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$E(s^2)$-OPTIMAL SUPERSATURATED DESIGNS

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Abstract: Tang and Wu (1997) derived a lower bound on the $E(s^2)$-value of an arbitrary supersaturated design, and described a method of constructing some $E(s^2)$-optimal designs achieving this lower bound. In this paper, we relate designs achieving Tang and Wu's bound to orthogonal arrays, and give a unified treatment of Tang and Wu's optimality result and the optimality of Lin's (1993) half Hadamard matrices. The optimality of designs obtained by adding one or two factors to (or by removing one or two factors from) those achieving Tang and Wu's bound is also proved. As an application, we give a complete solution of $E(s^2)$-optimal 8-run designs which can accommodate 8 to 35 factors.

Key words and phrases: Balanced incomplete block design, Hadamard matrix, Nearly balanced incomplete block design, orthogonal array.

1. Introduction

Recently there has been renewed interest in the study of supersaturated designs. An N-run design for k two-level factors is *saturated* if $N = k + 1$. Such designs have minimum number of runs for estimating all the main effects when the interactions are negligible, and are useful for screening experiments in the initial stage of an investigation where the primary goal is to identify the few active factors from a large number of potential factors. *Supersaturated* designs, with $N < k + 1$, provide more flexibility and cost saving. As with saturated designs, the assumption of effect sparsity is essential.

Let $\boldsymbol{X}$ be an $N \times k$ matrix of 1's and -1's, where $N < k + 1$. Each column of $\boldsymbol{X}$ corresponds to a factor, and each row defines a factor-level combination. Throughout this paper, as is usually done in the literature, it will be assumed that each column of $\boldsymbol{X}$ contains the same number of 1's and -1's. It is also necessary that all the columns of $\boldsymbol{X}$ are distinct. Booth and Cox (1962), in the first systematic construction of supersaturated designs, proposed the criterion of minimizing

$$E(s^2) = \sum_{1 \le i < j \le k} s_{ij}^2 \Big/ \binom{k}{2}, \tag{1.1}$$

where s_{ij} is the (i, j)th entry of $\boldsymbol{X}^T\boldsymbol{X}$. A supersaturated design minimizing (1.1) is called $E(s^2)$-optimal. Note that $s_{ij} = 0$ when the ith and jth columns of $\boldsymbol{X}$

are orthogonal. Thus $E(s^2)$ measures departure from orthogonality through the overall pairwise correlation among the k factors.

After Booth and Cox (1962), the subject of supersaturated designs remained dormant until the appearance of Lin (1993). Other recent works include, e.g., Wu (1993), Lin (1995), Tang and Wu (1997), Deng, Lin and Wang (1994) and Nguyen (1996). Lin (1993) proposed a method of constructing supersaturated designs from half fractions of Hadamard matrices. Without loss of generality, an $n \times n$ Hadamard matrix $\boldsymbol{H}$ can be expressed as

$$\boldsymbol{H} = \begin{bmatrix} \mathbf{1} & \mathbf{1} & \boldsymbol{H}^h \\ \mathbf{1} & -\mathbf{1} & * \end{bmatrix}, \tag{1.2}$$

where $\mathbf{1}$ is an $n/2 \times 1$ vector of 1's. If $\boldsymbol{H}^h$ contains no identical columns, then it is a supersaturated design with $N = n/2$ and $k = n - 2$.

Tang and Wu (1997) showed that for any supersaturated design with k factors and N runs,

$$E(s^2) \geq \frac{k - N + 1}{(k-1)(N-1)} N^2. \tag{1.3}$$

They also showed that the lower bound in (1.3) is achieved by the following construction. Suppose $k = m(N-1)$ and for $i = 1, \ldots, m$, there exists an $N \times N$ Hadamard matrix $\boldsymbol{H}_i = [\mathbf{1} \vdots \boldsymbol{H}_i^*]$ such that $\boldsymbol{H}_1^*, \ldots, \boldsymbol{H}_m^*$ have distinct columns. Then $[\boldsymbol{H}_1^* \cdots \boldsymbol{H}_m^*]$ achieves the lower bound and is an $E(s^2)$-optimal supersaturated design with $k = m(N-1)$.

