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D- and *MS*-optimal 2-Level Choice Designs for $N \equiv 0 \pmod 4$

Rakhi Singh[1], Feng-Shun Chai[2] and Ashish Das[1]

[1]Indian Institute of Technology Bombay, Mumbai, India
[2]Academia Sinica, Taipei, Taiwan

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Indian Institute of Technology Bombay
Powai, Mumbai-400 076, India

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[1]*Indian Institute of Technology Bombay, Mumbai, India*
[2]*Academia Sinica, Taipei, Taiwan*

Abstract

Street and Burgess (2007) present a comprehensive exposition of designs for choice experiments till then. Our focus is on choice experiments with two-level factors and a main effects model. We consider designs for choice experiment involving k attributes (factors) and all choice sets are of size m. We derive a simple form of the Information matrix of a choice design for estimating the factorial effects. For N being the number of choice sets in the design, we obtain D- and MS-optimal designs in the class of all designs with given N, k and $m = 2$. For given N and k, we show that in many situations D-optimal designs for $m = 2$ are superior than the optimal design for $m = 3$ and $m = 5$. Also, MS-optimal designs with $m = 2$ are always better than the best designs under the same optimality criteria for any odd m. Furthermore, with respect to *trace*-optimality, there is no optimal design for $m > 2$ which is better than the optimal design for $m = 2$.

Key words and phrases: choice sets; choice design; factorial design; main effects; Hadamard matrix.

1 INTRODUCTION

Discrete choice experiments are widely used in various areas including marketing, transport, environmental resource economics and public welfare analysis. A choice experiment consists of a number of choice sets, each containing several options (alternatives, profiles or treatment combinations). A respondent is shown each of the choice sets in turn and is asked for the preferred option as per his perceived utility. Each option in a choice set is described by a set of attributes (factors), where each attribute has two or more levels. We assume that there are no repeated options in a choice set. We consider choice experiments involving N choice sets with m options in each choice set. Furthermore, each option in a choice set is described by k attributes each at two levels, -1 and 1 (say). Thus there are a total of 2^k options. It is ensured that respondents choose one of the options in each choice set (termed forced choice in the literature). A choice design is a collection of choice sets employed in a choice experiment and may contain repeated choice sets. Though choice designs may contain repeated choice sets, one may desirably prefer that no two choice sets are repeated in the choice design.

We denote a choice set by $T_i = (t_{i1}, t_{i2}, \ldots, t_{im})$, where $t_{i\alpha}$ is the α-th option in the i-th choice set, $i = 1, 2, \ldots, N$ and $\alpha = 1, 2, \ldots, m$. Since each option in the choice set is a representation of k attributes, $t_{i\alpha}$ can be written as $(t_{i\alpha}^{(1)}t_{i\alpha}^{(2)}\cdots t_{i\alpha}^{(k)})$ where $t_{i\alpha}^{(q)}$ represents the level of the q-th factor in the α-th option of the i-th choice set. The collection of all such choice sets T_i, $i = 1, 2, \ldots, N$ is called a choice design, say T, with parameters N, k and m. Let the 2^k options be lexicographically arranged, i.e., first option being $(-1\ -1 \cdots -1\ -1)$, second option being $(-1\ -1 \cdots -1\ 1)$, $\ldots$ and the 2^k-th option being $(1\ 1 \cdots 1\ 1)$ and be labeled as $0, 1, 2, \ldots, 2^k - 1$ respectively. Then there is a one-to-one correspondence between the labels and their corresponding options through $\{l, (t_{i\alpha}^{(1)}t_{i\alpha}^{(2)}\cdots t_{i\alpha}^{(k)})\}$ where $l = (t_{i\alpha}^{(1)}+1)2^{k-2} + (t_{i\alpha}^{(2)}+1)2^{k-3} + \cdots + (t_{i\alpha}^{k}+1)2^{(-1)}$.

Street and Burgess (2007) present a comprehensive exposition of designs for choice experiments under multinomial logit (MNL) model. MNL model specifies the probability that an individual will choose one of the m alternatives from a choice set T_i. As in Burgess and Street (2005) (or Street and Burgess, 2007, Chapter 3), under the assumption of MNL model and equal choice probabilities, the information matrix of order 2^k of the options is $\Lambda = ((\Lambda(r, s)))$, with rows and columns of Λ being indexed by the option labels $0, 1, \ldots, 2^k - 1$. Here,

$$\Lambda(r, s) = \begin{cases} \dfrac{m-1}{m^2 N} n_r & \text{if r = s,} \\ \\ \dfrac{-1}{m^2 N} n_{r,s} & \text{if r} \neq \text{s} \end{cases}$$

with r and s being the labels of the corresponding options, n_r is the number of times option label r appears in the choice design and $n_{r,s}$ is the number of times option labels r and s occur together in choice sets of the design. Note that Λ can also be expressed as

$$\Lambda = \frac{1}{N}\sum_{i=1}^{N}\Lambda_i, \tag{1.1}$$

where Λ_i is the information matrix of the i-th choice set T_i. Also, for the i-th choice set $T_i = (t_{i\alpha})$, $\alpha = 1, 2, \ldots, m$, the information matrix Λ_i can be expressed as sum of $\binom{m}{2}$ matrices. For $\alpha \neq \alpha' = 1, 2, \ldots, m$, we define a matrix of order 2^k corresponding to α-th and α'-th options in the i-th choice set as $\Delta_{i(\alpha\alpha')} = ((\Delta_{i(\alpha\alpha')}(r, s)))$, with rows and columns of $\Delta_{i(\alpha\alpha')}$ being indexed by the option labels $0, 1, \ldots, 2^k - 1$. Here,

$$\Delta_{i(\alpha\alpha')}(r, s) = \begin{cases} n_r & \text{if r = s,} \\ \\ -n_{r,s} & \text{if r} \neq \text{s,} \end{cases}$$

and, as mentioned earlier, r and s are the labels of the corresponding options, n_r is the number of times option label r appears in the pair $(t_{i\alpha}, t_{i\alpha'})$ and $n_{r,s}$ is the number of times option labels r and s occur together in the pair $(t_{i\alpha}, t_{i\alpha'})$. Then,

$$\Lambda_i = \frac{1}{m^2} \sum_{\alpha=1}^{m-1} \sum_{\alpha'(>\alpha)=2}^{m} \Delta_{i(\alpha,\alpha')}. \tag{1.2}$$

We consider choice experiments where we restrict our interest to only main effects of the attributes. Under such a main effects model and with B representing the contrast matrix for the main effects of the 2^k choice experiment, the information matrix (also called the C-matrix) corresponding to the main effects is

$$C = B\Lambda B'. \tag{1.3}$$

We assume that rows of B represent a set of orthonormal contrasts. As defined in Burgess and Street (2005), B is a $k \times 2^k$ matrix given as,

$$B = \begin{pmatrix} B_2 \otimes \frac{1}{\sqrt{2}} 1_2 \otimes \cdots \otimes \frac{1}{\sqrt{2}} 1_2 \\ \frac{1}{\sqrt{2}} 1_2 \otimes B_2 \otimes \cdots \otimes \frac{1}{\sqrt{2}} 1_2 \\ \vdots \\ \frac{1}{\sqrt{2}} 1_2 \otimes \frac{1}{\sqrt{2}} 1_2 \otimes \cdots \otimes B_2 \end{pmatrix}$$

where $B_2 = \frac{1}{\sqrt{2}}(-1 \ 1)$, $1_2 = (1 \ 1)$ and $\otimes$ denotes the Kronecker product. Note that the columns of B are lexicographic arrangement of all 2^k options. A choice design for estimating the main effects is said to be *connected* if $rank(C) = k$. We restrict ourselves to the class of all *connected* designs. When a design is *connected*, it ensures that the main effects are estimable. In general, the main effects are estimable if and only if $rank(C) = k$. In what follows, the class of all connected choice designs involving k 2-level attributes and N choice sets each of size m is denoted by $\mathcal{D}_{N,k,m}$.

A choice design $T \in \mathcal{D}_{N,k,m}$ is said to be D-optimal for the estimation of the main effects if it minimizes the generalized variance of the parameter estimates; that is, if the determinant of the variance-covariance matrix of the parameter estimates, C^{-1}, is as small as possible in $\mathcal{D}_{N,k,m}$. Of course a choice design T which minimizes $det(C^{-1})$ is the one which maximizes $det(C)$ and the order of the choice sets within the choice design and the order of the options within each choice set is immaterial. Throughout this paper we will only be talking about optimality with respect to the estimation of the main effects.

