Optimality of multi-way designs

email of corresponding author : bhaskarbagchi53@gmail.com

Sunanda Bagchi and Bhaskar Bagchi*
1363, 10th cross, Kengeri Satellite Town,
Bangalore 560060
India

Abstract

In this paper we study optimality aspects of a certain type of designs in a multi-way heterogeneity setting. These are "duals" of plans orthogonal through the block factor (POTB). Here by the dual of a main effect plan (say ρ) we mean a design in a multi-way heterogeneity setting obtained from ρ by interchanging the roles of the block factors and the treatment factors. Specifically, we take up two series of universally optimal POTBs for symmetrical experiments constructed in Morgan and Uddin (1996). We show that the duals of these plans, as multi-way designs, satisfy M-optimality.

Next, we construct another series of multiway designs and proved their M-optimality, thereby generalising the result of Bagchi and Shah (1989). It may be noted that M-optimality includes all commonly used optimality criteria like A-, D- and E-optimality.

AMS Subject Classification : 62k05.

1 Introduction

An experimental unit subjected to more than one heterogeneity directions occurs in many situations. The search for optimal designs in a setting with two crossed nuisance (or blocking) factors began in Kiefer (1975). Later others joined the search and obtained optimal row-column designs [see Shah and Sinha (1989) for more details].

Optimality study in a general m-way heterogeneity setting was initiated by Cheng (1978). He assumed a model with no interaction among the blocking factors and considered a set up with constant number of level combinations of the blocking factors. Mukhopadhyay and Mukhopadhyay (1984) assumed the same model as Cheng (1978), but relaxed the complete crossing requirement on the block factors. Assuming that the level combinations of the block factors form an orthogonal array with variable number of symbols, they obtained optimality results very similar to those of Cheng (1978). Bagchi and Mukhopadhyay (1989) considered the situations where two factor interactions are present among the block factors and obtained optimality results. Morgan (1997) considered an m-way setting with t-factor interactions and generalised all the optimality results obtained so far.

The dual of an optimal block design often satisfies optimality property. In this paper we try to see whether that happens for a main effect plan (MEP) also. In this context we interpret duality as an interchange between the roles of the block factors and the treatment factors. Thus, dual of a blocked MEP is a design in a multi-way setting [see Definition 5.1]. We have taken up two series of universally optimal blocked MEPs constructed in Morgan and Uddin (1996) and proved that the duals of these plans are also optimal as multi-way designs, although the type of

optimality is different and the competing class of designs is smaller. We have also constructed a new series of multi-way designs and proved its optimality.

In section 2 we describe the set up we consider. In this section we also discuss the concept of adjusted orthogonality and its consequence [see Definition 2.3 and Lemma 2.1], which we used later. Discussion on optimality criteria is placed in Section 3. In Section 4 we describe three multiway settings and derive the information matrix (or C-matrix) of the treatment effects for a design in each of these settings [see Lemma 4.1]. We take up the designs of our interest in Section 5. We describe the duals of two series of plans of Morgan and Uddin (1996), study the properties of these multiway designs and then prove their optimality [see Theorems 5.1 and 5.2]. In Section 5.3 we construct a series of multiway designs satisfying adjusted orthogonality [see Theorem 5.3] and proved their optimality property [see Theorem 5.4].

2 Preliminaries

We shall consider designs in a multi-way heterogeneity setting, in which an experimental unit is subjected to more than one heterogeneity directions or blocking factors. An experimental design in a multi-way heterogeneity setting is completely specified by a quadruple $(U, \mathcal{F}, S, \eta)$, where U is the set of all units, $\mathcal{F} = \mathcal{B} \cup \{V, G\}$ is the set of factors. The distinguished factor V is called the treatment factor, the factors in $\mathcal{B}$ are called the block factors and G is the general effect. S represents the set of levels : S_A being the set of levels of the factor A, $A \in \mathcal{F}$. $s_A := |S_A|$. In particular, S_V is the set of treatments. We shall write v for s_V. We have $s_G = 1$.

The allotment function $\eta : U \times \mathcal{F} \to S$ specifies, for any unit u and factor A, the level $\eta(u, A)$ of A to be applied to the unit u. Thus, $\{\eta(u, A) : u \in U\} = S_A$, $A \in \mathcal{F}$.

m will denote $|\mathcal{B}|$ and n will denote $|U|$. We assume that $m \geq 3$.

