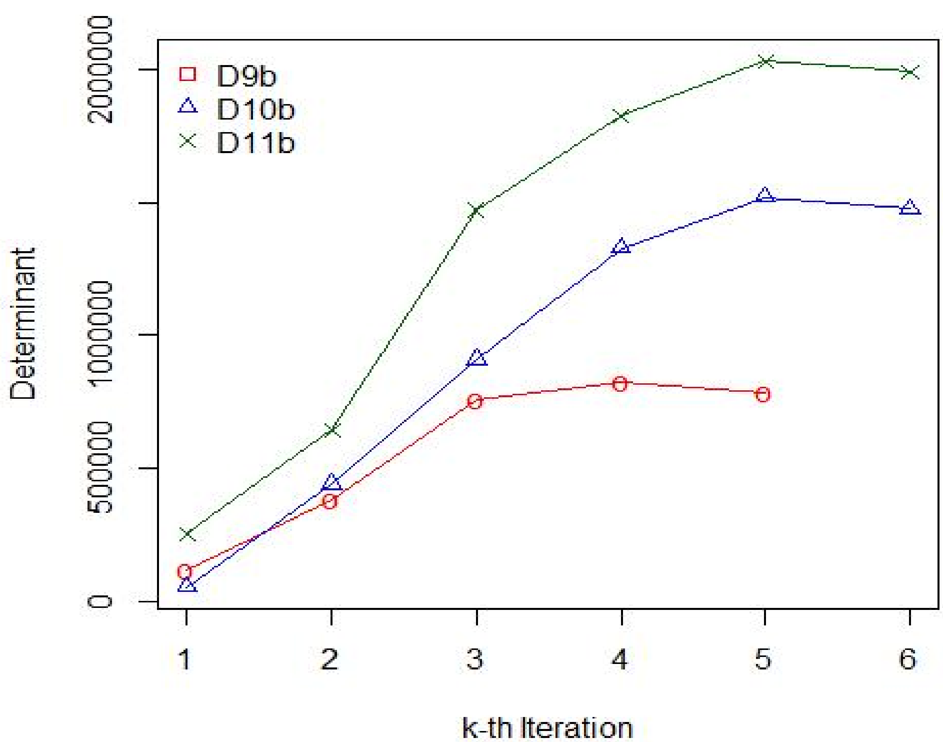

Figure 3: Influence of cycling on the determinants in quadratic component, N – point designs.

5.4 Influence of improved algorithm on cycling

Tables (1) – (3), give the values of the determinants for the $k-$iterations in each of the two-variable $9-$, $10-$ and $11-$point designs in linear, mixed and quadratic components up to the points of cycling. In this section, we apply the improved algorithm on the $(k+1)$th iteration in the different $N-$ point designs.

5.4.1 Linear order effect

The $(k+1)^{\text{th}}$ iteration for the $N-$point linear order effect designs are as follows

$$\xi_9^{(k+1)} = \begin{pmatrix} 1 & -2 & -1 \\ 1 & -2 & -0.5 \\ 1 & -2 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & 2 & -1 \\ 1 & 2 & -1 \\ 1 & 2 & -0.5 \\ 1 & 2 & 1 \end{pmatrix}, \quad \xi_{10}^{(k+1)} = \begin{pmatrix} 1 & -2 & -1 \\ 1 & -2 & 0.5 \\ 1 & -2 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & 2 & -1 \\ 1 & 2 & 0.5 \\ 1 & 2 & 1 \\ 1 & 2 & 1 \end{pmatrix}, \quad \xi_{11}^{(k+1)} = \begin{pmatrix} 1 & -2 & -1 \\ 1 & -2 & -0.5 \\ 1 & -2 & 0.5 \\ 1 & -2 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 2 & -1 \\ 1 & 2 & -0.5 \\ 1 & 2 & 0.5 \\ 1 & 2 & 1 \\ 1 & 2 & 1 \end{pmatrix}$$

The effects of the improved algorithm on rising determinants for the different $N-$point linear order effect designs are given in Table 4

Table 4: Rise in determinants on application of the improved algorithm in the linear order effect designs.

