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The modified balanced confounded design algorithm for constructing n-point d-optimal global designs

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Abstract
The Balanced Confounded Design Algorithm (BCDA) for constructing N-point D-optimal designs was used in constructing a 3^2, 2 x 3^2 and a 2^4 N-point D-optimal response surface designs. When the results were inspected, it was observed that in all, the global optimum could be located faster if all or more support points from G_1 are taken. Hence, a modification of the BCDA is proposed. The result of this work has shown that the Modified Balanced Confounded Design Algorithm (MBCDA) is superior in efficiency to the traditional BCDA.

Keywords: Balanced Designs, D-optimal, Global optimum, Symmetric and Asymmetric designs, Iterations

1. Introduction

It has been established that of all the N-point possible designs for both Symmetric and Asymmetric response surface designs that could be obtained by the Balanced Confounded Designs Algorithm (BCDA) for constructing N-point D-optimal designs proposed by (Umoren and Isaac, 2010) [4], the balanced confounded designs are indeed D-optimal. Thus, the search for D-optimal designs was to be restricted only to the class of balanced designs. However, we know that the aim of all iterative search procedures like the Variance Exchange Algorithm (Atkinson and Donev, 1992) [1], the Steepest Ascent Method (Pazman, 1986) [2], the Combinatorial Procedure (Onukogu and Iwundu, 2008) [3] and the most recent procedure, the Balanced Confounded Designs Algorithm (Umoren and Isaac, 2010) [4], is to locate the global optimum (best design) within the shortest possible moves or iterations in order to save cost, time and computer space and not just to locate an optimal design. This means that though a design may be balanced and hence, D-optimal, yet it may not be the best design (global optimum) among its class of designs. The BCDA though proved to be superior in efficiency to the Combinatorial Procedure, yet, did not take cognisance of which group of support points that should be taken while searching for global optimum so that the global optimum could be located within the shortest possible moves or iterations. This work which is indeed a modification of the Balanced Confounded Designs Algorithm, will take care of this drawback in order to ensure that the number of moves or iterations required to reach the global optimum (best design) is further reduced to the barest minimum.

2. Symmetric and Asymmetric Designs

Symmetric design is the design in which the factors $\{A, B, C......N\}$ appear at the same level. For example, 3^3 design. In this type of design, factor A appear at 3 levels $\{-, 0, +\}$, factor B appear at 3 levels $\{-, 0, +\}$ and factor C appear at 3 levels $\{-, 0, +\}$. On the other hand, Asymmetric design is the design in which the factors $\{A, B, C......N\}$ have different levels. Examples of such designs include $2x3^2$, 2^2x3^2, $2x3x5$ etc;

2.1 Algorithm for Constructing N-Point D-Optimal Designs

We will like to give a review of the Combinatorial Procedure as well as the Balance

Confounded Design Algorithm for constructing N –Point D-optimal designs.

2.1.1 The algorithm of the Combinatorial Procedure for Constructing N-Point D-Optimal Designs.

This procedure is as follows;

[Step1]: Group the support points according to the number of minus and plus $\{-+\}$ and zeros $\{0\}$ and number them as $G_1, G_2, G_3 \ldots G_k$

[Step 2]: Partition each group $G_i, i = 1, 2, 3 \ldots k$ into subgroups as $g_{i0}, g_{i1}, g_{i2} \ldots g_{ir}$ and $g_{k0}, g_{k1}, g_{k2} \ldots g_{kr}$ where the sub-groups are being referred to as sub-design measures.

[Step3]: Choose N number of support points that would go into the class. Let V_j be defined as a vector of points consisting of n_{11} selected from G_1, n_{22} selected from G_2 and n_{rr} selected from G_k where n_{11} is the number of support points from G_1 that will make the N number of support points and so on. For example, if N = 20, and we define a class of design as $V_{20}^{(1)} = 7:6:6:1$, this means that, take 7, 6, 6, and 1 support point from G_1, G_2, G_3 and G_4 respectively.

[Step4]: Using combination mathematics, determine the number of designs from that class and label them as $\xi_1^{(v_j)}, \xi_2^{(v_j)}, \xi_3^{(v_j)} \ldots\ldots \xi_n^{(v_j)}$

[Step5]: Obtain the information matrix $X'_{\xi_1^{(v_j)}} X_{\xi_1^{(v_j)}}$ for each of the design and compute its determinant as $d^*_{\xi_1^{(v_j)}}$. Similarly, obtain $d^*_{\xi_2^{(v_j)}}, d^*_{\xi_3^{(v_j)}} \ldots d^*_{\xi_n^{(v_j)}}$.