Notation 2.1. *η_1 (respectively η_2) will denote the restriction of the allotment function η to $U \times \{V\}$ (respectively to $U \times \mathcal{B}$). η_2 is called the experimental set up (and is viewed as given by nature) and η_1 is called the design (and is viewed as designed by the experimenter). Note that η_1 may be thought of as the function $x \mapsto \eta_1(x, V)$ from U to S_V. For ease of description, we shall describe a design by the allotment function η, which includes both the experimental set up and the allocation of treatments in a combined form.*

Notation 2.2. *(a) 1_n will denote the $n \times 1$ vector of all-ones, while $J_{m \times n}$ will denote the $m \times n$ matrix of all-ones. We shall write J_m for $J_{m \times m}$. The $n \times 1$ vector of responses will be denoted by Y.*

(b) Fix $A \in \mathcal{F}$. The design matrix X_A is the $n \times s_A$ matrix having the (u, p)th entry 1 if $\eta(u, A) = p$, and 0 otherwise ($u \in U, p \in S_A$). Clearly, $X_G = 1_n$. We shall use the following notations for the incidence matrices. For $A \neq B$ in $\mathcal{B}$, the A versus B incidence matrix is the matrix $M_{AB} = X'_A X_B$. Thus the (p, q)th entry of M_{AB} is $M_{AB}(p, q)$, which is the number of units u in which A is at level p and B is at level q, $p \in S_A$, $q \in S_B$. A is said to be equireplicate if the levels of A appear with equal frequency in the setting.

For $A \in \mathcal{B}$, the V versus A incidence matrix is the matrix $N_A = X'_V X_A$.

(c) The $s_A \times 1$ vector α^A will denote the vector of unknown effects of A, $A \in \mathcal{F}$.

The model is expressed in matrix form as

$$\mathbf{Y} = \mathbf{X}\alpha + \epsilon : \mathbf{X} = [X_A : A \in \mathcal{F}] \quad \alpha = [\alpha^A : A \in \mathcal{F}]', \quad \epsilon \sim N_n(0, \sigma^2 I_n). \qquad (2.1)$$

Here $Z \sim N_p(\mu, \Sigma)$ means that Z is a random variable following p-variate normal distribution with mean μ and covariance matrix Σ.

The normal equation for the least square estimates of the vector α of all effects is

$$\mathbf{X}'\mathbf{X}\,\widehat{\alpha} = \mathbf{X}'\mathbf{Y}. \qquad (2.2)$$

We shall use the following notations for the sake of compactness.

Notation 2.3. *(a) For any matrix M, P_M will denote the projection operator onto the column space of M. Thus, $P_M = M(M'M)^- M'$, where H^- denotes a g-inverse of the matrix H.*
(b) Let $T = \{A, B, \cdots\}$ be a subset of $\mathcal{F}$.
(i) X_T will denote $\begin{bmatrix} \mathbf{X}_A & \mathbf{X}_B & \cdots \end{bmatrix}$.
(ii) α^T will denote $[(\alpha^A)' : A \in T]'$. $\widehat{\alpha^T}$ will denote the least square estimate of α^T.
(iii) P_A will denote the projection operator onto the column space of $X_A, A \in \mathcal{F}$. Further, P_T will denote the projection operator onto the column space of X_T.

Consider $T \subset \mathcal{F}$ and let $\bar{T} = \mathcal{F} \setminus T$. The reduced normal equation for the vector α^T of all effects of all members in T after eliminating the effects of $\bar{T}$ from (2.2) is given by

$$\mathbf{C}_{T;\bar{T}}\widehat{\alpha^T} = \mathbf{Q}_{T;\bar{T}}, \text{ where} \qquad (2.3)$$

$$\begin{aligned}
\mathbf{C}_{T;\bar{T}} &= ((C_{AB;\bar{T}}))_{A,B \in T}, \ C_{AB;\bar{T}} = \mathbf{X}'_A(I - P_{\bar{T}})\mathbf{X}_B, & (2.4) \\
\mathbf{Q}_{T;\bar{T}} &= ((Q_{A;\bar{T}}))_{A \in T}, \ Q_{A;\bar{T}} = \mathbf{X}'_A(I - P_{\bar{T}})\mathbf{Y}. & (2.5)
\end{aligned}$$

Definition 2.1. *(a) For factors $A \neq B$, $Q_{A;B}$ will denote the vector $X'_A(I - P_B)Y$. It is commonly known as "the total for A, adjusted for B".*
(b) By the C-matrix of a multi-way design d we mean the $v \times v$ matrix $\mathbf{C}_{V;\bar{V}} = \mathbf{X}'_V(I - P_{\bar{V}})\mathbf{X}_V$, which we shall refer to as C_d. In order that every treatment contrast is estimable, rank of C_d must be $v - 1$. We, therefore, consider only the designs satisfying that condition. We shall refer to such designs as 'connected'.

Definition 2.2. *A multi-way design d is said to be equireplicate if every treatment (i.e. every member of S_V) occurs with equal frequency.*

Adjusted orthogonality : Following Eccleston and Russel (1977) we define the following.

