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Optimal Two-level Choice Designs for Estimating Specified Interaction Effects

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SUMMARY

This paper investigates optimal choice designs for models that include main effects and specified higher-order interaction effects. Existing optimal designs primarily focus on estimating all the main effects or all the two-factor interaction effects along with the main effects. However, in most practical choice experiments, only a limited number of two-factor and three-factor interactions are of substantive interest rather than the full set of possible interactions. Motivated by this practical consideration, we develop universally optimal choice designs that allow efficient estimation of main effects along with specified two- and three-factor interaction effects.

Keywords: Optimal choice designs, Main effects, Two-factor interactions, Three-factor interactions.

Dr. M.N. Dascentenary celebrations

To commemorate the centenary celebrations of Late Dr. M.N. Das, the Indian Society of Agricultural Statistics has brought out a special issue of the Journal comprising of invited papers from different parts of the globe. Dr. Das was a prolific researcher and contributed significantly to the theory of Statistics and its applications. Apart from being an outstanding researcher, he was also an excellent teacher. He had been a mentor to several Ph.D. students, and one among them was Dr. Aloke Dey. Among the authors here, Ashish Das had been a Ph.D. student of Dr. Dey while Soumen Manna had been a Ph.D. student of Dr. Ashish Das. Thus, here we have first, second and third generation Ph.D. students of Dr. M. N. Das who are contributing to honor Dr. M.N. Das through this special issue."Academic descendants" of Dr. M.N. Das are spread across the globe.

The contribution made here gels with Dr. Das's interest in application of design of experiments in varied fields of research. Market-research through choice experiments uses designs having interlinks with factorial designs-an area to which Dr. Das has contributed significantly. We present few results on optimal choice-designs as a tribute to Dr. M.N. Das.

1. INTRODUCTION

Discrete choice experiments are widely used to quantify consumer preferences across a broad range of application areas. A typical choice experiment consists of N choice sets, where each set contains m distinct options and no option is repeated within a set. Respondents are presented with the choice sets sequentially and are asked to select their most preferred option from each set based on their perceived utility. Each option in a choice set is characterized by n factors, with each factor taking two or more possible levels. In this paper, we focus on choice designs involving n two-level factors. Hence, each option corresponds to a treatment combination from a 2^n factorial experiment, and we refer to such an experiment as a 2^n choice experiment. A typical option (or treatment)in a 2^n choice experiment is denoted by

$$T_i = t_1^i \ldots t_x^i \ldots t_n^i,$$

where $t_x^i \in \{0, 1\}$, x=1, ..., n, represents the level of the xth factor. A choice design $d = d_{N,n,m}$ is defined as a

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collection of N choice sets, each containing m options, used in a 2^n choice experiment. The data obtained from such an experiment are then used to estimate the factorial effects of interest. For example, let us consider a 2^5 choice experiment where the five factors are the “Brand”, “Camera”, “Storage”, “Battery life” and “CT” (Cellular Technology) of a mobile. The levels of the factors areas follows.

Factors	*Brand*	*Camera*	*Storage*	*Battery*	*CT*
Level−0	*Apple*	20*MP*	64*GB*	16*H*	4*G*
Level−1	*Samsung*	25*MP*	128*GB*	24*H*	5*G*

An example of a choice design d for five factors, consisting of eight choice sets each containing four options, is given below:

$$d = d_{8,\,5,\,4} = \begin{pmatrix} 11111, & 00000, & 00111, & 11000 \\ 10110, & 01001, & 01110, & 10001 \\ 11010, & 00101, & 00010, & 11101 \\ 10011, & 01100, & 01011, & 10100 \\ 11100, & 00011, & 00100, & 11011 \\ 10101, & 01010, & 01101, & 10010 \\ 11001, & 00110, & 00001, & 11110 \\ 10000, & 01111, & 01000, & 10111 \end{pmatrix}$$
$$= (A_1,\, A_2,\, A_3,\, A_4)(say).$$

In this design, A_1, A_2, A_3, and A_4 are referred to as the component matrices of the design d, and the eight rows of d correspond to the eight choice sets. Respondents are presented with these choice sets and are asked to select their most preferred option from each set. The resulting choice data are then used to estimate the factorial effects of interest. Analyzing these estimates enables the researcher to determine which factorial effects have the greatest influence on respondents’ choice behavior. In general, a 2^n choice experiment allows for the estimation of at most 2^n-1 factorial effects. However, in practice, researchers are often not interested in estimating all possible interaction effects but rather a specified subset — for instance, interactions involving particular factors with the rest. In the above example, one may be interested in examining how each of the factors “Brand” and “Camera” interacts with the remaining three factors. In this paper, we discuss the construction of optimal choice designs for such specified interaction-effects models.