$\xi_N^{(k)}$	$\left\|M\left(\xi_9^{(k)}\right)\right\|$	$\left\|M\left(\xi_{10}^{(k)}\right)\right\|$	$\left\|M\left(\xi_{11}^{(k)}\right)\right\|$
1	887.75	1090.0	474
2	1116.00	1461.0	1203
3	1392.75	1774.5	1974
4	1608.00	2100.5	2501
5	1806.00	2349.0	2926
6	1806.00	2352.9	3204
7	-	2349.5	3204

$\xi_N^{(k+1)}$	1959.00	2587.5	3262

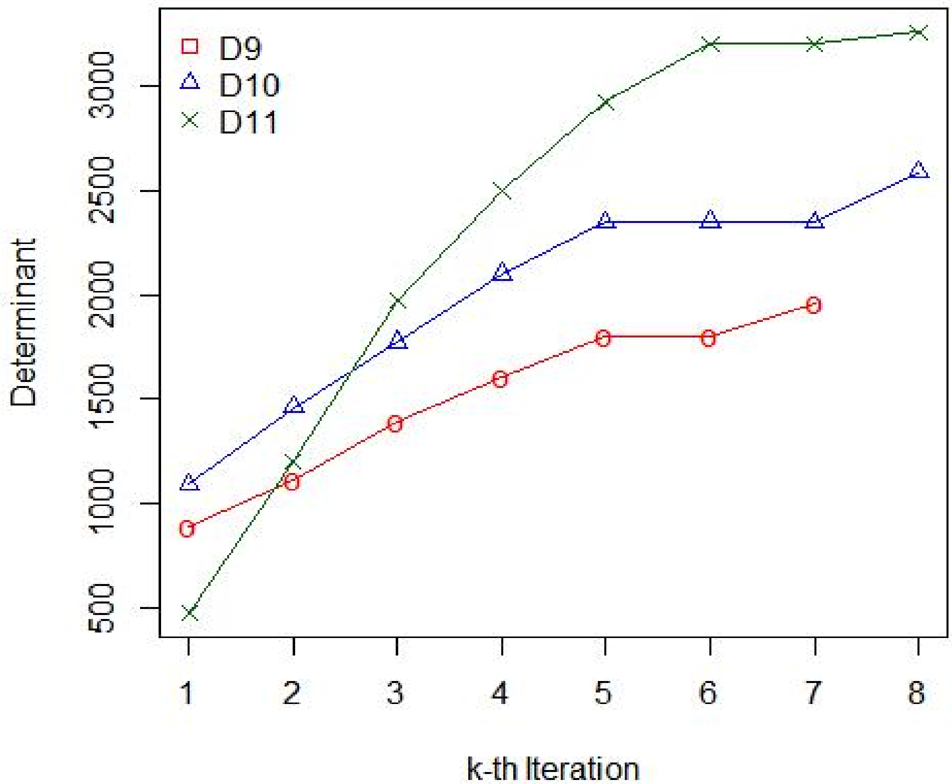

Figure 4: Impact of the improved algorithm on breaking cycling in linear component designs

5.4.2 Interactive order effect

The $(k+1)^{\text{th}}$ iteration for the $N-$point interactive order effect designs are as follows

.

$$\xi_9^{(k+1)} = \begin{pmatrix} 1 & -2 & -1 & 2 \\ 1 & -2 & -1 & 2 \\ 1 & -2 & 0.5 & -1 \\ 1 & -2 & 1 & -2 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & -1 & -2 \\ 1 & 2 & -0.5 & -1 \\ 1 & 2 & 1 & 2 \end{pmatrix}, \quad \xi_{10}^{(k+1)} = \begin{pmatrix} 1 & -2 & -1 & 2 \\ 1 & -2 & 0.5 & -1 \\ 1 & -2 & 1 & -2 \\ 1 & -2 & 1 & -2 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & -1 & -2 \\ 1 & 2 & 0.5 & 1 \\ 1 & 2 & & 2 \end{pmatrix}, \quad \xi_{11}^{(k+1)} = \begin{pmatrix} 1 & -2 & -1 & 2 \\ 1 & -2 & 0.5 & -1 \\ 1 & -2 & 1 & -2 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & 2 & -1 & -2 \\ 1 & 2 & -0.5 & -1 \\ 1 & 2 & 0.5 & 1 \\ 1 & 2 & 1 & 2 \\ 1 & 2 & 1 & 2 \end{pmatrix}$$

The effects of the improved algorithm on rising determinants for the different $N-$ point interactive order effect designs are given in Table 5

Table 5: Rise in determinants on application of the improved algorithm in the interactive order effect designs.