[Step6]: Define another vector of points for N and carry out [Step4] and [Step5] above.

[Step7]: Tabulate your result above as follows;

Table 1: Table for the Combinatorial Procedure for Constructing N-point D-Optimal Designs

Class (s)	Group	Class Size (s_j)	Max Det Value	Global Optimum

2.1.2 Balanced Confounded Design Algorithm for Constructing N-Point D-Optimal Designs.

[Step1]: Group the support points according to the number of minus and plus $\{-+\}$ and zeros $\{0\}$ and number them as $G_1, G_2, G_3 \ldots G_k$

[Step 2]: Partition each group $G_i, i = 1, 2, 3 \ldots k$ into subgroups as $g_{i0}, g_{i1}, g_{i2} \ldots g_{ir}$ and $g_{k0}, g_{k1}, g_{k2} \ldots g_{kr}$ where the sub-groups are being referred to as sub- design measures.

[Step3]: Choose N number of support points that would go into the class. Let V_j be defined as a vector of points consisting of n_{11} selected from G_1, n_{22} selected from G_2 and n_{rr} selected from G_k where n_{11} is the number of support points from G_1 that will make the N number of support points and so on. For example, if N = 20, and we define a class of design as $V_{20}^{(1)} = 7:6:6:1$, this means that, take 7, 6, 6, and 1 support point from G_1, G_2, G_3 and G_4 respectively.

[Step4]: Using combination mathematics, determine the number of designs from that class and label them as $\xi_1^{(v_j)}, \xi_2^{(v_j)}, \xi_3^{(v_j)} \ldots\ldots \xi_n^{(v_j)}$ without splitting the sub-design measures since they are already balanced.

[Step5]: Obtain the information matrix $X'_{\xi_1^{(v_j)}} X_{\xi_1^{(v_j)}}$ for each of the design and compute its determinant as $d^*_{\xi_1^{(v_j)}}$. Similarly, obtain $d^*_{\xi_2^{(v_j)}}, d^*_{\xi_3^{(v_j)}} \ldots d^*_{\xi_n^{(v_j)}}$ and test each design whether it is balanced or unbalanced. A design is tested for balance by calculating their loss of information L.I (See Umoren and Isaac, 2010) [4]

[Step6]: Tabulate your result as balanced and unbalanced designs.

[Step7] Define another vector of points for N and carry out [Step4] and [Step5] above.

The table of this Algorithm is given thus;

Table 2: Table for Balanced Confounded Designs Algorithm

Class (s)	Group	Class Size (s_j)	No of Balanced Designs	Max Det for Balanced Designs	No of Unbalanced Designs	Max Det for Unbalanced Designs

2.2 Numerical Illustration of the Combinatorial Procedure and the Balanced Confounded Design Algorithm for Constructing N-Point D-Optimal Designs.

Given the experimental area $\tilde{X} = \{x_1 = -,+; x_2 = -,0,+\}$. The support points are grouped as follows;

$$G_1: \begin{pmatrix} - - \\ \hline - + \\ + - \\ \hline + + \end{pmatrix} \begin{matrix} g_{10} \\ g_{11} \\ \\ g_{12} \end{matrix} \qquad G_2: \begin{pmatrix} -0 \\ \hline +0 \end{pmatrix} \begin{matrix} g_{20} \\ g_{21} \end{matrix}$$

$[S_1]$: Define a vector of points, V_j such as $V_5^{(1)} = 4:1$.

$$P = a_{00}x_0 + a_{10}x_1 + a_{20}x_2 + a_{12}x_1x_2 + a_{22}x_2^2 + \varepsilon$$