Most of the existing literature on choice experiments is developed under the multinomial logit framework of Street and Burgess (2007). The majority of research on optimal choice designs assumes, a priori, that either only the main effects or the main effects together with all two-factor interaction effects are of interest (see, for example, Graßhoff *et al.* (2003), Graßhoff *et al.* (2004), Street and Burgess (2007), Manna and Das (2016), Chai *et al.* (2019), and Großmann and Schwabe (2015)). In practice, however, many empirical studies do not consider the full set of possible interaction effects, but focus instead on a limited number of interactions that are substantively meaningful. Hence, there is clear practical value in developing choice designs that allow the estimation of specified interaction effects along side the main effects while requiring fewer choice sets. In many applied settings, the primary interest lies in estimating main effects together with selected two- and three-factor interaction effects.

Street and Burgess (2012) and Großmann and Schwabe (2015) noted that no general results exist for constructing optimal choice designs that accommodate main effects together with selected two- and three-factor interactions, although Street and Burgess (2007) previously illustrated the issue with a few examples. More recently, Chai *et al.* (2018) and Manna and Das (2024) proposed optimal choice designs under models restricted to main effects and a specified set of two-factor interactions. However, optimal designs for estimating three-factor interactions remain scarce, despite the fact that in many applications such effects are of substantive interest. For instance, in our earlier example, beyond the main effects one might wish to estimate two-factor interactions such as “Camera×Storage” or “Camera×Battery life,” as well as the three-factor interaction “Camera×Storage×Battery life.” This assumption is reasonable, since consumers seeking a high-quality camera typically also look for sufficient storage and battery capacity. In the literature, Jost and Möser (2023), Norman *et al.* (2023), and others have incorporated specific three-factor interactions in their choice models to improve model fit and stability. Motivated by these considerations, the present paper develops optimal choice designs for an extended specified model of Manna and Das (2024) that includes main effects, selected two- and three-factor interactions.

Let $f_1, ..., f_n$ denote the n factors in a 2^n choice experiment. The main effect associated with factor f_h is denoted by F_h, the two-factor interaction between factors f_h and f_g by F_{hg}, and the three-factor interaction among factors f_h, f_g, and f_l by F_{hgl}, where $h, g, l = 1, ..., n$. For notational convenience, we assume $h < g < l$ when defining the interaction effects F_{hg} and F_{hgl}.

We call our models 'specified choice models', which constitutes 'main effects plus specified two- and three-factor interaction effects'. To define specified interaction effects we consider two groups of factors, namely $\mathbf{f_1}$ and $\mathbf{f_2}$. Let $\mathbf{f_1}$ consist of k factors and $\mathbf{f_2}$ consist of the remaining $(n-k)$ factors. Without loss of generality, we assume $\mathbf{f_1} = \{f_1, ..., f_k\}$ and $\mathbf{f_2} = \{f_{(k+1)}, ..., f_n\}$. We denote F_{hg} be a two-factor interaction effect between the factors f_h and f_g, where $f_h \in \mathbf{f_1}$ and $f_g \in \mathbf{f_2}$. Similarly, we denote F_{hgl} be a three-factor interaction effects among the factors f_h, f_g and f_l, where $f_h \in \mathbf{f_1}$ and $f_g, f_l \in \mathbf{f_2}$. Thus, the factorial effects of interest in our model are $F = \{F_h, h = 1, ..., n; F_{hg}, h = 1, ..., k, g = k+1, ..., n; F_{hgl}, h = 1, ..., k, g < l, g, l = k+1, ..., n\}$. We call such a model as $\mathscr{T}_k$. Since the interaction effects in model $\mathscr{T}_k$ are specified by the first k factors of $\mathbf{f_1}$, we refer to $\mathbf{f_1}$ as the specified group of factors and to $\mathbf{f_2}$ as the unspecified group of factors. Therefore, in model, F consist of n main effects, $k(n-k)$ two-factor interaction effects and $k\binom{n-k}{2}$ three factor interaction effects. All the factorial effects in $F$are assumed to be arranged in lexicographical order. In this paper, we develop optimal choice designs for the model $\mathscr{T}_k$, where $k = 1, 2$.

As noted by Großmann and Schwabe (2015), choice sets of size $m = 2, 3,$ or 4 are generally preferred in practice, since $m \geq 5$ creates cognitive burden on respondents that can adversely affect response quality. Motivated by this consideration, the present paper develops universally optimal choice designs for estimating main effects together with a specified set of two- and three-factor interaction effects for choice set sizes $m = 3$ and $m = 4$, under the assumption that all remaining interaction effects are negligible. Universally optimal designs are, in particular, also A-, D-, and E-optimal.