$\xi_N^{(k)}$	$\left\|M\left(\xi_9^{(k)}\right)\right\|$	$\left\|M\left(\xi_{10}^{(k)}\right)\right\|$	$\left\|M\left(\xi_{11}^{(k)}\right)\right\|$
1	4258.50	10471.00	10435.50
2	11976.50	23228.25	22698.00
3	2710.87	37962.00	42623.13
4	32814.00	44381.25	49428.00
5	36000.00	50544.00	57011.62
6	36972.00	50400.00	63063.00
7	36972.00		68688.00
8			68688.00
$\xi_N^{(k+1)}$	44148.00	60363.00	82044.00

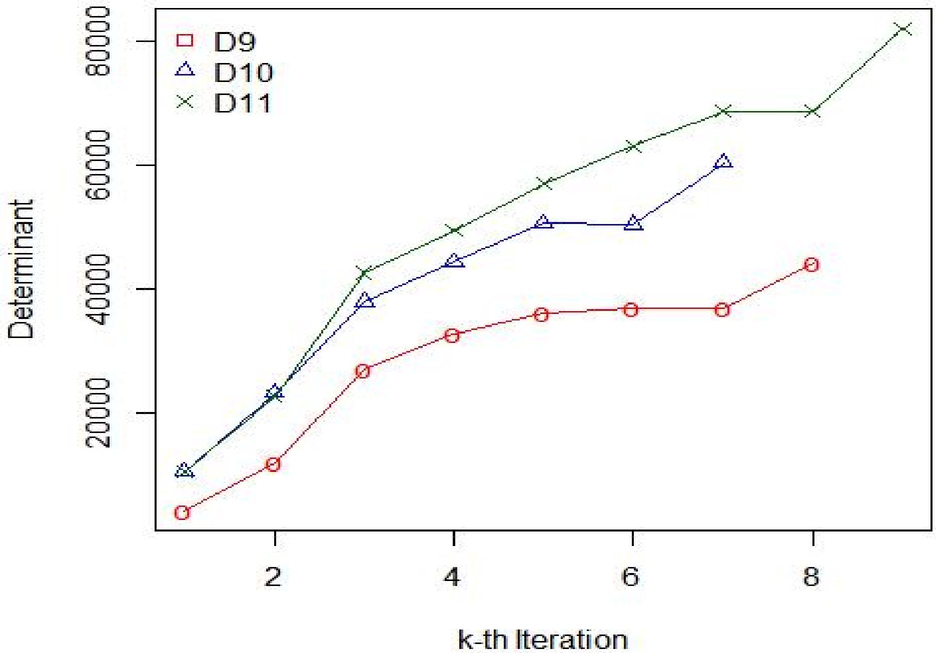

Figure5: Impact of the improved algorithm on breaking cycling in interactive order effect designs

5.4.3 Quadratic order effect

The $(k+1)^{\text{th}}$ iteration for the $N-$point quadratic order effect designs are as follows

$$X_9^{(k+1)} = \begin{pmatrix} 1 & -2 & -1 & 2 & 4 & 1 \\ 1 & -2 & -1 & 2 & 4 & 1 \\ 1 & -2 & 0.5 & -1 & 4 & 0.25 \\ 1 & -2 & 1 & -2 & 4 & 1 \\ 1 & 0 & -0.5 & 0 & 0 & 0.25 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 2 & -1 & -2 & 4 & 1 \\ 1 & 2 & 0.5 & 1 & 4 & 0.25 \\ 1 & 2 & 1 & 2 & 4 & 1 \end{pmatrix}, \quad X_{10}^{(k+1)} = \begin{pmatrix} 1 & -2 & -1 & 2 & 4 & 1 \\ 1 & -2 & -0.5 & 1 & 4 & 0.25 \\ 1 & -2 & 0.5 & -2 & 4 & 0.25 \\ 1 & -2 & 1 & -2 & 4 & 1 \\ 1 & 0 & -0.5 & 0 & 0 & 0.25 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 2 & -1 & -2 & 4 & 1 \\ 1 & 2 & -0.5 & -1 & 4 & 0.25 \\ 1 & 2 & 1 & 2 & 4 & 1 \\ 1 & 2 & 1 & 2 & 4 & 1 \end{pmatrix},$$

.

$$\xi_{11}^{(k+1)} = \begin{pmatrix} 1 & -2 & -1 & 2 & 4 & 1 \\ 1 & -2 & -0.5 & 1 & 4 & 0.25 \\ 1 & -2 & 0.5 & -1 & 4 & 0.25 \\ 1 & -2 & 1 & -2 & 4 & 1 \\ 1 & -2 & 1 & -1 & 1 & 1 \\ 1 & 0 & -1 & 0 & 0 & 1 \\ 1 & 1 & 0.5 & 0.5 & 1 & 0.25 \\ 1 & 2 & -1 & -2 & 4 & 1 \\ 1 & 2 & -0.5 & -1 & 4 & 0.25 \\ 1 & 2 & 1 & 2 & 4 & 1 \\ 1 & 2 & 1 & 2 & 4 & 1 \end{pmatrix}$$

The effects of the improved algorithm on rising determinantsfor the different $N-$point quadratic order effect designs are given in Table 6

Table 6: Rise in determinants on application of the improved algorithm on the quadratic order effect designs.