We now define some of the commonly used optimality criteria in terms of the eigenvalues of the C-matrix. For choice design $T \in \mathcal{D}_{N,k,m}$, let $0 < \gamma_1 \leq \gamma_2 \leq \cdots \leq \gamma_k$ be the eigenvalues of C. Then, $T^* \in \mathcal{D}_{N,k,m}$ is said to be

i) *trace*-optimal in $\mathcal{D}_{N,k,m}$ if $\left(\sum_{i=1}^{k}\gamma_i\right)^{-1}$ is minimum for the design T^*.

ii) D-optimal in $\mathcal{D}_{N,k,m}$ if $\prod_{i=1}^{k}\gamma_i^{-1}$ is minimum for the design T^*.

iii) A-optimal in $\mathcal{D}_{N,k,m}$ if $\sum_{i=1}^{k}\gamma_i^{-1}$ is minimum for the design T^*.

iv) E-optimal in $\mathcal{D}_{N,k,m}$ if γ_1^{-1} is minimum for the design T^*.

v) MS-optimal in $\mathcal{D}_{N,k,m}$ if $\sum_{i=1}^{k}\gamma_i^2$ is minimum for the design T^* among all trace-optimal designs $T \in \mathcal{D}_{N,k,m}$.

Demirkale, Donovan and Street (2013) considered the general setup of symmetric factorials at 2 or more levels and obtained D-optimal choice designs under main effects model. However, their results were restricted to situations where the C-matrix is necessarily a scalar multiple of identity matrix. Furthermore, their construction of 2^k D-optimal choice designs in N choice sets is restricted to N being a multiple of 4. Recently, Chai, Das and Manna (2014) derived a modified information matrix so as to overcome the shortcoming of decreasing information content with addition of choice sets. This modified information matrix (denoted by C_{mod}) is related to the classical C-matrix of (1.3) through $C_{mod} = NC$. As long as we compare designs in $\mathcal{D}_{N,k,m}$, we may use the C-matrix as in (1.3). However, while comparing designs with different N, one needs to work with the modified information matrix C_{mod}.

In Section 2, the C-matrix for general m is expressed as a function of the C-matrices of paired choice designs. Restricting ourselves to choice sets of size two, we derive a neat and simple form of the C-matrix in terms of the design matrix of the paired choice design. This allows us to see a one-one correspondence between paired choice designs and the chemical balance weighing designs. The D-optimality bounds obtained in Payne (1974) and Galil and Kiefer (1980, 1982) are used to construct new D-optimal choice designs in $\mathcal{D}_{N,k,2}$ with *distinct* choice sets. We also give some new constructions of paired choice designs.

In Section 3, to overcome situations where D-optimal designs are not known, we first obtain a lower bound to $\sum_{i=1}^{k}\gamma_i^2$ and then obtain MS-optimal designs in $\mathcal{D}_{N,k,2}$ for all N except $k = N \equiv 1 \pmod 4$.

Finally, in Section 4 we establish results to show that generally there is no optimal design for $m > 2$ which is better than the optimal paired choice design. Specifically, for given N and k, we show that there exists designs for $m = 2$ that are superior than the D-optimal designs for $m = 3$ and $m = 5$. Also, MS-optimal designs with $m = 2$ are always better than the best designs under the same optimality criteria for any odd m. Furthermore, with respect to *trace*-optimality, there is no optimal design for $m > 2$ which is better than the optimal design for $m = 2$. Since optimal designs with $m > 2$ are generally no better than optimal designs in $\mathcal{D}_{N,k,2}$, it provides more value to restrict ourselves to $m = 2$ while obtaining D- and MS-optimal designs.

2 INFORMATION MATRIX AND D-OPTIMAL DESIGNS

Let T be a paired choice design with parameters N and k. For options $\alpha = 1, 2$, define the $N \times k$ matrix $P_\alpha = ((t_{i\alpha}^{(j)}))$ such that $\{P_1, P_2\}$ represent the paired choice design. Also, let $X_{12} = \frac{1}{2}(P_1 - P_2)$. We henceforth call the matrix X_{12} as the paired choice design matrix. Since X_{12} is a matrix with elements ± 1 and 0, it is similar to chemical balance weighing design. To obtain P_1 and P_2 from X_{12}, for every elements ± 1 in X_{12}, entries in P_1 are same as X_{12} and entries in P_2 are negative of the entries in X_{12}. Also, for every element 0 in X_{12}, entries in P_1 and P_2 are either both 1 or both are -1.

In this section, we first derive the C-matrix for general m in terms of the paired choice design matrices. In particular, this provides a very simple form of the C-matrix for a paired choice design.

Lemma 2.1 Let T be a choice design with parameters N, k and m. For any $\alpha \neq \alpha' = 1, 2, \ldots, m$, define the $N \times k$ matrix $P_\alpha = ((t_{i\alpha}^{(j)}))$. Then,

$$B\Delta_{i(\alpha\alpha')}B' = \frac{1}{2^{k-2}} x'_{i\alpha\alpha'} x_{i\alpha\alpha'},$$

where $x_{i\alpha\alpha'}$ is the i-th row of $X_{\alpha\alpha'} = \frac{1}{2}(P_\alpha - P'_\alpha)$

Proof. Let $t_{i\alpha}$ and $t_{i\alpha'}$ be the i-th row of P_α and $P_{\alpha'}$ respectively. Without loss of generality, let $t_{i\alpha}$ and $t_{i\alpha'}$ correspond to the r-th and the s-th lexicographic label with $r < s$.

Let $B = \frac{1}{\sqrt{2^k}}[B_1 \mid b_r \mid B_2 \mid b_s \mid B_3]$, where B_1 is of order $k \times (r-1)$, B_2 is of order $k \times (s-r-1)$, and B_3 is of order $k \times (2^k - s)$. Since r-th and s-th column of B are the r-th and s-th treatment combinations in lexicographic order respectively, $b_r = t_{i\alpha}$ and $b_s = t_{i\alpha'}$.

Also, from definition, $\Delta_{i(\alpha\alpha')}$ is given by

$$\Delta_{i(\alpha\alpha')} = \left(\begin{array}{c|c|c|c|c} 0_{2^k \times (r-1)} & w'_{i\alpha\alpha'} & 0_{2^k \times (s-r-1)} & -w'_{i\alpha\alpha'} & 0_{2^k \times (2^k - s)} \end{array} \right)$$

where $w_{i\alpha\alpha'} = \begin{pmatrix} 0_{1\times(r-1)} & 1 & 0_{1\times(s-r-1)} & -1 & 0_{1\times(2^k-s)} \end{pmatrix}$.

Then,

$$\begin{aligned}
B\Delta_{i(\alpha\alpha')}B' &= \frac{1}{\sqrt{2^k}}\begin{pmatrix} 0_{k\times(r-1)} & | & (t'_{i\alpha}-t'_{i\alpha'}) & | & 0_{k\times(s-r-1)} & | & (t'_{i\alpha'}-t'_{i\alpha}) & | & 0_{k\times(2^k-s)} \end{pmatrix}B' \\
&= \frac{1}{\sqrt{2^k}}\begin{pmatrix} 0_{k\times(r-1)} & | & 2x'_{i\alpha\alpha'} & | & 0_{k\times(s-r-1)} & | & -2x'_{i\alpha\alpha'} & | & 0_{k\times(2^k-s)} \end{pmatrix}B' \\
&= \frac{1}{2^k}\begin{pmatrix} 0_{k\times(r-1)} & | & 2x'_{i\alpha\alpha'} & | & 0_{k\times(s-r-1)} & | & -2x'_{i\alpha\alpha'} & | & 0_{k\times(2^k-s)} \end{pmatrix}\begin{pmatrix} B'_1 \\ t_{i\alpha} \\ B'_2 \\ t_{i\alpha'} \\ B'_3 \end{pmatrix} \\
&= \frac{2}{2^k}(x'_{i\alpha\alpha'}t_{i\alpha} - x'_{i\alpha\alpha'}t_{i\alpha'}) = \frac{2}{2^k}x'_{i\alpha\alpha'}(t_{i\alpha}-t_{i\alpha'}) = \frac{4}{2^k}x'_{i\alpha\alpha'}x_{i\alpha\alpha'} \\
&= \frac{1}{2^{k-2}}x'_{i\alpha\alpha'}x_{i\alpha\alpha'}. \qquad \square
\end{aligned}$$

Using the above Lemma, we derive the C-matrix for general m and in particular for $m = 2$.

Theorem 2.2 Let T be a choice design with parameters N, k and m. Then,

$$C = \frac{1}{m^2N2^{k-2}}\sum_{\alpha=1}^{m-1}\sum_{\alpha'(>\alpha)=2}^{m} X'_{\alpha\alpha'}X_{\alpha\alpha'}.$$

Proof. From (1.1), (1.2) and (1.3),

$$\begin{aligned}
C &= B\Lambda B' = B\left\{\frac{1}{N}\sum_{i=1}^{N}\Lambda_i\right\}B' = \frac{1}{N}B\sum_{i=1}^{N}\left\{\frac{1}{m^2}\sum_{\alpha=1}^{m-1}\sum_{\alpha'(>\alpha)=2}^{m}\Delta_{i(\alpha,\alpha')}\right\}B' \\
&= \frac{1}{m^2N}\sum_{i=1}^{N}\sum_{\alpha=1}^{m-1}\sum_{\alpha'(>\alpha)=2}^{m} B\Delta_{i(\alpha,\alpha')}B'
\end{aligned}$$

Using Lemma 2.1, we get

$$\begin{aligned}
C &= \frac{1}{m^2N}\sum_{i=1}^{N}\sum_{\alpha=1}^{m-1}\sum_{\alpha'(>\alpha)=2}^{m}\left\{\frac{1}{2^{k-2}}x'_{i\alpha\alpha'}x_{i\alpha\alpha'}\right\} \\
&= \frac{1}{m^2N2^{k-2}}\sum_{\alpha=1}^{m-1}\sum_{\alpha'(>\alpha)=2}^{m}\left\{\sum_{i=1}^{N}x'_{i\alpha\alpha'}x_{i\alpha\alpha'}\right\} \\
&= \frac{1}{m^2N2^{k-2}}\sum_{\alpha=1}^{m-1}\sum_{\alpha'(>\alpha)=2}^{m} X'_{\alpha\alpha'}X_{\alpha\alpha'}. \qquad \square
\end{aligned}$$

Corollary 2.3 Let T be a paired choice design with parameters N and k. Then $C = \dfrac{1}{N2^k}X'_{12}X_{12}$.