Let $C = C_d$ denote the information matrix (Street and Burgess (2007)) associated with a choice design d, and let $D = D_{N, n, m}$ represent the class of all such designs $d = d_{N, n, m}$ used to estimate the factorial effects F. Following Kiefer (1975), we state the sufficient condition for universal optimality as follows:

Suppose $d^* \in \mathscr{D}$ and C_{d^*} satisfies (i) C_{d^*} is a scalar multiple of the identity matrix and, (ii) trace(C_{d^*})= $\max_{d \in \mathscr{D}}$ trace(C_d). Then, d^* is universally optimal in $\mathscr{D}$.

A detailed treatment of the C-matrix associated with a choice design d for estimating the factorial effects F is provided in the supplementary material of Manna and Das (2024). In this paper, we construct universally optimal choice designs for choice set sizes $m = 3$ and $m = 4$. For a given number of factors n, consider the following normalized Hadamard matrix of order 2^v, where $2^v \geq n$:

$$H = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \underbrace{\otimes \ldots \otimes}_{v\ times} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{1.1}$$

Let

$$A = \frac{H + J}{2}, \tag{1.2}$$

where J is the matrix of all ones. Let U and V be matrices formed from k and $(n-k)$ distinct columns of A, respectively. Define the four component matrices as

$$A_1 = [U \vdots V],\ A_2 = [\bar{U} \vdots \bar{V}],\ A_3 = [\bar{U} \vdots V],\ A_4 = [U \vdots \bar{V}],$$

where $\bar{U}$ and $\bar{V}$ denote the complement matrices obtained by interchanging 0 sand 1 sin U and V, respectively.

Using these component matrices, we consider two choice designs: $d_1^* \in \mathscr{D}_{2^v, n, 4}$ and $d_2^* \in \mathscr{D}_{2^{v+1}, n, 3}$, defined as follows:

$$d_1^* = (A_1, A_2, A_3, A_4) \tag{1.3}$$

and

$$d_2^* = \left(\begin{bmatrix} A_1 \\ A_1 \end{bmatrix}, \begin{bmatrix} A_2 \\ A_2 \end{bmatrix}, \begin{bmatrix} A_3 \\ A_4 \end{bmatrix} \right). \tag{1.4}$$

With an appropriate choice of U and V, we now demonstrate how to construct the optimal choice designs d_1^* and d_2^* for the specified choice models $\mathscr{T}_k$, $k = 1, 2$.

As with many related constructions, the proposed designs are developed under the multinomial logit framework and rely on the indifference assumption of equal choice probabilities. It means, before collecting data, we don't know real preferences. the assumption of equal choice probability ensures that the designs are not biased toward some particular outcomes. It gives a neutral starting point. The indifference assumption of equal choice probability is not only a behavioral baseline but also a technical tool that makes the information matrix symmetric and tractable, which is essential in constructing optimal choice designs. Designs constructed under this assumption are commonly referred to in the literature as *utility-neutral* designs (Huberand Zwerina (1996)).

2. OPTIMAL CHOICE DESIGNS UNDER THE MODEL $\mathscr{T}_1$

In the model $\mathscr{T}_1$, the specified group $\mathbf{f_1}$ contains only one factor and the unspecified group $\mathbf{f_2}$ contains the remaining $(n-1)$ factors, that is $\mathbf{f_1}=\{f_1\}$ and $\mathbf{f_2} = \{f_2, ..., f_n\}$. Under this model, we are interested in estimating n main effects $F_1, ..., F_n$, and $(n-1)$ specified two-factor interaction effects $F_{12}, ..., F_{1n}$, and $(n-1)(n-2)/2$ three-factor interaction effects $F_{123}, F_{124}, ..., F_{1(n-1)n}$. Therefore, in this section, we are interested in estimating $F = \{F_1, ..., F_n, F_{12}, ..., F_{1n}, F_{123}, F_{124}, F_{134}, ..., F_{1(n-1)n}\}$.

Statement 2.1. *Let* ν *be the smallest integer such that* $n \le 2^\nu$. *Then, optimal choice designs* d_1^* *and* d_2^* *can be constructed in* $\mathscr{D}_{2^\nu, n, 4}$ *and* $\mathscr{D}_{2^{\nu+1}, n, 3}$, *respectively, for estimating F.*

Construction 2.1. *Construct a Hadamard matrix H of order* 2^ν *according to (1.1) and take the corresponding Hadamard matrix A of (1.2). Let U consist of the first column of A while V consist of any* $(n-1)$ *remaining columns of A. Construct* d_1^* *and* d_2^* *of (1.3) and (1.4), respectively, using these U and V. The constructed designs* d_1^* *and* d_2^* *are then optimal in* $\mathscr{D}_{2^\nu, n, 4}$ *and* $\mathscr{D}_{2^{\nu+1}, n, 3}$, *respectively, for estimating F (refer to Appendix for the proof).*

