A Systematic Approach for the Construction of Definitive Screening Designs

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Abstract: Definitive screening (DS) designs, first proposed by Jones & Nachtsheim (2011), have received much attention due to its good design properties and run-size economy. This paper investigates the structure of three-level DS designs and suggests a theoretically-driven approach to construct DS designs for any number of run size. This construction method is computational efficient and universal to designs with even or odd number of factors. Many constructed DS designs possess high (if not optimal) D-efficiencies, which are comparable to those found in the literature.

Key words and phrases: Definitive Screening (DS) Designs, Conference Matrix, Circulant Matrix, D-optimal

1. Introduction

There is considerable scope for reducing resources used in research by designing more efficient studies. Experiments are increasingly complex, in addition to rising experimental cost and competing resources. Careful design considerations even with only minor variation in traditional designs can lead to a more efficient study in terms of more precise estimate or able to estimate more effects in the study at the same cost.

Traditionally, resolution III and IV two-level fractional factorial designs have been widely used for early-stage screening experimentation (Box & Hunter , 1961). However, resolution III designs fail to disentangle the confounding between main effects and two-factor interactions, while similar situations exist in resolution IV designs in a pair of two-factor interactions (Phoa, Wong & Xu , 2009). A nonregular design has the ability to disentangle the partial aliased structure, but it is not simple to construct and analyze (Phoa, Xu & Wong , 2009). Quaternary-code designs (Phoa & Xu , 2009; Phoa , 2012) possess similar structure to regular designs, but its structure-based analysis is still under investigation.

In addition to confounding, two-level designs have no capability for capturing curvature due to pure-quadratic effects, and it leads to the pioneered work of a new class of three-level screening designs called definitive screening (DS) designs (Jones & Nachtsheim , 2011). In essence, DS designs are 3-level designs for studying m quantitative factors with the following desired properties: (1) The number of required runs is $N = 2m + 1$, i.e., it is saturated for estimating the intercept, m main effects and m quadratic effects; (2) All main effects are orthogonal to other main effects, all quadratic effects and all two-factor interactions.

Stylianou (2011) and Xiao, Lin & Bai (2012) pointed out that the DS designs can be constructed by stacking a positive and a negative C, plus a row of zeros as the center points. C is generally known as a conference matrix of order m, which is an $m \times m$ matrix satisfying: (1) the diagonal entries of C vanish, while its off-diagonal entries lie in $\{-1, 1\}$; (2) $C'C = (m-1)I$, where I is the $m \times m$ identity matrix. The conference matrix is only available for even m. Nguyen & Stylianou (2012) connected the conference matrix to incomplete block designs and they proposed a general algorithm to construct an $m \times m$ $(0, \pm 1)$-matrix with zero diagonal. This method shrinked the searching space and it was certainly faster than the computerized enumeration in Jones & Nachtsheim (2011). However, it is still a purely computerized search without structural information.

In this paper, we propose a systematic approach to construct the $m \times m$ $(0, \pm 1)$-matrix with zero diagonal, or simply called C matrix in the paper, and its corresponding DS design. Section 2 gives the notations and definitions that are used in the paper. The general structure of C is also given in this section. Section 3 states the theoretical properties of the components in the structure of C. There, theorems describe the criteria on how the C matrix is generated and the D-efficiency of the corresponding DS designs is discussed. Section 4 compares the DS designs generated in this paper to the best DS designs found in the literature. Section 5 is the discussion and conclusion. All proofs are given in the Appendix.

2. Notations, Definitions and Structure

Let m be the number of factors. For a simplified presentation, set $m = 2n + 2$ for even m and $2n + 1$ for odd m. Before we define the structure of the C matrix, two additional matrices, T and S, need to be introduced. T can be obtained cyclically via a generator vector $\vec{t}$ as follows. Given $\vec{t} = (0, t_2, \ldots, t_n)'$, a lower-triangular matrix T_l can be expressed as

$$T_l = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ t_2 & 0 & 0 & \cdots & 0 & 0 \\ t_3 & t_2 & 0 & \cdots & 0 & 0 \\ t_4 & t_3 & t_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ t_n & t_{n-1} & t_{n-2} & \cdots & t_2 & 0 \end{pmatrix},$$

and $T = T_l + T_l'\delta$, where T_l' is the transpose of T and $\delta = 1$ when n is even and $\delta = -1$ when n is odd. Similarly, S can also be obtained cyclicly via a generator vector $\vec{s}$ as follows.