Proof. Since in a paired choice design, α =1, $\alpha' = 2$ and m=2, from Theorem 2.2, it follows that, $C = \dfrac{1}{N2^k}X'_{12}X_{12}$. $\square$

It follows from Corollary 2.3 that $rank(C) = k$ only if $k \leq N$. In the remaining paper we mostly discuss paired choice designs and thus for notational convenience write X_{12} as X. However, in Section 4, we give some remarks on how (for fixed k) the best designs with $m > 2$ are usually no better than the best design with $m = 2$.

We now provide D-optimal designs in $\mathcal{D}_{N,k,2}$. Corresponding to a paired choice design $T \in \mathcal{D}_{N,k,2}$, let $X = ((x_{ij}))$ be the paired choice design matrix. Let $\mathcal{Y}(N, k)$ denote the set of all such $N \times k$ full column rank matrices $X = ((x_{ij}))$ consisting entirely of entries ± 1 and 0. Also, let $\mathcal{X}(N, k)$ denote the set of all $N \times k$ full column rank matrices $X = ((x_{ij}))$ consisting entirely of entries ± 1 only. Clearly, $\mathcal{X} \subset \mathcal{Y}$. We restrict ourselves to the D-optimal design matrices in a sub-class $\mathcal{X}(N, k)$. This is because, Galil and Kiefer (1980) showed that if a design matrix $X \in \mathcal{Y} - \mathcal{X}$ is D-optimal in $\mathcal{Y}$, one can find a corresponding $X \in \mathcal{X}$ which is also D-optimal in $\mathcal{Y}$. To illustrate, consider two D-optimal design matrices W_1 and W_2 with $N = 3$ and $k = 3$ having the same D-value but $W_1 \in \mathcal{X}$ and $W_2 \in \mathcal{Y} - \mathcal{X}$. The design matrices are,

$$W_1 = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix} \text{ and } W_2 = \begin{pmatrix} -1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & -1 \end{pmatrix}.$$

$$\text{Also, } W_1'W_1 = \begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix} \text{ and } W_2'W_2 = \begin{pmatrix} 3 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 3 \end{pmatrix}.$$

Here, $\det(W_1'W_1) = \det(W_2'W_2) = 16$ while $trace(W_1'W_1) = 9 > 8 = trace(W_2'W_2)$.

From Corollary 2.3 it follows that finding optimal paired choice design T is equivalent to finding optimal paired choice design matrix X. Let I_p denote the identity matrix of order p and J_p a matrix of order p of all ones. Results on D-optimal paired choice designs in $\mathcal{D}_{N,k,m}$ for $N \equiv 0 \pmod 4$ follows from Demirkale, Donovan and Street (2013) and Chai, Das and Manna (2014). Let $H_{N,N}$ denote a Hadamard matrix of order N. From $H_{N,N}$, one can easily obtain a Hadamard matrix in its normal form having first row and first column of all 1s. Now, for every $k \leq N$, deleting any $N - k$ columns of $H_{N,N}$ we get $H_{N,k} \in \mathcal{X}(N, k)$ such that $H'_{N,k}H_{N,k} = NI_k$. In such a situation $H_{N,k}$ is A-, D-, E- and MS-optimal in $\mathcal{Y}(N, k)$. Galil and Kiefer (1980) showed that even for $k < N$, for which a Hadamard matrix of order N is not known, a D-optimal design matrix can be constructed in some cases.

We now present the D-optimality results for (i) $N \equiv 1 \pmod 4$, (ii) $N \equiv 2 \pmod 4$ and (iii) $N \equiv 3 \pmod 4$.

i) $N \equiv 1$ (mod 4) :

For $k = N$, Ehlich (1964a) established that an $X \in \mathcal{X}(N, N)$ with $X'X = (N-1)I_N + J_N$ is D-optimal in $\mathcal{X}(N, N)$. However, such a X exists only if $2N - 1$ is a perfect square. In general, no systematic constructions for D-optimal matrices are available when $k = N$.

Payne (1974) showed that for $k < N$, an $X \in \mathcal{X}(N,k)$ with $X'X = (N-1)I_k + J_k$ is D-optimal in $\mathcal{X}(N,k)$, with $\det(X'X) = (N-1+k)(N-1)^{(k-1)}$. Payne (1974) provided the construction for such an X by adding a row of all 1s to $H_{N-1,k}$. Cheng (1980) showed that such matrices are A- and E-optimal as well.

ii) $N \equiv 2$ (mod 4) :

For $k = N$, Ehlich (1964a) and Wojtas (1964) showed that an $X \in \mathcal{X}(N,N)$ with $X'X = \begin{pmatrix} Y & 0 \\ 0 & Y \end{pmatrix}$ is D-optimal in $\mathcal{X}(N,N)$, where $Y = (N-2)I_{k/2} + 2J_{k/2}$. For $k = N-1$, systematic results on optimal design matrices are not known. Also, no systematic constructions for D-optimal matrices are available for $k = N$ and $k = N-1$.

Payne (1974) showed that for $k < N-1$, an $X \in \mathcal{X}(N,k)$ with

$$X'X = \begin{pmatrix} Y1 & 0 \\ 0 & X1 \end{pmatrix} \tag{2.1}$$

is D-optimal in $\mathcal{X}(N,k)$, with $\det(X'X) = ((N-2+k)^2 - \mu)(N-2)^{k-2}$. Here, for k even, $X1 = Y1 = (N-2)I_{k/2} + 2J_{k/2}$ and $\mu = 0$, while for k odd, $X1 = (N-2)I_{(k\pm1)/2} + 2J_{(k\pm1)/2}$, $Y1 = (N-2)I_{(k\mp1)/2} + 2J_{(k\mp1)/2}$ and $\mu = 1$. Payne (1974) provided the construction for such an X by adding two rows to $H_{N-2,k}$, one consisting entirely of 1s and the other consisting of ±1s such that the number of 1s and -1s differ by atmost 1. Cheng (1980) showed that these designs are E-optimal as well.

iii) $N \equiv 3$ (mod 4) :

For $k = N$, though Ehlich (1964b) derived an upper bound for the D-value, no D-optimal designs have been obtained attaining the bound. For $(N+5)/2 < k < N$, theoretical upper bounds to the D-value is not known. Also no systematic constructions for D-optimal matrices are available for $(N+5)/2 < k \leq N$.

For $k \leq (N+5)/2$, Payne (1974) and Galil and Kiefer (1980) showed that an $X \in \mathcal{X}(N,k)$ with $X'X = (N-1)I_k + J_k$ is D-optimal in $X \in \mathcal{X}(N,k)$, with $\det(X'X) = (N+1-k)(N+1)^{k-1}$. Payne (1974) and Galil and Kiefer (1980) also provided the construction for such an X by deleting from a $H_{N+1,k}$ in its normal form, the row of all 1s.

Though in (i)-(iii) above, we have indicated situations where no systematic constructions are given, there are few stray cases where isolated D-optimal designs have been obtained. The link *http://www.indiana.edu/ maxdet/fullPage.shtml\#tableTop* provides few of such designs for $k = N \leq 119$.

As indicated in Section 1, though choice designs in $\mathcal{D}$ may contain repeated choice sets, one may desirably prefer that no two choice sets are repeated in the choice design.

Accordingly we provide choice design constructions where no two choice sets are repeated. Two rows of a choice design matrix $X \in \mathcal{X}(N,k)$ are said to be *distinct* if their inner product is less than k. In what follows, in partial modification to the constructions provided Payne (1974) and Galil and Kiefer (1980), we provide constructions such that the rows of X are all *distinct*. We take up the cases $N \equiv i \pmod 4$, $i = 0, 1, 2, 3$ separately.

Construction-(0) for $N \equiv 0$ (mod 4), $k \leq N$

We show that for $N \equiv 0 \pmod 4$, starting from $H_{N,N}$ one can randomly delete upto $N/2 - 1$ columns resulting in $H_{N,k}$ ($=X_0$, say) with $k > N/2$, such that no two rows have an inner product equal to $\pm k$ (i.e., all rows are *distinct*). However, for deleting $N/2$ or more columns, one would need to carefully delete columns so as to ensure that all rows are *distinct*. Though not explicitly required here, for ease of subsequent constructions, henceforth we always consider $H_{N,N}$ to be in its normal form.

