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MINIMUM ABERRATION DESIGNS FOR TWO-LEVEL FACTORIALS IN $N = 1$ (MOD 4) RUNS

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Abstract: Two-level minimum aberration (MA) designs in $N = 1$ (mod 4) runs are studied. For this purpose, we consider designs obtained by adding any single run to a two-symbol orthogonal array (OA) of strength two and then, among these designs, sequentially minimize a measure of bias due to interactions of successively higher orders. The reason for considering such OA plus one run designs is that they are optimal main effect plans in a very broad sense in the absence of interactions. Our approach aims at ensuring model robustness even when interactions are possibly present. It is shown that the MA criterion developed here has an equivalent formulation which is similar but not identical to the minimum moment aberration criterion. This formulation is utilized to derive theoretical results on and construct tables of MA designs in the present context.

Key words and phrases: Augmentation, bias, effect hierarchy, effect sparsity, Hadamard matrix, interaction, main effect, minimum moment aberration, nonorthogonality, orthogonal array.

1. Introduction

Optimal factorial fractions under the minimum aberration (MA) and related model robustness criteria have received much attention over the last two decades. See Mukerjee and Wu (2006) and Xu, Phoa, and Wong (2009) for reviews of regular and nonregular designs, respectively, and further references. Recall that regular designs are the ones that arise through a defining relation.

We consider two-level factorial designs which are of particular interest due to their popularity among practitioners. The number of runs in regular MA designs is a power of two, while nonregular MA designs have been studied more generally for $n = 4t$ runs, where $t \geq 1$ is an integer. Two symbol orthogonal arrays (OAs) play a key role in this context. An $\mathrm{OA}(n, m, 2, 2)$ of strength two, where $n = 4t$, is an $n \times m$ array with entries from a set of two symbols, say ± 1, such that in every $n \times 2$ subarray, all four possible pairs of symbols occur equally often as rows. The rows of such an OA, interpreted as treatment combinations, give a fraction of a 2^m factorial in n runs.

Following Tang and Deng (1999), a two-level nonregular MA design in $n = 4t$ runs sequentially minimizes, among designs given by $\mathrm{OA}(n, m, 2, 2)$, a certain measure of the bias due to interactions of successively higher orders in the estimation of the main effects. This adheres to the effect hierarchy principle (Wu and Hamada (2009, p.172)) that asserts that interactions of the same order are equally likely to be active and lower order interactions are more likely to be active than higher order ones. The MA designs so obtained have sound statistical motivation because (a) consideration of designs given by $\mathrm{OA}(n, m, 2, 2)$ ensures universal optimality, among all n-run designs, for the general mean and the main effects when interactions are absent (Cheng (1980a)), while (b) sequential minimization of bias among these designs as indicated above maximizes model robustness even in the presence of interactions. This is appealing because typically the main effects are of principal interest and only a small number of interactions are really active, by the principle of effect sparsity (Wu and Hamada (2009, p.173)). Indeed, the same statistical motivation applies to nonregular MA designs for more general factorials (Xu and Wu (2001)) and also to regular MA designs even though the original formulation of the MA criterion there looks combinatorial.

We focus on MA designs when the available resources allow $N = n + 1 (= 4t + 1)$ runs. Precisely along the lines of (a) and (b) above for $n = 4t$ runs, it makes sense to consider a design strategy that (i) starts with designs that are optimal for main effects in the absence of interactions, and then (ii) selects a design from amongst these so as to provide maximum protection, under the effect hierarchy principle, against bias even in possible presence of interactions. Now, analogously to the optimality of designs given by $\mathrm{OA}(n, m, 2, 2)$ in the n-run case, following Cheng (1980b), designs obtained by the addition of any one run to any such OA are optimal under a very wide range of criteria (including the well-known D-, A- or E-criteria), among all N-run designs, for the general mean and the main effects when interactions are absent. Therefore, in accordance with (i) and (ii) and resembling the literature for $n = 4t$ runs, our approach to finding an MA design in $N = n + 1 (= 4t + 1)$ runs starts with such OA plus one run designs and then sequentially minimizes, among these designs, a certain measure of the bias due to interactions of successively higher orders. The resulting MA designs can be quite attractive as screening designs where the main effects are of principal interest but it is also important to guard against the bias caused by interactions possibly present.

Although our approach to MA designs is inspired by that for $n = 4t$ runs, its implementation involves significantly new features because the OA plus one run designs we start with are themselves nonorthogonal even in the absence of interactions. This, in particular, leads to some counterintuitive results such as those for the 13-run case in Section 4 below.

2. Preliminaries

Denote the m two-level factors by $F_1, \ldots, F_m$, and the treatment combinations by $j_1 \cdots j_m$, where $j_i = -1$ or 1, $1 \leq i \leq m$. Let $\tau(j_1 \cdots j_m)$ be the treatment effect associated with $j_1 \cdots j_m$. Then, under the usual orthogonal parametrization and a full factorial model where no assumption is made about the absence of any interaction,

$$\tau(j_1 \cdots j_m) = \sum_{x \in \Omega} j_1^{x_1} \cdots j_m^{x_m} \beta(x), \tag{2.1}$$

for each $j_1 \cdots j_m$, where Ω is the set of binary m-tuples. For $\boldsymbol{x} = x_1 \cdots x_m \in \Omega$, the parameter $\beta(x)$ in (2.1) represents the general mean if $x = 0 \cdots 0$, or the factorial effect $F_1^{x_1} \cdots F_m^{x_m}$ otherwise. Clearly, any $\beta(x)$ represents a main effect if exactly one of $x_1, \ldots, x_m$ equals 1, or an interaction if two or more of $x_1, \ldots, x_m$ equal 1. In particular, if all interactions are absent, then (2.1) reduces to

$$\tau(j_1 \cdots j_m) = \beta_0 + j_1\beta_1 + \cdots + j_m\beta_m, \tag{2.2}$$

where we write $\beta_0 = \beta(0 \cdots 0)$, $\beta_1 = \beta(10 \cdots 0)$ etc. for notational simplicity.

Let $\boldsymbol{Q} = (q_{ui})$, $1 \leq u \leq n$, $1 \leq i \leq m$, be an OA$(n, m, 2, 2)$, and consider an $N(= n+1)$-run design obtained by adding a run, say $q_{01} \cdots q_{0m}$, to $\boldsymbol{Q}$. Let $\boldsymbol{q}_0 = (q_{01}, \ldots, q_{0m})^T$. Each element of $\boldsymbol{Q}$ and $\boldsymbol{q}_0$ is ± 1. Denote the vector of observations by $\boldsymbol{Y} = (Y_0, Y_1, \ldots, Y_n)^T$, where Y_0 arises from $q_{01} \cdots q_{0m}$ and $Y_1, \ldots, Y_n$ from the runs given by the rows of $\boldsymbol{Q}$. Then by (2.2), under the absence of all interactions,

$$E(\boldsymbol{Y}) = \boldsymbol{Z}\boldsymbol{\beta}^*, \tag{2.3}$$

where

$$\boldsymbol{Z} = \begin{bmatrix} 1 & \boldsymbol{q}_0^T \\ \boldsymbol{1}_n & \boldsymbol{Q} \end{bmatrix}, \qquad \boldsymbol{\beta}^* = \begin{pmatrix} \beta_0 \\ \boldsymbol{\beta}_{\text{main}} \end{pmatrix}, \tag{2.4}$$

$\boldsymbol{\beta}_{\text{main}} = (\beta_1, \ldots, \beta_m)^T$ the vector of the main effect parameters, and $\boldsymbol{1}_a$ the $a \times 1$ vector of ones. Assume as usual that the observations $Y_0, Y_1, \ldots, Y_n$ have equal variance and are uncorrelated.