In this paper, further results on $E(s^2)$-optimal supersaturated designs will be presented. First of all, there is an alternative proof of (1.3) which provides a simple characterization of the designs attaining the lower bound. From this not only Tang and Wu's (1997) optimality result, but also the $E(s^2)$-optimality of Lin's half Hadamard matrices follows immediately. It came to our knowledge that similar results had been obtained by Nguyen (1996), who also derived (1.3). Therefore this proof is omitted here. However, since Nguyen and Tang and Wu were apparently unaware of each other's work, in Section 2, we shall briefly discuss the optimality of Tang and Wu's construction. It is instructive to give a unified treatment of Tang and Wu's optimality result and the optimality of half Hadamard matrices. This is done by relating designs achieving the lower bound in (1.3) to orthogonal arrays. Section 3 is devoted to the $E(s^2)$-optimality of designs obtained by removing one or two factors from (or by adding one or two factors to) those achieving the lower bound in (1.3). These techniques are used in Section 4 to give a complete solution of $E(s^2)$-optimal designs with eight runs, which can accommodate from eight to thirty-five factors.

We end this section by recalling that a $(1, -1)$-matrix $\boldsymbol{X}$ is called a two-level *orthogonal array* with strength two if the four $1{\times}2$ vectors $(1,1), (1,-1), (-1,1)$

and $(-1,-1)$ appear equally often in any two columns of $\boldsymbol{X}$. A block design is called binary if every treatment appears in each block at most once. A balanced incomplete block design, denoted BIBD(t,b,q), is a binary block design with t treatments and b blocks of size q, where $q < t$, such that all the treatments appear the same number of times, and every pair of treatments appear together in the same number of blocks. The treatment-block incidence matrix of a binary incomplete block design with t treatments and b blocks is a $t \times b$ matrix such that the (i,j)th entry is equal to 1 if the ith treatment appears in the jth block, and is equal to -1 otherwise.

2. $E(s^2)$-Optimal Designs Constructed from Orthogonal Arrays and Block Designs

The key idea in Nguyen's (1996) and our alternative proof of (1.3) (and the development throughout this paper) is to utilize the identity $\mathrm{tr}(\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{X}^T\boldsymbol{X}) = \mathrm{tr}(\boldsymbol{X}\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{X}^T)$: instead of inner products of columns of $\boldsymbol{X}$, it is sufficient to consider inner products of rows of $\boldsymbol{X}$. Then it becomes a weighing design problem and techniques from weighing design literature can be applied. Another crucial point is that since each column of $\boldsymbol{X}$ has the same number of 1's and -1's, $\boldsymbol{X}\boldsymbol{X}^T$ has zero row sums. The lower bound in (1.3) follows easily from these two observations. Furthermore, this lower bound is achieved if and only if all the off-diagonal entries of $\boldsymbol{X}\boldsymbol{X}^T$ are equal to $-k/(N-1)$, which must be a negative integer. The readers are referred to Nguyen (1996) for the details. Let $m = k/(N-1)$ and $\widetilde{\boldsymbol{X}}$ be obtained by adding m columns of 1's to $\boldsymbol{X}$. Then clearly all the off-diagonal entries of $\boldsymbol{X}\boldsymbol{X}^T$ are equal to $-k/(N-1)$ if and only if any two rows of $\widetilde{\boldsymbol{X}}$ are orthogonal. We state this as

Theorem 2.1. *Suppose $N < k+1$. Then the equality holds in* (1.3) *if and only if $k = m(N-1)$ for some positive integer m and any two rows of the matrix obtained by adding m columns of* 1*'s to $\boldsymbol{X}$ are orthogonal.*

Now consider Tang and Wu's (1997) construction. If $\boldsymbol{H}$ is a Hadamard matrix, then $\boldsymbol{H}^T$ is also a Hadamard matrix. Suppose $\boldsymbol{H}_1, \ldots, \boldsymbol{H}_m$ are Hadamard matrices, where $\boldsymbol{H}_i = [\mathbf{1} \vdots \boldsymbol{H}_i^*]$. Then any two rows of $\boldsymbol{H}_i$ are orthogonal. Therefore any two rows of $[\underbrace{\mathbf{1}\cdots\mathbf{1}}_{m}\ \boldsymbol{H}_1^* \cdots \boldsymbol{H}_m^*]$ are also orthogonal. It follows from Theorem 2.1 that $[\boldsymbol{H}_1^* \cdots \boldsymbol{H}_m^*]$ is $E(s^2)$-optimal. For half Hadamard matrices, any two rows of the Hadamard matrix (1.2) are orthogonal. In particular, any two rows of $[\mathbf{1}\ \mathbf{1}\ \boldsymbol{H}^h]$ are orthogonal. Since each column of $\boldsymbol{H}^h$ contains the same number of 1's and -1's, it again follows from Theorem 2.1 that $\boldsymbol{H}^h$ is an $E(s^2)$-optimal supersaturated design if all of its columns are distinct. The same argument also shows the $E(s^2)$-optimality of quarter- or higher fractions of