$[S_2]$: The possible designs using the Combinatorial Procedure will be 4 since the search sweeps through all possible combinations and the sub design measures are splits. They are;

$$\xi_1^{(5)} = \begin{pmatrix} g_{10} \\ g_{11} \\ g_{20} \\ g_{21} \end{pmatrix}; \quad \xi_2^{(5)} = \begin{pmatrix} g_{11} \\ -+ \\ ++ \\ g_{20} \\ g_{21} \end{pmatrix}; \quad \xi_3^{(5)} = \begin{pmatrix} g_{10} \\ +- \\ ++ \\ g_{20} \\ g_{21} \end{pmatrix}; \quad \xi_4^{(5)} = \begin{pmatrix} g_{11} \\ g_{12} \\ g_{20} \\ g_{21} \end{pmatrix}$$

For the Balanced Confounded Design Algorithm, the possible designs will be 2 since the sub-design measures are not split and they are;

$$\xi_1^{(5)} = \begin{pmatrix} g_{10} \\ g_{11} \\ g_{20} \\ g_{21} \end{pmatrix} \qquad \xi_2^{(5)} = \begin{pmatrix} g_{11} \\ g_{12} \\ g_{20} \\ g_{21} \end{pmatrix}$$

$[S_3]$: We obtain the information matrix ($X'_{\xi_n^{(5)}} X_{\xi_n^{(5)}}$) for each of the designs as follows;

$$X_{\xi_1^{(5)}} = \begin{pmatrix} x_0 & x_1 & x_2 & x_1x_2 & x_2^2 \\ 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{pmatrix}$$

and

$$X'_{\xi_1^{(5)}} X_{\xi_1^{(5)}} = \begin{pmatrix} x_0 & x_1 & x_2 & x_1x_2 & x_2^2 \\ 5 & -1 & -1 & -1 & 3 \\ & 5 & -1 & -1 & -1 \\ & & 3 & -1 & -1 \\ & & & 3 & -1 \\ & & & & 3 \end{pmatrix}$$

$[S_4]$: Compute $d_1^* = \dfrac{\det(X'_{\xi_1^{(5)}} X_{\xi_1^{(5)}})}{N^P}$; where N = Number of support points and P = number of the parameters in the designs.

Hence we have; $d_1^* = 2.048x10^{-2}$; $d_2^* = 8.182x10^2$

$[S_5]$: Define another vector of points, V_j such as $V_5^{(1)} = 3:2$ and carry out $[S_2]$;$[S_3]$ and $[S_4]$ above. Their determinants are given as follows; $d_1^* = 2.048x10^{-2}$; $d_2^* = 2.048x10^{-2}$; $d_3^* = 2.048x10^{-2}$ and $d_4^* = 2.048x10^{-2}$

$[S_6]$: Tabulate the result thus;

Table 3: Table for the result of Constructing N-point D-Optimal Designs using the Combinatorial Procedure

Class (s)	**Group**	**Class Size** (s_j)	**Max Det Value**	**Global Optimum**
1	3:2	4	$2.048x10^{-2}$	
2	4:1	4	$8.182x10^{2}$	$8.182x10^{2}$
Total		8		

Table 4: Table for the result of Constructing N-point D-Optimal Balanced Designs using the BCD Algorithm

Class (s)	**Group**	**Class Size** (s_j)	**No of Balanced Designs**	**Max Det for Balanced Designs**	**No of Unbalanced Designs**	**Max Det for Unbalanced Design**
1	3:2	2	2	$2.048x10^{-2}$	-	-
2	4:1	2	2	$8.182x10^{2}$	-	-
Total		4				

The results from table 2.1 and 2.2 above showed that for the Combinatorial Procedure, it took 8 moves or iterations to locate the global optimum whereas, using the BCDA, only 4 moves were used in locating the global optimum. More so, the BCDA showed that the global optimum was among the balanced designs. It was therefore concluded that the BCDA was superior in efficiency when compared with the Combinatorial Procedure, thus, the search for global designs was to be restricted to the class of balanced design using the BCDA..

3. Exploration with the Balanced Confounded Design Algorithm

Since it has been established that the Balanced Confounded Design Algorithm (BCDA) is superior in efficiency to the Combinatorial Procedure, we thus work with the BCDA for both the symmetric and the asymmetric designs using the examples of Umoren and Isaac, 2010 [4].