We now focus attention on the main effect parameters as given by $\boldsymbol{\beta}_{\text{main}}$. Let $\hat{\boldsymbol{\beta}}_{\text{main}}$ be the best linear unbiased estimator (BLUE) of $\boldsymbol{\beta}_{\text{main}}$ under (2.3). Clearly

$$\hat{\boldsymbol{\beta}}_{\text{main}} = \boldsymbol{L}\boldsymbol{Y}, \tag{2.5}$$

where $\boldsymbol{L}$ is the $m \times N$ submatrix of $(\boldsymbol{Z}^T\boldsymbol{Z})^{-1}\boldsymbol{Z}^T$ formed by the last m rows of the latter. To find $\boldsymbol{L}$ more explicitly, we write $\boldsymbol{I}_m$for the identity matrix of order m and use the facts that

$$\boldsymbol{Q}^T\boldsymbol{1}_n = \boldsymbol{0}, \qquad \boldsymbol{Q}^T\boldsymbol{Q} = n\boldsymbol{I}_m, \qquad N = n+1, \qquad \boldsymbol{q}_0^T\boldsymbol{q}_0 = m, \tag{2.6}$$

the first two of which are consequent on $\boldsymbol{Q}$ being an OA$(n, m, 2, 2)$ with elements ± 1. Hence by (2.4) and (2.6), after some simplification,

$$\boldsymbol{L} = \{n(N+m)\}^{-1}[n\boldsymbol{q}_0 \quad \{(N+m)\boldsymbol{I}_m - \boldsymbol{q}_0\boldsymbol{q}_0^T\}\boldsymbol{Q}^T - \boldsymbol{q}_0\boldsymbol{1}_n^T]. \tag{2.7}$$

3. Formulating the Minimum Aberration Criterion

3.1. MA criterion via consideration of bias

If the assumption of absence of all interactions is dropped, then the BLUE $\hat{\boldsymbol{\beta}}_{\text{main}}$ of $\boldsymbol{\beta}_{\text{main}}$, arising under (2.3) and shown in (2.5), becomes biased. We now quantify this bias with a view to controlling it and thus discriminating amongst the OA plus one run designs from the perspective of model robustness. So we return to the representation (2.1) for the $\tau(j_1 \cdots j_m)$, where no assumption about the absence of interactions is made. For $2 \le i \le m$, let $\Omega(i)$ be the set of binary m-tuples with exactly i ones. Then for any $x = x_1 \cdots x_m \in \Omega(i)$, the parameter $\beta(x)$ in (2.1) represents the i-factor interaction $F_1^{x_1} \cdots F_m^{x_m}$, and it is not hard to see that under (2.1), the expression for $E(\boldsymbol{Y})$ in (2.3) gets modified to

$$E(\boldsymbol{Y}) = \boldsymbol{Z}\boldsymbol{\beta}^* + \sum_{i=2}^{m} \sum_{x \in \Omega(i)} \boldsymbol{\varphi}(x)\beta(x),$$

where

$$\boldsymbol{\varphi}(x) = (q_{01}^{x_1} \cdots q_{0m}^{x_m}, q_{11}^{x_1} \cdots q_{1m}^{x_m}, \ldots, q_{n1}^{x_1} \cdots q_{nm}^{x_m})^T. \tag{3.1}$$

Therefore, by (2.5), the bias vector of $\hat{\boldsymbol{\beta}}_{\text{main}}$ under (2.1), as an estimator of $\boldsymbol{\beta}_{\text{main}}$, is

$$\sum_{i=2}^{m} \sum_{x \in \Omega(i)} \boldsymbol{L}\boldsymbol{\varphi}(x)\beta(x) = \sum_{i=2}^{m} \boldsymbol{\Delta}(i)\boldsymbol{\theta}(i), \tag{3.2}$$

where $\boldsymbol{\Delta}(i)$ is the matrix with columns $\boldsymbol{L}\boldsymbol{\varphi}(x)$, $x \in \Omega(i)$, and correspondingly, $\boldsymbol{\theta}(i)$ is the column vector of the i-factor interaction effects $\beta(x)$, $x \in \Omega(i)$. By (3.2), the i-factor interactions collectively contribute a term $\boldsymbol{\Delta}(i)\boldsymbol{\theta}(i)$ to the bias vector of $\hat{\boldsymbol{\beta}}_{\text{main}}$. Note that $\boldsymbol{\Delta}(i)$ is the alias matrix associated with the i-factor interactions. As an effective strategy for controlling the bias of $\hat{\boldsymbol{\beta}}_{\text{main}}$ in the possible presence of interactions, invoking the effect hierarchy principle, it makes sense to look for a design that sequentially minimizes the "sizes" of $\boldsymbol{\Delta}(2), \ldots, \boldsymbol{\Delta}(m)$. This is in the spirit of Tang and Deng (1999) and Xu and Wu (2001) who explored nonregular designs represented by OAs. Following these authors, for $2 \le i \le m$, we take

$$G_i = \text{tr}\{\boldsymbol{\Delta}(i)\boldsymbol{\Delta}(i)^T\}, \tag{3.3}$$

as a very reasonable measure of the size of $\boldsymbol{\Delta}(i)$. Then the MA criterion calls for finding an OA plus one run design that sequentially minimizes $G_2, \ldots, G_m$ among all such designs.

Along the lines of Mukerjee and Tang (2012) who studied two-level factorial designs under a baseline parametrization different from the one considered here, Bayesian-inspired considerations further justify sequential minimization of $G_2, \ldots, G_m$. Let μ_i be number of active i-factor interactions, $i \geq 2$. In the absence of any knowledge about which μ_i of the i-factor interactions are active or their exact magnitudes, suppose (i) for each $i \geq 2$, all possibilities about the μ_i active i-factor interactions are equally likely, and (ii) the active interactions are uncorrelated, each with mean zero and a constant variance. Let $\mathcal{E}$ denote the expected trace, under (ii) and then simply averaged as per (i), of the mean squared error matrix of $\hat{\boldsymbol{\beta}}_{\text{main}}$ as an estimator of $\boldsymbol{\beta}_{\text{main}}$. As in Mukerjee and Tang (2012), then from (3.2) and (3.3) one can check that bias due to interactions accounts for a term proportional to $\sum_{i=2}^{m} \pi_i G_i$ in the expression for $\mathcal{E}$, where $\pi_i = \mu_i / \binom{m}{i}$ is the proportion of active i-factor interactions. Through the π_i's are not exactly known in practice, the two principles of effect sparsity and effect hierarchy suggest that they are small and that they decrease rapidly with increase in i. Hence it is sensible to sequentially minimize $G_2, \ldots, G_m$ so as to control $\mathcal{E}$.

3.2. Further simplification

In order to streamline the subsequent development, we now obtain an equivalent version of the MA criterion introduced above. Since $\boldsymbol{\Delta}(i)\boldsymbol{\Delta}(i)^T = \sum_{x \in \Omega(i)} \boldsymbol{L}\boldsymbol{\varphi}(x)\boldsymbol{\varphi}(x)^T \boldsymbol{L}^T$ by the definition of $\boldsymbol{\Delta}(i)$, from (3.3) we get

$$G_i = \operatorname{tr}\{\boldsymbol{L}^T \boldsymbol{L} \boldsymbol{\Phi}(i)\}, \qquad 2 \leq i \leq m, \tag{3.4}$$

where

$$\boldsymbol{\Phi}(i) = \sum_{x \in \Omega(i)} \boldsymbol{\varphi}(x)\boldsymbol{\varphi}(x)^T. \tag{3.5}$$

Recall that $\boldsymbol{Q} = (q_{ui})$, $1 \leq u \leq n$, $1 \leq i \leq m$, and that $\boldsymbol{q}_0 = (q_{01}, \ldots, q_{0m})^T$. Let

$$p_{uw} = \sum_{i=1}^{m} q_{ui} q_{wi}, \qquad 0 \leq u, w \leq n, \tag{3.6}$$

and, for $0 \leq s \leq m$, define the $N \times N$ matrices $\boldsymbol{P}^{(s)} = (p_{uw}^s)_{u,w=0,1,\ldots,n}$, where the s in p_{uw}^s is a power index. Write

$$R_s = \operatorname{tr}\{\boldsymbol{L}^T \boldsymbol{L} \boldsymbol{P}^{(s)}\}, \qquad 0 \leq s \leq m. \tag{3.7}$$

Then the following lemmas, proved in Appendix A, hold.

Lemma 1. *For* $2 \leq i \leq m$, $\boldsymbol{\Phi}(i) = \sum_{s=0}^{i} k_{is} \boldsymbol{P}^{(s)}$, *where the* k_{is} *are constants which depend on* i, s, m *but not on the design, and* $k_{ii} > 0$.