Example 2.1. *Consider the case where* $n = 4$, *and the objective is to estimate all main effects together with all two- and three-factor interaction effects involving the first factor. So,* $\mathbf{f_1} = \{f_1\}$, $\mathbf{f_2} = \{f_2, f_3, f_4\}$ *and* $F = \{F_1, F_2, F_3, F_4, F_{12}, F_{13}, F_{14}, F_{123}, F_{124}, F_{134}\}$. *Here,*

$$A = \begin{pmatrix} 1111 \\ 1010 \\ 1100 \\ 1001 \end{pmatrix}, \; U = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \; and \; V = \begin{pmatrix} 111 \\ 010 \\ 100 \\ 001 \end{pmatrix}.$$

Hence,

$$A_1 = \begin{pmatrix} 1111 \\ 1010 \\ 1100 \\ 1001 \end{pmatrix}, \; A_2 = \begin{pmatrix} 0000 \\ 0101 \\ 0011 \\ 0110 \end{pmatrix}, \; A_3 = \begin{pmatrix} 0111 \\ 0010 \\ 0100 \\ 0001 \end{pmatrix}, \; and$$

$$A_4 = \begin{pmatrix} 1000 \\ 1101 \\ 1011 \\ 1110 \end{pmatrix}.$$

Therefore, the designs

$$d_1^* = \begin{pmatrix} 1111, & 0000, & 0111, & 1000 \\ 1010, & 0101, & 0010, & 1101 \\ 1100, & 0011, & 0100, & 1011 \\ 1001, & 0110, & 0001, & 1110 \end{pmatrix} \text{ and}$$

$$d_2^* = \begin{pmatrix} 1111, & 0000, & 0111 \\ 1010, & 0101, & 0010 \\ 1100, & 0011, & 0100 \\ 1001, & 0110, & 0001 \\ 1111, & 0000, & 1000 \\ 1010, & 0101, & 1101 \\ 1100, & 0011, & 1011 \\ 1001, & 0110, & 1110 \end{pmatrix}$$

are optimal in $\mathscr{D}_{4, 4, 4}$ *and* $\mathscr{D}_{8, 4, 3}$, *respectively, for estimating* $F = \{F_1, F_2, F_3, F_4, F_{12}, F_{13}, F_{14}, F_{123}, F_{124}, F_{134}\}$.

3. OPTIMAL CHOICE DESIGNS UNDER THE MODEL $\mathscr{T}_2$

We now focus on the model $\mathscr{T}_2$, in which the specified group $\mathbf{f}_1$ consists of two factors, while the unspecified group $\mathbf{f}_2$ comprises the remaining $(n-2)$ factors. Hence, $\mathbf{f_1} = \{f_1, f_2\}$, $\mathbf{f_2} = \{f_3, ..., f_n\}$, and we are interested in estimating n main effects, $2(n-2)$ two-factor interaction effects, and $2\binom{n-2}{2}$ three factor interaction effects. Therefore, the factorial effects of interest are $F = \{F_1, \ldots, F_n, F_{13}, \ldots, F_{1n}, F_{23}, \ldots, F_{2n}, F_{134}, F_{135}, \ldots, F_{1(n-1)n}, F_{234}, F_{235}, \ldots, F_{2(n-1)n}\}$.

Statement 3.1. *Let* ν *be the smallest integer such that* $2(n-1) \leq 2^{\nu}$*. Then, optimal choice designs* d_1^* *and* d_2^* *can be constructed in* $\mathscr{D}_{2^{\nu}, n, 4}$ *and* $\mathscr{D}_{2^{\nu+1}, n, 3}$*, respectively, for estimating F.*

Construction 3.1. *Construct a Hadamard matrix H of order* 2^{ν} *according to (1.1) and take the corresponding (0, 1) matrix A of (1.2) as* $A = [a_1 a_2 \cdots a_{2^{\nu}}]$*, where* a_i *denotes the i-th column of A. Consider* $U = [a_1 a_2]$ *and choose the columns* $a_{(2i-1)}, i = 2, \ldots, (n-1)$*, and construct V. Construct* d_1^* *and* d_2^* *of (1.3) and (1.4), respectively, using these U and V. The constructed designs* d_1^* *and* d_2^* *are then optimal in* $\mathscr{D}_{2^{\nu}, n, 4}$ *and* $\mathscr{D}_{2^{\nu+1}, n, 3}$*, respectively, for estimating F(refer to Appendix for the proof).*

Example 3.1. *Suppose* $n = 5$ *and the objective is to estimate all main effects together with all two-and three-factor interaction effects involving the first two factors. Accordingly, the specified group is* $\mathbf{f}_1 = \{f_1, f_2\}$ *and the unspecified group is* $\mathbf{f}_2 = \{f_3, f_4, f_5\}$*. These to f factorial effects of interest is therefore*

$F = \{F_1, F_2, F_3, F_4, F_5, F_{13}, F_{14}, F_{15}, F_{23}, F_{24}, F_{25}, F_{134}, F_{135}, F_{145}, F_{234}, F_{235}, F_{245}\}$.

