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On the Optimality of Blocked Main Effects Plans

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***Abstract*—**In this article, experimental situations are considered where a main effects plan is to be used to study m two-level factors using n runs which are partitioned into b blocks, not necessarily of same size. Assuming the block sizes to be even for all blocks, for the case $n \equiv 2$ (mod 4), optimal designs are obtained with respect to type 1 and type 2 optimality criteria in the class of designs providing estimation of all main effects orthogonal to the block effects. In practice, such orthogonal estimation of main effects is often a desirable condition. In the wider class of all available m two level even sized blocked main effects plans, where the factors do not occur at high and low levels equally often in each block, E-optimal designs are also characterized. Simple construction methods based on Hadamard matrices and Kronecker product for these optimal designs are presented.

***Keywords*—**Design matrix, Hadamard matrix, Kronecker product, type 1 criteria, type 2 criteria.

I. Introduction

THE study of optimal orthogonal and nonorthogonal blocked main effects plans involving 2-level factors have attracted quite a number of researchers in recent decades, for example, [1], [3], [6]-[12]. All these studies were carried out for the blocks of equal sizes. In practice, experimental situations may demand more relaxations leading to the use of blocks of unequal sizes. Raghavarao and Pearce have pointed out the need for blocks of unequal sizes for agronomic and biological experiments (see [14] and [13] respectively). Thus, it is worthwhile to consider wider experimental situations in which a main effect plan involving m two-level factors is to be studied using n runs, partitioned into b blocks of sizes $k_1, k_2, \ldots, k_b$, k_i's need not be equal. It is also pertinent to assume that the block sizes do not differ substantially as it has been pointed out by Raghavarao (see [14]) that in such cases it is reasonable to consider a model with the same intrablock error variance for blocks of all sizes. Very few papers have been addressed in this direction viz. [4], [10]. In particular, for n odd, Dutta and SahaRay considered experimental situations where blocks can have both even and odd sizes and obtained D- and E-optimal designs (see [4]). The optimal designs suggested in [10] are of two types: Either the design has a group of blocks of different sizes, where in each group, the number of blocks is necessarily a multiple of 4, or the blocks of the design are of two different sizes, k_1 and $k_1 + 1$. Thus, the practical applicability of the suggested optimal designs is limited, quite often requiring a large number of runs partitioned into a large number of blocks. The present paper aims at relaxing such conditions on block numbers and block sizes to make the designs more practical. Whenever each factor occurs at its high and low levels equally often within each block, the main effect parameters can be estimated orthogonally to the block effects which is often a desirable condition in practice. Under such situations, for the case $n \equiv 2$ (mod 4) and k_i even for all $i = 1, 2, \ldots, b$, optimal designs are obtained with respect to very general classes of optimality criteria, viz. generalised type 1 and generalised type 2 criteria as defined in [2]. E- optimal designs are also characterised in the wider class of all available m two level, unequal even sized blocked main effects designs, which do not necessarily have all factors occurring at high and low levels equally often within each block. Thus the findings generalize some of the previously established results given in [6], [7]. In the process of derivation it has been established that E-optimal design is not unique.

The paper has been organised as follows. In Section II, the notations and basic definitions are dealt with. Optimality results are given in Section III and the constructions of optimal designs are presented in Section IV. Concluding remarks are made in Section V.

II. Basic Notation and Definitions

Throughout the sequel, let d denote a design used to study m two level factors in n runs partitioned into b blocks of sizes $k_1, k_2, \ldots, k_b$, k_i's even, $\sum_{i=1}^{b} k_i = n$. Let $D(n, m, b, k_1, k_2, \ldots, k_b)$ be the class of all such available designs. Without loss of generality it can be assumed that $k_1 \leq k_2 \leq \ldots \leq k_b$. Let $\bar{D}(n, m, b, k_1, k_2, \ldots, k_b)$ denote a subclass of designs within $D(n, m, b, k_1, k_2, \ldots, k_b)$ where each factor occurs at its high and low levels equally often within each block. In this article only main effects plans are considered. The model for analyzing the data under the design $d \in D(n, m, b, k_1, k_2, \ldots, k_b)$ is assumed to be