Given $\vec{s} = (s_1, \ldots, s_n)'$, S can be expressed as

$$S = \begin{pmatrix} s_1 & s_2 & s_3 & \cdots & s_{n-1} & s_n \\ s_2 & s_3 & s_4 & \cdots & s_n & s_1 \\ s_3 & s_4 & s_5 & \cdots & s_1 & s_2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ s_n & s_1 & s_2 & \cdots & s_{n-2} & s_{n-1} \end{pmatrix}.$$

The C matrix can be written in the following structure:

$$C = \begin{pmatrix} 0 & \delta & \vec{\delta}' & \vec{\delta}' \\ 1 & 0 & \vec{\delta}' & -\vec{\delta}' \\ \vec{1} & \vec{1} & T & S\delta \\ \vec{1} & -\vec{1} & S & -T\delta \end{pmatrix}; \text{when } m \text{ is even;}$$

and

$$C = \begin{pmatrix} 0 & -\vec{\delta} & -\vec{\delta} \\ \vec{1} & T & S\delta \\ -\vec{1} & S & -T\delta \end{pmatrix}; \text{when } m \text{ is odd,}$$

where $\vec{1}$ and $\vec{\delta}$ are column vectors of length n that all entries of $\vec{1}$ and $\vec{\delta}$ are 1 and δ respectively. The design matrix D for the DS designs can be constructed as

$$D = \begin{pmatrix} C \\ -C \\ \vec{0}' \end{pmatrix}$$

where $\vec{0}$ is a column vector of length m that all entries are 0 and C is $m \times m$ $(0, \pm 1)$-matrix with zero diagonal. Ideally C is a conference matrix. For m even, an $m \times m$ matrix C is a conference matrix if it satisfies $C'C = (m-1)I_{m \times m}$, with $C_{ii} = 0$ and $C_{ij} \in \{-1, 1\}$ for $i \neq j$, $i, j = 1, 2, \ldots, m$.

We denote D_o as a hypothetical D-optimal design of order m. For a fair comparison with DS designs in the literature, we adapt the D-efficiency criterion defined in Jones & Nachtsheim (2011).

$$d_e(D, D_o) = \left(\frac{|X(D)'X(D)|}{|X(D_o)'X(D_o)|} \right)^{1/p}$$

where $X(D)$ and $X(D_o)$ are the design matrices of designs D and D_o respectively, $|M|$ is the determinant of a matrix M, p is the number of terms in the model which consists of the intercept term and all linear effects.

3. Main Theorems

Some lemmas about the properties of T and S are stated for the convenience in explainations and notations in the theorems.

Lemma 1. S is back-circulant and symmetric.

The back-circulant property of S is obvious from its structure, which implies that the sums of columns and rows of S are all equal (i.e., symmetry property), and we denote $s = \sum_{i=1}^{n} s_i$. In addition, it is well-known that a back-circulant matrix is always symmetric.

Lemma 2. For $t_i = t_{n+2-i}\delta$ in $\vec{t}$, (a) T is back-circulant and symmetric when n is even, and (b) T is back-circulant and anti-symmetric when n is odd.

The symmetric property of T is obvious from its definition and it implies $T = T'$. When $t_i = t_{n+2-i}$, $\vec{t} = (0, t_2, t_3, \ldots, t_{(n-1)/2}, t_{n/2}, t_{(n-1)/2}, \ldots, t_3, t_2)$ if n is odd, and $\vec{t} = (0, t_2, t_3, \ldots, t_{n/2-1}, -t_{n/2-1}, \ldots, -t_3, -t_2)$ if n is even. T is circulant no matter which $\vec{t}$ is used as the generator. The circulant property implies that the sums of columns and rows of T are all equal, and we denote $t = \sum_{i=1}^{n} t_i$.

The following theorem states the criteria on $\vec{s}$ and $\vec{t}$ for C being a conference matrix with even number of factors.

Theorem 1. Given $\vec{s}$ and $\vec{t}$ as the generators of S and T and m is even. If the following condition holds:

1. $t_i = t_{n+2-i}$ in $\vec{t}$;
2. $(s, t) = (0, -1)$ for even n or $(1, 0)$ for odd n;
3. $\sum_i (s_i s_{(i \bmod n)+k} + t_i t_{(i \bmod n)+k}) = -2$ for all integers $k < \frac{n+1}{2}$,

then C is a $(2n+2) \times (2n+2)$ conference matrix.

