TWO-LEVEL MINIMUM ABERRATION DESIGNS UNDER A CONDITIONAL MODEL WITH A PAIR OF CONDITIONAL AND CONDITIONING FACTORS

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Abstract: Two-level factorial designs are considered under a conditional model with a pair of conditional and conditioning factors. Such a pair can arise in many practical situations. With properly defined main effects and interactions, an appropriate effect hierarchy is introduced under the conditional model. A complementary set theory as well as an efficient computational procedure, supported by a powerful recursion relation, are developed to implement the resulting design strategy, leading to minimum aberration designs. This calls for careful handling of many new and subtle features of the conditional model as compared to the traditional one.

Key words and phrases: Bias, complementary set, effect hierarchy, model robustness, orthogonal array, regular design, universal optimality, wordlength pattern.

1. Introduction

Fractional factorial designs are of significant interest due to their wide applicability to diverse fields. Exploration of these designs under the minimum aberration (MA) and related model robustness criteria has received much attention and the two-level case has been particularly focused on because of its popularity among practitioners. We refer to Mukerjee and Wu (2006), Wu and Hamada (2009), Xu, Phoa and Wong (2009), and Cheng (2014) for surveys and further references.

In this paper, we consider two-level factorials but the setting is different from the traditional one. Among the factors, there is a pair, F_1 and F_2 , such that the main and interaction effects involving F_1 are defined conditionally on each fixed level of F_2 . To motivate the ideas, suppose there are only two factors F_1 and F_2 , each at levels 0 and 1. With the treatment effects denoted by $\tau(00)$, $\tau(01)$, $\tau(10)$ and $\tau(11)$, main effect of F_1 is traditionally defined in terms of the arithmetic mean of the simple effects $\tau(00) - \tau(10)$ and $\tau(01) - \tau(11)$. One can view (Wu and Hamada, 2009, p. 164) these simple effects as conditional main effects of F_1 , for F_2 held fixed at levels 0 and 1, respectively. There are practical situations, however, where these conditional effects, which compare the levels of F_1 separately at each fixed level of F_2 , are themselves of interest rather than the traditional main effect of F_1 . A conditional model, with F_1 and F_2 as the conditional and conditioning factors, respectively, is appropriate in situations of this kind.

The interests in a given context determine a choice between the traditional and conditional models as well as the specification in advance of the conditional and conditioning factors in the latter model. For example, if motor and speed are two factors in an industrial experiment on fuel consumption, there being two motors each of which can be run at two speeds, say 1,500 rpm and 2,500 rpm, and interest lies in comparing the speeds separately for each motor, then the conditional model is relevant, with speed and motor as the conditional and conditioning factors respectively. Their roles get reversed if, on the other hand, comparison of the motors separately at each speed is of interest. Any other factor can be handled in the traditional way and termed a traditional factor if there is no particular interest in comparing its levels separately at each fixed level of another factor. We refer to the Fisher lecture paper of Wu (2015) for further examples of situations from social sciences or on comparison of genotypes within environmental conditions where the conditional model is appropriate.

Some work has been reported in the literature on the analysis aspects of the conditional model. Wu (2015) initiated work in this direction and the ideas were developed to a much fuller extent in Su and Wu (2017). But the design issues under this model, taking due cognizance of the objects of interest, have not so far been attended to. The present paper initiates a systematic study of the design problem with one pair of conditional and conditioning factors, the other factors being traditional. This is the case in many practical situations which warrant the use of the conditional model. We begin by rigorously defining the main effects and interactions under this model and observe that even with a single pair of conditional and conditioning factors, as many as half of these effects differ from the traditional ones. Thus a new effect hierarchy is called for, which is introduced through a prior specification on treatment effects and found to match our intuition. This paves the way for a sensible design strategy along with a minimum aberration criterion which aims at sequentially minimizing the bias caused in the estimation of the main effects by successive interactions in the effect hierarchy. A complementary set theory as well as an efficient computational procedure, supported by a powerful recursion relation, are developed to implement the design

strategy. In the process, many new features and complexities of the conditional model, compared to the traditional one, come to the fore. For example, not all main effects are seen to enjoy the same status, successive terms in the wordlength pattern (WLP) do not always involve words of progressively higher lengths, and new identities emerge in the complementary set theory.

2. Parametrization and Effect Hierarchy

2.1. Parametrization

Consider a 2^n factorial with $n \geq 3$ factors, each at levels 0 and 1. Define Ω as the set of the $\nu = 2^n$ binary *n*-tuples. For $i_1 \dots i_n \in \Omega$, let $\tau(i_1 \dots i_n)$ be the treatment effect of treatment combination $i_1 \dots i_n$. Similarly, in a traditional factorial setup, for $j_1 \dots j_n \in \Omega$, we write $\theta(j_1 \dots j_n)$ to denote the parameter representing factorial effect $F_1^{j_1} \dots F_n^{j_n}$ when $j_1 \dots j_n$ is nonnull, and $\theta(0 \dots 0)$ to denote the general mean. Let τ and θ be $\nu \times 1$ vectors with elements $\tau(i_1 \dots i_n)$ and $\theta(j_1 \dots j_n)$, respectively, arranged in the lexicographic order; e.g., if n = 3, then

$$\theta = (\theta(000), \theta(001), \theta(010), \theta(011), \theta(100), \theta(101), \theta(110), \theta(111))',$$

where the prime indicates transpose. Then the traditional full factorial model is

$$\tau = H^{\otimes n}\theta,\tag{2.1}$$

where \otimes represents Kronecker product and $H^{\otimes n}$ denotes the *n*-fold Kronecker product of

$$H = \begin{pmatrix} 1 & 1\\ 1 & -1 \end{pmatrix}, \tag{2.2}$$

a Hadamard matrix of order two. Let $H(0) = (1 \quad 1)$ and $H(1) = (1 \quad -1)$ stand for the top and bottom rows of H, respectively.

Continuing with n two-level factors F_1, \ldots, F_n , now consider a conditional model with a pair of conditional and conditioning factors, say F_1 and F_2 , respectively. The other factors remain traditional. Then the $\nu/2$ parameters $\theta(0j_2 \ldots j_n)$ not involving F_1 stay unchanged but are now denoted by $\beta(0j_2 \ldots j_n)$; in particular, $\beta(0 \ldots 0)$, which equals $\theta(0 \ldots 0)$, continues to represent the general mean. If we write β_- for the $(\nu/2) \times 1$ vector of these parameters, arranged lexicographically, then

$$\beta_{-} = \nu^{-1} \{ H(0) \otimes H^{\otimes (n-1)} \} \tau, \qquad (2.3)$$

because $\theta = \nu^{-1}(H^{\otimes n})\tau$ by (2.1) and (2.2), and β_{-} consists of the top $\nu/2$

elements of θ .