Note that $2(n-1) = 8 \leq 2^3$*, and hence* $\nu = 3$*.We therefore construct a Hadamard matrix of order* $2^3 = 8$ *using* (1.1)*, and obtain the corresponding matrix A in* (1.2) *as*

$A = [a_1\, a_2\, a_3\, a_4\, a_5\, a_6\, a_7\, a_8]$,

where a_i *denotes the ith column of A for* $i = 1, \ldots, 8$.

Here, $U = [a_1 a_2]$ *and* $V = [a_3 a_5 a_7]$*. Hence,* $A_1 = [a_1\, a_2\, a_3\, a_5\, a_7]$, $A_2 = [\bar{a}_1\, \bar{a}_2\, \bar{a}_3\, \bar{a}_5\, \bar{a}_7]$, $A_3 = [\bar{a}_1\, \bar{a}_2\, a_3\, a_5\, a_7]$, *and* $A_4 = [a_1\, a_2\, \bar{a}_3\, \bar{a}_5\, \bar{a}_7]$*. Therefore, the designs*

$$d_1^* = \begin{pmatrix} 11111, & 00000, & 00111, & 11000 \\ 10111, & 01000, & 01111, & 10000 \\ 11010, & 00101, & 00010, & 11101 \\ 10010, & 01101, & 01010, & 10101 \\ 11100, & 00011, & 00100, & 11011 \\ 10100, & 01011, & 01100, & 10011 \\ 11001, & 00110, & 00001, & 11110 \\ 10001, & 01110, & 01001, & 10110 \end{pmatrix} \text{ and}$$

$$d_2^* = \begin{pmatrix} 11111, & 00000, & 00111 \\ 10111, & 01000, & 01111 \\ 11010, & 00101, & 00010 \\ 10010, & 01101, & 01010 \\ 11100, & 00011, & 00100 \\ 10100, & 01011, & 01100 \\ 11001, & 00110, & 00001 \\ 10001, & 01110, & 01001 \\ 11111, & 00000, & 11000 \\ 10111, & 01000, & 10000 \\ 11010, & 00101, & 11101 \\ 10010, & 01101, & 10101 \\ 11100, & 00011, & 11011 \\ 10100, & 01011, & 10011 \\ 11001, & 00110, & 11110 \\ 10001, & 01110, & 10110 \end{pmatrix}$$

are optimal in $\mathscr{D}_{8, 5, 4}$ *and* $\mathscr{D}_{16, 5, 3}$*, respectively, for estimating* $F = \{F_1, F_2, F_3, F_4, F_5, F_{13}, F_{14}, F_{15}, F_{23}, F_{24}, F_{25}, F_{134}, F_{135}, F_{145}, F_{234}, F_{235}, F_{245}\}$.

4. DISCUSSION AND CONCLUSIONS

Constructing optimal choice designs becomes particularly challenging when practitioners seek to estimate higher-order interaction effects along side main effects. In practice, interest typically extends to interaction effects involving at most three factors, as interactions of higher order rarely have meaningful practical interpretation. Under the utility-neutral modeling framework, Street and Burgess (2004) and Großmann *et al.* (2012) developed optimal paired choice designs for estimating main effects together with all two-factor inter-action effects. However, these designs require a large number of choice sets, which limits their applicability in real-world choice experiments.

In many choice investigation problems, researchers are interested not in all possible higher-order interactions, but only in a small, substantively meaningful subset. To address this issue, Chai *et al.* (2018) and Manna and Das (2024) proposed optimal choice designs for models that include main effects and specified two-factor interaction effects, using relatively fewer choice sets. Nevertheless, there exist important choice situations in which selected three-factor interaction effects are also of interest, yet optimal designs for such models have not been available to date. The present paper fills this gap by developing optimal choice designs for models that include main effects together with specified two- and three-factor interaction effects.