Definition 2.3. *For three distinct factors A, B, T we say that A and B are adjusted orthogonal with respect to T if $Cov(Q_{A;T}, Q_{B;T}) = 0$.*
If T is equireplicate, then $Cov(Q_{A;T}, Q_{B;T}) = M_{AB} - r^{-1}M_{AT}M_{TB}$, where r is the replication number of T. Therefore, in this case, A and B are adjusted orthogonal with respect to T, if and only if $M_{AT}M_{TB} = rM_{AB}$.

Shah and Eccleston (1986) proved a few interesting properties of a row-column design, in which the factors row and column are adjusted orthogonal with respect to the treatment factor. Those results can be easily generalized to a multi-way heterogeneity setting. Among those, we present one result, restricting to the designs in the equireplicate class.

Lemma 2.1. *Consider an equireplicate multi-way design d. Suppose $A, B \in \mathcal{B}$ are such that $M_{AB} = J_{s_A \times s_B}$. Consider the $v \times v$ matrices $T_A = N_A N_A'$ and $T_B = N_B N_B'$. If A and B are adjusted orthogonal with respect to V, then the following holds.*
Suppose $x' 1_v = 0$ and x is an eigenvector of T_A with non-zero eigenvalue. Then $T_B x = 0$.

Proof : Since d is equireplicate, 1_v is an eigenvector of T_A as well as of T_B corresponding to their maximum eigenvalue. Again, by the hypothesis, $T_A T_B = r^3 J_v = T_B T_A$, where r is the replication number (for the treatments). Thus, T_A and T_B are commuting matrices and hence there is an orthonormal basis (including 1_v) consisting of common eigenvectors of these two matrices. Therefore, $\mathcal{C}(T_A) \cap \mathcal{C}(T_B) = \mathcal{C}(T_A T_B) = \mathcal{C}(J_v) = \langle 1_v \rangle$. Hence the result. $\square$

3 Optimality Tools

We define a class of optimality criteria which are functions of the eigenvalues of the C-matrix of a design d [see Definition 2.1].

Notation 3.1. *For a real symmetric $n \times n$ matrix A,*
(a) $\mu_0(A) \leq \cdots \leq \mu_{n-1}(A)$ will denote the eigenvalues of A.
(b) $\mu(A) = (\mu_0(A), \cdots \mu_{n-1}(A))'$ will denote the vector of eigenvalues of A.
(c) Consider a connected design d. C_d will denote its C-matrix. By the vector of eigenvalues of d we shall mean the vector of positive eigenvalues of C_d in the nondecreasing order and it will be denoted by $\mu(d)$.

Notation 3.2. Φ *will denote the class of all non-increasing convex real valued functions on $\mathbb{R}^+ = (0, \infty)$.*
For $f \in \Phi$, $\Psi_f : (\mathbb{R}^+)^n \to \mathbb{R}$ is defined by $\Psi_f(x) = \sum_{i=1}^{n} f(x_i)$.

Definition 3.1. *(a) For $x, y \in (\mathbb{R})^n$, x is said to be Ψ_f-better than y if*

$$\Psi_f(x) \leq \Psi_f(y). \tag{3.1}$$

(b) Consider a class $\mathcal{D}$ of connected designs with a common set up and a member d^* of $\mathcal{D}$. If $\mu(d^*)$ is Ψ_f-better than $\mu(d)$ for every $d \in \mathcal{D}$, then d^* is said to be Ψ_f-optimal in $\mathcal{D}$.

The following members of Φ are of special interest as the corresponding Ψ_f criteria have important statistical interpretation [see Shah and Sinha (1989) for more details]. These are the functions $f(u) \equiv u^{-1}$ corresponding to A-optimality and $f(u) \equiv -log(u)$ corresponding to D-optimality. Another popular optimality criterion is E-optimality, which may be obtained as the limit of a class of Ψ_f criteria.

A powerful approach to design optimality problems is through the concept of majorization.

Notation 3.3. $(\mathbb{R}^n)^{\uparrow}$ *will denote the set of vectors $x = (x_1, \cdots x_n) \in \mathbb{R}^n$, such that $x_1 \leq \cdots \leq x_n$.*

Definition 3.2. *(Marshall, Olkin and Arnold(2011)) For $x, y \in (\mathbb{R}^n)^{\uparrow}$, x is said to be weakly majorized from above by y (in symbols, $x \prec^w y$) if*

$$\sum_{i=1}^{k} x_i \geq \sum_{i=1}^{k} y_i, \quad k = 1, 2, \cdots, n, \tag{3.2}$$

See Marshall, Olkin and Arnold (2011) for a comprehensive treatment of majorization concepts and results.

Following Bagchi and Bagchi (2001) we define the following.