The remaining $\nu/2$ factorial effect parameters $\theta(1j_2 \dots j_n)$ which involve F_1 are, however, replaced in the conditional model by their conditional counterparts, namely,

$$\beta(1j_2...j_n) = \nu^{-1} 2^{1/2} \{ H(1) \otimes e(j_2) \otimes H(j_3) \otimes ... \otimes H(j_n) \} \tau, \qquad (2.4)$$

where $e(0) = (1 \ 0)$ and $e(1) = (0 \ 1)$. Any such $\beta(1j_2...j_n)$ represents a conditional main effect of F_1 , if $j_3...j_n = 0...0$, and a conditional interaction involving F_1 and one or more of $F_3, ..., F_n$, otherwise. From (2.4), observe that each $\beta(1j_2...j_n)$ is a contrast of the treatment effects with the level of the conditioning factor F_2 held fixed at j_2 ; e.g., with n = 3,

$$\beta(1j_20) = 2^{-5/2} \{ \tau(0j_20) + \tau(0j_21) - \tau(1j_20) - \tau(1j_21) \}, \beta(1j_21) = 2^{-5/2} \{ \tau(0j_20) - \tau(0j_21) - \tau(1j_20) + \tau(1j_21) \}.$$

This justifies their description as conditional main effects or interactions, conditioning on the level at which F_2 is held fixed. Moreover, by (2.4), in each $\beta(1j_2...j_n)$, the coefficient vector of τ has norm $\nu^{-1/2}$, which is precisely the same as what happens with the $\beta(0j_2...j_n)$ in view of (2.3). Let β_+ denote the $(\nu/2) \times 1$ vector of parameters $\beta(1j_2...j_n)$, arranged lexicographically. Then by (2.4),

$$\beta_{+} = \nu^{-1} \{ H(1) \otimes (2^{1/2} I_2) \otimes H^{\otimes (n-2)} \} \tau,$$

where I_l is the identity matrix of order *l*. This, in conjunction with (2.3), yields

$$\beta = \nu^{-1} \{ W \otimes H^{\otimes (n-2)} \} \tau, \qquad (2.5)$$

where $\beta = (\beta'_{-}, \beta'_{+})'$ is the $\nu \times 1$ vector of all the β -parameters and by (2.2),

$$W = \begin{pmatrix} H(0) \otimes H \\ H(1) \otimes 2^{1/2} I_2 \end{pmatrix} = \begin{pmatrix} H & H \\ 2^{1/2} I_2 & -2^{1/2} I_2 \end{pmatrix}.$$
 (2.6)

It will be useful to cluster the $\beta(j_1 \dots j_n)$, $j_1 \dots j_n \neq 0 \dots 0$, into parametric vectors representing unconditional and conditional factorial effects of various orders. For s = 0, 1, and $1 \leq l \leq n - 1$, let β_{sl} be the vector with elements $\beta(j_1 \dots j_n), j_1 \dots j_n \in \Omega_{sl}(\subset \Omega)$, where

$$\Omega_{0l} = \{j_1 \dots j_n : j_1 = 0 \text{ and } l \text{ of } j_2, \dots, j_n \text{ equal } 1\}, 1 \le l \le n - 1,$$

$$\Omega_{1l} = \{j_1 \dots j_n : j_1 = 1, j_2 = 0 \text{ or } 1 \text{ and } l - 1 \text{ of } j_3, \dots, j_n \text{ equal } 1\},$$

$$1 \le l \le n - 1.$$
(2.7)

By (2.7), β_{01} consists of the (unconditional) main effects of F_2, \ldots, F_n , while β_{11} incorporates the conditional main effects of F_1 . Similarly, for $2 \leq l \leq n-1$,

 β_{0l} and β_{1l} account for the unconditional and conditional *l*-factor interactions, respectively.

2.2. Effect hierarchy

Equation (2.5) helps us to define effect hierarchy under the β -parametrization via a prior specification on τ in terms of a Gaussian random function such that $\operatorname{cov}(\tau) = \sigma^2 R^{\otimes n}$, where $\sigma^2 > 0$ and

$$R = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix},$$

with $0 < \rho < 1$. This covariance structure is equivalent to the one considered by Joseph (2006) for two-level factorials in his equation (4), with $\rho = \psi_0(2)$ in his notation; see Joseph (2006) for earlier references in this connection. The above correlation structure induces a correlation ρ^l between the effects of any two treatment combinations which differ from each other in the levels of l out of the n factors, $0 \le l \le n$. By (2.5), then the prior covariance matrix of β is given by

$$\operatorname{cov}(\beta) = \sigma^2 \nu^{-2} (WR^{\otimes 2}W') \otimes (HRH')^{\otimes (n-2)}$$

Since by (2.2) and (2.6), $WR^{\otimes 2}W' = 4\text{diag}\{(1/2)(1+\rho)HRH', (1-\rho)R\}$ and $HRH' = 2\text{diag}\{1+\rho, 1-\rho\}$, from (2.7) one can now check that each $\beta(j_1 \dots j_n)$ in β_{sl} has prior variance V_{sl} , where

$$V_{0l} = \sigma^2 \nu^{-1} (1+\rho)^{n-l} (1-\rho)^l, V_{1l} = \sigma^2 \nu^{-1} (1+\rho)^{n-l-1} (1-\rho)^l, 1 \le l \le n-1.$$

Clearly, for every $\rho \in (0,1)$,

$$V_{01} > V_{11} > V_{02} > V_{12} > \ldots > V_{0n-1} > V_{1n-1}.$$
 (2.8)

In view of (2.8), defining effect hierarchy in order of prior variance, the unconditional main effects of F_2, \ldots, F_n appear at the top, while the conditional main effects of F_1 are positioned next; then come the unconditional two-factor interactions (2fis), followed by the conditional 2fis, and so on. Obviously, the β 's in the same β_{sl} enjoy the same status.

The effect hierarchy obtained above perfectly matches our intuition and can be viewed as a translation of that in the traditional model to our setup. Thus here too, it turns out that lower order factorial effects are positioned above higher order ones. Furthermore, unconditional factorial effects are positioned above conditional factorial effects of the same order which is again natural, because by (2.3) and (2.4), the former is the same as the corresponding traditional factorial effect whereas the latter is a linear combination of two traditional factorial effects, one of the same order and the other of the next higher order; cf. (3.1) below.

In conformity with traditional factorials (see e.g., Tang and Deng (1999)), the current effect hierarchy suggests a sensible design strategy under the conditional model. We first identify a class of designs which ensure optimal inference on β_{01} and β_{11} , i.e., the unconditional and conditional main effects representing the two highest placed classes of factorial effects, in the absence of all interactions. Then from consideration of model robustness, among these designs we find one which sequentially minimizes a suitably defined measure of bias in the estimation of β_{01} and β_{11} , caused by successive interactions in the effect hierarchy, i.e., interactions in β_{02} , β_{12} , β_{03} , β_{13} ,..., in that order, with precedence given at each stage on the bias in the estimation of β_{01} over that in estimating β_{11} which comes next to it.