Hadamard matrices discussed in Deng, Lin and Wang (1994) if such designs can be constructed.

Remark 1. In Theorem 2.1, we may normalize $\widetilde{\boldsymbol{X}}$ so that its first row consists of 1's. This can be achieved by changing the signs of all the entries in the same column if necessary. It is clear that when $N \geq 3$, any two rows of $\widetilde{\boldsymbol{X}}$ are orthogonal if and only if the transpose of the array obtained by deleting the first row of this normalized version of $\widetilde{\boldsymbol{X}}$ is an orthogonal array with strength two.

Remark 2. Since the size of an orthogonal array with strength 2 is a multiple of 4, it follows from Remark 1 that if N is not a multiple of 4, then the lower bound in (1.3) can be achieved only when k is an even multiple of $N-1$.

Nguyen (1996) proposed a method of constructing supersaturated designs with $2(N-1)$ factors in N runs by using balanced incomplete block designs. As mentioned earlier, for any supersaturated design $\boldsymbol{X}$, by changing the signs of all the entries in the same column if necessary, we may normalize it so that all the entries of its first row are equal to 1. Let $\boldsymbol{Z}$ be obtained from such a normalized version of $\boldsymbol{X}$ by deleting the first row. Then $\boldsymbol{Z} = [z_{ij}]_{(N-1)\times k}$ can be considered as the treatment-block incidence matrix of a binary incomplete block design with $N-1$ treatments and k blocks of size $N/2-1$, where the ith treatment appears in the jth block if and only if $z_{ij} = 1$. For convenience, denote this block design by $d_{\boldsymbol{X}}$. It follows immediately from Theorem 2.1 that a supersaturated design $\boldsymbol{X}$ attains the lower bound in (1.3) if and only if $d_{\boldsymbol{X}}$ is a balanced incomplete block design. This equivalence of the existence of a BIBD$(N-1, m(N-1), N/2-1)$ and that of an $N \times m(N-1)$ supersaturated design $\boldsymbol{X}$ attaining lower bound (1.3) extends the well known result that the existence of a BIBD$(N-1, N-1, N/2-1)$ is equivalent to that of an $N \times N$ Hadamard matrix. Note that for $\boldsymbol{X}$ to have no identical columns, all the blocks of $d_{\boldsymbol{X}}$ must be distinct. Conversely, from a binary block design d with t treatments and b distinct blocks of size $(t-1)/2$, one can construct a supersaturated design with b factors in $t+1$ runs by adding one row of 1's to the treatment-block incidence matrix of d. Such a design will be denoted by $\boldsymbol{X}_d$.

In $d_{\boldsymbol{X}}$, let r_i be the number of replications of treatment i, $i = 1, \ldots, N-1$, and let λ_{ij} be the number of times treatments i and j appear together in the same block, $1 \leq i \neq j \leq N-1$. Then

$$\begin{aligned}\operatorname{tr}(\boldsymbol{X}\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{X}^T) &= Nk^2 + 2\sum_{i=1}^{N-1}(2r_i - k)^2 + \sum_{1\leq i\neq j\leq N-1}(4\lambda_{ij} + k - 2r_i - 2r_j)^2 \\ &= C + 8\sum_{i=1}^{N-1} r_i^2 + \sum_{1\leq i\neq j\leq N-1}(4\lambda_{ij} - 2r_i - 2r_j)^2\end{aligned}$$

for some constant C. Therefore the search of an $E(s^2)$-optimal supersaturated design with k factors in N runs is equivalent to that of a binary incomplete block design with $N-1$ treatments and k distinct blocks of size $N/2-1$ which minimizes $2\sum_{i=1}^{N-1} r_i^2 + \sum_{1\le i\ne j\le N-1}(2\lambda_{ij} - r_i - r_j)^2$. This quantity is minimized, for instance, when all the r_i's are equal and all the λ_{ij}'s are also equal. Once again this establishes the $E(s^2)$-optimality of $\boldsymbol{X}$ when $d_{\boldsymbol{X}}$ is a BIBD.