Lemma 2.4 When *any* $N - k$ columns of a Hadamard matrix $H_{N,N}$ are deleted to obtain X_0, the rows of X_0 are *distinct* if and only if $k > N/2$.

Proof. Interchanging the columns of $H_{N,N}$ retains the Hadamard property of $H_{N,N}$. Therefore, without loss of generality let,

$$H_{N,N} = (X_0 \mid H_{N,N-k}) . \tag{2.2}$$

Therefore

$$X_0X_0' + H_{N,N-k}H_{N,N-k}' = H_{N,N}H_{N,N}' = NI_N. \tag{2.3}$$

Let $X_0X_0' = ((u_{ij}))$ and $H_{N,N-k}H_{N,N-k}' = ((w_{ij}))$. Then from (2.3), it follows that

$$u_{ij} + w_{ij} = 0 \text{ or } |u_{ij}| = |w_{ij}|. \tag{2.4}$$

and

$$|u_{ij}| \leq k \text{ and } |w_{ij}| \leq N - k, \tag{2.5}$$

Only if condition : Let X_0 has *distinct* rows. Then, for $i \neq j$, $|u_{ij}| < k$. Thus from (2.4) $|w_{ij}| < k$, or from (2.5) $N - k < k$, i.e., $k > N/2$.

If condition : Let $k > N/2$. If possible let $|u_{ij}| = k$ for some (i,j), say (i_0, j_0). Then from (2.4) and (2.5) $|u_{i_0j_0}| = k = |w_{i_0j_0}| \leq N - k$. Thus $k \leq N - k$, or, $k \leq N/2$, which is not possible. Therefore, $|u_{ij}| < k$ for all (i,j), and hence the rows of X_0 are *distinct*. $\square$

Remark 2.1 If $k > N/2$ then choosing any k columns of $H_{N,N}$ would suffice. Let w be an integer and $[x]$ denotes the largest integer less than or equal to x. For $N = 2^w$, we can always obtain $H_{N,w}$ directly by listing all possible options as rows. Here, to get *distinct* rows, number of factors $k \geq w = log_2N$. When $2^w < N < 2^{w+1}$, N *distinct* rows can be obtained provided $k \geq [log_2N] + 1$.

Remark 2.2 We also did a complete enumeration on $H_{N,N}$, $4 \leq N \leq 128$, to find out the least number of columns k required so as to have N *distinct* rows in $H_{N,k}$. Results showed that,
(A) for $N = 2^w$,
a) For $N = 4$, 8, 16, 32 and 64: $k \geq [log_2 N] + 1$,
b) For $N = 128$: $k \geq [log_2 N] + 2$,
and
(B) for $N \neq 2^w$
c) For $N \leq 44$ (except $N = 12, 24$ and 28) or $N = 80$ and 88: $k \geq [log_2 N] + 2$,
d) For $48 \leq N \leq 96$ (except $N = 80$ and 88) or $N = 12, 24$ and 28: $k \geq [log_2 N] + 3$
e) For $100 \leq N \leq 124$: $k \geq [log_2 N] + 4$.

Construction-(I) for $N \equiv 1$ (mod 4), $k < N$

Consider $H_{N-1,k}$ of Construction-(0). To ensure that no two choice sets are repeated, one may add to $H_{N-1,k}$ any row of ±1s not present in $H_{N-1,k}$ or $-H_{N-1,k}$ to get a design matrix, say X_0. We now show that the resultant X_0 is also D-optimal.

Theorem 2.5 For $k < N$ one can add *any* row consisting of entries ±1 to $H_{N-1,k} \in \mathcal{X}(N-1, k)$ and the resultant paired choice design d_0 corresponding to X_0 satisfies $\det(X_0'X_0) = (N-1+k)(N-1)^{k-1}$ and thus, is D-optimal in $\mathcal{D}_{N,k,2}$.

Proof. Let $H_{N-1,N-1}$ be a Hadamard matrix of order $N-1$ and a be column vector of order k consisting entirely of entries ±1. Keeping any k columns of $H_{N-1,N-1}$, a $(N-1) \times k$ matrix $H_{N-1,k}$ is obtained. Then, $H'_{N-1,k}H_{N-1,k} = (N-1)I_k$. Let X_0 be a $N \times k$ matrix with $k \leq N$ such that $X_0 = \begin{pmatrix} H_{N-1,k} \\ a' \end{pmatrix}$. Then, $X_0'X_0 = H'_{N-1,k}H_{N-1,k} + aa'$, or

$$X_0'X_0 = (N-1)I_k + aa' \tag{2.6}$$

.

Since $(N-1)I_k$ and aa' commute,
Eigenvalues of $X_0'X_0$ = Eigenvalues of $(N-1)I_k$ + Eigenvalues of aa'.

Since, the eigenvalues of $(N-1)I_k$ are $N-1$ with multiplicity k and the eigenvalues of aa' are 0 and $a'a$ with respective multiplicities $k-1$ and 1, therefore eigenvalues of $X_0'X_0$ are $N-1$ and $N-1+a'a$ with respective multiplicities $k-1$ and 1. Thus, $\det(X_0'X_0) = (N-1+k)(N-1)^{k-1}$ which is attaining the theoretical bound as obtained in Payne(1974). Therefore, X_0 is D-optimal in $\mathcal{X}(N,k)$. □

This result allows us to broaden the selection of the D-optimal paired choice design by adding any one of the $2^k - 2(N-1)$ possible options which are not there as options in the rows of $\pm H_{N-1,k}$.

Construction-(II) for $N \equiv 2 \pmod 4$, $k \leq N$

For $k \leq N-2$, consider $H_{N-2,k}$ of Construction-(0). Then to obtain $X_0 \in \mathcal{X}(N,k)$, we add to $H_{N-2,k}$ two rows as follows. Multiply any column of $H_{N-2,k}$ by -1 and add a row of all 1s. As second row, one can add *any* row consisting of entries ± 1 such that number of 1s and -1s differ by atmost 1 and is *distinct* from the other $N-1$ rows. The resultant paired choice design (d_0, say) corresponding to the design matrix X_0 would be D-optimal in $\mathcal{D}_{N,k,2}$, as multiplying any column by -1 doesn't change the Hadamard properties of $H_{N-2,k}$.

For, $k = N$ and $N-1$, consider $H_{N+2,k}$ of Construction-(0). Then from $H_{N+2,k}$ delete the first row of all 1s and a row such that number of 1s and -1s differ by atmost 1. This results in $X_0 \in \mathcal{X}(N,k)$ corresponding to a paired choice design d_0. Note that Payne (1974) and Galil and Kiefer (1980) did not provide any constructions for $k = N$ and $N-1$, since D-optimality bounds were not established in these cases.

Construction-(III) for $N \equiv 3 \pmod 4$, $k \leq N$

For $k \leq N$, consider $H_{N+1,k}$ of Construction-(0). Delete *any* row from $H_{N+1,k}$ to get a design matrix, say X_0. This would sometimes facilitate to get distinct N rows of X_0. We now show that the resultant X_0 is also D-optimal in the cases where D-optimality bounds have already been found.

Theorem 2.6 For $k \leq N$, one can delete *any* row from $H_{N+1,k} \in \mathcal{X}(N+1,k)$ and the resultant paired choice design d_0 corresponding to X_0 satisfies $\det(X_0'X_0) = (N+1-k)(N+1)^{k-1}$ and is D-optimal in $\mathcal{D}_{N,k,2}$ for $k \leq (N+5)/2$.

Proof. Let $H_{N+1,N+1}$ be a Hadamard matrix of order $N+1$ and a be column vector of order k consisting entirely of entries ± 1. Keeping any k columns of $H_{N+1,N+1}$, a $(N+1) \times k$ matrix $H_{N+1,k}$ is obtained. Then, $H_{N+1,k}'H_{N+1,k} = (N+1)I_k$. Let X_0 be a $N \times k$ matrix with $k \leq N$ such that $H_{N+1,k} = \begin{pmatrix} X_0 \\ a' \end{pmatrix}$. Then, $H_{N+1,k}'H_{N+1,k} = X_0'X_0 + aa'$, or

$$X_0'X_0 = (N+1)I_k - aa' \tag{2.7}$$

.

Since $(N+1)I_k$ and aa' commute,
Eigenvalues of $X_0'X_0$ = Eigenvalues of $(N+1)I_k$ - Eigenvalues of aa'.

Since, the eigenvalues of $(N+1)I_k$ are $N+1$ with multiplicity k and the eigenvalues of aa' are 0 and $a'a$ with respective multiplicities $k-1$ and 1, therefore eigenvalues of $X_0'X_0$ are $N+1$ and $N+1-a'a$ with respective multiplicities $k-1$ and 1. Thus, $\det(X_0'X_0) = (N+1-k)(N+1)^{(k-1)}$ which is attaining the theoretical bound as obtained in Payne(1974) and Galil and Kiefer(1980) for $k \leq (N+5)/2$. Therefore, X_0 is D-optimal in $\mathcal{X}(N,k)$ for $k \leq (N+5)/2$. $\square$

This result allows us to broaden the selection of the D-optimal paired choice design by deleting any one of the $N+1$ possible options which are there as options in the rows of $H_{N+1,k}$.