For ease of reference, we denote the papers by Chai *et al.* (2018), Manna and Das (2024), and the present work as CDS18, MD24, and MDC25, respectively. Table 4.1 summarizes the design parameters of the optimal choice designs proposed in CDS18 and MD24 for models involving main effects and up to specified two-factor interaction effects. The optimal design parameters reported under MDC25 correspond to models with $k = 1$ and $k = 2$, which include main effects and upto specified three-factor interaction effects. For a given number of factors n (upto $n = 9$), were port two key characteristics of the proposed designs: P, the maximum number of factorial effects included in the model, and N, the number of choice sets required for the corresponding optimal design. The subscript k in column P denotes the specified model, where $k \in \{1, 2\}$ for CDS18 and MDC25, and $k \in \{1, 2, 3, 4\}$ for MD24.

The designs proposed under MDC25 extend existing results by accommodating main effects together with specified three-factor interaction effects, whereas the designs in CDS18 and MD24 are restricted to main effects and specified two-factor interactions. These extensions provide greater flexibility for practitioners in constructing optimal choice designs across a wider range of choice models. Moreover, since the proposed designs are straight forward to construct and do not require advanced expertise in statistical design theory, they are well suited for applied researchers who use choice experiments to study behavioral decision-making problems.

Despite their advantages, the proposed designs are subject to several limitations. First, our attention is restricted to designs involving two-level attributes. Extending the results to three-level or mixed-level attributes would broaden their applicability. Second, we focus on two specified model configurations. Developing optimal designs with more than two factors in the specified group would further enhance modeling flexibility. Third, the current framework considers two- and three-factor interactions between factors in $\mathbf{f}_1$ and those in $\mathbf{f}_2$. Future research could explore optimal designs that also allow interaction effects within $\mathbf{f}_1$ and/or within $\mathbf{f}_2$. Finally, our specified-model approach assumes prior knowledge of which two- and three-factor interaction effects are relevant. In situations where such prior information is unavailable, this assumption may be restrictive. In the design literature, optimal designs for classes of candidate models sharing common main effects but differing in interaction structures have been studied under the framework of Common Variance Designs (Chowdhury *et al.* (2020); Mandal and Mukerjee (2005)). It will be interesting to see how to obtain Common Variance Choice Designs for a set of candidate choice models.

Table 4.1. Comparison of the optimal designs proposed by CDS18, MD24 and MDC25

n	*m* = 3						*m* = 4					
	CDS18		**MD24**		**MDC25**		**CDS18**		**MD24**		**MDC25**	
	P	*N*	*P*	*N*	*P*	*N*	*P*	*N*	*P*	*N*	*P*	*N*
3	5_1	8	5_1	8	6_1	8	5_1	4	5_1	4	6_1	4
	5_2	16	5_2	8	5_2	8	5_2	8	5_2	4	5_2	4
	7_1	8	7_1	8	10_1	8	7_1	4	7_1	4	10_1	4
4	8_2	16	8_2 7_3	16 16	10_2	16	8_2	8	8_2 7_3	8 8	10_2	8
	9_1	16	9_1	16	15_1	16	9_1	8	9_1	8	15_1	8
5	11_2	32	11_2 11_3	16 32	17_2	16	11_2	16	11_2 11_3	8 16	17_2	8
			9_4	16					9_4	8		
	11_1	16	11_1	16	21_1	16	11_1	8	11_1	8	21_1	8
6	14_2	32	14_2 15_3	32 32	26_2	32	14_2	16	14_2 15_3	16 16	26_2	16
			14_4	32					14_4	16		
	13_1	16	13_1	16	28_1	16	13_1	8	13_1	8	28_1	8
7	17_2	32	17_2 19_3	32 64	37_2	32	17_2	16	17_2 19_3	16 32	37_2	16
			19_4	32					19_4	16		
	15_1	16	15_1	16	36_1	16	15_1	8	15_1	8	36_1	8
8	20_2	32	20_2 23_3	32 64	50_2	32	20_2	16	20_2 23_3	16 32	50_2	16
			24_4	64					24_4	32		
	17_1	24	17_1	32	45_1	32	17_1	12	17_1	16	45_1	16
9	23_2	48	23_2 27_3	32 64	65_2	32	23_2	24	23_2 27_3	16 32	65_2	16
			29_4	64					29_4	32		

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APPENDIX

Proof: d_1^* and d_2^* are optimal for estimating F under the model $\mathscr{T}_u$, u=1, 2

Note that this paper is an extension of the work by Mannaand Das (2024). In their study, the authors obtained the optimal designs d_1^* and d_2^* for estimating the main effects and a specified set of two-factor interaction effects. In contrast, the present paper extends their model to additionally allow the estimation of specified three-factor interactions.

Accordingly, the only modification in the current setup is that, while Fin Manna and Das (2024) consisted of n main effects and $k\binom{n-k}{2}$ two-factor interactions, here F further includes $kn-k$ three-factor interaction effects.