When k is not a multiple of $N-1$ (or when it is an odd multiple of $N-1$ and N is not a multiple of 4 (see Remark 2)), the lower bound in (1.3) can be improved upon. One can minimize $\sum_{i=1}^{N-1} r_i^2$ and $\sum_{1\le i\ne j\le N-1}(2\lambda_{ij} - r_i - r_j)^2$ separately by making the r_i's as equal as possible, and the $(2\lambda_{ij} - r_i - r_j)$'s also as equal as possible. Form this, a general lower bound better than (1.3) can be obtained, but we shall not pursue it here. Generally, one would expect a supersaturated design $\boldsymbol{X}$ to perform well under the $E(s^2)$-criterion when $d_{\boldsymbol{X}}$ is a nearly balanced incomplete block design in the sense of Cheng and Wu (1981), although it may not be $E(s^2)$-optimal (see Example 2 in Section 3.)

3. $E(s^2)$-Optimal Designs with $k = m(N-1) \pm 1$ or $m(N-1) \pm 2$

Suppose there exists an $E(s^2)$-optimal supersaturated design with $m(N-1)$ factors in N runs which attains the lower bound in (1.3). We shall present rules for constructing supersaturated designs for $k = m(N-1)\pm 1$ and $m(N-1)\pm 2$, and show that the resulting designs are $E(s^2)$-optimal.

Write k as $m(N-1)+e$. For any supersaturated design $\boldsymbol{X}$ with k factors in N runs, let $\widetilde{\boldsymbol{X}}$ be obtained by adding m columns of 1's to $\boldsymbol{X}$ as in the paragraph preceding Theorem 2.1. Then $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T = \boldsymbol{X}\boldsymbol{X}^T + m\boldsymbol{J}_N$,and since $\boldsymbol{X}\boldsymbol{X}^T$ has zero row sums, $\mathrm{tr}[\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T]^2 = \mathrm{tr}(\boldsymbol{X}\boldsymbol{X}^T)^2 + m^2N^2$. It follows that $\boldsymbol{X}$ is $E(s^2)$-optimal if and only if it minimizes $\mathrm{tr}[\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T]^2$. Furthermore, since $\boldsymbol{X}\boldsymbol{X}^T$ has zero row sums,

$$\text{all the row sums of } \widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T \text{ are equal to } mN \tag{3.1}$$

and

$$\text{all the diagonal entries of } \widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T \text{ are equal to } k+m = mN+e. \tag{3.2}$$

3.1. $k = m(N-1)+1$

In this case, we show that an $E(s^2)$-optimal design can be obtained by adding any column with the same number of 1's and -1's to an $E(s^2)$-optimal design with $m(N-1)$ factors in N runs which attains the lower bound in (1.3). Of course, to avoid duplicated columns, the new column cannot be any of the $m(N-1)$ columns in the initial design. Denote a design so constructed by $\boldsymbol{X}^*$ and an arbitrary design with $m(N-1)+1$ factors in N runs by $\boldsymbol{X}$. Then since $\widetilde{\boldsymbol{X}}$ has an odd number ($k+m=mN+1$) of columns, all the off-diagonal entries of $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ must be odd integers. On the other hand, all the off-diagonal entries of $\widetilde{\boldsymbol{X}}^*(\widetilde{\boldsymbol{X}}^*)^T$ are equal to 1 or -1. It follows that $\boldsymbol{X}^*$ minimizes $\text{tr}[\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T]^2$, and is therefore $E(s^2)$-optimal.

In other words, if d is a BIBD$(N-1, m(N-1), N/2-1)$ with distinct blocks supplemented by an arbitrary block not appearing in the BIBD, then $\boldsymbol{X}_d$ is $E(s^2)$-optimal.

3.2. $k=m(N-1)-1$, $m>1$

By the same argument as in the previous case, an $E(s^2)$-optimal design can be obtained by deleting any column from an $E(s^2)$-optimal design with $m(N-1)$ factors in N runs which attains the lower bound in (1.3). Or, equivalently, if d is obtained by deleting an arbitrary block from a BIBD$(N-1, m(N-1), N/2-1)$ with distinct blocks, then $\boldsymbol{X}_d$ is $E(s^2)$-optimal.