$\xi_N^{(k)}$	$\left\|M\left(\xi_9^{(k)}\right)\right\|$	$\left\|M\left(\xi_{10}^{(k)}\right)\right\|$	$\left\|M\left(\xi_{11}^{(k)}\right)\right\|$
1	119749.5	53230.5	254229.8
2	380515.5	441414.6	643248.0
3	755712.0	910818.0	1472981.0
4	823680.0	1329552.0	1827636.0
5	787392.0	1521792.0	2033151.0
6		1475712.0	1992587.0
$\xi_N^{(k+1)}$	882432	1533312.0	2416492.0

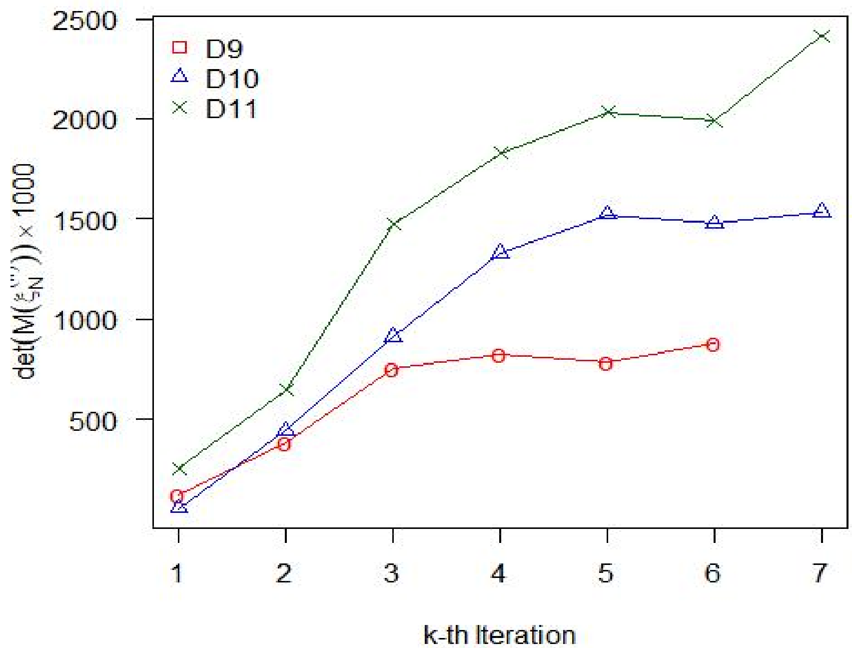

Figure 6: Impact of improved algorithm on breaking cycling in quadratic order effect designs

6. Discussion

In this work, we considered constructing an improved algorithm to eliminate cycling, when it occurs, in a variance exchange process searching for a D-optimal design. The structure of a variance exchange algorithm was given from which an improved version was built upon. The improved algorithm was subjected to test by conducting analysis with data generated using two-variable response function in linear, interactive and quadratic order effect designs.

The results of Tables 1 – 3 and of Figures1 – 3, show that the determinants of the information matrices for all the two-variable $9-$, $10-$ and $11-$point designs stagnate at the k^{th} step. That is,

$$\left|M\left(\xi_N^{(k)}\right)\right| \leq \left|M\left(\xi_N^{(k-1)}\right)\right|.$$

Also, the results of Tables 4 – 6 and Figures.4 – 6, indicate that all the determinants of the information matrices for the two-variable $9-$, $10-$ and $11-$ point designs at the $\left(k+1\right)^{\text{th}}$ step, are greater than the $(k-1)^{\text{th}}$ step when the improved algorithm was employed. That is,

$$\left|M\left(\xi_N^{(k+1)}\right)\right| > \left|M\left(\xi_N^{(k)}\right)\right|.$$

7. Conclusion

We have demonstrated in this paper that whichever the design, whether it is of linear, interactive, or quadratic order effect, applying the improved algorithm will break cycling and improve upon the determinants of the information matrices of the designs. The effect of breaking cycling will help to increase the rate of convergence of the design to the desired D-optimum. We recommend the use of the improved algorithm when cycling presents impediments to the rate of convergence in an iterative search for D-optimality.

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