The next theorem states how efficient a design D is when it is constructed via the conference matrix C in Theorem 1.

Theorem 2. Consider $D = (C, -C, \vec{0})'$, where C is the $(2n+2) \times (2n+2)$ conference matrix in Theorem 1. Then the D-efficiency of D is optimal and $d_e(D, D_0) = (\frac{2n+1}{2n+2})^{\frac{2n+2}{2n+3}}$.

Notice that D-optimal matrix does not exist when a conference matrix structure is assumed. It is mainly because of the existence of zero entries in each column of C. If D-optimal matrix exists, all entries have to be $+1$ or -1 (because $0 \times 0 = 0$ not 1). In this sense, such design is two-level with no zero entry. To justify the case of next best possible D-efficiency, adding more zero entries in each column of C reduces the value of determinant of $C'C$, so a fewer number of zero entries maximizes the determinant. Therefore, the best case is to add only one zero in each column of C. An example on the uses of Theorems 1 and 2 to construct DS designs with even m is illustrated below.

Example 1. Consider a construction of DS designs with $m = 12$, i.e., a 25×12 matrix. An example of this kind is given as D, the formula (1) in Xiao, Lin & Bai (2012). For

$m = 12$, $n = 5$. In order to fulfill conditions (1) - (3) in Theorem 1, only two combinations are possible:

$$\vec{t} = (0, 1, 1, -1, -1) \text{ and } \vec{s} = c(1, 1, -1, 1, -1)$$

or

$$\vec{t} = (0, 1, -1, 1, -1) \text{ and } \vec{s} = c(1, 1, 1, -1, -1).$$

If we choose the first combination, then

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

and $D = (C, -C, \vec{0}_{12})'$, where $\vec{0}_{12}$ is a vector of length 12 that all entries are zeros and C is a 12×12 conference matrix. According to Theorem 2, D is a DS design with D-efficiency 92.2823%, which is optimal and equivalent to those in Jones & Nachtsheim (2011), Xiao, Lin & Bai (2012) and Nguyen & Stylianou (2012).

If the second coombination is chosen instead, a different 12×12 matrix C is resulted due to different T and S matrices. However, C is still a conference matrix and thus the resulting DS design has the optimal D-efficiency.

Although the conference matrices do not exist when number of columns is odd, the next theorem describes the property of $C'C$ where C is constructed in a specific structure proposed in the previous section.

Theorem 3. Given $\vec{s}$ and $\vec{t}$ as the generators of S and T and m is odd. If all three conditions stated in Theorem 1 hold, then $C'C$ has the following structure:

$$C'C = \begin{pmatrix} 2n & -\vec{1}' & -\vec{1}' \\ -\vec{1} & A & 1_{n\times n} \\ -\vec{1} & 1_{n\times n} & A \end{pmatrix},$$

where $\vec{1}$ is a vector of length n that all entries are 1, $1_{n\times n}$ is a $n \times n$ matrix that all entries are 1, and A is a $n \times n$ matrix such that the diagonal entries of A are $2n$ and the off-diagonal entries of A are -1.

Let $\{a_i\}$ be a sequence of length $n+1$, $\{o_i\}$ be sequences of length n, and $\{b_i\}$ be sequences of length $2n+1$. Their initial values are taken as follows: $a_0 = b_0 = 2n$,

$a_1 = b_1 = 2n - (1/2n)$ and $o_1 = 1 - (1/2n)$. For $i = 2, \dots, n+1$, the elements in the sequences are defined

$$a_i = (2n+1)(2 - \frac{2n+1}{a_{i-1}})$$
$$o_i = o_{i-1}\frac{2n+1}{a_{i-1}}$$
$$b_i = b_{i-1} - \frac{o_i^2 a_{i-1}}{(2n+1)^2}$$

For $i = n+2, \dots, 2n$,

$$b_i = (2n+1)(2 - \frac{2n+1}{b_{i-1}})$$

The next theorem states the D-efficiency of a design D constructed from C in Theorem 3.

Theorem 4. Consider $D = (C, -C, \vec{0})'$, where C is the $(2n+1) \times (2n+1)$ matrix in Theorem 3. Then the D efficiency of D is $(\frac{|C'C|}{(2n)^{2n+1}})^{\frac{1}{2n+2}}$, where $|C'C|$ is the determinant of $C'C$ and it equals to $\prod_{i=0}^{2n} a_i I(i \leq n) + b_i I(i > n)$.