$$\mathbf{Y} = \mathbf{X}_d\boldsymbol{\tau} + \mathbf{B}_d\boldsymbol{\beta} + \boldsymbol{\epsilon} \quad (1)$$

where $\mathbf{Y}$ is an $n \times 1$ vector of observations, $\boldsymbol{\tau}' = (\tau_1, \tau_2, \ldots, \tau_m)$ is the vector of main effect parameters, $\boldsymbol{\beta}' = (\beta_1, \beta_2, \ldots, \beta_b)$ is the vector of block effect parameters, $\mathbf{X}_d$ is the design matrix corresponding to the main effect parameters, $\mathbf{B}_d$ is the design matrix corresponding to the block effects and $\boldsymbol{\epsilon}$ is a vector of random errors which are uncorrelated with zero mean and constant variance σ^2. It is assumed that the observations are arranged block wise and the block sizes do not vary substantially so that the assumption of homogeneity of experimental units within blocks and similar variability of experimental units between blocks is reasonable. Let $\mathbf{X}_d = (x_{dij})$, where x_{dij}=1 or -1 depending on whether in run i, j^{th} factor occurs at high or low level, $i = 1, 2, \ldots, n$, $j = 1, 2, \ldots, m$ and $\mathbf{B}_d = (b_{dij})$, where b_{dij}=1 or 0 depending on whether run i occurs in block j^{th} or not, $i = 1, 2, \ldots, n$, $j = 1, 2, \ldots, b$. Quite often in the following a design d is interchangeably represented by $\mathbf{X}_d$ defined above.

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Under Model (1), for any design $d \in D(n,m,b,k_1,k_2,\ldots,k_b)$, the least square estimate for $\boldsymbol{\tau}$ is any solution to the reduced normal equation for main effects given by

$$\mathbf{M}_d\hat{\boldsymbol{\tau}} = \mathbf{Q} \tag{2}$$

where

$$\mathbf{M}_d = \mathbf{X}_d'\mathbf{X}_d - \mathbf{X}_d'\mathbf{B}_d\left(\mathbf{B}_d'\mathbf{B}_d\right)^{-1}\mathbf{B}_d'\mathbf{X}_d \tag{3}$$

and $\mathbf{Q} = \mathbf{X}_d'\left(\mathbf{I}_n - \mathbf{B}_d\left(\mathbf{B}_d'\mathbf{B}_d\right)^{-1}\mathbf{B}_d'\right)\mathbf{Y}$ and $\mathbf{I}_n$ is the $n \times n$ identity matrix. Whenever the information matrix $\mathbf{M}_d$ is nonsingular, then the dispersion matrix of $\hat{\boldsymbol{\tau}}$ is $\sigma^2\mathbf{M}_d^{-1}$. Note that $\mathbf{B}_d'\mathbf{B}_d$ is a diagonal matrix of entries $k_1,\ k_2,\ldots,k_b$. For any design $d \in \bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$, $\mathbf{X}_d'\mathbf{B}_d$ is a null matrix and the information matrix for the main effect parameters $\boldsymbol{\tau}$ takes the form $\mathbf{M}_d = \mathbf{X}_d'\mathbf{X}_d$. Thus for such designs, the main effect parameters are estimated orthogonally to the block effects, which is an important desirable condition in practice.

A design d^* is said to be Φ-optimal if it minimizes some functional Φ of the information matrix $\mathbf{M}_d$. Φ is called an optimality criterion. In this paper, the following two types of optimality criteria defined in [2] are considered.

Definition 1: Let $\mathcal{M}_{\mathcal{D}} = \max_{d\in D}\ tr\left(\mathbf{M}_d\right)$ where D is the class of all designs under consideration. Then a Type 1 criterion Φ_f is defined by $\Phi_f(\mathbf{M}_d) = \sum_{i=1}^{n} f(\lambda_{di})$ where $\lambda_{d1} \leq \lambda_{d2} \leq \ldots \leq \lambda_{dn}$ are eigenvalues of $\mathbf{M}_d$, and f is a real valued function defined on $[0,\mathcal{M}_{\mathcal{D}}]$ such that

1) f is continuous, strictly convex, and strictly decreasing on $[0,\mathcal{M}_{\mathcal{D}}]$. Included here is the possibility that $\lim_{x\to 0^+} f(x) = f(0) = \infty$.
2) f is continuously differentiable on $(0,\mathcal{M}_{\mathcal{D}})$ and f' is strictly concave on $(0,\mathcal{M}_{\mathcal{D}})$.