As we have already noted that there are several situations where D-optimal design matrices in $\mathcal{X}(N,k)$ are not available, we now summarize below the cases where theoretical D-optimality upper bounds are not available or, there exists no constructions for a D-optimal design.

a) When $N \equiv 1 \pmod 4$: No systematic construction is available for $k = N$ except when $2N-1$ is a perfect square.
b) When $N \equiv 2 \pmod 4$: No systematic construction is available for $k = N$ and $k = N-1$.
c) When $N \equiv 3 \pmod 4$: No systematic construction is available for $(N+5)/2 < k \leq N$.

Given that systematic constructions are not available for the above cases, in the next Section we obtain MS-optimality bounds and then show that the paired choice design d_0 corresponding to Constructions(I-III) are MS-optimal in $\mathcal{D}_{N,k,2}$.

3 MS-OPTIMAL DESIGNS

As seen in Section 2, bounds and systematic constructions for D-optimal designs do not exist for several parameter sets. In order to address the situation, we now find MS-optimal designs in $\mathcal{D}_{N,k,2}$. Following Chai, Das and Manna (2014), and denoting the C-matrix (as given in (1.3)) involving k attributes of N choice sets of size m by C_m, the upper bound to $trace(C_m)$ is

$$trace(C_m) \leq \begin{cases} \dfrac{k}{2^k} & \text{for } m \text{ even} \\[2ex] \dfrac{k(m^2-1)}{2^k m^2} & \text{for } m \text{ odd} \end{cases} \tag{3.1}$$

Thus, it follows that for $m=2$, a paired choice design in $\mathcal{D}_{N,k,2}$ having maximum $trace(C_2)$ has a design matrix necessarily belonging to $\mathcal{X}(N,k)$. From Corollary 2.3 it follows that finding MS-optimal paired choice design is equivalent to finding a paired choice design matrix $X \in \mathcal{X}(N,k)$ such that $\sum_{i=1}^{k} \lambda_i^2$ is minimum where $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k$ are the eigenvalues of $X'X$. Note that the eigenvalues of C_2 are $\gamma_i = \dfrac{1}{N2^k}\lambda_i$ for $i = 1, 2, \ldots, k$.

In what follows, we study the MS-optimality of designs in $\mathcal{X}(N,k)$. First we obtain a lower bound to $\sum_{i=1}^{k} \lambda_i^2$.

Theorem 3.1 Let $X \in \mathcal{X}(N,k)$. Then $\sum_{i=1}^{k} \lambda_i^2 \geq N^2k + L$, where

$$L = \begin{cases} 0 & \text{for } N \equiv 0 \pmod 4, \\ 4\big(\frac{k^2}{2} - k\big) & \text{for } N \equiv 2 \pmod 4 \text{ and } k \text{ even}, \\ 4\big(\frac{k^2}{2} - k + \frac{1}{2}\big) & \text{for } N \equiv 2 \pmod 4 \text{ and } k \text{ odd}, \\ k(k-1) & \text{for } N \equiv 1 \pmod 4 \text{ or } N \equiv 3 \pmod 4. \end{cases}$$

Proof. Let $X'X = M = ((m_{ij}))$. Then

$$\sum_{i=1}^{k} \lambda_i^2 = trace(M^2) = N^2k + \sum_{i=1}^{k} \sum_{j(\neq i)=1}^{k} m_{ij}^2. \tag{3.2}$$

For every given row of X the four possible values for the i-th and j-th column entries are $(1,1)$, $(1,-1)$, $(-1,1)$ and $(-1,-1)$. Let,
f_1 = number of rows of X with $(1,1)$ in the i-th and j-th columns respectively,
f_2 = number of rows of X with $(1,-1)$ in the i-th and j-th columns respectively,
f_3 = number of rows of X with $(-1,1)$ in the i-th and j-th columns respectively,
f_4 = number of rows of X with $(-1,-1)$ in the i-th and j-th columns respectively.

Then,

$$f_1 + f_2 + f_3 + f_4 = N, \tag{3.3}$$

and

$$(f_1 + f_4) - (f_2 + f_3) = m_{ij}. \tag{3.4}$$

Now, (3.3) and (3.4) implies

$$f_1 + f_4 = \frac{(m_{ij} + N)}{2} \text{ and } f_2 + f_3 = \frac{(N - m_{ij})}{2}. \tag{3.5}$$

Since $f_1 + f_4$ is an integer, m_{ij} is even when N is even and m_{ij} is odd when N is odd.
Now we define,

$$e_{ij} = (-1)^{(2f_1 + f_2 + f_3)}. \tag{3.6}$$

Hence, $e_{ij} = -1$ if f_2 is odd and f_3 is even, or vice versa. In another words, $e_{ij} = -1$ if one column has even number of +1s and another column has odd number of +1s, otherwise $e_{ij} = 1$.

For N even, we have the two cases, (i) $N \equiv 0 \pmod 4$ and (ii) $N \equiv 2 \pmod 4$. As seen above, for N even, m_{ij} is always even and thus m_{ij} can either be of type $0 \pmod 4$ or $2 \pmod 4$.

Case (i) $N \equiv 0 \pmod 4$:

When $m_{ij} \equiv 0 \pmod 4$:
Let $N = 4v$ and $m_{ij} = 4w$ where v and w are integers. Using (3.5) and (3.6) we see that $f_2 + f_3 = 2(v - w)$ and $e_{ij} = 1$.

When $m_{ij} \equiv 2 \pmod 4$:
Let $N = 4v$ and $m_{ij} = 4w + 2$ where v and w are integers. Using (3.5) and (3.6) we see that $f_2 + f_3 = 2(v - w) - 1$ and $e_{ij} = -1$.

In order to get a lower bound for $\sum_{i=1}^{k} \sum_{j(\neq i)=1}^{k} m_{ij}^2$, since $e_{ij} = +1$ for $m_{ij} \equiv 0 \pmod 4$, and $e_{ij} = -1$ for $m_{ij} \equiv 2 \pmod 4$, therefore, there exists a matrix X such that $\mid m_{ij} \mid \geq 0$ for all i, j. Hence, $\sum_{i=1}^{k} \sum_{j(\neq i)=1}^{k} m_{ij}^2 \geq 0$. Thus from (3.2), we get $\sum_{i=1}^{k} \lambda_i^2 \geq N^2 k$.

Note that $m_{ij} = 0$ for all i, j when all columns of X have +1s even number of times or all columns of X have +1s odd number of times.

Case (ii) $N \equiv 2 \pmod 4$:

When $m_{ij} \equiv 0 \pmod 4$:
Let $N = 4v + 2$ and $m_{ij} = 4w$ where v and w are integers. Using (3.5) and (3.6) we see that $f_2 + f_3 = 2(v - w) + 1$ and $e_{ij} = -1$.

When $m_{ij} \equiv 2 \pmod 4$:
Let $N = 4v + 2$ and $m_{ij} = 4w + 2$ where v and w are integers. Using (3.5) and (3.6) we see that $f_2 + f_3 = 2(v - w)$ and $e_{ij} = 1$.

Again, we work on getting a lower bound for $\sum_{i=1}^{k} \sum_{j(\neq i)=1}^{k} m_{ij}^2$ using the fact that $e_{ij} = -1$ for $m_{ij} \equiv 0 \pmod 4$, and $e_{ij} = +1$ for $m_{ij} \equiv 2 \pmod 4$. We observe that, for $k \geq 3$, there is no matrix X such that $m_{ij} = 0$ (or equivalently e_{ij} is -1) for all i, j, since out of k ($\geq$ 3) columns there will be atleast 2 columns that either have odd number of +1s or even number of +1s. Thus, we minimize the number of m_{ij}'s taking the value 2.

Now, since there are k columns in the matrix X, it can either have:

k (and 0) columns with even (odd) number of +1s,
$k-1$ (and 1) columns with even (odd) number of +1s,
$\vdots$
$\frac{k}{2}$ (and $\frac{k}{2}$) columns with even (odd) number of +1s, for k even or,
$\frac{k+1}{2}$ (and $\frac{k-1}{2}$) columns with even (odd) number of +1s, for k odd
$\vdots$
0 (and k) columns with even (odd) number of +1s.

We now consider the two cases based on k being even or odd.

Case: k even
Two columns such that $e_{ij}=1$ can be selected in either $\binom{k}{2}$ or $\binom{k-1}{2}$ or $\left(\binom{k-2}{2}+\binom{2}{2}\right)$ or $\cdots$ or $\left(\binom{k/2}{2}+\binom{k/2}{2}\right)$ ways.
Since,

$$\binom{k}{2} \geq \binom{k-1}{2} \geq \left(\binom{k-2}{2}+\binom{2}{2}\right) \geq \cdots \geq \left(\binom{k/2}{2}+\binom{k/2}{2}\right),$$

the minimum number of cases for $e_{ij}=1$ and $e_{ji}=1$ are $2\left(\binom{k/2}{2}+\binom{k/2}{2}\right) = \left(\frac{k^2}{2}-k\right)$ and for each such case $\mid m_{ij} \mid \geq 2$ for all i,j. Hence, $\sum_{i=1}^{k} \sum_{j(\neq i)=1}^{k} m_{ij}^2 \geq 4\big(\frac{k^2}{2}-k\big)$. Thus from (3.2), we get $\sum_{i=1}^{k} \lambda_i^2 \geq N^2k + 4\left(\frac{k^2}{2}-k\right)$.