Due to the non-existence of conference matrices when the number of factors is odd, the D-efficiency of a DS design never reaches the hypothetical D-optimal value. An example on the uses of Theorems 3 to 5 to construct DS designs with odd m is illustrated below.

Example 2. Consider a construction of DS designs with $m = 11$, i.e., a 23×11 matrix. Similar to Example 1, the first combination of $\vec{t}$ and $\vec{s}$ is used for design construction and thus according to Theorem 3,

$$C'C = \begin{pmatrix} 10 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & 10 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 10 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 10 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 10 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 & 10 & 1 & 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 & 1 & 1 & 10 & -1 & -1 & -1 & -1 \\ -1 & 1 & 1 & 1 & 1 & 1 & -1 & 10 & -1 & -1 & -1 \\ -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & 10 & -1 & -1 \\ -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & 10 & -1 \\ -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 10 \end{pmatrix}$$

Although C is not a conference matrix, its generated D possesses good D-efficiency. We obtain two sequences $\{a\} = \{10.0000, 9.9000, 9.7778, 9.6250, 9.4286, 9.1667\}$ and $\{b\} = \{10.0000, 9.9000, 9.8182, 9.7159, 9.5844, 9.4091, 9.1636, 8.7956, 8.2432, 7.3212, 5.4726\}$. The total product of six entries of $\{a\}$ and the last five entries of $\{b\}$ is 21435888100. Then the D-efficiency of the DS design D can be obtained via Theorem 4 and it is 87.9553%.

4. A Table of Suggested DS Designs

Table 1 suggested some DS designs constructed via the method proposed in this paper. In Table 1, the first column (n) is the length of the generator vectors, which is also the dimension of the circulant matrix. The second column (m) is the numbers of column of the three-level DS designs, and it is either $2n+1$ or $2n+2$. The third and fourth columns state the D-efficiencies of the corresponding DS designs. The last column lists the vectors $\vec{t}$ and $\vec{s}$ for generating the circulant matrices T and S, which are the essential components of the conference matrix C in the proposed method.

Table 4.1: Some suggested DS designs for $n = 3, \ldots, 15$

n	m	$d_e(D, D_0)$	Generators
3	7	86.339	$\vec{t} = (0+-)$
	8	88.808	$\vec{s} = (++-)$
4	9	87.173	$\vec{t} = (0-+-)$
	10	90.866	$\vec{s} = (++--)$
5	11	87.955	$\vec{t} = (0++--)$
	12	92.282	$\vec{s} = (++-+-)$
6	13	88.664	$\vec{t} = (0+---+)$
	14	93.317	$\vec{s} = (++-+--)$
7	15	89.298	$\vec{t} = (0++-+--)$
	16	94.107	$\vec{s} = (+++-+--)$
8	17	89.863	$\vec{t} = (0+--+--+)$
	18	94.729	$\vec{s} = (+++-+---)$
9	19	90.369	$\vec{t} = (0+++-+---)$
	20	95.232	$\vec{s} = (++-+-++--)$
10	21	85.386	$\vec{t} = (0+--+-+--+)$
	22	90.163	$\vec{s} = (+++-+---+-)$
11	23	91.233	$\vec{t} = (0+++-+-+---)$
	24	95.997	$\vec{s} = (++-++-++---)$
12	25	91.604	$\vec{t} = (0-++--+--++-)$
	26	96.293	$\vec{s} = (++++-+-+----)$
13	27	91.942	$\vec{t} = (0+++-++--+---)$
	28	96.550	$\vec{s} = (++++--+-+-+--)$
14	29	92.251	$\vec{t} = (0++---+-+---++)$
	30	96.772	$\vec{s} = (+++-++-+--+---)$
15	31	92.534	$\vec{t} = (0+++-++-+--+---)$
	32	96.968	$\vec{s} = (+++-+---+-+++--)$

For each n, or each pair of $\vec{t}$ and $\vec{s}$, it results in two DS designs. The first DS design is generated via the method when C is odd, while the second DS design is generated via the method when C is even. For example, in the case of $n = 5$, i.e., $\vec{t} = (0++--)$ and

$\vec{s} = (++-+-)$, the DS design with 11 columns (and 23 rows) is generated via the method when C is odd, and the entries of C, the D- and T-efficiencies of D can be referred to Example 2. On the other hand, the DS design with 12 columns (and 25 rows) is generated via the method when C is even, and the entries of C, the D- and T-efficiencies of D can be referred to Example 1.