Definition 2: Let $\mathcal{M}_{\mathcal{D}} = \max_{d\in D}\ tr\left(\mathbf{M}_d\right)$ where D is the class of all designs under consideration. Then a Type 2 criterion Φ_f is defined by $\Phi_f\left(\mathbf{M}_d\right) = \sum_{i=1}^{n} f\left(\lambda_{di}\right)$ where $\lambda_{d1} \leq \lambda_{d2} \leq \ldots \leq \lambda_{dn}$ are eigenvalues of $\mathbf{M}_d$, and f is a real valued function defined on $[0,\mathcal{M}_{\mathcal{D}}]$ such that

1) f is continuous, strictly convex, and strictly decreasing on $[0,\mathcal{M}_{\mathcal{D}}]$. Included here is the possibility that $\lim_{x\to 0^+} f(x) = f(0) = \infty$.
2) f is continuously differentiable on $(0,\mathcal{M}_{\mathcal{D}})$ and f' is strictly convex on $(0,\mathcal{M}_{\mathcal{D}})$.

A generalized criterion of type i $(i = 1,2)$ is defined to be the point wise limit of a sequence of type i criteria. It is easy to verify that the well-known D-optimality criterion is of type 1, by taking $f(x) = -\log x$. Also the E-criterion is a generalized type 1 criterion.

III. Main Results

The main results of this article are presented in this section. To start with, some theorems and lemma given in [2] and [5] which are useful for the derivation of the main results are quoted.

Theorem 1: ([2]) Let $\mathcal{C} = \{\mathbf{M}_d\}_{d\in D}$ be a class of $n \times n$ symmetric non negative definite matrices.

(a) Suppose $\mathbf{M}_{d^*} \in \mathcal{C}$ is either a multiple of $\mathbf{I}_n$ or has two distinct eigenvalues $\lambda > \lambda'$ such that the multiplicity of λ' is $n-1$, and

$$\mathbf{M}_{d^*}\ maximizes\ tr(\mathbf{M}_d)\ over\ \mathcal{C} \tag{4}$$

$$tr(\mathbf{M}_{d^*}^2) < (tr(\mathbf{M}_{d^*}))^2/(n-1). \tag{5}$$

$$\begin{aligned}&\mathbf{M}_{d^*}\ maximizes\\ &tr(\mathbf{M}_d) - [n/(n-1)]^{\frac{1}{2}}\left[tr(\mathbf{M}_d^2) - \left(tr(\mathbf{M}_d)\right)^2/n\right]^{\frac{1}{2}}\\ &over\ \mathcal{C}.\end{aligned} \tag{6}$$

Then, $\mathbf{M}_{d^*}$ is optimal over $\mathcal{C}$ with respect to any generalized criterion of type 1.

(b) Suppose $\mathbf{M}_{d^*} \in \mathcal{C}$ is either a multiple of $\mathbf{I}_n$ or has two distinct eigenvalues $\lambda > \lambda'$ such that the multiplicity of λ is $n-1$, and

$$\mathbf{M}_{d^*}\ maximizes\ tr(\mathbf{M}_d)\ over\ \mathcal{C} \tag{7}$$

$$\begin{aligned}&\mathbf{M}_{d^*}\ maximizes\\ &tr(\mathbf{M}_d) - [n/(n-1)]^{\frac{1}{2}}\left[tr(\mathbf{M}_d^2) - \left(tr(\mathbf{M}_d)\right)^2/n\right]^{\frac{1}{2}}\\ &over\ \mathcal{C}.\end{aligned} \tag{8}$$

Then $\mathbf{M}_{d^*}$ is optimal over $\mathcal{C}$ with respect to any generalized criterion of type 2.