A comparison of prior variances as in (2.8), which forms the basis of effect hierarchy, is meaningful only when the coefficient vectors of τ in all the $\beta(j_1 \dots j_n)$ have the same norm, as achieved by the scaling in (2.4). This scaling will play no further role in the rest of the paper. Indeed, changing the multiplier $\nu^{-1}2^{1/2}$ in (2.4) to some other constant would amount to replacing $\beta_{11}, \beta_{12}, \beta_{13}$ etc. by some scalar multiples thereof. One can readily check that the optimality result on β_{11} in Theorem 1 below will continue to hold even for inference on such a scalar multiple of β_{11} . Also, the bias terms indicated above and summarized later in equation (4.2) will each get multiplied by a positive constant, without any impact on their sequential minimization.

3. Universally Optimal Designs in the Absence of Interactions

3.1. Linking the traditional and conditional models

A linkage with the traditional model facilitates the study of designs under the conditional model. We begin by connecting the θ -parameters in the former with the β -parameters in the latter. By (2.2) and (2.6), $HH = 2I_2$ and $WH^{\otimes 2} =$ diag($4I_2, 2^{3/2}H$). Hence from (2.1) and (2.5),

$$\beta = \nu^{-1} \{ WH^{\otimes 2} \otimes (HH)^{\otimes (n-2)} \} \theta = \operatorname{diag}(I_2^{\otimes (n-1)}, 2^{-1/2}H \otimes I_2^{\otimes (n-2)}) \theta.$$

Since the block diagonal matrix in the extreme right is symmetric and orthogonal, the roles of β and θ can be interchanged in the above. Recalling (2.2), this yields

$$\theta(0j_2\dots j_n) = \beta(0j_2\dots j_n), \theta(10j_3\dots j_n) = 2^{-1/2} \{\beta(10j_3\dots j_n) + \beta(11j_3\dots j_n)\},\\ \theta(11j_3\dots j_n) = 2^{-1/2} \{\beta(10j_3\dots j_n) - \beta(11j_3\dots j_n)\},$$
(3.1)

for each j_2, \ldots, j_n . The first identity in (3.1) is in agreement with the definition

of $\beta(0j_2\ldots j_n)$.

Consider now an N-run design which may be represented by an $N \times n$ array $D = (d_{ui})$ where d_{ui} equals 1 if factor F_i is at level 0 in the *u*th run, and -1 otherwise, $1 \leq u \leq N$, $1 \leq i \leq n$. If Y denotes the $N \times 1$ observational vector arising from the design D, then by (2.1) and (2.2), the traditional model retaining all factorial effects is given by $E(Y) = \sum_{\Omega} x(j_1 \dots j_n) \theta(j_1 \dots j_n)$, where \sum_{Ω} denotes sum over all binary *n*-tuples and, for any $j_1 \dots j_n \in \Omega$, the $N \times 1$ vector $x(j_1 \dots j_n)$ has elements

$$x(u; j_1 \dots j_n) = d_{u1}^{j_1} \dots d_{un}^{j_n}, 1 \le u \le N.$$
(3.2)

Hence by (3.1), under the conditional model, $E(Y) = \sum_{\Omega} z(j_1 \dots j_n) \beta(j_1 \dots j_n)$, or equivalently,

$$E(Y) = z(0...0)\beta(0...0) + \sum_{s=0}^{1} \sum_{l=1}^{n-1} Z_{sl}\beta_{sl},$$
(3.3)

where for each $j_2 \ldots j_n$,

$$z(0j_2...j_n) = x(0j_2...j_n), z(10j_3...j_n) = 2^{-1/2} \{ x(10j_3...j_n) + x(11j_3...j_n) \}, z(11j_3...j_n) = 2^{-1/2} \{ x(10j_3...j_n) - x(11j_3...j_n) \},$$
(3.4)

and, in conformity with β_{sl} , the matrix Z_{sl} consists of columns $z(j_1 \dots j_n)$, $j_1 \dots j_n \in \Omega_{sl}$. As usual, it is assumed that the random observational errors have the same variance and are uncorrelated.

3.2. Universally optimal designs

If all interactions are assumed to be absent, then the model (3.3) reduces to

$$E(Y) = z(0...0)\beta(0...0) + Z_{01}\beta_{01} + Z_{11}\beta_{11}, \qquad (3.5)$$

where β_{01} and β_{11} are the vectors of the unconditional and conditional main effect parameters and accordingly the matrices Z_{01} and Z_{11} , of orders $N \times (n-1)$ and $N \times 2$, are given by

$$Z_{01} = [z(010\dots 0)\dots z(000\dots 1)], Z_{11} = [z(100\dots 0)\dots z(110\dots 0)].$$
(3.6)

We are now in a position to present Theorem 1. Requirement (i) of this theorem makes D an orthogonal array of strength two with symbols ± 1 and is commonly imposed also in traditional factorials. On the other hand, requirement (ii) caters to the conditional model where the first two factors play a special role. We refer to Kiefer (1975) for more details on universal optimality as considered in Theorem 1 but note that it implies, in particular, the well-known D-, A- and E-optimality, which entail maximization of det(J), $-tr(J^{-1})$ and $\mu_{\min}(J)$, respectively, where

J denotes the information matrix of the parametric vector of interest and $\mu_{\min}(J)$ is its smallest eigenvalue.

Theorem 1. An N-run design D where (i) all four pairs of symbols occur equally often as rows in every two-column subarray of D, and (ii) all eight triplets of symbols occur equally often as rows in every three-column subarray of D which includes the first two columns, is universally optimal among all N-run designs for inference on both β_{01} and β_{11} under the absence of all unconditional and conditional interactions.

Proof. For h = 0, 1, let J_h denote the information matrix for β_{h1} under model (3.5). As $Z'_{h1}Z_{h1} - J_h$ is nonnegative definite, we obtain for every N-run design,

$$\operatorname{tr}(J_0) \le \operatorname{tr}(Z'_{01}Z_{01}) = N(n-1), \operatorname{tr}(J_1) \le \operatorname{tr}(Z'_{11}Z_{11}) = 2N.$$
 (3.7)

The identities in (3.7) hold because by (3.2), every $x(j_1 \dots j_n)$ has squared norm N and hence by (3.4), each column of Z_{01} in (3.6) has squared norm N, whereas the squared norms of the two columns of Z_{11} in (3.6) add up to 2N. For any design meeting (i) and (ii), from (3.2) now observe that the vectors $x(j_1 \dots j_n)$ with at most one of j_1, \dots, j_n equal to 1 are mutually orthogonal and that all these vectors are orthogonal to $x(110\dots 0)$ as well; so, by (3.2), (3.4) and (3.6),

$$Z'_{h1}z(0\dots 0) = 0(h=0,1), Z'_{01}Z_{11} = 0, Z'_{01}Z_{01} = NI_{n-1}, Z'_{11}Z_{11} = NI_2.$$
(3.8)

Thus by (3.5), for any such design, $J_0 = NI_{n-1}$ and $J_1 = NI_2$, and $tr(J_0)$ and $tr(J_1)$ attain the upper bounds in (3.7). The result now follows from Kiefer (1975).