Case: k odd
Two columns such that $e_{ij}=1$ can be selected in either $\binom{k}{2}$ or $\binom{k-1}{2}$ or $\left(\binom{k-2}{2}+\binom{2}{2}\right)$ or $\cdots$ or $\left(\binom{(k+1)/2}{2}+\binom{(k-1)/2}{2}\right)$ ways.
Since,

$$\binom{k}{2} \geq \binom{k-1}{2} \geq \left(\binom{k-2}{2}+\binom{2}{2}\right) \geq \cdots \geq \left(\binom{(k+1)/2}{2}+\binom{(k-1)/2}{2}\right),$$

the minimum number of cases for $e_{ij}=1$ and $e_{ji}=1$ are $2\left(\binom{(k+1)/2}{2}+\binom{(k-1)/2}{2}\right)$

$= \left(\frac{k^2}{2} - k + \frac{1}{2}\right)$ and for each such case $| m_{ij} | \geq 2$ for all i, j. Hence, $\sum_{i=1}^{k} \sum_{j(\neq i)=1}^{k} m_{ij}^2 \geq 4\left(\frac{k^2}{2} - k + \frac{1}{2}\right)$. Thus from (3.2), we get $\sum_{i=1}^{k} \lambda_i^2 \geq N^2 k + 4\left(\frac{k^2}{2} - k + \frac{1}{2}\right)$.

In addition to the cases where N is even, we now consider the case where N is odd.

Case (iii) $N \equiv 1 \pmod 4$ or $N \equiv 3 \pmod 4$:

We have already seen that for N odd, m_{ij} is always odd implying that $| m_{ij} | \geq 1$ for all i, j. In other words, for each of the $k(k-1)$ entries, m_{ij} is atleast ± 1 and hence, $\sum_{i=1}^{k} \sum_{j(\neq i)=1}^{k} m_{ij}^2 \geq k(k-1)$. Thus from (3.2), we get $\sum_{i=1}^{k} \lambda_i^2 \geq N^2 k + k(k-1)$. ☐

Corollary 3.2 An $X \in \mathcal{X}(N, k)$ will attain the MS-optimality lower bound value if the off-diagonal elements of $X'X$,

i) for $N \equiv 0 \pmod 4$, are 0 for all elements,

ii) for $N \equiv 2 \pmod 4$, k even, are ± 2 for $\left(\frac{k^2}{2} - k\right)$ elements,

iii) for $N \equiv 2 \pmod 4$, k odd, are ± 2 for $\left(\frac{k^2}{2} - k + \frac{1}{2}\right)$ elements,

iv) for $N \equiv 1 \pmod 4$ and $N \equiv 3 \pmod 4$, are ± 1 for all elements.

Proof. Follows directly from the bounds obtained in Theorem 3.1. ☐

Recall the Constructions(I-III) of $X_0 \in \mathcal{X}(N, k)$ for all N and k except $k = N \equiv 1 \pmod 4$. The Constructions X_0 correspond to D-optimal designs matrices in $\mathcal{X}(N, k)$ for $N \equiv 1 \pmod 4$ $(k < N)$, for $N \equiv 2 \pmod 4$ $(k < N - 1)$ and for $N \equiv 3 \pmod 4$ $(k \leq (N+5)/2)$, respectively. We now show that X_0 is MS-optimal in $\mathcal{X}(N, k)$ for all N and $k \leq N$.

Theorem 3.3 A paired choice design d_0 corresponding to the design matrix $X_0 \in \mathcal{X}(N, k)$, as given in Constructions(I-III), are MS-optimal in $\mathcal{D}_{N,k,2}$.

Proof. We take up the cases $N \equiv i \pmod 4$, $i = 1, 2, 3$.

For $N \equiv 1 \pmod 4$ $(k < N)$, using (2.6), it follows that $X_0'X_0 = (N-1)I_k + aa'$, where a is a column vector of all ± 1s. Thus, off-diagonal elements of $X_0'X_0$ are all ± 1s. Therefore, from Corollary 3.2, design matrix X_0 and hence the paired choice design d_0 is MS-optimal.

For $N \equiv 2 \pmod 4$ $(k < N - 1)$, using (2.1), it follows that $X_0'X_0 = \begin{pmatrix} Y1 & 0 \\ 0 & X1 \end{pmatrix}$ where, for k even, $X1 = Y1 = (N-2)I_{k/2} + 2J_{k/2}$, while for k odd, $X1 = (N-2)I_{(k\pm1)/2} + 2J_{(k\pm1)/2}$

and $Y1 = (N-2)I_{(k\mp1)/2} + 2J_{(k\mp1)/2}$. From here, it is evident that there are $\left(\frac{k^2}{2} - k\right)$ ±2s in off-diagonal positions for k even and $\left(\frac{k^2}{2} - k + \frac{1}{2}\right)$ ±2s for k odd. Therefore, from Corollary 3.2, design matrix X_0 and hence the paired choice design d_0 is MS-optimal.

For $N \equiv 2 \pmod 4$ $(k = N-1, N)$, recall from Construction(II) that two rows from $H_{N+2,k}$ are deleted such that the inner product of each of their columns contribute to $\frac{k^2}{2}$ (or, $\left(\frac{k^2-1}{2}\right)$ for k odd) 0s in off-diagonal positions. Note that off-diagonal elements of $H'_{N+2,k}H_{N+2,k}$ were all 0 and hence deleting two rows as above would lead to $\frac{k^2}{2}$ (or, $\left(\frac{k^2-1}{2}\right)$ for k odd) $0s$ and $\left(\frac{k^2}{2} - k\right)$ (or, $\left(\frac{k^2}{2} - k + \frac{1}{2}\right)$ for k odd) $\pm2s$ to the off-diagonal elements of X'_0X_0. Therefore, from Corollary 3.2, design matrix X_0 and hence the paired choice design d_0 is MS-optimal.

For $N \equiv 3 \pmod 4$ $(k \leq N)$, using (2.7), it follows that $X'_0X_0 = (N+1)I_k - aa'$, where a is a column vector of all ±1s. Thus, off-diagonal elements of X'_0X_0 are all ±1s. Therefore, from Corollary 3.2, design matrix X_0 and hence the paired choice design d_0 is MS-optimal.
□

Thus, from above, we obtain MS-optimal designs for each N and $k \leq N$ except $k = N \equiv 1 \pmod 4$.

4 COMPARING DESIGNS WITH $m = 2$ AND WITH $m > 2$

Generally there is no optimal design for $m > 2$ which is better than the optimal paired choice design. For given N and k, with respect to maximum of $trace(C)$, (i) all designs with m even are equivalent and (ii) a design with m odd is always inferior to a design with m even. For given N and k, we show that there exists designs for $m = 2$ that are superior than the D-optimal design for $m = 3$ and $m = 5$. Also, MS-optimal designs with $m = 2$ are always better than the best designs under the same optimality criteria for any odd m. Thus for given N and k, it follows that a D-, MS- and $trace$-optimal 2^k choice design in $\mathcal{D}_{N,k,2}$ is also D-, MS- and $trace$-optimal respectively, in a more broader class of all connected choice designs involving N choice sets.

As a counter example for m even, consider two designs $d_1 \in \mathcal{D}_{5,5,2}$ and $d_2 \in \mathcal{D}_{5,5,4}$. Let, $d_1 = ((P \mid p),\ (-P \mid -p))$ and $d_2 = ((P \mid p),\ (-P \mid -p),\ (P \mid -p),\ (-P \mid p))$ where

$$P = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & -1 & -1 \end{pmatrix} \text{ and } p = (-1\ 1\ 1\ 1\ -1)'. \text{ Then,}$$

$$160C_{2d_1} = 32C_{mod,2d_1} = \begin{pmatrix} 5 & -1 & -1 & -1 & 1 \\ -1 & 5 & 1 & 1 & -1 \\ -1 & 1 & 5 & 1 & -1 \\ -1 & 1 & 1 & 5 & -1 \\ 1 & -1 & -1 & -1 & 5 \end{pmatrix}$$

$$\text{and } 160C_{4d_2} = 32C_{mod,4d_2} = \begin{pmatrix} 5 & -1 & -1 & -1 & 0 \\ -1 & 5 & 1 & 1 & 0 \\ -1 & 1 & 5 & 1 & 0 \\ -1 & 1 & 1 & 5 & 0 \\ 0 & 0 & 0 & 0 & 5 \end{pmatrix}.$$

Also, since $det(160C_{4d_2}) = 2560 > 2304 = det(160C_{2d_1})$ and the sum of squares of the off-diagonal elements of $160C_{2d_2}$ is less than the sum of squares of the off-diagonal elements of $160C_{2d_1}$, therefore $d_2 \in \mathcal{D}_{5,5,4}$ is D- and MS-better than $d_1 \in \mathcal{D}_{5,5,2}$.