Example 1. Let $\boldsymbol{H}$ be a 12×12 Hadamard matrix and

$$\boldsymbol{X}=\begin{bmatrix}\boldsymbol{H} & \boldsymbol{H}\\ \boldsymbol{H} & -\boldsymbol{H}\end{bmatrix}.$$

Then $\boldsymbol{X}$ is a 24×24 Hadamard matrix. The 12×22 arrays obtained by applying Lin's (1993) method to $\boldsymbol{X}$ achieve the lower bound in (1.3). Except for one choice of the branching column, each of such arrays contains two identical columns. To have a legitimate supersaturated design, one needs to delete one of the duplicated columns. This results in a design with 21 factors in 12 runs. It no longer attains the bound in (1.3), but is $E(s^2)$-optimal.

3.3. $k=m(N-1)+2$

In this case, an $E(s^2)$-optimal design can be obtained by adding two columns to a design with $m(N-1)$ factors in N runs which attains the lower bound in (1.3). However, these two columns are not arbitrary and need to be selected carefully. We divide the discussion into two cases according to whether N is a multiple of 4.

Case 1. N is a multiple of 4

In this case, these two supplemented columns can be any pair of orthogonal columns (i.e., each of $(1,1), (1,-1), (-1,1)$ and $(-1,-1)$ appears $N/4$ times as row vectors in these two columns) as long as they do not appear in the initial design. In other words, when N is a multiple of 4, if d is a BIBD$(N-1$, $m(N-1)$, $N/2-1)$ with distinct blocks supplemented by two blocks of the forms $\{1,2,\ldots,N/2-1\}$ and $\{1,2,\ldots,N/4-1, N/2, N/2+1,\ldots,3N/4-1\}$ which do not appear in the BIBD, then $\boldsymbol{X}_d$ is $E(s^2)$-optimal.

To see that this produces an $E(s^2)$-optimal design, denote by $\boldsymbol{X}^*$ a design constructed as described in the previous paragraph. Also, denote an arbitrary design with $m(N-1)+2$ factors in N runs by $\boldsymbol{X}$. Rearrange the rows so that the two supplemented columns have the same sign in the first $N/2$ rows and opposite signs in the last $N/2$ rows. Then

$$\widetilde{\boldsymbol{X}}^*(\widetilde{\boldsymbol{X}}^*)^T = \begin{bmatrix} \boldsymbol{A}^* & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{B}^* \end{bmatrix}, \tag{3.3}$$

where all the diagonal entries of $\boldsymbol{A}^*$ and $\boldsymbol{B}^*$ are $mN+2$, all the off-diagonals are equal to 2 or -2, and both $\boldsymbol{A}^*$ and $\boldsymbol{B}^*$ are $N/2 \times N/2$. Clearly $mN+2 \equiv 2(\text{mod } 4)$. Without loss of generality, we may assume that the last p rows of $\widetilde{\boldsymbol{X}}$ have odd numbers of entries equal to 1 and the first $N-p$ rows have even numbers of entries equal to 1, where $p \leq N/2$. Then since $mN+2 \equiv 2\,(\text{mod } 4)$, $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ can be written as

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{C} \\ \boldsymbol{C}^T & \boldsymbol{B} \end{bmatrix}, \tag{3.4}$$

where $\boldsymbol{B}$ is $p \times p$, all the entries of $\boldsymbol{C}$ are multiples of 4 and all the entries of $\boldsymbol{A}$ and $\boldsymbol{B}$ are congruent to 2 mod 4. From this it follows that

$$\text{tr}[\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T]^2 \geq \text{tr} \begin{bmatrix} \boldsymbol{A} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{B} \end{bmatrix}^2. \tag{3.5}$$

For fixed p, the right-hand side of (3.5) is minimized when all the off-diagonal entries of $\boldsymbol{A}$ and $\boldsymbol{B}$ are equal to 2 or -2, and for such $\boldsymbol{A}$ and $\boldsymbol{B}$, the right-hand side of (3.5) is a decreasing function of p for $p \leq N/2$. This shows that $\boldsymbol{X}^*$ is $E(s^2)$-optimal when N is a multiple of 4, since in this case $\boldsymbol{B}^*$ is $N/2 \times N/2$.