In a design D meeting (i) and (ii) of Theorem 1, factors F_1 and F_2 can be replaced by a four level factor to yield a mixed level orthogonal array; see Wu (1989). However, the effect hierarchy in such mixed factorials (Wu and Zhang , 1993) is different from ours due to the distinction between the unconditional and conditional factorial effects here. Consequently, neither the model robustness criteria nor the associated results there apply to our setup. Only a technical tool from there is of possible use in Section 5 while developing our complementary set theory.

4. Minimum Aberration Criterion

Hereafter, to avoid trivialities, let $n \ge 4$. We consider designs meeting (i) and (ii) of Theorem 1 and proceed to discriminate among these with regard to model robustness. For h = 0, 1, by (3.5) and (3.8), $\hat{\beta}_{h1} = N^{-1}Z'_{h1}Y$ is the best linear unbiased estimator of β_{h1} in any such design under the reduced model

(3.5). To assess the impact of possible presence of interactions on $\widehat{\beta}_{h1}$, we revert back to the full model (3.3). Then by (3.8), $\widehat{\beta}_{h1}$ no longer remains unbiased but is seen to have bias $N^{-1} \sum_{s=0}^{1} \sum_{l=2}^{n-1} Z'_{h1} Z_{sl} \beta_{sl}$. So, as in traditional factorials (Tang and Deng, 1999), a very reasonable measure of the bias in $\widehat{\beta}_{h1}$ caused by the interaction parameters in β_{sl} emerges as

$$K_{sl}(h) = N^{-2} \operatorname{tr}(Z'_{h1} Z_{sl} Z'_{sl} Z_{h1}) = N^{-2} \operatorname{tr}(X'_{h1} X_{sl} X'_{sl} X_{h1}), \qquad (4.1)$$

where X_{sl} , like Z_{sl} , is a matrix with columns $x(j_1 \dots j_n)$, $j_1 \dots j_n \in \Omega_{sl}$. The last step in (4.1) follows because by (2.7) and (3.4), $Z_{0l} = X_{0l}$ and $Z_{1l} = X_{1l}\Gamma_l$, the matrix Γ_l being orthogonal, $1 \leq l \leq n-1$.

Recalling the effect hierarchy introduced in Section 2, the biases caused by the interactions in $\beta_{02}, \beta_{12}, \beta_{03}, \beta_{13}, \ldots$, are successively positioned in order of priority. At the same time, the bias due to any such β_{sl} in $\hat{\beta}_{01}$ gets precedence over that in $\hat{\beta}_{11}$. From this perspective, we will explore an MA design minimizing

$$K = \{K_{02}(0), K_{02}(1), K_{12}(0), K_{12}(1), K_{03}(0), K_{03}(1), K_{13}(0), K_{13}(1), \ldots\}$$
(4.2)

in a sequential manner from left to right. Such a design is also known as a minimum contamination design in the sense of sequentially minimizing the contamination or bias due to successive interactions in the effect hierarchy, with the bias in $\hat{\beta}_{01}$ getting priority over that in $\hat{\beta}_{11}$ at each stage.

5. Regular Designs: Complementary Set Theory

We now focus attention on regular designs under the conditional model. This is motivated by several reasons, in addition to their popularity among practitioners. First, as seen below, requirements (i) and (ii) of Theorem 1 can be readily met with these designs. Second, the rich literature on regular traditional designs is useful in our setup. Third, regular designs are very promising; for run size 16, nonregular designs will be seen to entail no further gain. Finally, the findings on regular designs provide an important benchmark for assessing any future work on nonregular designs.

In what follows, all operations with binary vectors are over the finite field GF(2). Let Δ_r be the set of nonnull $r \times 1$ binary vectors. A regular 2^n traditional factorial design in $N = 2^r (r < n)$ runs is given by n distinct vectors b_1, \ldots, b_n from Δ_r such that the matrix $B = [b_1 \ldots b_n]$ has full row rank. The design consists of the N treatment combinations a'B, where $a \in \Delta_r \cup \{0\}$. Clearly, such a design meets (i) of Theorem 1. Similarly, (ii) is also met if

$$b_1 + b_2 \neq b_s, 3 \le s \le n.$$
 (5.1)

Here b_1 and b_2 correspond to the conditional and conditioning factors, F_1 and F_2 , respectively, and b_3, \ldots, b_n to the traditional factors F_3, \ldots, F_n . Because of (5.1), we get $n \leq 2^r - 2$, as b_3, \ldots, b_n are different from b_1, b_2 and $b_1 + b_2$.

All regular designs as above enjoy the universal optimality property of Theorem 1. To discriminate among them under the MA criterion given by (4.2), we first convert (4.2) to a WLP appropriate for the conditional model. For $1 \leq l \leq n-1$, define $A_l^{(0)}$ as the number of ways of choosing l out of b_2, \ldots, b_n such that the sum of the chosen l equals 0, and $A_l^{(1)}$ as the number of ways of choosing l-1 out of b_3, \ldots, b_n such that the sum of the chosen l-1 is in the set $\{b_1, b_1 + b_2\}$. Similarly, for $2 \leq l \leq n-1$, let $A_l^{(2)}$ denote the numbers of ways of choosing l-1 out of b_3, \ldots, b_n such that the sum of the chosen l-1 is in the set $\{0, b_2\}$. These quantities resemble the terms in the traditional WLP with the major difference that now b_1 and b_2 , representing F_1 and F_2 , are separately taken care of. For example, $A_l^{(0)}$ is the number of words of length l in the defining relation which involve l out of F_2, \ldots, F_n , while $A_l^{(1)}$ is the number of words of lengths l or l+1 in the defining relation which involve l-1 of F_3, \ldots, F_n in addition to F_1 and may or may not involve F_2 as well. Clearly,

$$A_1^{(0)} = A_2^{(0)} = A_1^{(1)} = A_2^{(1)} = A_2^{(2)} = 0, (5.2)$$

where $A_2^{(1)} = 0$, by (5.1). The next result gives expressions for the $K_{sl}(h)$ in (4.1) in terms of the quantities just introduced. Its proof is sketched in the appendix.

Theorem 2. For $2 \le l \le n-1$, (a) $K_{0l}(0) = (n-l)A_{l-1}^{(0)} + (l+1)A_{l+1}^{(0)}$, (b) $K_{0l}(1) = A_l^{(1)} + A_{l+1}^{(1)}$, (c) $K_{1l}(0) = (n-l)A_{l-1}^{(1)} + A_l^{(1)} + lA_{l+1}^{(1)}$, (d) $K_{1l}(1) = 2A_l^{(2)}$, where $A_n^{(0)}$ and $A_n^{(1)}$ are interpreted as zeros.