Lemma 2. (a) $R_0 = 0$, $R_1 = m$.
(b) *For* $2 \leq s \leq m$,

$$R_s = \{n(N+m)\}^{-2}[n^2 m^{s+1} + 2n \sum_{u=1}^{n} (Np_{0u} - m) p_{0u}^s + \sum_{u=1}^{n} \sum_{w=1}^{n} \{(N+m)^2 p_{uw} - (2N+m) p_{0u} p_{0w} - 2Np_{0u} + m\} p_{uw}^s].$$

For $2 \leq i \leq m$, by (3.4), (3.7), and Lemma 1, $G_i = \sum_{s=0}^{i} k_{is} R_s$, where the k_{is} are constants that depend on i, s, m but not on the design, and $k_{ii} > 0$. Since by Lemma 2(a), R_0 and R_1 do not depend on the design, it follows that sequential minimization of $G_2, \ldots, G_m$, as demanded by the MA criterion, is equivalent to that of $R_2, \ldots, R_m$. However, by Lemma 2(b), consideration of $R_2, \ldots, R_m$ rather than $G_2, \ldots, G_m$ entails much more computational efficiency, because the p_{uw} are simply scalar products of the experimental runs. As seen in the Appendix, this also facilitates the derivation of theoretical results.

3.3. Comparison with other criteria

We now discuss how the MA criterion developed in the last two subsections compares with commonly used criteria like (a) minimum G_2 aberration (Tang and Deng (1999); this G_2 is unrelated to our G_i), (b) generalized minimum aberration (Xu and Wu (2001)), and (c) minimum moment aberration (MMA; Xu (2003)). As noted in Xu and Wu (2001) and Xu (2003), these three criteria are equivalent in the two-level case. Hence for two-level designs in $n = 4t$ runs as given by OAs of strength two, following Tang and Deng (1999), they all sequentially minimize a measure of bias caused by interactions of successively higher orders and thus have nice statistical justification even though their definitions are somewhat combinatorial. It is precisely this statistical reasoning that was followed to develop our MA criterion for $N = 4t + 1$ runs. One may wonder if the criteria in (a)$-$(c) also have the same statistical justification in our setup. In view of the aforesaid equivalence of (a)$-$(c), it suffices to consider only MMA criterion in (c) for this purpose.

Let $c(u, w)$ be the number of coincidences between the runs $(q_{u1}, \ldots, q_{um})$ and $(q_{w1}, \ldots, q_{wm})$, and write

$$C_i = \left\{\frac{N(N-1)}{2}\right\}^{-1} \sum\sum_{0 \leq u < w \leq n} \{c(u, w)\}^i, \qquad 1 \leq i \leq m.$$

Then the MMA criterion sequentially minimizes $C_1, \ldots, C_m$, or equivalently $R_1^*, \ldots, R_m^*$, where $R_s^* = \sum_{u=0}^{n} \sum_{w=0}^{n} p_{uw}^s$, $1 \leq s \leq m$, because by (3.6),

$$p_{uw} = 2c(u, w) - m, \qquad 0 \leq u, w \leq n, \tag{3.8}$$

i.e., $c(u, w) = (1/2)(p_{uw} + m)$. The R_s^* are, however, different from the R_s shown in Lemma 2(b) and obtained directly from consideration of bias. Hence, in our setup, there is no guarantee in general that the MMA criterion, or equivalently the criteria in (a) and (b), sequentially minimize the bias due to interactions of successively higher orders as the MA criterion developed in the last two subsections does.

Nevertheless, for smaller values of N, namely $N = 5, 9, 13$ and 17, we checked computationally that the MMA criterion and our MA criterion lead to identical optimal designs. For the nearly saturated cases $m = n - 1$ and $m = n - 2$, this happens because both the R_s^* and R_s have simplified versions − see e.g., (B.2) and (B.3) in the Appendix − so that sequential minimization of one can be shown to be equivalent to that of the other. While such simplification does not take place for other values of m, a heuristic explanation arises from the fact that R_{s+1}^* is the sum of pure $(s + 1)$th degree terms p_{uw}^{s+1} while, by Lemma 2(b), our R_s involves sth, $(s+1)$th, and $(s+2)$th degree terms in the p_{uw} but the coefficients of the pure $(s + 1)$th degree terms among them typically dominate those of the other terms. Thus, although the MMA criterion is not formally equivalent to our MA criterion arising directly from statistical considerations, the two appear to be good surrogates for each other.

4. Minimum Aberration Designs

Theorem 1 presents necessary and sufficient conditions for OA plus one run designs, obtained by adding a single run $\boldsymbol{q}_0^T$ to an OA$(n, m, 2, 2)$ denoted by $\boldsymbol{Q}$, to have MA in the sense of sequentially minimizing $G_2, \ldots, G_m$, or equivalently $R_2, \ldots, R_m$, for $m = n-1, n-2$, or $n-3$. These are practically important cases where the OA that one starts with is saturated or nearly saturated.

Theorem 1. *Let $m(\geq 3)$ equal $n-1, n-2$, or $n-3$, and suppose an* OA$(n, m, 2, 2)$ *exists. Then an OA plus one run design has MA if and only if $\boldsymbol{Q}$ is any* OA$(n, m, 2, 2)$ *and $\boldsymbol{q}_0^T$ is the negative of some row of $\boldsymbol{Q}$.*

Theorem 1 is proved in Appendix B. As hinted earlier, the proofs for $m = n-1$ or $n-2$ show that the MA designs reported in Theorem 1 for these two cases have MMA as well. However one can check that these designs are not necessarily OAs of weak strength three as defined in Xu (2003), and hence cannot be obtained using the sufficient condition in Theorem 3 of his paper.

Theorem 1 settles the case $n = 4$, $m = 3$. Similarly, for $n = 8$, it settles the cases $m = 5, 6, 7$, while the case $m = 4$ is treated here.

Example 1. Let $N = 9$, $n = 8$, $m = 4$. Then there are two nonisomorphic choices of $\boldsymbol{Q}$ both of which correspond to regular fractions. A complete search of all possibilities for the added run, in conjunction with both these choices of $\boldsymbol{Q}$, shows that an MA design is given by $\boldsymbol{q}_0^T = (- - - +)$ and

$$\boldsymbol{Q} = \begin{matrix} - - - - \\ + + - - \\ + - + - \\ + - - + \\ - + + - \\ - + - + \\ - - + + \\ + + + + \end{matrix}$$

where $+$ and $-$ stand for $+1$ and -1 respectively. The search further reveals that augmentation of neither of the two nonisomorphic choices of $\boldsymbol{Q}$ by the negative of any row therein leads to an MA design with $N = 9$ runs.

Example 1 shows that the conclusion of Theorem 1 does not remain valid for arbitrary n and $m(\leq n-4)$. There are many other instances of this kind – e.g., with $n = 12$ and $4 \leq m \leq 8$, the consequence of augmenting $\boldsymbol{Q}$ by the negative of one of its rows depends on the specific $\boldsymbol{Q}$ and the specific row considered, and no general pattern emerges. Indeed, the proof of Theorem 1 shows that for $m = n-1, n-2$, and $n-3$, the quantities $R_2, \ldots, R_m$ are determined by p_{0u}, $1 \leq u \leq n$. The possible lack of this feature for $m \leq n-4$ precludes further extension of this theorem.

In the rest of this section, we computationally find and tabulate MA designs for $N = 13$ and 17, i.e., $n = 12$ and 16, and $m \leq n-4$. The following facts are useful for this purpose.

(a) For $n = 12$, there are two nonisomorphic OAs if $m = 5$ or 6, and only one such array if $m = 4$ or $m \geq 7$; see Deng and Tang (2002).

(b) For $n = 16$ and each m, a complete listing of nonisomorphic OAs can be obtained from Hall (1961) together with Sun, Li, and Ye (2008).

We now employ steps to obtain MA designs for $N = 13$ and 17. Certain simplifying features that can be incorporated in this procedure are indicated in the next section.

Step I. Given $N(= n+1)$ and m, follow (a) or (b) to list all nonisomorphic choices of $\boldsymbol{Q}$, say $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_g$.

Step II. For every fixed j, $1 \leq j \leq g$, consider each of the 2^m possibilities for the added run and use Lemma 2, or directly (3.7), to find a run whose addition to $\boldsymbol{Q}_j$ sequentially minimizes $R_2, \ldots, R_m$. Let d_j be the best N-run design so obtained from $\boldsymbol{Q}_j$.