Case 2. N is not a multiple of 4

When N is not a multiple of 4, orthogonal columns with the same number of 1's and -1's do not exist. In this case, an $E(s^2)$-optimal design can be obtained by supplementing a design attaining the lower bound in (1.3) with any two columns in which $(1,1)$ and $(-1,-1)$ each appears $(N+2)/4$ times, and both of $(-1,1)$ and $(1,-1)$ appear $(N-2)/4$ times. In other words, when N is not a multiple of 4, if d is a BIBD$(N-1, m(N-1), N/2-1)$ with distinct blocks supplemented by two blocks of the forms $\{1, 2, \ldots, N/2-1\}$ and $\{1, 2, \ldots, (N-2)/4, N/2, N/2+1, \ldots, (3N-6)/4\}$ which do not appear in the BIBD, then $\boldsymbol{X}_d$ is $E(s^2)$-optimal.

The proof is similar to that of Case 1 except that in (3.3), $\boldsymbol{A}^*$ is $(N/2+1) \times (N/2+1)$ and $\boldsymbol{B}^*$ is $(N/2-1) \times (N/2-1)$. By Remark 2, the lower bound in (1.3) can be achieved only when m is even. Therefore $mN+2 \equiv 2\,(\text{mod } 4)$, and again we may assume that for an arbitrary $\boldsymbol{X}$, $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ can be written as in (3.4), where $\boldsymbol{B}$ is $p \times p$, all the entries of $\boldsymbol{C}$ are multiples of 4 and all the entries of $\boldsymbol{A}$ and $\boldsymbol{B}$ are congruent to 2 mod 4. Another difference from Case 1 is that it is not possible to have $p = N/2$. This is because, by (3.1) and (3.2), the sum of all the off-diagonal entries of any row of $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ must be equal to -2. If $p = N/2$, then since $N/2-1$ is even, the sum of all the off-diagonal entries of any row of $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ would be a multiple of 4. This is a contradiction, and we must have $p \leq N/2-1$. Since $\boldsymbol{B}^*$ is $(N/2-1) \times (N/2-1)$, we conclude that $\boldsymbol{X}^*$ is $E(s^2)$-optimal.

Example 2. A BIBD$(11, 22, 5)$ with distinct blocks can be constructed by using the two initial blocks $\{1, 3, 4, 5, 9\}$ and $\{2, 6, 7, 8, 10\}$. Note that the first block consists of the quadratic residues mod 11, and the second block contains the non-quadratic residues (a positive integer y, $y < t$, is called a quadratic residue mod t if $y \equiv x^2 \pmod{t}$ for some x). Add to this BIBD the two blocks $\{1, 2, 3, 4, 5\}$ and $\{1, 2, 6, 7, 8\}$, and let $\boldsymbol{X}$ be the $(1, -1)$ treatment-block incidence matrix of the resulting design. Then an $E(s^2)$-optimal supersaturated design with 24 factors in 12 runs can be obtained by adding one row of ones to $\boldsymbol{X}$. This design has an $E(s^2)$-value of 180/23. Nguyen (1996) reported a design with $E(s^2)$ value 7.83, which appears to be optimal. Similarly, an $E(s^2)$-optimal supersaturated design with 36 factors in 18 runs can be constructed by supplementing the two blocks $\{1, 2, 3, 4, 5, 6, 7, 8\}$ and $\{1, 2, 3, 4, 9, 10, 11, 12\}$ to the BIBD$(17, 34, 8)$ constructed from the initial blocks $\{1, 2, 4, 8, 9, 13, 15, 16\}$ and $\{3, 5, 6, 7, 10, 11, 12, 14\}$. Let this block design be denoted by d_1, and let d_2 be the same BIBD supplemented by $\{1, 2, 3, 4, 5, 6, 7, 8\}$ and $\{9, 10, 11, 12, 13, 14, 15, 16\}$. Then d_2 has the most uniform distributions of r_i's and λ_{ij}'s, and is a nearly balanced incomplete block design. The $E(s^2)$ values of $\boldsymbol{X}_{d_1}$ and $\boldsymbol{X}_{d_2}$ are 10.806 and 11.111, respectively. We already know that $\boldsymbol{X}_{d_1}$ is $E(s^2)$-optimal even though d_1 is not as balanced as d_2. The design reported by Nguyen (1996) has $E(s^2) = 10.96$ and is not $E(s^2)$-optimal.