In view of (5.2) and Theorem 2, sequential minimization of the terms of K in (4.2) is equivalent to that of the terms of

$$A = (A_3^{(0)}, A_3^{(1)}, A_4^{(0)}, A_4^{(1)}, A_3^{(2)}, A_5^{(0)}, A_5^{(1)}, A_4^{(2)}, \ldots).$$
(5.3)

The sequence A, so arising from K, takes due care of sequential bias minimization under the present effect hierarchy and can be interpreted as the WLP under the conditional model. While the successive terms in its traditional counterpart involve words of progressively higher lengths, A is more complex because it follows this pattern only on the whole but not strictly. For example, the words of length four potentially involved in $A_3^{(1)}$ get priority over the words of same length in $A_4^{(0)}$. Even more conspicuously, $A_4^{(1)}$ appears before $A_3^{(2)}$ in A, but $A_4^{(1)}$ involves words of lengths four and five as against words of length three only in $A_3^{(2)}$.

t	b_1	b_2	Т
0	δ	$\alpha\delta$	Empty set
1	λ	$\alpha\lambda$	$\{\delta\}$
2	λ	$\alpha\lambda$	$\{\delta, \alpha\delta\}$
3	$\alpha\lambda$	$\alpha\delta\lambda$	$\{\alpha, \alpha\delta, \lambda\}$
4	$\delta\lambda$	$\alpha\delta\lambda$	$\{\delta, \alpha \delta, \lambda, \alpha \lambda\}$
5	ζ	$\alpha\delta\zeta$	$\{\alpha, \delta, \lambda, \alpha\lambda, \delta\lambda\}$
6	ζ	$\alpha\zeta$	$\{\delta, \alpha\delta, \lambda, \alpha\lambda, \delta\lambda, \alpha\delta\lambda\}$
7	ζ	$\delta \zeta$	$\{\alpha, \alpha\delta, \lambda, \alpha\lambda, \delta\lambda, \alpha\delta\lambda, \alpha\zeta\}$
8	ζ	$\lambda\zeta$	$\{\alpha, \delta, \alpha\delta, \alpha\lambda, \delta\lambda, \alpha\delta\lambda, \alpha\zeta, \delta\zeta\}$
9	$\alpha\delta\lambda$	$\delta\lambda\zeta$	$\{\alpha, \delta, \alpha\delta, \lambda, \alpha\lambda, \delta\lambda, \zeta, \delta\zeta, \lambda\zeta\}$
10	$\alpha\delta\lambda\zeta$	$\delta\lambda\zeta$	$\{\delta, \alpha\delta, \lambda, \alpha\lambda, \delta\lambda, \alpha\delta\lambda, \zeta, \alpha\zeta, \delta\zeta, \lambda\zeta\}$
11	$lpha\delta\zeta$	$\delta\lambda\zeta$	$\{\alpha, \delta, \alpha\delta, \lambda, \delta\lambda, \alpha\delta\lambda, \zeta, \alpha\zeta, \delta\zeta, \lambda\zeta, \alpha\delta\lambda\zeta\}$
12	$\lambda\zeta$	$\alpha\delta\lambda\zeta$	$\{\alpha, \delta, \lambda, \alpha\lambda, \delta\lambda, \alpha\delta\lambda, \zeta, \alpha\zeta, \delta\zeta, \alpha\delta\zeta, \alpha\lambda\zeta, \delta\lambda\zeta\}$

Table 1. Regular MA designs under conditional model via complementary sets.

We now develop a complementary set theory with a view to exploring the practically important saturated or nearly saturated cases where n equals or is close to the upper bound $2^r - 2$ and hence, as seen below, it suffices to consider at most the first three terms of the sequence A. This is in the spirit of the corresponding work in traditional deigns (Tang and Wu, 1996), but many new features emerge. Let \widetilde{T} be the complement of $\{b_2, \ldots, b_n\}$ in Δ_r . By (5.1), \widetilde{T} includes both b_1 and $b_1 + b_2$. Write T for the set obtained by excluding b_1 and $b_1 + b_2$ from \widetilde{T} , and t = #T, where # denotes the cardinality of a set. Then $t = 2^r - n - 2 \geq 0$. For l = 3, 4, define $A_l(\widetilde{T})$ as the number of ways of choosing l members of \widetilde{T} such that the sum of the chosen l equals 0. Similarly, let $A_2(T)$ denote the number of pairs arising from T such that the members of each pair add up to b_1 or $b_1 + b_2$. Then for the first three terms in the sequence A, we have

$$A_3^{(0)} = \text{constant} - A_3(\widetilde{T}), A_3^{(1)} = \text{constant} + A_2(T),$$

$$A_4^{(0)} = \text{constant} + A_3(\widetilde{T}) + A_4(\widetilde{T}),$$
(5.4)

where the constants may depend on r and n but not on the specific design. The first and third equations in (5.4) follow from Tang and Wu (1996), while the second equation can be deduced from either first principles or Lemmas 1 and 3(ii) in Mukerjee and Wu (2001). The key differences between (5.4) and the corresponding equations in traditional designs are that the second equation in (5.4) does not arise there and that neither \tilde{T} nor T is the complement of $\{b_1, \ldots, b_n\}$ in Δ_r which is actually given by $\tilde{T} \setminus \{b_1\} [= T \cup \{b_1 + b_2\}]$. Example 1 below illustrates the implications. For $0 \le t \le 12$, Table 1 shows regular MA designs, obtained via (5.4) under the conditional model, by displaying the associated b_1, b_2 and T. Given these, $\{b_3, \ldots, b_n\}$ can be readily obtained as the complement of $\{b_1, b_2, b_1 + b_2\} \cup T$ in Δ_r . For N = 8, 16, 32, 64 and 128, Table 1 applies to $4 \le n \le 6, 5 \le n \le 14,$ $18 \le n \le 30, 50 \le n \le 62$ and $114 \le n \le 126$, respectively. Hence it covers all possible *n* for run sizes 8 and 16.

In Table 1, all three equations in (5.4) are required for t = 9, and all other cases settled from the first or first two equations there. In addition to these equations, the following facts help:

- (I) The set \widetilde{T} is not closed under addition of distinct members, because $b_1, b_1 + b_2 \in \widetilde{T}$ but $b_2 \notin \widetilde{T}$.
- (II) By Theorem 2, the sequence K and hence the sequence A remain unaltered if the roles of b_1 and $b_1 + b_2$ are interchanged.

Thus any pair from \widetilde{T} with sum outside \widetilde{T} can potentially represent $(b_1, b_1 + b_2)$, the ordering within such a pair being immaterial to us. Example 1 illustrates the construction of Table 1. In this example as well as Table 1, α, δ, λ and ζ are any four linearly independent vectors from Δ_r and for brevity, we write $\delta \lambda = \delta + \lambda$, $\alpha \delta \zeta = \alpha + \delta + \zeta$, and so on.