Step III. Find the N-run MA design as one that sequentially minimizes $R_2, \ldots, R_m$ among $d_1, \ldots, d_g$.

The results for $N = 13$ and 17 are summarized in Tables 1 and 2 which show $\boldsymbol{Q}$ and the added run, denoted by 'Add', for the MA designs. In the tables, we write $+$ and $-$ for $+1$ and -1 respectively. The tables along with the process of their construction shed light on an issue of both theoretical and computational interest. Since we are considering designs obtained via the addition of a single run to $\boldsymbol{Q}$, an OA with n rows, does it suffice for our purpose to restrict attention to only such $\boldsymbol{Q}$ as having MA as an n-run design? In other words, do the $N(= n+1)$-run designs with $\boldsymbol{Q}$ itself having MA form an essentially complete class in our context? The answer to this question is in the affirmative in Example 1 where the $\boldsymbol{Q}$, shown for our MA design, itself has MA as an 8-run design. The cases $N = 13$ (i.e., $n = 12$) and $m = 5$ or 6, however, demonstrate the nonexistence of any general result in this direction. With $n = 12$ and $m = 5$, there are two nonisomorphic choices of $\boldsymbol{Q}$, say $\boldsymbol{Q}_1$ and $\boldsymbol{Q}_2$, as given by columns 1,2,3,4,5 and 2,4,5,6,10 of the OA$(12, 11, 2, 2)$ shown as $\boldsymbol{B}_{12}$ in Table 1. Note that $\boldsymbol{Q}_1$ has MA as a 12-run design and $\boldsymbol{Q}_2$ does not enjoy this property. However, $\boldsymbol{Q}_1$ never yields an MA design in our setup irrespective of the run added, while $\boldsymbol{Q}_2$ does so upon addition of a run as indicated in Table 1. The same phenomenon holds for $n = 12$, $m = 6$. For $N = 17$ (i.e., $n = 16$), on the other hand, each MA design shown in Table 2 is based on a $\boldsymbol{Q}$ which is itself a 16-run regular MA design; see e.g., Mukerjee and Wu (2006, Chap. 3). This happens presumably because the MA property of $\boldsymbol{Q}$ exerts, for relatively large n, a greater impact on that of the final design obtained by the addition of one run.

5. Some Computational Issues

The main obstacle to finding MA designs for values of $N(= n + 1)$ higher than those in Tables 1 and 2 is that for larger n, often a complete list of all nonisomorphic OA$(n, m, 2, 2)$, $3 \leq m \leq n - 4$, is not yet available. As with the case of $n(= 4t)$ runs, this prevents one from obtaining an N-run design which is perfectly guaranteed to have the MA property among all possible OA plus one run designs. Given N and m, from a practical point of view, in such a situation it makes sense to consider the known nonisomorphic OA$(n, m, 2, 2)$ or a reasonable subclass thereof in Step I of Section 4 and then apply Steps II and III to reach a design that can be expected to behave well under the MA criterion. For example, the fact that all MA designs in Table 2 are augmentations of 16-run regular OAs may encourage one to consider all regular nonisomorphic OA$(n, m, 2, 2)$ in Step

Table 1. MA designs for $N = 13$.

$m = 4$ Add: $- - + -$

$\boldsymbol{Q}$: Keep the first four columns of B_{12}.

$m = 5$ Add: $+ + + + +$

$\boldsymbol{Q}$: Keep columns 2,4,5,6,10 of B_{12}.

$m = 6$ Add: $+ + + + + +$

$\boldsymbol{Q}$: Keep columns 2,4,5,6,10,11 of B_{12}.

$m = 7$ Add: $- - - + - - +$

$\boldsymbol{Q}$: Keep the first seven columns of B_{12}.

$m = 8$ Add: $- - + - - + - +$

$\boldsymbol{Q}$: Keep the first eight columns of B_{12}.

$$\boldsymbol{B}_{12} : \begin{array}{ccccccccccc}
- & - & - & - & - & - & - & - & - & - & - \\
+ & - & + & - & - & - & + & + & + & - & + \\
+ & + & - & + & - & - & - & + & + & + & - \\
- & + & + & - & + & - & - & - & + & + & + \\
+ & - & + & + & - & + & - & - & - & + & + \\
+ & + & - & + & + & - & + & - & - & - & + \\
+ & + & + & - & + & + & - & + & - & - & - \\
- & + & + & + & - & + & + & - & + & - & - \\
- & - & + & + & + & - & + & + & - & + & - \\
- & - & - & + & + & + & - & + & + & - & + \\
+ & - & - & - & + & + & + & - & + & + & - \\
- & + & - & - & - & + & + & + & - & + & +
\end{array}$$

Table 2. MA designs for $N = 17$.

$m = 5$ Add: $- - - - +$

$\boldsymbol{Q}$: Keep columns 1, 2, 4, 8, 15 of B_{16}.

$m = 6$ Add: - - - - - +

$\boldsymbol{Q}$: Keep columns 1, 2, 4, 7, 8, 11 of B_{16}.

$m = 7$ Add: $- - - - - - +$

$\boldsymbol{Q}$: Keep columns 1, 2, 4, 7, 8, 11, 13 of B_{16}.

$m = 8$ Add: $- - - - - - ++$

$\boldsymbol{Q}$: Keep columns 1, 2, 4, 7, 8, 11, 13, 14 of B_{16}.

$m = 9$ Add: $- - + - + - + + -$

$\boldsymbol{Q}$: Keep columns 1-5, 8, 9,14,15 of B_{16}.

$m = 10$ Add: $- - + - + + - + -+$

$\boldsymbol{Q}$: Keep columns 1-6, 8, 9, 14, 15 of B_{16}.

$m = 11$ Add: $- - + - + + - + + - -$

$\boldsymbol{Q}$: Keep columns 1−6, 8−10, 13,14 of B_{16}.

$m = 12$ Add: $- - + - + + - + + - -+$

$\boldsymbol{Q}$: Keep columns 1-6, 8-10 and 13-15 of B_{16}.

$$\boldsymbol{B}_{16} : \begin{array}{ccccccccccccccc}
+ & + & - & + & - & - & + & + & - & - & + & - & + & + & - \\
+ & + & - & + & - & - & + & - & + & + & - & + & - & - & + \\
+ & + & - & - & + & + & - & + & - & - & + & + & - & - & + \\
+ & + & - & - & + & + & - & - & + & + & - & - & + & + & - \\
+ & - & + & + & - & + & - & + & - & + & - & - & + & - & + \\
+ & - & + & + & - & + & - & - & + & - & + & + & - & + & - \\
+ & - & + & - & + & - & + & + & - & + & - & + & - & + & - \\
+ & - & + & - & + & - & + & - & + & - & + & - & + & - & + \\
- & + & + & + & + & - & - & + & + & - & - & - & - & + & + \\
- & + & + & + & + & - & - & - & - & + & + & + & + & - & - \\
- & + & + & - & - & + & + & + & + & - & - & + & + & - & - \\
- & + & + & - & - & + & + & - & - & + & + & - & - & + & + \\
- & - & - & + & + & + & + & + & + & + & + & - & - & - & - \\
- & - & - & + & + & + & + & - & - & - & - & + & + & + & + \\
- & - & - & - & - & - & - & + & + & + & + & + & + & + & + \\
- & - & - & - & - & - & - & - & - & - & - & - & - & - & -
\end{array}$$

Note: $\boldsymbol{B}_{16}$ is the regular OA(16, 15, 2, 2).

I, when n is a power of two and a complete list of such regular nonisomorphic OAs exists.

We now indicate how, for larger N, a two-stage execution of Step II can considerably reduce the computing time while implementing Steps I-III as above. Recall that Step II finds the best augmentation, in the sense of sequential minimization of $R_2, \ldots, R_m$, of each OA$(n, m, 2, 2)$ considered in Step I. For any given OA$(n, m, 2, 2)$, say $\boldsymbol{Q}$, let $D(\boldsymbol{Q})$ be the set of n runs formed by the negatives of the n rows of $\boldsymbol{Q}$. As seen in Section 4, any arbitrary run in $D(\boldsymbol{Q})$ does not necessarily yield the best augmentation of $\boldsymbol{Q}$ among all the 2^mpossible runs that could be added. However, our computations reveal that almost invariably there exists a run in $D(\boldsymbol{Q})$ which either entails the best augmentation or comes quite close. This prompts execution of Step II in two stages as shown below. The $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_g$ of Step I are now the known nonisomorphic OA$(n, m, 2, 2)$ considered in a given context.