3.4. $k = m(N-1) - 2$, $m > 1$

By the same argument as in the previous case, an $E(s^2)$-optimal design can be obtained by deleting two columns from a design with $m(N-1)$ factors in N runs which attains the lower bound in (1.3). As in the previous case, when N is a multiple of 4, they can be any pair of orthogonal columns, and when N is not a multiple of 4, they can be any two columns in which $(1, 1)$ and $(-1, -1)$ each appears $(N+2)/4$ times, and both of $(-1, 1)$ and $(1, -1)$ appear $(N-2)/4$ times. Or, they can be constructed from a BIBD$(N-1, m(N-1), N/2-1)$ with distinct blocks by removing two blocks of the forms $\{1, 2, \ldots, N/2-1\}$ and $\{1, 2, \ldots, N/4-1, N/2, N/2+1, \ldots, 3N/4-1\}$ when N a multiple of 4, or $\{1, 2, \ldots, N/2-1\}$ and $\{1, 2, \ldots, (N-2)/4, N/2, N/2+1, \ldots, (3N-6)/4\}$ when N is not a multiple of 4.

4. $E(s^2)$-Optimal Designs with Eight Runs

We conclude this paper by a complete solution of $E(s^2)$-optimal designs with eight runs. Utilizing the connection with block designs, we see that since, for seven treatments, there are at most 35 distinct blocks of size 3, a supersaturated design with eight runs can accommodate at most 35 factors.

When $k = 7m, 1 \leq m \leq 5$, a BIBD$(7, k, 3)$ with distinct blocks exists. A BIBD$(7, 7, 3)$ with distinct blocks can be obtained by developing the initial block $\{1, 2, 4\}$ cyclically. The two initial blocks $\{1, 2, 4\}$ and $\{3, 5, 6\}$ together generate a BIBD$(7, 14, 3)$ with distinct blocks. For $b = 35$, we use all the 35 possible blocks of size 3. Deleting from this design the BIBD generated by $\{1, 2, 4\}$ (or $\{1, 2, 4\}$ and $\{3, 5, 6\}$), we obtain a BIBD$(7, 28, 3)$ (or BIBD$(7, 21, 3)$, respectively) with distinct blocks. From these BIBD's, we can write down 8-run supersaturated designs with 7, 14, 21, 28 and 35 factors which achieve the lower bound in (1.3). The methods in Section 3 can be used to construct $E(s^2)$-optimal designs for $k = 7m \pm e$, $e = 1, 2$. This covers designs with 8, 9, 12, 13, 15, 16, 19, 20, 22, 23, 26, 27, 29, 30, 33 and 34 factors. It can be verified that *any* two blocks in the BIBD generated by the initial block $\{1, 2, 4\}$ (or $\{3, 5, 6\}$) give a pair of orthogonal columns in the corresponding supersaturated design, and therefore can be used in the deleting or supplementing process. Among the blocks which cannot be generated by $\{1, 2, 4\}$ or $\{3, 5, 6\}$, $\{1,\ 2,\ 3\}$ and $\{3, 4, 5\}$ can be used to produce a pair of orthogonal columns.

It remains to consider designs with $k = 7m \pm 3$. We show that in these two cases, $E(s^2)$-optimal designs can be obtained by adding three appropriate columns to or by deleting three columns from designs attaining the lower bound in (1.3). They can be any three 8×1 columns, say $\boldsymbol{a}, \boldsymbol{b}$ and $\boldsymbol{c}$ such that

$$\text{in each row of } \boldsymbol{Y}\boldsymbol{Y}^T, \text{ there are three 1's, three } -1\text{'s, one 3 and one } -3, \quad (4.1)$$

where $\boldsymbol{Y} = [\ \boldsymbol{a} \vdots\ \boldsymbol{b}\ \vdots\ \boldsymbol{c}\ ]$. We point out that such columns $\boldsymbol{a}, \boldsymbol{b}$ and $\boldsymbol{c}$ can always be found (see Remark 3 at the end of this section).