Example 1. (a) Let t = 5, i.e., $\#\widetilde{T} = 7$. By the first equation in (5.4), \widetilde{T} should maximize $A_3(\widetilde{T})$, subject to (I) above. Up to isomorphism, the unique \widetilde{T} doing so is $\{\alpha, \delta, \alpha\delta, \lambda, \alpha\lambda, \delta\lambda, \zeta\}$. For this \widetilde{T} , in view of (II), it suffices to consider only two choices of $(b_1, b_1 + b_2)$, namely, $(\alpha, \delta\lambda)$ and $(\zeta, \alpha\delta)$, having $A_2(T)$ values 4 and 2 respectively. Other possible $(b_1, b_1 + b_2)$ are isomorphic to one of these two; e.g., the choice (ζ, α) reduces to $(\zeta, \alpha\delta)$ if we replace $\alpha, \delta, \lambda, \zeta$ by $\alpha\delta, \delta, \delta\lambda, \zeta$, respectively, which leaves \widetilde{T} unchanged. By the second equation in (5.4), therefore, \widetilde{T} as above, coupled with $(b_1, b_1 + b_2) = (\zeta, \alpha\delta)$ gives an MA design. Then $b_1 = \zeta$, $b_2 = \alpha\delta\zeta$ and $T = \{\alpha, \delta, \lambda, \alpha\lambda, \delta\lambda\}$, as shown in Table 1.

(b) Let t = 8, i.e., $\#\tilde{T} = 10$. By the first equation in (5.4), following Tang and Wu (1996), the only two nonisomorphic \tilde{T} that need be considered are $\tilde{T}_1 = \{\alpha, \delta, \alpha\delta, \lambda, \alpha\lambda, \delta\lambda, \zeta, \alpha\zeta, \delta\zeta, \lambda\zeta\}$ and $\tilde{T}_2 = \{\alpha, \delta, \alpha\delta, \lambda, \alpha\lambda, \delta\lambda, \alpha\delta\lambda, \zeta, \alpha\zeta, \delta\zeta\}$, both of which meet (I). Every possible $(b_1, b_1 + b_2)$ entails $A_2(T) = 6$ for \tilde{T}_1 , and $A_2(T) = 5$ or 6 for \tilde{T}_2 . So, we need to consider only \tilde{T}_2 , along with $(b_1, b_1 + b_2)$ such that $A_2(T) = 5$. Recalling (II), as in (a) above, all such $(b_1, b_1 + b_2)$ are isomorphic to (ζ, λ) . Therefore, \tilde{T}_2 , together with $(b_1, b_1 + b_2) = (\zeta, \lambda)$ yields an MA design. Then $b_1 = \zeta$, $b_2 = \lambda\zeta$, $T = \{\alpha, \delta, \alpha\delta, \alpha\lambda, \delta\lambda, \alpha\delta\lambda, \alpha\zeta, \delta\zeta\}$, as recorded in Table 1. The outcome here may be contrasted with what happens

in traditional factorials where the second equation in (5.4) does not arise and, as a complementary set of size 10, \tilde{T}_1 turns out to be superior to \tilde{T}_2 because of a smaller $A_4(\tilde{T})$ (Tang and Wu (1996)). At the same time, in our setup, the complement of $\{b_1, \ldots, b_n\}$ in Δ_r is not really \tilde{T} but $T \cup \{b_1 + b_2\}$, which equals $\{\alpha, \delta, \alpha\delta, \lambda, \alpha\lambda, \delta\lambda, \alpha\delta\lambda, \alpha\zeta, \delta\zeta\}$ for the design obtained here, has size 9, and agrees with the complementary set of the corresponding traditional MA design. Thus the case t = 8 brings out the subtleties of the conditional model showing how the associated complementary set theory can differ from or agree with the traditional one.

More generally, for $0 \le t \le 12$, a comparison of the complementary set $T \cup \{b_1 + b_2\}$ with its counterpart in the traditional setup (Tang and Wu, 1996) shows that all designs in Table 1 have MA also as traditional designs. At the same time, if the roles of b_1 and $b_1 + b_2$ are interchanged in these designs, then by (II) above, the resulting designs are equally good under the conditional model, but one can check that several of these cease to remain so in the traditional setup. Thus no general result connecting MA designs under the conditional and traditional models is anticipated, though some useful patterns come to light in the next section.

6. An Efficient Computational Procedure

Starting from an alternative version of the $K_{sl}(h)$ in (4.1), we now propose, with the development of necessary theory, a fast computational procedure which covers even nonregular designs for N = 16, supplements Table 1 for N = 32, and indicates a very promising design strategy for larger N. By (4.1), for any design, whether regular or not,

$$K_{sl}(h) = N^{-2} \operatorname{tr}(X_{h1} X'_{h1} X_{sl} X'_{sl}).$$
(6.1)

The above is reminiscent of minimum moment aberration in traditional factorials (Xu, 2003) and very helpful in our context too. To see this, for $0 \le c \le n-2$, let

$$Q_0(c) = 1, Q_1(c) = 2c - (n-2), Q_{n-1}(c) = 0,$$
(6.2)

$$Q_l(c) = l^{-1}[\{2c - (n-2)\}Q_{l-1}(c) - (n-l)Q_{l-2}(c)], 2 \le l \le n-2.$$
(6.3)

Write \widetilde{D} for the subarray given by the last n-2 columns of D meeting (i) and (ii) of Theorem 1. For $1 \leq u, w \leq N$, let c_{uw} be the number of positions where the *u*th and *w*th rows of \widetilde{D} have the same entry, and $q_{sl}(u, w)$ be the (u, w)th element of $X_{sl}X'_{sl}$. Then the following result, proved in the Appendix, holds.

Theorem 3. For $1 \le u, w \le N$ and $1 \le l \le n-1$, (a) $q_{0l}(u, w) = d_{u2}d_{w2}Q_{l-1}(c_{uw})$

+ $Q_l(c_{uw})$, (b) $q_{1l}(u, w) = d_{u1}d_{w1}(1 + d_{u2}d_{w2})Q_{l-1}(c_{uw})$.

Note that c_{uw} is easy to obtain as $c_{uw} = (f_{uw} + n - 2)/2$, where f_{uw} is the scalar product of the *u*th and *w*th rows of \tilde{D} . Moreover, the $Q_l(.)$ can be found very fast using the recursion relation (6.3). Thus Theorem 3 greatly simplifies the computation of the $q_{sl}(u, w)$ and hence, by (6.1) via direct matrix multiplication, that of the $K_{sl}(h)$ appearing in (4.2).

We now show how the above ideas enable us to find regular MA designs under the conditional model using the existing catalogs of regular traditional designs. Given $N(=2^r)$ and $n(\leq 2^r-2)$, suppose a complete list of nonisomorphic regular traditional designs is available as given by the corresponding choices of n distinct vectors b_1, \ldots, b_n from Δ_r . As in Section 5, any such design meets (i) and (ii) of Theorem 1 and hence qualifies for consideration under the conditional model if and only if the columns of $B = [b_1 \ldots b_n]$ are arranged such that the sum of the first two columns is different from every other column. This leads to Steps 1-3 below which search all regular designs under the conditional model and yield an MA design among them.