Remark 1: In settings where $tr(\mathbf{M}_d)$ is a constant, for all $d \in D$, (4) and (6) (or (7) and (8)) can be replaced by

$$\mathbf{M}_{d^*}\ minimizes\ tr(\mathbf{M}_d^2)\ over\ \mathcal{C}. \tag{9}$$

and the condition "$f' < 0$" in the definitions of type 1 and type 2 criteria can be dropped.

Remark 2: It is clear that "$\mathbf{M}_{d^*}$ is optimal over $\mathcal{C}$" is equivalent to saying that "d^* is optimal in the competing class D."

Lemma 1: ([5]) Suppose $\mathbf{x}$ and $\mathbf{y}$ are $p \times 1$ vectors whose entries are all ± 1. Also assume that $\mathbf{x}$ has p_1 entries equal to 1 and $\mathbf{y}$ has p_2 entries equal to 1. If $p \equiv 2$ (mod 4) and p_1, p_2 are both even or odd, then $|\mathbf{x}'\mathbf{y}| \geq 2$.

Theorem 2: Let $\bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$ be such that $n \equiv 2$ (mod 4) and $n > 2(m-1)$. Suppose there exists a design $d^* \in \bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$ such that $\mathbf{M}_{d^*} = (n-2)\mathbf{I}_m + 2\mathbf{J}_m$, where $\mathbf{J}_m$ is an $m \times m$ matrix of all ones. Then d^* is optimal in $\bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$ with respect to any generalized criterion of type 1.

Proof: For any $d \in \bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$, it follows that

$$\mathbf{M}_d = \mathbf{X}_d'\mathbf{X}_d \quad (\text{since}\ \ \mathbf{X}_d'\mathbf{B}_d = \mathbf{0}). \tag{10}$$

Let the $(i,j)^{\text{th}}$ element of $\mathbf{M}_d$ be denoted by $m_{d_{ij}}$. It is easy to see that

$$\left.\begin{array}{rcll} m_{d_{ii}} & = & n & \forall i = 1,2,\ldots,n \\ |m_{d_{ij}}| & \geq & 2 & \text{for } i \neq j \qquad\qquad (\text{using Lemma 1}) \end{array}\right\} \tag{11}$$

Therefore, for all $d \in \bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$ $tr(\mathbf{M}_d)$ is constant and

$$\begin{aligned} tr(\mathbf{M}_d^2) &\geq tr\left((n-2)\mathbf{I}_m + 2\mathbf{J}_m\right)^2 \\ &= n^2m + 4m(m-1) = tr(\mathbf{M}_{d^*}^2). \end{aligned} \tag{12}$$

Now

$$\begin{aligned} &\left(tr(\mathbf{M}_{d^*})\right)^2/(m-1) - tr(\mathbf{M}_{d^*}^2) \\ &= \tfrac{(nm)^2}{m-1} - n^2m - 4m(m-1) \\ &= \tfrac{m(n+2(m-1))(n-2(m-1))}{m-1} \\ &> 0 \qquad \text{as} \quad n > 2(m-1). \end{aligned}$$

Thus in view of Theorem 1 (a), the result follows.

Remark 3: E-optimality and D-optimality of $d^* \in \bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$ follow as special cases of Theorem 2 (see for a similar remark in [2]). The next Theorem obtains E-optimal designs over the wider class $D(n,m,b,k_1,k_2,\ldots,k_b)$.

Theorem 3: Let $D(n,m,b,k_1,k_2,\ldots,k_b)$ be such that $n \equiv 2 \pmod 4$ and $m \geq 3$. Suppose there exists a design $d_0^* \in D(n,m,b,k_1,k_2,\ldots,k_b)$ such that $\lambda_{d_0^*1} = n-2$. Then $d_0{}^*$ is E-optimal in $D(n,m,b,k_1,k_2,\ldots,k_b)$.