Except the case when $n = 10$, all $\vec{t}$ and $\vec{s}$ listed in Table 1 fulfill the conditions stated in Theorem 1. This implies that the D-efficiencies (as displayed in the third column) of all listed DS designs with even m are optimal. The D-efficiencies of all DS designs with odd m are high but not optimal. The case of $n = 10$ is special, because the pair of $\vec{t}$ and $\vec{s}$ that fulfills all conditions of Theorem 1 does not exist. Our suggested $\vec{t}$ and $\vec{s}$ in Table 1 fulfills the first two conditions. For the third condition, the summations are all -2 for $k = 2, \ldots, 5$, but -6 for $k = 1$. This results in some nonzero values in the off-diagonal entries of $D'D$. Thus, the DS design with $m = 22$ may not be D-optimal.

5. Discussions and Concluding Remarks

When C has odd number of factors, the proposed method clearly does not lead to a DS design with optimal D-efficiency, and one can search for some DS designs with better D-efficiencies than ours, see the results in Jones & Nachtsheim (2011) and Nguyen & Stylianou (2012). However, our proposed method is suggested mainly because of its simple construction method, its guaranteed high (although not optimal) D-efficiency and its universality on all matrix orders.

Consider the case $n = 20$ for example. It is easy to find that only 8 pairs of $\vec{t}$ and $\vec{s}$ fulfill the conditions in Theorem 1. If one of these 8 pairs is chosen to be the generator vectors, for example, $\vec{t} = (0+-+++----+-----+++-+)$ and $\vec{s} = (+--+--+++-+---++-++-)$, the constructed DS designs with 42 columns and 85 rows has optimal D-efficiency 97.674% and that with 41 columns and 83 rows has high D-efficiency 93.661%.

When the dimension of DS designs increases, the computer search is generally inefficient due to the increasingly large search space. Our construction method reduces the search space to a manageable size via the conditions in Theorem 1, and the D-efficiency of the DS design can be calculated by the product of two simple sequences rather than taking the determinant of a matrix, which involves a cross product of two matrices. Finally, our construction method is universal to all matrix orders, no matter it is odd or even, and no matter if the conference matrix exists in the given order. In contrast, the method in Xiao, Lin & Bai (2012) is workable only when the conference matrix exists, and the method in Georgiou, Stylianou & Aggarwal (2013) allows matrix of all even orders to be constructed using weighing matrix $W(m, m-1)$ with $s = 1$. Although the method in Nguyen & Stylianou (2012) allows matrix of even or odd orders to be constructed, it is not a universal method (see $m =, 10, 12, 20, 22, 24, 26, 28, 34, 36, 44, 48, 50$ in their Table 1) for even order and it is a computational intensive search for odd order.

One may notice that some of $\vec{t}$ and $\vec{s}$ are similar to modified Legendre sequences suggested in Fletcher, Gysin & Seberry (2001). In specific, Fletcher, Gysin & Seberry (2001) provided a list of GL(q)-pair from $n = 3$ to 55 via exhaustive computer searches. Some of them are similar to our reported vectors $\vec{t}$ and $\vec{s}$, with a modification that the first entry in the first sequence of GL(q)-pair changes from 1 to 0 in our $\vec{t}$ in order to cooperate with the zero-diagonal property of conference matrix. However, there are some importances of our results.

1. All GL(q)-pair sequences reported in Fletcher, Gysin & Seberry (2001) have odd number of length, because GL(q)-pairs do not exist for even lengths. However, following our conditions mentioned in Theorem 1, $\vec{t}$ and $\vec{s}$ can be found in any number of lengths (both odd and even).

2. The condition in Theorem 1 greatly reduces the search space of obtaining our vectors, while Fletcher, Gysin & Seberry (2001) find their GL(q)-pairs exhaustively via computer searches.

3. Even though Hadamard matrix is constructed via GL(q)-pairs, a conference matrix can only be obtained from a skew symmetric Hadamard matrix via $C = H - I_n$. This is only possible for even number of factors. However, conference matrices with both odd and even number of factors are ready to be constructed using the proposed construction method.

Acknowledgment The authors would like to thank the associate editor and two reviewers for their consructive comments and suggestions. This work was supported by National Science Council of Taiwan ROC grant numbers 100-2118-M-001-002-MY2 and 102-2628-M-001-002-MY3 and Thematic Research Program of Academia Sinica (Taiwan) grant number AS-103-TP-C03.

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