Step II. For every fixed j, $1 \leq j \leq g$, find the best N-run design d_j, among those obtained by adding one run to $\boldsymbol{Q}_j$, as follows.

(A) Among the n runs in $D(\boldsymbol{Q}_j)$, find one whose addition to $\boldsymbol{Q}_j$ sequentially minimizes $R_2, \ldots, R_m$. Record this run and the corresponding $R_2, \ldots, R_m$, say $R_{20}, \ldots, R_{m0}$, for comparative purpose while implementing (B) below.

(B) Next consider all the 2^m possibilities for the added run and, from amongst these, find one whose addition to $\boldsymbol{Q}_j$ sequentially minimizes $R_2, \ldots, R_m$.

Execution of (A) is almost instantaneous even for large $N(= n + 1)$ because there are only n runs in $D(\boldsymbol{Q}_j)$. On the other hand, the sequence $R_{20}, \ldots, R_{m0}$ emerging from (A) acts as a benchmark when (B) begins, and it remains so until even better and hence even more stringent augmentations possibly emerge. Now, typically, the sequence $R_{20}, \ldots, R_{m0}$ is itself quite stringent in view of the points noted above regarding the addition of runs from $D(\boldsymbol{Q}_j)$. As a result, a vast majority of the 2^m possible augmentations in (B) get eliminated very quickly on the basis of R_2, or at most R_3, alone. In this way, the two-stage implementation of Step II significantly enhances the speed of computation.

Example 2. Let $N = 33$, $n = 32$ and, for illustration, consider $m = 10$ and 25. To the best of our knowledge, for neither m, does a complete list of all nonisomorphic OA$(32, m, 2, 2)$ exist. So, we focus attention on designs obtained by adding one run to 32-run regular OAs for which a complete catalog of nonisomorphic solutions is available from D.X. Sun as an expanded version Table 3 in Chen, Sun, and Wu (1993). In order to describe the designs for $m = 10$ and 25, let $\boldsymbol{V}$ be the 5×31 matrix with columns given by the points of the finite projective geometry PG(4,2) in Yates order, i.e., in the order $(1, 0, 0, 0, 0)^T$, $(0, 1, 0, 0, 0)^T$, $(1, 1, 0, 0, 0)^T$, $\ldots$, and let $\boldsymbol{B}_{32}$ be the regular OA$(32, 31, 2, 2)$, obtained by replacing each 0 by -1 in the 32×31 array with rows spanned by those of $\boldsymbol{V}$ over GF(2).

(a) For $m = 10$, there are 46 nonisomorphic regular OA(32,10,2,2) which we consider in Step I. Then Steps II and III, with II executed in two stages as above, show that the design obtained by adding the run

$$- - - - - - - - + - +$$

to the regular OA, say $\boldsymbol{Q}^*$, as given by columns 1, 2, 4, 7, 8, 11, 16, 19, 29, 30 of $\boldsymbol{B}_{32}$ has MA among all augmentations of 32×10 regular OAs by one run.

(b) For $m = 25$, there are 9 nonisomorphic regular OA(32,25,2,2) which are considered in Step I. Then as before it is seen that the design obtained by adding the run

$$+ - - + + - - - - + + - - - - + + - - - - + + - -$$

to the regular OA, say $\boldsymbol{Q}^{**}$, as given by columns 1−13, 16−21, 26−31 of $\boldsymbol{B}_{32}$ has MA among all augmentations of 32×25 regular OAs by one run.

Interestingly, for $m = 25$, the added run in (b) is the negative of a row of $\boldsymbol{Q}^{**}$, while for $m = 10$, the best design among the augmentations of $\boldsymbol{Q}^*$ by the negative of a row of itself comes quite close to the one reported in (a) in the sense of having the same R_2 and an only 2% larger R_3. This is in agreement with the rationale behind the two-stage execution of Step II as proposed above.

The OAs $\boldsymbol{Q}^*$ and $\boldsymbol{Q}^{**}$ in Example 2 represent 32-run regular MA designs for the respective values of m; see e.g., Mukerjee and Wu (2006, Chap. 3). This lends further support to the point noted earlier in connection with Table 2 that, for relatively large n, the behavior of an OA$(n, m, 2, 2)$ under the MA criterion tends to exert an influence on that of its best augmentation. Therefore, one may wonder about the possible existence of a general result in this direction. For instance, given a class of nonisomorphic OA$(n, m, 2, 2)$ and their best augmentations, will the ranking of these best augmentations as $N(= n + 1)$-run designs be the same as that of the OAs themselves as n-run designs under the MA criterion, when n is relatively large? Our computations show that for $n = 32$ and $m = 25$, this is indeed the case with the 9 nonisomorphic regular OAs in Example 2(b) and their best augmentations. On the other hand, for $n = 32$ and $m = 10$, the rankings of the 46 nonisomorphic regular OAs in Example 2(a) and their best augmentations turn out to be quite similar but not identical. Thus even for $n = 32$, no general result emerges, which is not entirely unexpected given the somewhat involved form of $R_2, \ldots, R_m$.

Nevertheless, the present computations as well as many others not reported here suggest that, for relatively large n, if out of the nonisomorphic OA$(n, m, 2, 2)$, say $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_g$, considered in a given context, only the top few, say the top four or five, under the MA criterion are included in Step I and then Steps II and III are employed, then the resulting design is the same as what one would obtain by including all of $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_g$ in Step I. In other words, for larger n, consideration of only the top few of $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_g$ rather than all of them for the purpose of augmentation should yield at least highly efficient $N(= n+1)$-run designs under the MA criterion, while at the same time entailing further significant reduction of computing time.

6. Concluding Remarks

Several open issues emerge from the present work. Although the conclusion of Theorem 1 does not hold for arbitrary n and $m(\leq n-4)$, our computations show that augmentation of specific choices of $\boldsymbol{Q}$ by the negatives of some specific, but not all, rows therein may lead to MA designs even for $m \leq n-4$. It would be of interest to obtain systematic results in this direction. However, given the complexities and multitude of steps already encountered in the proof of Theorem 1 for $m = n-3$, this problem looks quite formidable.

Further improvement in the computational procedure also deserves attention. For instance, in the spirit of the two-stage execution of Step II proposed in Section 5, one may wish to explore if some other modification of this step can reduce the computing time to an even greater extent.

Following Mukerjee (1999), main effect plans obtained via the augmentation of an OA by one run enjoy wide-ranging optimality properties in the absence of interactions, not only for two-level factorials but also for general symmetric factorials and certain asymmetric factorials. Extension of the present ideas and results to more general factorials of this kind is of interest. A Kronecker representation for the factorial effects should be useful for this purpose.

Back to 2^m factorials, the present work on $N(4t+1)$-run designs supplements the existing results on $n(= 4t)$-run designs. This leaves open the cases of designs with $4t+2$ and $4t+3$ runs. In either case, from a statistical perspective, one may in principle consider employing the same basic ideas as here to formulate the design problem: (i) start with designs which are optimal under a broad range of criteria for the main effects when interactions are absent, and then (ii) among these designs, find one which sequentially minimizes the bias caused by the possible presence of interactions of successively higher orders. With $4t+2$ runs, following Jacroux, Wong, and Masaro (1983), OA plus two run designs have wide-ranging optimality properties for the general mean and the main effects in the absence of interactions, provided the number of coincidences between the two added runs equals $[m/2]$, the greatest integer in $m/2$. Therefore, in accordance with (i) above, it makes sense to start with OA plus two run designs of this kind. Preliminary studies show that the counterparts of $R_2, \ldots, R_m$ are then even more involved. Additional complexities arise in the derivation of theoretical results because the two added runs have to be handled simultaneously subject to the aforesaid constraint on the number of coincidences between them. Work is currently underway on this problem and will be reported elsewhere. The case of $4t+3$ runs, however, looks far more intractable at this stage because then, to the best of our knowledge, even in the absence of interactions, sufficiently general optimality results as envisaged in (i) above are not yet available.