We now show how by meaningfully utilizing the options in a design with $m = 4$, one can reconstruct a new design with $m = 2$ having greater information content. Consider a design $d_3 \in \mathcal{D}_{10,5,2}$ obtained from the options in design $d_2 \in \mathcal{D}_{5,5,4}$. With

$$d_3 = \begin{pmatrix} (P \mid p), & (-P \mid -p) \\ (P \mid -p), & (-P \mid p) \end{pmatrix},$$

we have

$$320C_{2d_3} = 32C_{mod,2d_3} = \begin{pmatrix} 10 & -2 & -2 & -2 & 0 \\ -2 & 10 & 2 & 2 & 0 \\ -2 & 2 & 10 & 2 & 0 \\ -2 & 2 & 2 & 10 & 0 \\ 0 & 0 & 0 & 0 & 10 \end{pmatrix}.$$

Since d_2 is based on $N = 5$ while d_3 is based on $N = 10$, we evaluate determinant of $32C_{mod,4d_2}$ and $32C_{mod,2d_3}$. It is seen that $\det(32C_{mod,2d_3}) = 32768 > 2560 = \det(32C_{mod,4d_2})$. Also, $trace(C_{mod,2d_3}) > trace(C_{mod,4d_2})$. Thus, it may be more meaningful to utilize the resources available, in form of options, by employing a design with $m = 2$ rather than a design with $m = 4$, unless there are extraneous reasons which forces one to use a design with $m = 4$.

Under the premise that designs with $m > 5$ are expected not to have much practical utility when there exists optimal designs with $m \leq 5$, we now concentrate on designs X_0

($m = 2$), constructed in Section 2, and show that they are D-better than the best possible designs with $m = 3$ and $m = 5$.

Comparing designs with $m = 2$ and $m = 3$

From (3.1), for $m = 3$ we have $trace(C_3) \leq \frac{2}{9}\left(\frac{k}{2^{k-2}}\right)$ and for $m = 5$, we have $trace(C_5) \leq \frac{6}{25}\left(\frac{k}{2^{k-2}}\right)$. Since, sum of eigenvalues is equal to trace of matrix, $det(C_3) \leq \left\{\frac{2}{9}\left(\frac{1}{2^{k-2}}\right)\right\}^k = det_{m=3,max}$ and $det(C_5) \leq \left\{\frac{6}{25}\left(\frac{1}{2^{k-2}}\right)\right\}^k = det_{m=5,max}$. We now show that there exists a choice design d_0 (with corresponding design matrix X_0) in $\mathcal{D}_{N,k,2}$ such that $\det(C_2) > det_{m=3,max}$.

Now since for the choice design d_0, $C_2 = \frac{1}{N2^k}X_0'X_0$, we can write $N2^kC_2 = X_0'X_0$. Also, $det(N2^kC_3) \leq \left\{\frac{8N}{9}\right\}^k$ and $det(N2^kC_5) \leq \left\{\frac{24N}{25}\right\}^k$. Thus, to show that the D-optimal design with $m = 3$ is inferior to d_0 it suffices to show $\det(N2^kC_2) > \left\{\frac{8N}{9}\right\}^k$.

We consider three cases based on the values of N,
a) $N \equiv 1 \pmod 4$, b) $N \equiv 2 \pmod 4$ and c) $N \equiv 3 \pmod 4$.

Theorem 4.1 For $N \equiv 1 \pmod 4$ and $k < N$, $d_0 \in \mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,3}$.

Proof. We know that for $k \leq N - 1$, eigenvalues of $X_0'X_0$ are $(N - 1 + k)$ and $(N - 1)$ with multiplicity 1 and $k - 1$ respectively. We now show that $\det(N2^kC_2) = (N - 1 + k)(N - 1)^{k-1} > \left\{\frac{8N}{9}\right\}^k$.

For a fixed N, let $f(k) = (N-1+k)(N-1)^{k-1} - (8N/9)^k$. While proving by induction, first note that $f(1) = N - (8N/9) > 0$. Now, let $f(k) > 0$ be true. Then we prove that $f(k+1) = (N - 1 + k)(N - 1)^k - (8N/9)^{k+1} > 0$. Now, since $f(k) = (N - 1 + k)(N - 1)^{k-1} - (8N/9)^k$, therefore,

$$f(k+1) > \frac{\{(N+k)(N-1)^k\}\{(8N/9)^k\} - \{(8N/9)^{k+1}\}\{(N-1+k)(N-1)^{k-1}\}}{(N-1+k)(N-1)^{k-1}(8N/9)^k} = A.$$

Now

$$A = \frac{(N+k)(N-1)^k}{(N-1+k)(N-1)^{k-1}} - \frac{(8N/9)^{k+1}}{(8N/9)^k} = \frac{(N+k)(N-1)}{(N-1+k)} - \frac{8N}{9} = \frac{N(N-1) + k(N-9)}{9(N-1+k)}$$

Thus, $A > 0$, for $N \geq 9$. For $N = 5$, $A > 0$ for $k < 5$. □

Thus, we have shown that for $N \equiv 1 \pmod 4$, $d_0 \in \mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,3}$.

Theorem 4.2 For $N \equiv 2 \pmod 4$ and $k < N-1$, $d_0 \in \mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,3}$.

Proof. Let $k \leq N-2$. We consider the cases k even and k odd separately.

<u>k even</u>. For the design d_0, $\det(N2^kC_2) = (N-2+k)^2(N-2)^{k-2}$. We now show that $(N-2+k)^2(N-2)^{k-2} > (8N/9)^k$.

For a fixed N, let $f(k) = (N-2+k)^2(N-2)^{k-2} - (8N/9)^k$. To prove by induction, first note that $f(2) = N^2 - (8N/9)^2 > 0$. Now, let $f(k) > 0$ be true. Then, since k is even, we prove that $f(k+2) = (N+k)^2(N-2)^k - (8N/9)^{k+2} > 0$. Now, since $f(k) = (N-2+k)^2(N-2)^{k-2} - (8N/9)^k > 0$, therefore,

$$f(k+2) > \frac{\{(N+k)^2(N-2)^k\}\{(8N/9)^k\} - \{(8N/9)^{k+2}\}\{(N-2+k)^2(N-2)^{k-2}\}}{(N-2+k)^2(N-2)^{k-2}(8N/9)^k} = A.$$

Now,

$$A = \frac{(N+k)^2(N-2)^k}{(N-2+k)^2(N-2)^{k-2}} - \frac{(8N/9)^{k+2}}{(8N/9)^k} = \frac{(N+k)^2(N-2)^2}{(N-2+k)^2} - \left(\frac{8N}{9}\right)^2.$$

To show $A > 0$, we may equivalently show that $\dfrac{(N+k)(N-2)}{(N-2+k)} > \dfrac{8N}{9}$,

or, show $9(N+k)(N-2) > 8N(N-2+k)$,

or, show $N(N-2) + k(N-18) > 0$. But this is always true for $N \geq 18$. For $N = 10$ and $N = 14$, since $k \leq N-2$, it is easy to see that the above inequality is always true.

For $N = 6$, we have to show that $4^{k-2}(4+k)^2 > (16/3)^k$, $k = 2, 4$. Putting the values in expression, we see that the inequality holds.

<u>k odd</u>. For the design d_0, $\det(N2^kC_2) = ((N-2+k)^2 - 1)(N-2)^{k-2}$. We now show that $((N-2+k)^2 - 1)(N-2)^{k-2} > (8N/9)^k$.

For a fixed N, let $f(k) = ((N-2+k)^2-1)(N-2)^{k-2} - (8N/9)^k$. To prove by induction, first note that $f(1) = ((N-1)^2-1)/(N-2) - (8N/9) = N - (8N/9) > 0$. Now, let $f(k) > 0$ be true. Then, since k is odd, we prove that $f(k+2) = ((N+k)^2-1)(N-2)^k - (8N/9)^{k+2} > 0$. Now, since $f(k) = ((N-2+k)^2-1)(N-2)^{k-2} - (8N/9)^k > 0$, therefore,

$$f(k+2) > \frac{\{((N+k)^2-1)(N-2)^k\}\{(8N/9)^k\} - \{(8N/9)^{k+2}\}\{((N-2+k)^2-1)(N-2)^{k-2}\}}{((N-2+k)^2-1)(N-2)^{k-2}(8N/9)^k} = A.$$

Now,

$$A=\frac{((N+k)^2-1)(N-2)^k}{((N-2+k)^2-1)(N-2)^{k-2}}-\frac{(8N/9)^{k+2}}{(8N/9)^k}=\frac{((N+k)^2-1)(N-2)^2}{((N-2+k)^2-1)}-\left(\frac{8N}{9}\right)^2,$$

or,

$$A=\frac{(N+k-1)(N+k+1)(N-2)^2}{(N-3+k)(N-1+k)}-\left(\frac{8N}{9}\right)^2=\frac{(N+k+1)(N-2)^2}{(N-3+k)}-\left(\frac{8N}{9}\right)^2.$$

Since $(N+k+1)>(N-3+k)$, to show $A>0$, it is sufficient to show that $9(N-2)\geq 8N$. But this is always true for $N\geq 18$. For $N=10$ and $N=14$, since $k\leq N-2$, it is easy to see that $A>0$.