Proof: For any design $d \in D(n,m,b,k_1,k_2,\ldots,k_b)$ from (3) it follows that

$$\mathbf{M}_d \leq \mathbf{X}_d'\mathbf{X}_d.$$

Let $\mathbf{X}_d'\mathbf{X}_d = (p_{ij})$. Since $m \geq 3$, there must exist two columns, say column 1 and column 2 in $\mathbf{X}_d'\mathbf{X}_d$ satisfying the conditions of Lemma 1. Thus $|p_{12}| \geq 2$. Whenever $p_{12} \geq 2$, choosing a $m \times 1$ vector $\mathbf{q}' = (1,-1,0,\ldots,0)$, it follows that

$$\begin{aligned} \lambda_{d1} &\leq (1/2)\ \mathbf{q}'\ \mathbf{M}_d\ \mathbf{q} \leq (1/2)\ \mathbf{q}'\left(\mathbf{X}_d'\mathbf{X}_d\right)\ \mathbf{q} \\ &= (p_{11} + p_{22} - 2p_{12}) = (1/2)(n + n - 2p_{12}) \\ &\leq n-2 = \ \lambda_{d_0^*1}. \end{aligned}$$

Whenever $p_{12} \leq -2$, choosing $\mathbf{q}' = (1,1,0,\ldots,0)$, the above result can be obtained.

Remark 4: It can be seen that E-optimal design in $D(n,m,b,k_1,k_2,\ldots,k_b)$ is not unique. Besides d^* with $\mathbf{M}_{d^*} = (n-2)\mathbf{I}_m + 2\mathbf{J}_m$ being E-optimal in $D(n,m,b,k_1,k_2,\ldots,k_b)$ there exists other E-optimal designs as well in this wider class.

Theorem 4: Let $\bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$ be such that $n \equiv 2 \pmod 4$. Suppose there exists a design $\tilde{d}^* \in \bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$ such that $\mathbf{M}_{\tilde{d}^*} = (n+2)\mathbf{I}_m - 2\mathbf{J}_m$. Then $\tilde{d}^*$ is optimal in $\bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$ with respect to any generalized criterion of type 2.

Proof: Note that $tr(\mathbf{M}_{\tilde{d}^*}^2) = n^2m + 4m(m-1)$ and thus using (11) for any $d \in \bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$ $tr(\mathbf{M}_d^2) \geq n^2m + 4m(m-1) = tr(\mathbf{M}_{\tilde{d}^*}^2)$. In view of part (b) of Theorem 1 and Remark 1, the result now follows.

IV. Constructions

The methods of construction presented in this section rely on the well known $N \times N$ matrices such as Hadamard matrix $\mathbf{H}_N$, Identity matrix $\mathbf{I}_N$ and $M \times N$ matrix $\mathbf{J}_{M\times N}$, a matrix with all elements equal to one.

Case I: Construction of d^* with $\mathbf{M}_{d^*} = (n-2)\mathbf{I}_m + 2\mathbf{J}_m$

Let $\mathbf{n = 8q + 2}$, for some integer $\mathbf{q \geq 1}$.

Step 1: Let $\mathbf{H}_{\frac{n}{2}-1}$ exist and let

$$\mathbf{A}_1 = \begin{pmatrix} \mathbf{H}_{\frac{n}{2}-1} \\ \mathbf{1}'_{\frac{n}{2}-1} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

where $\otimes$ denotes the Kronecker product and $\mathbf{1}_{\frac{n}{2}-1}$ is a vector of order $1 \times \frac{n}{2} - 1$ with all elements one. **Step 2:** Obtain $d^* \in \bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$ having $\mathbf{X}_{d^*}$ formed from $\mathbf{A}_1$ by selecting any m $(1 \leq m \leq \frac{n}{2} - 1)$ columns, where sets of successive k_i rows correspond to the i^{th} block of d^*, $i = 1,2,\ldots,b$.

Now considering the maximum possible number of factors as discussed above, some examples of classes of designs are noted below in which the optimal design d^* can be constructed. It immediately follows that an optimal blocked main effects plan with the number of factors less than m, as shown in Example 1 can also be constructed with the given number of observations and block sizes.