We conclude with the hope that the present work will generate interest in these and related problems.

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Appendices

Appendix A: Proofs of Lemmas 1 and 2

Proof of Lemma 1. The proof follows essentially from Xu (2003) though, for completeness, we indicate it briefly. By (3.1) and (3.5), the (u,w)th element of $\mathbf{\Phi}(i)$ is

$$\begin{aligned}\Phi_{uw}(i) &= \sum_{x\in\Omega(i)} (q_{u1}q_{w1})^{x_1}\cdots(q_{um}q_{wm})^{x_m} \\ &= \sum_{h=0}^{i} \binom{c(u,w)}{h}\binom{m-c(u,w)}{i-h}(-1)^{i-h}. \qquad \text{(A.1)}\end{aligned}$$

where, for integers $a, b(\geq 0)$, $\binom{a}{b}$ equals 1 if $b=0$, and $a(a-1)\cdots(a-b+1)/b!$ if $b>0$. Since by (3.8), $c(u,w)=(p_{uw}+m)/2$, it is not hard to see from (A.1) that $\Phi_{uw}(i)$ is an ith degree polynomial in p_{uw}, where the coefficients depend on i and m but not on u, w, or the design, and the coefficient of the ith degree term is positive. Hence the result follows.

Proof of Lemma 2. Clearly, by (2.6) and (2.7), $\boldsymbol{L}\mathbf{1}_N=\mathbf{0}$ and $\boldsymbol{L}\widetilde{\boldsymbol{Q}}=\boldsymbol{I}_m$, where $\widetilde{\boldsymbol{Q}}=[\boldsymbol{q}_0\ \boldsymbol{Q}^T]^T$. Since by definition $\boldsymbol{P}^{(0)}=\mathbf{1}_N\mathbf{1}_N^T$ and $\boldsymbol{P}^{(1)}=\widetilde{\boldsymbol{Q}}\widetilde{\boldsymbol{Q}}^T$, part (a) follows from (3.7). Using (2.6) and (2.7) again,

$$\boldsymbol{L}^T\boldsymbol{L}=\{n(N+m)\}^{-2}\begin{bmatrix} n^2m & \boldsymbol{\gamma}^T \\ \boldsymbol{\gamma} & \mathbf{\Gamma}\end{bmatrix},$$

where $\boldsymbol{\gamma} = n(N\boldsymbol{Q}\boldsymbol{q}_0 - m\mathbf{1}_n)$, and

$$\boldsymbol{\Gamma} = (N+m)^2\boldsymbol{Q}\boldsymbol{Q}^T - (2N+m)\boldsymbol{Q}\boldsymbol{q}_0\boldsymbol{q}_0^T\boldsymbol{Q}^T - N(\boldsymbol{Q}\boldsymbol{q}_0\mathbf{1}_n^T + \mathbf{1}_n\boldsymbol{q}_0^T\boldsymbol{Q}^T) + m\mathbf{1}_n\mathbf{1}_n^T.$$

Hence (b) follows from (3.7) and the facts that

$$\begin{array}{ll} p_{uu} = m, \qquad p_{uw} = p_{wu}, & 0 \le u, w \le n, \\ \boldsymbol{Q}\boldsymbol{q}_0 = (p_{01}, \ldots, p_{0n})^T, & \boldsymbol{Q}\boldsymbol{Q}^T = (p_{uw})_{u,w=1,\ldots,n}, \end{array} \tag{A.2}$$

which are evident from (3.6) and the definitions of $\boldsymbol{Q}$ and q_0.

Appendix B: Proof of Theorem 1

Case 1: $\boldsymbol{m = n - 1}$.

Lemma B.1. *If $m = n-1$, then the following are equivalent:* (a) *for* $1 \le u \le n$, $p_{0u} \in \{-(n-1), -1, 1\}$, (b) *one of* $p_{01}, \ldots, p_{0n}$ *equals* $-(n-1)$ *and the rest equal* 1, (c) *the vector* $\boldsymbol{q}_0^T$, *representing the added run, is the negative of some row of* $\boldsymbol{Q}$.

Proof. Since $m = n-1$, by (2.6) and (A.2),

$$\sum_{u=1}^{n} p_{0u} = \mathbf{1}_n^T\boldsymbol{Q}\boldsymbol{q}_0 = 0, \qquad \sum_{u=1}^{n} p_{0u}^2 = \boldsymbol{q}_0^T\boldsymbol{Q}^T\boldsymbol{Q}\boldsymbol{q}_0 = nm = n(n-1). \tag{B.1}$$

Suppose (a) holds. Let f_0, f_1, and f_2 of $p_{01} \ldots, p_{0n}$ equal $-(n-1)$, -1, and 1 respectively. Then $f_0 + f_1 + f_2 = n$, while by (B.1), $-(n-1)f_0 - f_1 + f_2 = 0$ and $(n-1)^2 f_0 + f_1 + f_2 = n(n-1)$. These equations have the unique solution $f_0 = 1$, $f_1 = 0$, $f_2 = n-1$. Hence (a) implies (b). Trivially, (b) implies (c) because if one of $p_{01}, \ldots, p_{0n}$, say p_{01}, equals $-(n-1)(= -m)$, then $\boldsymbol{q}_0^T$ must be the negative of the first row of $\boldsymbol{Q}$. It remains to show that (c) implies (a). To that effect, note that $m = n-1$ and hence $\boldsymbol{H} = [\mathbf{1}_n \ \boldsymbol{Q}]$ is a Hadamard matrix of order n. Let (c) hold with $\boldsymbol{q}_0^T$ as the negative of, say, the first row of $\boldsymbol{Q}$. Then $(-1, \boldsymbol{q}_0^T)$ equals the negative of the first row of $\boldsymbol{H}_n$, so that

$$\boldsymbol{Q}\boldsymbol{q}_0 = [\mathbf{1}_n \ \boldsymbol{Q}]\begin{pmatrix} -1 \\ \boldsymbol{q}_0 \end{pmatrix} + \mathbf{1}_n = \boldsymbol{H}_n\begin{pmatrix} -1 \\ \boldsymbol{q}_0 \end{pmatrix} + \mathbf{1}_n = \begin{pmatrix} -n \\ \mathbf{0} \end{pmatrix} + \mathbf{1}_n = \begin{pmatrix} -(n-1) \\ \mathbf{1}_{n-1} \end{pmatrix},$$

i.e., by (A.2), (a) holds. Therefore, (c) implies (a), completing the proof.

Proof of Theorem 1 for $\boldsymbol{m = n-1}$. Clearly, $p_{uu} = m$ for every u, while $p_{uw} = -1$, for every $1 \le u \ne w \le n$, because $\boldsymbol{H}_n = [\mathbf{1}_n \ \boldsymbol{Q}]$ is a Hadamard matrix. Hence from (B.1) and Lemma 2(b),

$$R_2 = \text{constant} + 2Nn^{-1}(N+m)^{-2}\sum_{u=1}^{n} p_{0u}^3, \tag{B.2}$$

$$R_s = \text{constant} + 2n^{-1}(N+m)^{-2}\sum_{u=1}^{n}(Np_{0u} - m)p_{0u}^s, \quad 3 \le s \le m, \tag{B.3}$$

where the constants do not depend on the design. We now proceed to minimize R_2, or equivalently $\sum_{u=1}^n p_{0u}^3$; see (B.2). By (3.8) and the fact that $m(=n-1)$ is odd, $p_{0u} \geq -(n-1)$ and $|p_{0u}| \geq 1$, $1 \leq u \leq n$. Hence $\sum_{u=1}^n (p_{0u}+n-1)(p_{0u}^2-1) \geq 0$, i.e., $\sum_{u=1}^n p_{0u}^3 \geq -n(n-1)(n-2)$, using (B.1). Clearly, this lower bound is attained if and only if (a), or equivalently (b), of Lemma B.1 holds. But (b) of Lemma B.1 uniquely determines $R_3, \ldots, R_m$; see (B.3). The result now follows, recalling the equivalence of (b) and (c) of Lemma B.1.

Case 2: $\boldsymbol{m = n - 2}$.