To prove that the procedure described above indeed produces $E(s^2)$-optimal designs, denote a design so constructed by $\boldsymbol{X}^*$. Due to similarity in the proofs, only that for the case $k = 7m + 3$ will be presented. For an arbitrary supersaturated design $\boldsymbol{X}$ with $7m + 3$ factors in 8 runs, let $\widetilde{\boldsymbol{X}}$ be obtained by adding $m - 1$ columns of 1's to $\boldsymbol{X}$. As in Section 3, $\boldsymbol{X}^*$ is $E(s^2)$-optimal if and only if it minimizes $\text{tr}[\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T]^2$ Since among the off-diagonal entries of each row of $\widetilde{\boldsymbol{X}}^*(\widetilde{\boldsymbol{X}}^*)^T$, three are equal to -2, one is equal to -4, and all the others are equal to 0, the sum of squares of all the off-diagonal entries of $\widetilde{\boldsymbol{X}}^*(\widetilde{\boldsymbol{X}}^*)^T$ is equal to 224. It is sufficient to show that the sum of squares of all the off-diagonal entries of any $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ is at least 224.

Since $\boldsymbol{X}\boldsymbol{X}^T$ has zero row sums, the sum of all the off-diagonal entries in each row of $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ must be equal to -10. Furthermore, $\widetilde{\boldsymbol{X}}$ has $8m+2$ columns, where $8m + 2 \equiv 2 \pmod 4$; therefore as in Section 3.3, $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ can be written as in (3.4), where $\boldsymbol{B}$ is $p \times p$, $0 \leq p \leq 4$, all the entries of $\boldsymbol{C}$ are multiples of 4 and all the entries of $\boldsymbol{A}$ and $\boldsymbol{B}$ are congruent to 2 mod 4.

Case 1. $p = 0$. In this case, the sum of squares of all the off-diagonal entries of $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ is at least $56 \cdot 4 = 224$.

Case 2. $p = 1$, 3, or 4. Since the sum of all the off-diagonal entries in each row of $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ must be equal to -10, clearly each row of $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ has at least one off-diagonal entry with absolute value > 2. Then the sum of squares of all the off-diagonal entries of $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ is at least $[\,p(p-1)+(8-p)(7-p)]\cdot 2^2+8\cdot 4^2 \geq 224$.

Case 3. $p = 2$. In this case, $\boldsymbol{A}$ is 6×6, and the sum of squares of all its off-diagonal entries is at least $30 \cdot 2^2 = 120$. It follows that we only need to consider the case where the two off-diagonal entries of $\boldsymbol{B}$ have absolute values equal to 2 or 6. If they are 6, then since the sum of all the off-diagonal entries in each row of $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ is equal to -10, $\boldsymbol{C}$ must have at least two entries with absolute values greater than or equal to 4. Then the sum of squares of all the off-diagonal entries of $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ is at least $30 \cdot 2^2 + 2 \cdot 6^2 + 4 \cdot 4^2 > 224$. On the other hand, if the two off-diagonal entries of $\boldsymbol{B}$ have absolute values equal to 2, then similarly one can argue that one of the following holds: (i) $\boldsymbol{C}$ has at least one entry with absolute value greater than or equal to 8, or (ii) $\boldsymbol{C}$ has at least four entries with absolute values greater than or equal to 4. In both cases, the sum of squares of all the off-diagonal entries of $\widetilde{\boldsymbol{X}}(\widetilde{\boldsymbol{X}})^T$ is at least 224.

Remark 3. It can be verified that *any* three blocks in the BIBD generated by the initial block $\{1, 2, 4\}$ (or $\{3, 5, 6\}$) produce three columns satisfying (4.1), and therefore can be used in the deleting or supplementing process. Among the blocks which cannot be generated by $\{1, 2, 4\}$ or $\{3, 5, 6\}$, $\{1, 2, 3\}$, $\{3, 4, 5\}$ and $\{2, 5, 6\}$can be used. For instance, an $E(s^2)$-optimal design with 17 factors in 8 runs can be constructed from the block design d which is the union of $\{1, 2, 3\}$, $\{3, 4, 5\}$ and $\{2, 5, 6\}$ and the BIBD(7, 14, 3) generated by the two initial blocks $\{1, 2, 4\}$ and $\{3, 5, 6\}$, while an $E(s^2)$-optimal design with 18 factors in 8 runs can be constructed from the block design which consists of all the blocks not in d.

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