3.1 Exploration with the 3^K Series (Symmetric design)

Given

$$f(x_1x_2) = a_{00}x_0 + a_{10}x_1 + a_{20}x_2 + a_{12}x_1x_2 + a_{11}x_1^2 + a_{22}x_2^2 + \varepsilon$$

to be the experimental model for the 3^K series, for 3^2 designs, the support points are grouped as;

$$G_1: \begin{pmatrix} -- \\ \hline -+ \\ +- \\ \hline ++ \end{pmatrix} \begin{matrix} g_{10} \\ g_{11} \\ \\ g_{12} \end{matrix} \qquad G_2: \begin{pmatrix} -0 \\ 0- \\ \hline +0 \\ 0+ \end{pmatrix} \begin{matrix} g_{20} \\ \\ g_{21} \end{matrix} \qquad G_3: \begin{pmatrix} 00 \end{pmatrix} g_{30}$$

A tabulation of the result of the analysis for a 7 point, 3^2 response surface design is given as

Table 5: Table of the result for constructing 7-point D-Optimal Designs for 3^2 Response surface designs using BCD algorithm

Class (s)	**Group**	**Class Size** (s_j)	**No of Balanced Designs**	**Max Det for Balanced Designs**	**No of Unbalanced Designs**	**Max Det for Unbalanced Design**
1	3:4:0	2	2	$3.26x10^{-3}$	-	-
2	4:2:1	2	2	$8.155x10^{-3}$	-	-
Total		4	4			

3.2 Exploration with the Mixed Series (Asymmetric design)

Given

$f(x_1, x_2, x_3) = a_{00}x_0 + a_{10}x_1 + a_{20}x_2 + a_{30}x_2 + a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3 + a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^3 + \varepsilon$

Given $\tilde{X} = \{x_1 = -,+; x_2 = -,0,+; x_3 = -,0,+\}$ to be the experimental region, the support points are grouped as;

$$G_1 = \begin{pmatrix} - - - \\ \hline - - + \\ - + - \\ + - - \\ \hline + + - \\ + - + \\ - + + \\ \hline + + + \end{pmatrix} \begin{matrix} g_{10} \\ g_{11} \\ g_{12} \\ g_{13} \end{matrix} \qquad G_2 = \begin{pmatrix} - - 0 \\ - 0 - \\ \hline - + 0 \\ - 0 + \\ \hline + 0 - \\ + - 0 \\ \hline + 0 + \\ + + 0 \end{pmatrix} \begin{matrix} g_{20} \\ g_{21} \\ g_{22} \\ g_{33} \end{matrix} \qquad G_3 = \begin{pmatrix} - 0 0 \\ + 0 0 \end{pmatrix} \begin{matrix} g_{30} \\ g_{31} \end{matrix}$$

A tabulation of the result of the analysis is given in the table below;

Table 6: Table for the Result of Constructing 13-Point D-Optimal Designs for 2 X 3^2 Response Surface Design Using Bcda

Class (s)	Group	Class Size (s_j)	No of Balanced Designs	Max Det for Balanced Designs	No of Unbalanced Designs	Max Det for Unbalanced Design
1	7:6:0	6	4	$2.88x10^{-3}$	2	$2.66x10^{-3}$
	7:4:2	12	4	$3.32x10^{-3}$	8	$2.66x10^{-3}$
2	8:4:1	12	4	$5.78x10^{-3}$	8	$4.26x10^{-3}$
Total		30	12		18	

3.3 Exploration with 2^k series:

Let $f(x_1, x_2, x_3) = a_{00}x_0 + a_{10}x_1 + a_{20}x_2 + a_{30}x_2 + a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3 + a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^3 + \varepsilon$

Give $\tilde{X} = \{x_1, x_2, x_3, x_4 = -,+\}$ to be the experimental region, the support points are grouped as;

$$G_1 = \begin{pmatrix} - - - - \\ \hline - - - + \\ - - + - \\ - + - - \\ + - - - \\ \hline - - + + \\ - + - + \\ - + + - \\ + - - + \\ + - + - \\ + + - - \\ \hline + + + - \\ + + - + \\ + - + + \\ - + + + \\ \hline + + + + \end{pmatrix} \begin{matrix} g_{10} \\ g_{11} \\ g_{12} \\ g_{13} \\ g_{14} \end{matrix}$$

A tabulation of the result for balanced and unbalanced designs for a 12-point designs for a 2^4 response surface design is given in the table below;

Table 7: Table for the Result of Constructing 12-Point, D-Optimal Balanced and Unbalanced Designs for 2^4 Response Surface Design Using BCDA