Lemma B.2. *If $m = n-2$, then the following are equivalent:* (a) *for* $1 \leq u \leq n$, $p_{0u} \in \{-(n-2), 0, 2\}$, (b) *one of $p_{01}, \ldots, p_{0n}$ equals $-(n-2)$ and, among the rest, there are $n/2$ and $n/2-1$ which equal* 0 *and* 2 *respectively,* (c) *the vector $\boldsymbol{q}_0^T$, representing the added run, is the negative of some row of $\boldsymbol{Q}$.*

Proof. Since $m = n-2$, analogously to (B.1),

$$\sum_{u=1}^n p_{0u} = 0, \qquad \sum_{u=1}^n p_{0u}^2 = n(n-2). \tag{B.4}$$

Hence as with Lemma B.1, it follows that (a) implies (b), and (b) implies (c).

We next show that (c) implies (a). Note that $m = n-2$ and hence $\boldsymbol{Q}$ can be embedded in a saturated OA$(n, n-1, 2, 2)$; cf., Mukerjee and Wu (1995). Thus there exists a vector $\boldsymbol{\varepsilon} = (\varepsilon_1, \ldots, \varepsilon_n)^T$, with half of its elements 1 and the rest -1, such that $\boldsymbol{H}_n = [\boldsymbol{1}_n \ \boldsymbol{\varepsilon} \ \boldsymbol{Q}]$ is a Hadamard matrix of order n. Let (c) hold with $\boldsymbol{q}_0^T$ as the negative of, say, the first row of $\boldsymbol{Q}$. Then $(-1, -\varepsilon_1, \boldsymbol{q}_0^T)$ equals the negative of the first row of $\boldsymbol{H}_n$ so that, as in the proof of Lemma B.1,

$$\boldsymbol{Q}\boldsymbol{q}_0 = \begin{pmatrix} -n \\ \boldsymbol{0} \end{pmatrix} + \boldsymbol{1}_n + \varepsilon_1 \boldsymbol{\varepsilon}.$$

Since each of $\varepsilon_1, \ldots, \varepsilon_n$ is 1 or -1, it follows that the first element of $\boldsymbol{Q}\boldsymbol{q}_0$ is $-(n-2)$ and the remaining elements are 0 or 2, i.e., by (A.2), (a) holds. Hence (c) implies (a), completing the proof.

Proof of Theorem 1 for $\boldsymbol{m = n-2}$. Since $\boldsymbol{H}_n = [\boldsymbol{1}_n \ \boldsymbol{\varepsilon} \ \boldsymbol{Q}]$ is a Hadamard matrix, p_{uw} equals -2 if ε_u and ε_w have the same sign, and 0 otherwise, $1 \leq u \neq w \leq n$. Moreover, $\boldsymbol{1}_n^T \boldsymbol{Q}\boldsymbol{q}_0 = \boldsymbol{\varepsilon}^T \boldsymbol{Q}\boldsymbol{q}_0 = 0$, as the columns of $\boldsymbol{H}_n$ are mutually orthogonal. Hence by (A.2), $\Sigma_+ p_{0w} = \Sigma_- p_{0w} = 0$, where Σ_+ and Σ_- denote sums on u over $\{u : 1 \leq u \leq n, \varepsilon_u = 1\}$ and $\{u : 1 \leq u \leq n, \varepsilon_u = -1\}$, respectively. Since $p_{uu} = m$ for each u, from these facts together with (B.4) and Lemma 2(b), one can check that (B.2) and (B.3) continue to hold. In view of (B.2), minimization of R_2 amounts to that of $\sum_{u=1}^n p_{0u}^3$. By (3.8), $p_{0u} \geq -(n-2)$

and each p_{0u} is even, because $m = n-2$ is even. Therefore, as the product of two consecutive integers is nonnegative, $\sum_{u=1}^{n}(p_{0u}+n-2)(p_{0u}/2)(p_{0u}/2-1) \geq 0$, i.e., $\sum_{u=1}^{n} p_{0u}^3 \geq -n(n-2)(n-4)$, using (B.4). Clearly, this lower bound is attained if and only if (a) of Lemma B.2 holds. The result now follows as in Case 1, using Lemma B.2 in place of Lemma B.1.

Case 3: $\boldsymbol{m = n - 3}$.

The proofs in Cases 1 and 2 were facilitated by the fact that, for $m = n-1$ and $m = n-2$, if $\boldsymbol{q}_0^T$ is the negative of some row of $\boldsymbol{Q}$ then at most three of $p_{01}, \ldots, p_{0n}$ are distinct; see Lemmas B.1 and B.2. As Lemma B.6 below demonstrates, this simplifying feature ceases to hold for $m = n - 3$. Consequently, the proof now gets quite involved. If $n = 8$ or 12 and $m = n - 3$, then there is a unique choice of $\boldsymbol{Q}$ up to isomorphism and the proof in Case 3 follows via a complete enumeration of all possibilities for the added run. Therefore, in what follows, we consider $m = n - 3$ and $n \geq 16$

Since $m = n - 3$, following Vijayan (1976), there exist vectors $\boldsymbol{\varepsilon}^{(1)} = (\varepsilon_{11}, \ldots, \varepsilon_{1n})^T$ and $\boldsymbol{\varepsilon}^{(2)} = (\varepsilon_{21}, \ldots, \varepsilon_{2n})^T$ with elements ± 1 such that each of the sets

$$
\begin{aligned}
&J_1 = \{u : 1 \leq u \leq n, \varepsilon_{1u} = \varepsilon_{2u} = 1\}, \qquad J_2 = \{u : 1 \leq u \leq n, \varepsilon_{1u} = 1, \varepsilon_{2u} = -1\}, \\
&J_3 = \{u : 1 \leq u \leq n, \varepsilon_{1u} = -1, \varepsilon_{2u} = 1\}, \quad J_4 = \{u : 1 \leq u \leq n, \varepsilon_{1u} = \varepsilon_{2u} = -1\},
\end{aligned} \tag{B.5}
$$

has cardinality $n/4$ and

$$\boldsymbol{H}_n = [\boldsymbol{1}_n \ \boldsymbol{\varepsilon}^{(1)} \ \boldsymbol{\varepsilon}^{(2)} \ \boldsymbol{Q}] \tag{B.6}$$

is a Hadamard matrix of order n. Let

$$\xi_l = \sum_{u \in J_l} p_{0u}. \tag{B.7}$$

Lemma B.3. $\xi_1 = -\xi_2 = -\xi_3 = \xi_4$.

Proof. By (B.6), each of $\boldsymbol{1}_n$, $\boldsymbol{\varepsilon}^{(1)}$, and $\boldsymbol{\varepsilon}^{(2)}$ is orthogonal to $\boldsymbol{Q}\boldsymbol{q}_0$. So, by (A.2), (B.5), and (B.7), $\xi_1 + \xi_2 + \xi_3 + \xi_4 = \xi_1 + \xi_2 - \xi_3 - \xi_4 = \xi_1 - \xi_2 + \xi_3 - \xi_4 = 0$, and the lemma follows.

Lemma B.4. (a) $R_s = \textit{constant} + \{n(N+m)\}^{-2}[2n\sum_{u=1}^{n}(Np_{0u}-m)p_{0u}^s - (2N+m)\alpha_s\xi_1^2]$, $2 \leq s \leq m$, *where* $\alpha_s = 4\{1+(-3)^s - 2(-1)^s\}$ *and the constants do not depend on the design.*
(b) *Minimization* R_2 *of is equivalent to minimizing*

$$W = 2n(n+1)\sum_{u=1}^{n} p_{0u}^3 - 32(3n-1)\xi_1^2. \tag{B.8}$$

Proof. Since $\boldsymbol{H}_n$ as shown in (B.6) is a Hadamard matrix of order n, from (B.5) we get

$$\begin{aligned} p_{uw} &= -3, \text{ if } u \neq w \text{ and } u, w \text{ belong to the same } J_l, \\ &= -1, \text{ if one of } u, w \text{ belongs to } J_1 \text{ or } J_4 \text{ and the other to } J_2 \text{ or } J_3. \\ &= \ \ 1, \text{ if one of } u, w \text{ belongs to } J_1 \text{ and the other to } J_4 \\ &\qquad \text{or if one of } u, w \text{ belongs to } J_2 \text{ and the other to } J_3. \end{aligned} \tag{B.9}$$

Also, $p_{uu} = n - 3$, $1 \leq u \leq n$, and analogously to (B.1),

$$\sum_{u=1}^{n} p_{0u} = 0, \qquad \sum_{u=1}^{n} p_{0u}^2 = n(n-3). \tag{B.10}$$

Part (a) follows from Lemmas 2(b) and B.3, using relationships such as

$$\sum_{u=1}^{n}\sum_{w=1}^{n} p_{0u}p_{0w}p_{uw}^{s} = \text{constant} + \alpha_s\xi_1^2 \quad \text{and} \quad \sum_{u=1}^{n}\sum_{w=1}^{n} p_{0u}p_{uw}^{s} = 0,$$

which are consequent on (B.7), (B.9), and (B.10). Part (b) then follows from (a) using (B.10) and the facts that $N = n + 1$, $m = n - 3$, and $\alpha_2 = 32$.