Since the proof of optimality for the proposed designs follows the same line of argument as that presented in the supplementary notes of Manna and Das (2024), we do not reproduce the complete proof here. Instead, we outline only the additional cases that need to be incorporated into the earlier proof of Manna and Das (2024). Interested readers are referred to the supplementary material of Manna and Das (2024) for the detailed proof. For consistency and simplicity, we adopt the same notation as used in Manna and Das(2024).

Outline for additional changes

1. The total number of factorial effects Q in F now become $n+k(n-k)+k\binom{n-k}{2}$ instead of $n+k(n-k)$.
2. The new definition of τ_q^i of the equation (0.1) will now be

$$\tau_q^i = \begin{cases} t_q^i & \text{when } q \in \{1, \ldots, n\}, \\ t_h^i + t_g^i + 1 \pmod 2 & \text{when } q \in \{n+1, \ldots, n+ \\ & k(n-k)\} \text{ and } F_{(q)} = F_{hg}, \\ t_h^i + t_g^i + t_l^i \pmod 2 & \text{when } q \in \{n+k(n-k)+ \\ & 1, \ldots, Q\} \text{ and } F_{(q)} = F_{hgl}. \end{cases}$$

3. The models $\mathscr{M}_u$, $u = 1, 2, 3, 4$ now be called $\mathscr{T}_k$, k=1, 2.

   In section 3:

4. The notations N_u, $\bar{N}u$, now becomes N_k, $\bar{N}k$, k=1, 2.
5. Under the **Part 1** of the proof (d_1^* is optimal for estimating F under the model $\mathscr{T}_k$), add the following three additional cases:

   Case 4: when $q \in \{1, ..., n\}$ and $r \in \{n+k(n-k)+1, ..., Q\}$.

   Under this case, we can consider $F_{(q)}=F_q$ and $F_{(r)}=F_{hgl}$. Based on the value of q, we get the following two sub cases.

   Subcase 4.1: when q, $h \in N_k$, g, $l \in \bar{N}k$.

   Here, $z_{p1} = t_{pq}$ and $z_{p2} = t_{ph}+t_{pg}+t_{pl}$ (mod 2). Then, from (3.1), we observe that all effective choice sets $S_p(q, r)$ are of the following type:

   $S_p(q, r) = (z_{p1}z_{p2}, \bar{z}_{p1}\bar{z}_{p2}, \bar{z}_{p1}\bar{z}_{p2}, z_{p1}z_{p2})_{q,r}$

   Subcase 4.2: when $h \in N_k$, q, g, $l \in \bar{N}k$.

   Here, $z_{p1} = t_{pq}$ and $z_{p2} = t_{ph}+t_{pg}+t_{pl}$ (mod 2). Then, from (3.1), we observe that all effective choice sets $S_p(q, r)$are of the following type:

   $S_p(q, r) = (z_{p1}z_{p2}, \bar{z}_{p1}\bar{z}_{p2}, z_{p1}\bar{z}_{p2}, \bar{z}_{p1}z_{p2})_{q,r}$

   Case 5: when $q \in \{n+1, ..., k(n-k)\}$ and $r \in \{n+k(n-k)+1, ..., Q\}$.

   Under this case, we can consider $F_{(q)}=F_{hg}$ and $F_{(r)} = F_{uxy}$. According to the choice of F, h, $u \in N_k$, g, x, $y \in \bar{N}k$. Here, $z_{p1} = t_{ph}+t_{pg}+1$ (mod2) and $z_{p2} = t_{pu}+t_{px}+t_{py}$ (mod2). Then, from(3.1), we observe that all effective choice sets $S_p(q, r)$ are of the following type:

   $S_p(q, r) = (z_{p1}z_{p2}, z_{p1}\bar{z}_{p2}, \bar{z}_{p1}\bar{z}_{p2}, \bar{z}_{p1}z_{p2})_{q,r}$

   Case 6: when both q, $r \in \{n+k(n-k)+1, ..., Q\}$.

   Under this case, we can consider $F_{(q)}=F_{hgl}$ and $F_{(r)}=F_{uxy}$. According to the choice of F, h, $u \in N_k$, g, l, x, $y \in \bar{N}k$. Here, $z_{p1} = t_{ph}+t_{pg}+t_{pl}$(mod2) and $z_{p2}=t_{pu}+t_{px}+t_{py}$(mod2). Then, from(3.1), we observe that all effective choice sets $S_p(q, r)$ are of the following type:

   $S_p(q, r)=(z_{p1}z_{p2}, \bar{z}_{p1}\bar{z}_{p2}, \bar{z}_{p1}\bar{z}_{p2}, z_{p1}z_{p2})_{q,r}$
6. Under the **Part 1** of the proof, in **Category 1**, change the first line as if q, r fall under Subcases 1.3, 2.1, 2.2, 4.2, or Case 5, ...
7. Under the **Part 1** of the proof, in **Category 2**, change the first line as if q, r fall under Subcases 1.1, 1.2, 4.1, or Cases 3, 6, ...