- <u>Step 1</u>. Given N and n, start with a list of all nonisomorphic regular traditional designs as given by the corresponding choices of b_1, \ldots, b_n . For N = 16 and 32, this can be done using the catalogs in Chen, Sun and Wu (1993) and Xu (2009).
- Step 2. For each choice of b_1, \ldots, b_n in Step 1, identify all pairs (b_i, b_j) , i < j, such that $b_i + b_j \neq b_s$ for every $s \neq i, j$. For every such pair, let \widetilde{B} be the matrix with columns $b_s, s \neq i, j$, and consider designs $[b_i \quad b_j \quad \widetilde{B}]$ and $[b_j \quad b_i \quad \widetilde{B}]$; both need to be taken into account because, by (6.1) and Theorem 3, factors F_1 and F_2 affect the $K_{sl}(h)$ differently and hence are not interchangeable.
- <u>Step 3</u>. For every design obtained through Steps 1 and 2, use (6.1) and Theorem 3 to obtain the sequence K in (4.2), and hence find an MA design.

Table 2 exhibits the results of Steps 1-3 for N = 32 and $6 \le n \le 17$, showing in each case, the *n* vectors specifying the design. A vector $b = (b(1), \ldots, b(r))'$ is written as the number $\sum_{l=1}^{r} b(l)2^{l-1}$ to save space; e.g., (1, 1, 0, 0, 1)' is denoted simply by 19. The first two vectors for any design correspond to factors F_1 and F_2 , respectively. As hinted in Step 2, these two are not interchangeable. For example, with N = 32 and n = 7, 8, 9 or 12, if the first two vectors in the design shown in Table 2 are interchanged, then the resulting design no longer has MA.

n	MA design
6	1, 2, 4, 8, 16, 31
7	1, 4, 2, 8, 15, 16, 19
8	1, 8, 2, 4, 15, 16, 19, 21
9	1, 15, 2, 4, 8, 16, 19, 21, 25
10	1, 2, 4, 8, 15, 16, 19, 21, 25, 30
11	1, 2, 4, 7, 8, 11, 13, 16, 21, 25, 31
12	1, 16, 2, 4, 7, 8, 11, 13, 14, 21, 25, 31
13	1, 2, 4, 7, 8, 11, 13, 14, 16, 19, 21, 25, 31
14	1, 2, 4, 7, 8, 11, 13, 14, 16, 19, 21, 22, 25, 31
15	1, 2, 4, 7, 8, 11, 13, 14, 16, 19, 21, 22, 25, 26, 31
16	1, 2, 4, 7, 8, 11, 13, 14, 16, 19, 21, 22, 25, 26, 28, 31
17	1, 4, 2, 3, 7, 8, 11, 13, 14, 16, 19, 21, 22, 25, 26, 28, 31

Table 2. Regular MA designs under conditional model for N = 32.

Tables 1 and 2 together cover all possible n for N = 32. A comparison with Xu (2009) shows that all designs in Table 2 also have MA as traditional designs.

For N = 16, 32, and every n, we had actually employed Steps 1-3 to obtain all regular MA designs. Most of these were found to enjoy the same property as traditional designs and the rest were among the top few in this sense. In the absence of a general result connecting the two models due to reasons explained in Section 5, the point just noted can be useful in finding good designs under the conditional model for larger N where a complete list of all nonisomorphic regular traditional designs is not yet available but the top few of them may be known. Our computations as indicated above suggest that consideration of only these top few in Step 1 should yield a very good design, if not an MA design, also under the conditional model. An example follows.

Example 2. For N = 64 and n = 20, Xu (2009) lists the top 24 regular traditional designs. If we include these 24 in Step 1 and then employ Steps 2 and 3 above, then all the resulting designs, one of which is given by

1, 2, 4, 8, 11, 13, 16, 21, 22, 25, 28, 31, 32, 39, 41, 46, 51, 52, 58, 61,

are seen to originate only from the best traditional design. This reinforces our findings for N up to 32 and makes us hopeful that the designs so found should continue to have MA under the conditional model or at least come very close to doing so even if all nonisomorphic regular traditional designs were known and could be incorporated in Step 1.

We next discuss, for smaller N, the consequences of entertaining nonregular

designs. For N = 8, all two-symbol orthogonal arrays are regular and hence so are all designs as envisaged in Theorem 1. For N = 16 and each n, a list of all nonisomorphic two-symbol orthogonal arrays, regular as well as nonregular, can be found from Sun, Li and Ye (2008) together with Hall (1961). With all such designs included in Step 1 of our procedure, we employed Steps 2 and 3, with appropriate adjustments in Step 2 as dictated by (ii) of Theorem 1, to find MA designs under the conditional model in the class of all designs regular or not. It was seen that all the regular designs obtained from Table 1 continue to have MA even when nonregular designs are allowed. Moreover, for n = 5 and 8, all nonregular designs turned out to be worse than these regular designs. This is quite reassuring, and in keeping with other situations such as factorial designs under a baseline parametrization; cf. Mukerjee and Tang (2012).

7. An Alternative Wordlength Pattern

For traditional factorial designs, the MA criterion was formulated originally in the regular case (Fries and Hunter, 1980) in terms of sequential minimization of A_3, A_4, \ldots , where A_l is the number of words of length l in the defining relation. This was motivated by the effect hierarchy there without explicit consideration of bias control, but shown later by Tang and Deng (1999) to be equivalent to sequentially minimizing the bias caused in the estimation of the main effects by interactions of successively higher orders. Indeed, Tang and Deng (1999) propounded this idea of bias control while extending the MA criterion to the nonregular case and we have followed their approach because of its applicability to both regular and nonregular designs. However, it is of interest to examine how this compares in the regular case with an alternative approach which is driven, in the spirit of Fries and Hunter (1980)'s original formulation, purely by the present effect hierarchy without direct reference to bias control for main effects.