Lemma B.5. (a) *For* $1 \leq u \leq n$, p_{0u} *is an odd integer which is greater than or equal to* $-(n-3)$. (b) *The minimum of* p_{0u}, *over* $1 \leq u \leq n$, *equals* $-(n-3)$ *if and only if* $\boldsymbol{q}_0^T$ *is the negative of some row of* $\boldsymbol{Q}$.

Proof. This is evident from (3.8) noting that here $m = n - 3$ is odd.

Lemma B.6. *Consider designs where* $\boldsymbol{q}_0^T$ *is the negative of some row of* $\boldsymbol{Q}$.

(a) *For every such design, one* p_{0u}, $1 \leq u \leq n$, *equals* $-(n-3)$ *and, among the rest, there are* $n/4 - 1$, $n/2$, *and* $n/4$ *which equal* 3, 1, *and* -1, *respectively.*

(b) *Every such design has* $\xi_1^2 = n^2/16$ *and* $W = W_0$, *where*

$$W_0 = -2n^2(n+1)(n-4)(n-5) - 2n^2(3n-1). \tag{B.11}$$

(c) *All such designs have the same sequence* $R_2, \ldots, R_m$.

Proof. Without loss of generality, let $\boldsymbol{q}_0^T$ be the negative of the first row of $\boldsymbol{Q}$ and suppose $1 \in J_1$. Then $p_{0u} = -p_{1u}$, $1 \leq u \leq n$, so that by (B.9), $p_{01} = -(n-3)$, $p_{0u} = 3$, for $u (\neq 1) \in J_1$, and among p_{0u}, $u \notin J_1$, there are $n/2$ and $n/4$ which equal 1 and -1 respectively. Thus (a) follows. Next, from (B.7) and the proof of (a), $\xi_1 = -n/4$, i.e., $\xi_1^2 = n^2/16$. The rest of (b) follows from (a) and (B.8). Finally, (c) follows from (a), (b), and Lemma B.4(a).

Lemma B.7. *Let* $n \geq 16$. *If* $\min\{p_{0u} : 1 \leq u \leq n\} > -(n-3)$, *then* $W > W_0$.

Proof. Without loss of generality, let $p_{01} = \min\{p_{0u} : 1 \leq u \leq n\}$ and $1 \in J_1$. Since p_{01} is odd by Lemma B.5(a), it suffices to consider the three cases in (i)−(iii) below.

(i) Let $p_{01} = -(n-5)$. Then by (3.8), $\boldsymbol{q}_0^T$ has exactly one coincidence with $\boldsymbol{q}_1^T$, where $\boldsymbol{q}_1^T$ is the first row of $\boldsymbol{Q}$. If this coincidence is in the ith position, then $\boldsymbol{q}_0^T = -\boldsymbol{q}_1^T + 2q_{1i}\boldsymbol{e}_i^T$, where $\boldsymbol{e}_i^T$is the $1 \times m$ unit vector with 1 in the ith position and zeros elsewhere. Hence $p_{0u} = -p_{1u} + 2q_{1i}q_{ui}$, i.e., $p_{0u} = -p_{1u} \pm 2$, $1 \leq u \leq n$, as each element of $\boldsymbol{Q}$ is ± 1. Consequently, as $1 \in J_1$, it follows from (B.9) that $p_{0u} \in \{1, 5\}$ for $u(\neq 1) \in J_1$, $p_{0u} \in \{-1, 3\}$ for $u \in J_2 \cup J_3$, and $p_{0u} \in \{1, -3\}$ for $u \in J_4$. Hence if y_1, y_2, y_3, and y_4 denote the cardinalities of the sets $\{u : u(\neq 1) \in J_1, p_{0u} = 1\}$, $\{u : u \in J_2, p_{0u} = -1\}$, $\{u : u \in J_3, p_{0u} = -1\}$, and $\{u : u \in J_4, p_{0u} = 1\}$, then from (B.7) and the fact that $p_{01} = -(n-5)$, we get $\xi_1 = n/4 - 4y_1$, $\xi_2 = 3n/4 - 4y_2$, $\xi_3 = 3n/4 - 4y_3$, and $\xi_4 = 4y_4 - 3n/4$. Writing $y_4 = y$ for notational simplicity, Lemma B.3 now yields $y_1 = n/4 - y$, $y_2 = y_3 = y$, where $1 \leq y \leq n/4$ because $0 \leq y_1 \leq n/4 - 1$. From (B.8), (B.11) and the facts just noted, $W - W_0 = 2n^2(6n^2 - 66n - 40) - 512(3n-1)y^2 + 768n^2y$ after some algebra. The right-hand side of the expression for $W - W_0$ is increasing in y over $1 \leq y \leq n/4$, and hence is minimized at $y = 1$. Therefore, $W - W_0 \geq 4(n-4)(3n^3 - 21n^2 + 88n - 32) > 0$, for $n \geq 16$.

(ii) Let $p_{01} = -(n-7)$. Then $\boldsymbol{q}_0^T$ has exactly two coincidences with the first row of $\boldsymbol{Q}$, say in positions i_1 and i_2. As in (i) above, then $p_{0u} = -p_{1u} + 2(q_{1i_1}q_{ui_1} + q_{1i_2}q_{ui_2})$, i.e., $p_{0u} = -p_{1u}$ or $-p_{1u} \pm 4$, $1 \leq u \leq n$. Hence, noting that $1 \in J_1$ and using (B.9), $p_{0u} \in \{7, 3, -1\}$ for $u(\neq 1) \in J_1$. Since $n \geq 16$ and $p_{01} = -(n-7)$, from (B.7) one can now check that $|\xi_1| \leq 5n/4 - 8$. Also, each p_{0u} is odd by Lemma B.5(a), and $p_{0u} \geq -(n-7)$, $1 \leq u \leq n$, so that $\sum_{u=1}^{n}(p_{0u} + n - 7)(p_{0u}^2 - 1) \geq 0$, i.e., $\sum_{u=1}^{n} p_{0u}^3 \geq -n(n-4)(n-7)$, invoking (B.10). From these facts, together with (B.8) and (B.11), $W - W_0 \geq 4(n^4 - 39n^3 + 488n^2 - 1696n + 512) > 0$, for $n \geq 16$.

(iii) Let $p_{01} \geq -(n-9)$. As in (ii) above, then $\sum_{u=1}^{n} p_{0u}^3 \geq -n(n-4)(n-9)$. Also, by Lemma B.3, (B.7), (B.10), and the Cauchy-Schwarz inequality,

$$\xi_1^2 = \frac{1}{4}\sum_{l=1}^{4}\xi_l^2 \leq \frac{1}{4}\sum_{l=1}^{4}\Big(\sum_{u \in J_l} p_{0u}^2\Big)(\frac{1}{4}n) = \frac{1}{16}n\sum_{u=1}^{n} p_{0u}^2 = \frac{1}{16}n^2(n-3).$$

Therefore, by (B.8) and (B.11), $W - W_0 \geq 2n^2(n-4)(n+5) > 0$, for $n \geq 16$.

Proof of Theorem 1 for $\boldsymbol{m = n-3}$. As mentioned earlier, for $n = 8$ or 12, the result follows by complete enumeration of all possibilities for the added run. Let, therefore, $n \geq 16$. By Lemma B.4(b), Lemma B.5, Lemma B.6(b) and Lemma B.7, then R_2, or equivalently W, is minimized if and only if $\boldsymbol{q}_0^T$ is the negative of some row of $\boldsymbol{Q}$. Lemma B.6(c) now completes the proof.

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