8. Under the **Part 2** of the proof (d_2^* is optimal for estimating F under the model $\mathscr{T}_k$), add the following three additional cases:

Case 4: when $q \in \{1, ..., n\}$ and $r \in \{n+k(n-k)+1, ..., Q\}$.

Under this case, we can consider $F_{(q)}=F_q$ and $F_{(r)}=F_{hgl}$. Based on the value of q, we get the following two sub cases.

Subcase 4.1: when $q, h \in N_k$, $g, l \in \bar{N}k$.

Here, $z_{p1} = t_{pq}$ and $z_{p2} = t_{ph} + t_{pg} + t_{pl}$ (mod2). Then, from (3.2) and (3.3), we observe that all effective choice sets $S_p(q, r)$ are of the following type:

$$Sp(q,\ r) = \begin{cases} (z_{p1}z_{p2},\ \bar{z}_{p1}\bar{z}_{p2},\ \bar{z}_{p1}\bar{z}_{p2})_{q,r}, & p = 1,\dots,N/2, \\ (z_{p1}z_{p2},\ \bar{z}_{p1}\bar{z}_{p2},\ z_{p1}z_{p2})_{q,r}, & p = N/2+1,\dots,N. \end{cases}$$

Subcase 4.2: when $h \in N_k$, $q, g, l \in \bar{N}k$.

Here, $z_{p1} = t_{pq}$ and $z_{p2} = t_{ph} + t_{pg} + t_{pl}$ (mod2). Then, from (3.2) and (3.3), we observe that all effective choice sets $S_p(q, r)$ are of the following type:

$$Sp(q,\ r) = \begin{cases} (z_{p1}z_{p2},\ \bar{z}_{p1}\bar{z}_{p2},\ z_{p1}\bar{z}_{p2})_{q,r}, & p = 1,\dots,N/2, \\ (z_{p1}z_{p2},\ \bar{z}_{p1}\bar{z}_{p2},\ \bar{z}_{p1}z_{p2})_{q,r}, & p = N/2+1,\dots,N. \end{cases}$$

Case 5: when $q \in \{n + 1, ..., k(n - k)\}$ and $r \in \{n + k(n - k) + 1, ..., Q\}$.

Under this case, we can consider $F_{(q)} = F_{hg}$ and $F_{(r)} = F_{uxy}$. According to the choice of F, $h, u \in N_k$, $g, x, y \in \bar{N}k$. Here, $z_{p1} = t_{ph} + t_{pg} + 1$ (mod2) and $z_{p2} = t_{pu} + t_{px} + t_{py}$ (mod2). Then, from (3.2) and (3.3), we observe that all effective choice sets $S_p(q, r)$ are of the following type:

$$Sp(q,\ r) = \begin{cases} (z_{p1}z_{p2},\ z_{p1}\bar{z}_{p2},\ \bar{z}_{p1}\bar{z}_{p2})_{q,r}, & p = 1,\dots,N/2, \\ (z_{p1}z_{p2},\ z_{p1}\bar{z}_{p2},\ \bar{z}_{p1}z_{p2})_{q,r}, & p = N/2+1,\dots,N. \end{cases}$$

Case 6: when both $q, r \in \{n + k(n - k) + 1, ..., Q\}$.

Under this case, we can consider $F_{(q)} = F_{hgl}$ and $F_{(r)} = F_{uxy}$. According to the choice of F, $h, u \in N_k$, $g, l, x, y \in \bar{N}k$. Here, $z_{p1} = t_{ph} + t_{pg} + t_{pl}$ (mod2) and $z_{p2} = t_{pu} + t_{px} + t_{py}$ (mod2). Then, from (3.2) and (3.3), we observe that all effective choice sets $S_p(q, r)$ are of the following type:

$$Sp(q,\ r) = \begin{cases} (z_{p1}z_{p2},\ \bar{z}_{p1}\bar{z}_{p2},\ \bar{z}_{p1}\bar{z}_{p2})_{q,r}, & p = 1,\dots,N/2, \\ (z_{p1}z_{p2},\ \bar{z}_{p1}\bar{z}_{p2},\ z_{p1}z_{p2})_{q,r}, & p = N/2+1,\dots,N. \end{cases}$$

9. Under the **Part 2** of the proof, in **Category 1**, change the first line as when q, r fall under Subcases 1.1, 1.2, 4.1 or Cases 3, 6.

10. Under the **Part 2** of the proof, in **Category 3**, change the first line as when q, r fall under Subcases 4.2 or Case 2, 5.