Class (s)	Group	Class Size (s_j)	No of Balanced Designs	Max Det For Balanced Designs	No of Unbalanced Designs	Max Det For Unbalanced Design
1	12	2	2	$1.8x10^{-1}$	-	-

4. Proposed Modification

From Table 3.1, Table 3.2 and Table 3.3, remove 2 columns, that is, the columns for Unbalanced Designs and Max determinant for Unbalanced Designs respectively since the global design does not come from the unbalanced set.. In its place, add a column for Global Optimum, the result are summarized in the tables below;

Table 8: Showing Summary for Constructing 7-Point D-Optimal Designs for 3^2 Response Surface Designs Using the Modified Table

Class (s)	Group	Class Size (s_j)	No of Balanced Designs	Max Det For Balanced Designs	Global Optimum
1	3:4:0	2	2	$3.26x10^{-3}$	
2	4:2:1	2	2	$8.155x10^{-3}$	$8.155x10^{-3}$
Total		4	4		

Table 9: Showing Summary for the Constructing of 13-Point D-Optimal Balanced Designs for 2 X 3^2 Response Surface Designs Using the Modified Table.

Class (s)	Group	Class Size (s_j)	No of Balanced Designs	Max Det For Balanced Designs	Global Optimum
1	7:6:0	6	4	$2.88x10^{-3}$	
	7:4:2	12	4	$3.32x10^{-3}$	
2	8:4:1	12	4	$5.78x10^{-3}$	$5.78x10^{-3}$
Total		30	12		

Table 10: Showing Summary for Constructing 12-Point, D-Optimal Designs for 2^4 Response Surface Design Using the Modified Table

Class (s)	Group	Class Size (s_j)	No of Balanced Designs	Max Det For Balanced Designs	Global Optimum
1	12	2	2	$1.8x10^{-1}$	$1.8x10^{-1}$

5. Findings

A careful examination of table 4.1 shows that in Constructing a 7-point D-Optimal Designs for 3^2 response surface designs using the Balanced Confounded Design Algorithm, the Global optimum is found in the set of balanced designs in which all the support points from G_1 were taken. If we restrict the search for the global optimum to the class of designs in which all the support points from G_1 are taken, it will take only 2 iterations or moves as against 4 iterations to locate the global optimum. Again, from table 4.2, it could also be observed that in Constructing a 13-point D-Optimal Balanced Designs for 2 x 3^2 response surface design using the Balanced Confounded Design Algorithm, the global optimum is found in the set of balanced designs in which all the support points from G_1 were taken. If we restrict the search for the global optimum to the class of designs in which all the support points from G_1 are taken, it will take only 12 moves or iterations as against 30 moves which the Balanced Confounded Design Algorithm used before locating the global optimum. Finally, in Constructing a 12-point D-Optimal Designs for 2^4 response surface design using the Balanced Confounded Design Algorithm; the global optimum is found in the set of balanced designs in which all the support points came from G_1. In this case, 2 moves are required to reach the global optimum, the same number of moves the Balanced Confounded Design Algorithm used.

6. Conclusion

We have shown that in constructing a 3^2, 2 x 3^2 and a 2^4 N-point D-optimal response surface designs using the Balanced Confounded Design Algorithm (BCDA), it will take fewer moves or iterations to locate the global optimum if we restrict the search for global optimum to the class of designs in which all or more support points from G_1 are taken as against the traditional Balanced Confounded Design Algorithm (BCDA). This algorithm is called the Modified Balanced Confounded Design Algorithm (MBCDA). The result of this work has shown that the Modified Balanced Confounded Design Algorithm (MBCDA) is superior in efficiency to the Balanced Confounded Design Algorithm (BCDA) because in Constructing a 7-point D-Optimal Designs for 3^2 response surface designs, by using the BCDA, it will take 4 moves to locate the global optimum whereas by using the MBCDA, it will take only 2 iterations or moves to locate the global optimum. Again, in Constructing a 13-point D-Optimal Balanced Designs for 2 x 3^2 response surface design, if the MBCDA is used, the global optimum will be reached after only 12 moves or iterations as against 30 moves if the Balanced Confounded Design Algorithm is used. Finally, in Constructing a 12-point D-Optimal Designs for 2^4 response surface design, by using the MBCDA,, the global optimum is found after just 2 moves, the same number of moves the BCDA will take.

7. References

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