The quantities $A_l^{(0)}$ and $A_l^{(1)}$, $1 \leq l \leq n-1$, introduced in Section 5, play a key role in this regard. Recall that $A_l^{(0)}$ is the number of words of length l in the defining relation which involve l out of F_2, \ldots, F_n , while $A_l^{(1)}$ is the number of words of lengths l or l+1 in the defining relation which involve l-1of F_3, \ldots, F_n in addition to F_1 and may or may not involve F_2 as well. Thus, in view of (2.7) and the representation (3.1) of the factorial effect parameters under the traditional model in terms of those under the conditional model, the words involved in $A_l^{(0)}$ and $A_l^{(1)}$ correspond to $\beta(j_1 \ldots j_n)$ for $j_1 \ldots j_n$ in Ω_{0l} and Ω_{1l} , respectively. As a result, if one goes purely by the present effect hierarchy

as dictated by (2.8), then because of (5.2), one needs to sequentially minimize the terms of $A_{\text{alt}} = (A_3^{(0)}, A_3^{(1)}, A_4^{(0)}, A_4^{(1)}, A_5^{(0)}, A_5^{(1)}, \ldots)$, which differs from the previously considered A in (5.3) in that the $A_l^{(2)}$ in the latter are dropped. Note that the first four terms of A_{alt} and A are identical. Thus, the designs summarized in Table 1, as given by the complementary set theory and determined by at most the first three terms of A, continue to have MA under A_{alt} . The same is seen to happen also with the 32-run designs in Table 2. Moreover, one can check that A_{alt} and A lead to the same class of regular MA designs for each n in Table 2, except n = 12 when the MA designs via A form a subclass of those via A_{alt} . Thus, even if one goes purely by the present effect hierarchy without explicit consideration of bias control, the outcome remains essentially the same as reported earlier.

8. Concluding Remarks

In this paper, we initiated a systematic investigation of MA designs under a conditional model with a pair of conditional and conditioning factors. After properly introducing effect hierarchy in our setup, we developed a complementary set theory as well as a fast computational procedure for this purpose. There is scope of extending the present work in several directions.

(a) For larger run sizes, it will be of interest to obtain theoretical results which can supplement the findings in Section 6. A related question concerns possible connection between an MA design under the conditional model with N runs and n factors and an MA design under the traditional model with N/2 runs and n-1 factors. While a neat general result in this direction is not anticipated, even partial results along the lines of Butler (2004) will be illuminating.

(b) A more detailed study of nonregular designs will also be welcome. Although the case N = 16 does not hold out much promise for such designs, it will be of importance to know if this pattern persists for larger N as well.

(c) Another possible extension concerns the case of more than one pairs of conditional and conditioning factors. The number of such pairs will seldom exceed two in practice. The case of several factors conditional on the same conditioning factor can also be of interest. Both with two pairs of conditional and conditioning factors and several factors conditional on the same conditioning factor, initial studies show that effect hierarchy can be defined via a chain of inequalities similar to (2.8). Thus, our techniques should work at the expense of heavier notation and algebra.

We hope that the present endeavour will generate interest in these and related

open issues.

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Appendix: Proofs of Theorems 2 and 3

Proof of Theorem 2

Part (a) is evident from Section 2 of Tang and Deng (1999). We sketch the proof of (c). In a regular design specified by distinct nonnull binary vectors b_1, \ldots, b_n , with the array $D = (d_{ui})$ as introduced in Section 3, it is well known that for any binary *n*-tuple $j_1 \ldots j_n$, the quantity $|N^{-1} \sum_{u=1}^n d_{u1}^{j_1} \ldots d_{un}^{j_n}|$ equals 1 if $j_1b_1 + \ldots + j_nb_n = 0$, and 0 otherwise. Hence, considering the elements of $x(010\ldots 0)'X_{1l}, 2 \le l \le n-1$, by (2.7), (3.2) and the definitions of X_{1l} and $A_l^{(1)}$,

$$N^{-2}x(010\ldots 0)'X_{1l}X'_{1l}x(010\ldots 0) = A_l^{(1)}.$$

Similarly, if \widetilde{X}_{01} consists of the n-2 columns $x(00j_3 \dots j_n)$ with one of j_3, \dots, j_n equal to 1 and the rest zeros, then considering the elements of $\widetilde{X}'_{01}X_{1l}$,

$$N^{-2} \operatorname{tr}(\widetilde{X}_{01}' X_{1l} X_{1l}' \widetilde{X}_{01}) = (n-l) A_{l-1}^{(1)} + l A_{l+1}^{(1)}$$

Since $X_{01} = [x(010...0) \ \widetilde{X}_{01}]$, now (c) follows from (4.1). The proofs of (b) and (d) are similar.

Proof of Theorem 3

For $0 \leq l \leq n-2$, let $\Sigma^{(l)}$ denote sum over binary tuples $j_3 \dots j_n$ such that l of j_3, \dots, j_n equal 1. By (2.7), (3.2) and the definition of X_{sl} , we get for $1 \leq u, w \leq N$ and $1 \leq l \leq n-1$,

$$q_{0l}(u,w) = \Sigma^{(l-1)} x(u;01j_3...j_n) x(w;01j_3...j_n) + \Sigma^{(l)} x(u;00j_3...j_n) x(w;00j_3...j_n) = d_{u2} d_{w2} \Psi_{l-1}(u,w) + \Psi_l(u,w),$$
(A.1)
$$q_{1l}(u,w) = \Sigma^{(l-1)} \{ x(u;10j_3...j_n) x(w;10j_3...j_n) + x(u;11j_3...j_n) x(w;11j_3...j_n) \} = d_{u1} d_{w1} (1 + d_{u2} d_{w2}) \Psi_{l-1}(u,w),$$
(A.2)

where

$$\Psi_l(u,w) = \Sigma^{(l)} (d_{u3}d_{w3})^{j_3} \dots (d_{un}d_{wn})^{j_n}, 0 \le l \le n-2,$$
(A.3)

and $\Psi_{n-1}(u, w) = 0$, because the second term on the right-hand side of (A.1) does not arise when l = n - 1. In view of (A.1) and (A.2), the result will follow if we can show that $\Psi_l(u, w) = Q_l(c_{uw})$, a relationship which clearly holds for l = 0, 1 and n - 1, by (6.2) and (A.3). Thus it remains to show that $\Psi_l(u, w)$ satisfies the recursion relation (6.3) for $2 \le l \le n - 2$.

To that end, let $\Phi(\xi) = \prod_{i=3}^{n} (1 + \xi d_{ui} d_{wi})$ and let $\Phi_l(\xi)$ be the *l*th derivative of $\Phi(\xi)$. Differentiation of log $\Phi(\xi)$ yields

$$\Phi_1(\xi) = \left(\sum_{i=3}^n \frac{d_{ui}d_{wi}}{1+\xi d_{ui}d_{wi}}\right)\Phi(\xi) = \left(\frac{c_{uw}}{1+\xi} - \frac{n-2-c_{uw}}{1-\xi}\right)\Phi(\xi),$$

or, $(1 - \xi^2)\Phi_1(\xi) = \{2c_{uw} - (n - 2)(1 + \xi)\}\Phi(\xi)$. Differentiating this l - 1 times and taking $\xi = 0$,

$$\Phi_{l}(0) - (l-1)(l-2)\Phi_{l-2}(0) = \{2c_{uw} - (n-2)\}\Phi_{l-1}(0) - (n-2)(l-1)\Phi_{l-2}(0).$$
(A.4)

Now, by (A.3), $\Psi_l(u, w)$ is the coefficient of ξ^l in the expansion of $\Phi(\xi)$, i.e., it equals $\Phi_l(0)/l!$. Hence (A.4) implies that $\Psi_l(u, w)$ satisfies the recursion relation (6.3).

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