Example 1: $\bar{D}(10,5,3;2,4,4)$, $\bar{D}(18,8,5;2,4,4,4,4)$, $\bar{D}(26,12,6;4,4,4,4,4,6)$, $\bar{D}(42,20,7;6,6,6,6,6,6,6)$, $\bar{D}(42,20,6;6,6,6,8,8,8)$.

Case II: Construction of d^* with $\mathbf{M}_{d^*} = (n+2)\mathbf{I}_m - 2\mathbf{J}_m$

Let $\mathbf{n = 8q + 6}$, for some integer $\mathbf{q \geq 1}$.

Step 1: Let the Hadamard matrix $\mathbf{H}_{\frac{n}{2}+1}$ exist and can be written as follows:

$$\mathbf{H}_{\frac{n}{2}+1} = \begin{pmatrix} \mathbf{H}^*_{\frac{n}{2}+1} \\ \mathbf{1}'_{\frac{n}{2}+1} \end{pmatrix}.$$

Step 2:

$$\mathbf{A} = \mathbf{H}^*_{\frac{n}{2}+1} \otimes \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

Obtain $\tilde{d}^* \in \bar{D}(n,m,b,k_1,k_2,\ldots,k_b)$ having $\mathbf{X}_{\tilde{d}^*}$ formed from $\mathbf{A}$ by selecting any m $(1 \leq m \leq \frac{n}{2} + 1)$ columns, where sets of successive k_i rows correspond to the i^{th} block of $\tilde{d}^*$, $i = 1,2,\ldots,b$.

Now considering the maximum possible number of factors as discussed above, some examples of classes of designs are given below in which the optimal design $\tilde{d}^*$ can be constructed. It immediately follows that an optimal blocked main effects plan with the number of factors less than m, as shown in Example 2 can also be constructed with the given number of observations and block sizes.

Example 2: $\bar{D}(14,8,3;4,4,6)$, $\bar{D}(22,12,5;4,4,4,4,6)$, $\bar{D}(30,16,5;6,6,6,6,6)$, $\bar{D}(38,20,5;6,8,8,8,8)$, $\bar{D}(44,23,5;8,8,8,10,10,)$.

Case III: Construction of E-optimal d_0^* with $\lambda_{d_0^*} = n-2$.

Step 1: Let $\mathbf{B}$ be the $(n-2)\times(n-2)$ matrix given by

$$\mathbf{B} = \mathbf{H}_{\frac{n}{2}-1} \otimes \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{13}$$

Step 2: let

$$\mathbf{B}_1 = \begin{pmatrix} \mathbf{B} \\ \mathbf{J}_{2\times\frac{n}{2}-1} \end{pmatrix}$$

Step 3: Now obtain $d_0^* \in D(n, m, b, k_1, k_2, \ldots, k_b)$ having $\mathbf{X}_{d_0^*}$ formed from $\mathbf{B_1}$ by selecting any m $(1 \leq m \leq \frac{n}{2} - 1)$ columns, where sets of successive k_i rows correspond to the i^{th} block of d_0^*, $i = 1, 2, \ldots$

Now considering the maximum possible number of factors as discussed above, some examples of classes of designs are given below in which the optimal design $\tilde{d}^*$ can be constructed. It immediately follows that an optimal blocked main effects plan with the number of factors less than m, as shown in Example 3 can also be constructed with the given number of observations and block sizes.

Example 3: D(34,16,5;,6,6,6,8,8), D(50,24,4;12,12,12,14), D(58,29,7;8,8,8,8,8,8,10)

V. Conclusion

In this article, the problem of identification of optimal orthogonal blocked main effects plan with m two-level factors, using n runs, n odd, partitioned into b blocks of sizes k_1, k_2, $\ldots$, k_b, where k_i's are not necessarily equal, has been taken up with respect to very general classes of optimality criteria viz. type 1 and type 2. E-optimality result of [10] in the wider class of designs where all the factors do not necessarily occur at high and low levels equally often in each block has been generalised. Different methods of construction of such optimal designs are illustrated. A number of examples are presented to show existence of such optimal designs in appropriate classes with a reasonable number of factors and block sizes not varying substantially. Depending on the practical need many more such optimal designs can also be constructed.

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