For $N=6$, we have to show that $4^{k-2}((4+k)^2-1)>(16/3)^k$, $k=3$. Putting the values in expression, we see that the inequality holds. □

Thus, we have shown that for $N\equiv 2 \pmod 4$, $d_0\in\mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,3}$.

Theorem 4.3 For $N\equiv 3 \pmod 4$ and $k<N$, $d_0\in\mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,3}$.

Proof. We know that for $k\leq N-1$, eigenvalues of $X_0'X_0$ are $(N+1-k)$ and $(N+1)$ with multiplicity 1 and $k-1$ respectively. We now show that $\det(N2^kC_2)=(N+1-k)(N+1)^{k-1}>\left\{\frac{8N}{9}\right\}^k$.

We first prove that the above inequality holds for $k\leq N-8$ and then we separately treat the cases for remaining $k=N-7,N-6,\ldots,N-1$. For a fixed N, let $f(k)=(N+1-k)(N+1)^{k-1}-(8N/9)^k$. While proving by induction, first note that $f(1)=N-(8N/9)>0$. Now, let $f(k)>0$ be true. Then we prove that $f(k+1)=(N-k)(N+1)^k-(8N/9)^{k+1}>0$. Now, since $f(k)=(N+1-k)(N+1)^{k-1}-(8N/9)^k$, therefore,

$$f(k+1)>\frac{\{(N-k)(N+1)^k\}\{(8N/9)^k\}-\{(8N/9)^{k+1}\}\{(N+1-k)(N+1)^{k-1}\}}{(N+1-k)(N+1)^{k-1}(8N/9)^k}=A.$$

Now

$$A=\frac{(N-k)(N+1)^k}{(N+1-k)(N+1)^{k-1}}-\frac{(8N/9)^{k+1}}{(8N/9)^k}=\frac{(N-k)(N+1)}{(N+1-k)}-\frac{8N}{9}=\frac{N(N+1)-k(N+9)}{9(N+1-k)}.$$

Putting $k=N-8$, we see that $A=8/9>0$ for any N. Thus, we have shown that for $k\leq N-8$, the above inequality holds.

Now, we look into other cases $k=N-7,N-6,\ldots,N-1$. Let $k=N-\alpha$, $\alpha=1,2,\ldots,7$. Hence, $(N+1-k)(N+1)^{k-1}-\left\{\frac{8N}{9}\right\}^k=9^{N-\alpha}(\alpha+1)(N+1)^{N-\alpha-1}-8^{N-\alpha}NN^{N-\alpha-1}$.

Since $N+1 > N$, it suffices to show that for each k, $9^{N-\alpha}(\alpha+1) > 8^{N-\alpha}N$. It can be easily seen that $f_1(N,\alpha) = 9^{N-\alpha}(\alpha+1) - 8^{N-\alpha}N$ is an increasing function in N for $N \geq 23$ and $f_1(23,\alpha) > 0$ for $\alpha = 1, 2, \ldots, 7$. Thus, for $k = N-7, N-6, \ldots, N-1$ and $N \geq 23$, the inequality holds. Complete enumeration also shows that for $k \leq N-1$ and $N = 7$, 11, 15 and 19, $(N+1-k)(N+1)^{k-1} > \left\{\dfrac{8N}{9}\right\}^k$. □

Thus, we have shown that for $N \equiv 3 \pmod 4$, $d_0 \in \mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,3}$.

Comparing designs with $m = 2$ and $m = 5$

As seen above, for $m = 2$, $\det(N2^{k-2}C) = \dfrac{1}{4^k}\prod_{i=1}^{k} eig(X'X)$. Also, $det(N2^kC_5) \leq \left\{\dfrac{24N}{25}\right\}^k$. Thus, to show that the D-optimal design with $m = 5$ is inferior to d_0 it suffices to show $\det(N2^kC_5) > \left\{\dfrac{24N}{25}\right\}^k$.

We will divide this case further into three cases based on the values of N,
a) $N \equiv 1 \pmod 4$, b) $N \equiv 2 \pmod 4$ and c) $N \equiv 3 \pmod 4$.

Theorem 4.4 For $N \equiv 1 \pmod 4$ and $k < N$, $d_0 \in \mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,5}$ except $k = 4$ and $N = 5$.

Proof. We know that for $k \leq N-1$, eigenvalues of $X_0'X_0$ are $(N-1+k)$ and $(N-1)$ with multiplicity 1 and $k-1$ respectively. We now show that $\det(N2^kC_2) = (N-1+k)(N-1)^{k-1} > \left\{\dfrac{24N}{25}\right\}^k$. Doing this case on exactly similar lines as for $m = 3$, we get $25(N-1+k)A = N(N-1) + k(N-25)$. Thus, $A > 0$, for $N \geq 25$. For $N = 9$, 13, 17 and 21, $A > 0$ for $k < N-1$ and for $N = 5$, $A > 0$ for $k < N-2$. □

Thus, we have shown that for $N \equiv 1 \pmod 4$, $d_0 \in \mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,5}$ except $k = 4$ and $N = 5$.

Theorem 4.5 For $N \equiv 2 \pmod 4$ and $k < N-1$, $d_0 \in \mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,5}$ except when i) $N = 6$, $k = 4$ and ii) $N = 10$, $k = 7$, 8.

Proof. Let $k \leq N-2$. We consider the cases k even and k odd separately.

<u>k even</u>. For the design d_0, $\det(N2^kC_2) = (N-2+k)^2(N-2)^{k-2}$. We now show that $(N-2+k)^2(N-2)^{k-2} > (24N/25)^k$. Doing this case on exactly similar lines as for $m = 3$,

we only have to show that $N(N-2)+k(N-50)>0$, which is always true for $N \geq 50$. For $N = 14-42$, since $k \leq N-2$, it is easy to see that the above inequality is always true. For $N = 10$, the above inequality is only positive for $k \leq 6$ and for $N = 6$, it only holds for $k \leq 3$.

<u>k odd</u>. For the design d_0, $\det(N2^kC_2) = ((N-2+k)^2-1)(N-2)^{k-2}$. We now show that $((N-2+k)^2-1)(N-2)^{k-2} > (24N/25)^k$. Doing this case on exactly similar lines as for $m = 3$, we only have to show that $25(N-2) \geq 24N$, which is always true for $N \geq 50$. For $N = 14-42$, since $k \leq N-2$, it is easy to see that the above inequality is always true. For $N = 10$, the above inequality is only positive for $k \leq 6$ and for $N = 6$, it only holds for $k \leq 3$. □

Thus, we have shown that for $N \equiv 2 \pmod 4$, $d_0 \in \mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,5}$ except when i) $N = 6$, $k = 4$ and ii) $N = 10$, $k = 7, 8$.

Theorem 4.6 For $N \equiv 3 \pmod 4$ and $k < N$, $d_0 \in \mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,5}$ except when i) $N \leq 59$, $k = N-1$ ii) $N \leq 43$, $k = N-2$ iii) $11 \leq N \leq 31$, $k = N-3$ and iv) $15 \leq N \leq 19$, $k = N-4$.

Proof. We know that for $k \leq N-1$, eigenvalues of $X_0'X_0$ are $(N+1-k)$ and $(N+1)$ with multiplicity 1 and $k-1$ respectively. We now show that $\det(N2^kC_2) = (N+1-k)(N+1)^{k-1} > \left\{\dfrac{24N}{25}\right\}^k$.

We first prove that the above inequality holds for $k \leq N-24$ and then we separately treat the cases for remaining $k = N-\alpha$, $\alpha = 1, 2, \ldots, 23$. On exactly similar lines as for $m = 3$, we get $25(N+1-k)A = N(N+1) - k(N+25)$.

Putting $k = N-24$, we see that $A = 24/25 > 0$ for any N. Thus, we have shown that for $k \leq N-24$, the above inequality holds.

Now, for other cases $k = N-23, N-22, \ldots, N-1$. Let $k = N-\alpha$, $\alpha = 1, 2, \ldots, 23$, on similar lines as $m = 3$, we see that the inequality holds for $N \geq 59$ and $k = N-23, N-22, \ldots, N-2$ and for $N \geq 63$ and $k = N-1$. Complete enumeration for remaining $N \leq 59$ shows that $(N+1-k)(N+1)^{k-1} > \left\{\dfrac{24N}{25}\right\}^k$ for all N and $k \leq N-1$ except when i) $N \leq 59$, $k = N-1$ ii) $N \leq 43$, $k = N-2$ iii) $11 \leq N \leq 31$, $k = N-3$ and iv) $15 \leq N \leq 19$, $k = N-4$. □

Thus, we have shown that for $N \equiv 3 \pmod 4$, $d_0 \in \mathcal{D}_{N,k,2}$ is D-better than the D-optimal design in $\mathcal{D}_{N,k,5}$ except when i) $N \leq 59$, $k = N-1$ ii) $N \leq 43$, $k = N-2$ iii) $11 \leq N \leq 31$, $k = N-3$ and iv) $15 \leq N \leq 19$, $k = N-4$.

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