Definition 3.3. *For $d, d' \in \mathcal{D}$, d is said to be better than d' in the sense of majorization (in short M-better), if $\mu(C_d) \prec^w \mu(C_{d'})$, equivalently if $\mu(d) \prec^w \mu(d')$. A design d^* is said to be optimal in $\mathcal{D}$ in the sense of majorization (or, in short, d^* is M-optimal in $\mathcal{D}$) if it is M-better than every member of $\mathcal{D}$.*

In view of a theorem in Tomic (1949), we have the following useful result. [See Proposition B.2 of chapter 4 of Marshall, Olkin and Arnold (2011) for the theorem of Tomic].

Theorem 3.1. *A design $d^* \in \mathcal{D}$ is M-optimal in $\mathcal{D}$ if and only if d^* is Ψ_f-optimal in $\mathcal{D}$ for every $f \in \Phi$.*

By the discussion after Definition 3.1, M-optimality implies A-, D- and E-optimality, among many other optimality criteria.

Sufficient conditions for majorization :. It is easy to verify the following.

Lemma 3.1. *Suppose A and B are real symmetric matrices. If $A \geq B$, then $\mu(A) \prec^w \mu(B)$.*

The following is another useful result.

Lemma 3.2. *Let $m < n$. Consider $x \in (\mathbb{R}^n)^{\uparrow}$, such that m of the x_i's are $= a$ and the remaining $n - m$ of them are $= b$, where $a < b$. Suppose $y \in (\mathbb{R}^n)^{\uparrow}$ satisfies $(1) : \sum_{i=1}^{n} y_i \leq \sum_{i=1}^{n} x_i$ and $(2) : y_{m+1} \geq b$. Then, $x \prec^w y$.*

Proof : We shall use the fact that for an $n \times 1$ vector $y \in (\mathbb{R}^n)^{\uparrow}$, $(3) : (1/i) \sum_{j=1}^{i} y_j$ is increasing in i.

(1) and (2) together implies that $\sum_{j=1}^{m} y_j \leq ma$. This, in view of (3) implies that $\sum_{j=1}^{i} y_j \leq ia$, for $1 \leq i \leq m$.

Next, let $m + 1 \leq i \leq n$. Since $y \in (\mathbb{R}^n)^{\uparrow}$, (2) implies $\sum_{j=i+1}^{n} y_j \geq (n-i)b$. Subtracting this inequality from (1), we get $\sum_{j=1}^{i} y_j \leq ma + (i-m)b$. $\square$

4　C-matrices of multi-way designs in a nearly orthogonal set up

Our aim is to study the performances of a few multi-way designs. For that we need the C-matrix of the reduced normal equations for the BLUEs of the treatment effects for designs in the appropriate settings, (which is $\mathbf{C}_{V;\bar{V}}$ in Definition 2.1 (b)). The C-matrix of a design in a multi-way set up has been derived in Mukhopadhyay and Mukhopadhyay (1981), under the assumption that blocking factors are orthogonal to each other. This condition is not satisfied in any of the

experimental set ups we consider here and so those results are not applicable. However, they satisfy certain other conditions, which may be described as 'near orthogonality', as the incidence matrix of every pair of blocking factors is of the form $aI + bJ$. Here a and b are integers varying from one type of setting to another.

We now describe three different types of settings. In this description, the number of blocking factors is assumed to be an arbitrary integer $m \geq 3$.

Notation 4.1. *(a) By setting of type 1 we mean a setting with $n = s(s-1)$ units, in which each blocking factor has s levels. Moreover, $M_{BB'} = J_s - I_s$ for any two distinct block factors B, B'.*

(b) A setting of type 2 has $n = s(p+s)$ for an integer p, s levels for each blocking factor and $M_{BB'} = pI_s + J_s$, $B' \neq B, \in \mathcal{B}$.

(c) A setting of type 3 has $n = s(s+1)$, one (blocking) factor (say E) having $s+1$ levels, while the other ones have s levels each. Let $\tilde{\mathcal{B}} = \mathcal{B} \setminus \{E\}$. The incidence matrices are as follows.

$$M_{BB'} = I_s + J_s, \quad B' \neq B \in \tilde{\mathcal{B}}, \tag{4.1}$$

$$M_{BE} = J_{s \times s+1}, \qquad B \in \tilde{\mathcal{B}}, . \tag{4.2}$$

We proceed to obtain the reduced normal equation for the treatment effects. For the sake of compactness, we shall use the following notations in the statement of Lemma 4.1 (the original notations of Section 2 will be used whenever necessary).

Notation 4.2. *(a) $C_0 = C_{VV;G}$ [see (2.4)]. Thus, C_0 is the $v \times v$ matrix $R - (1/n)\mathbf{r}\mathbf{r}'$. Here $\mathbf{r} = (r_1, \cdots r_v)'$ is the vector of replication numbers of the treatments and R is the diagonal matrix with diagonal entries same as the entries of $\mathbf{r}$ in the same order.*

(b) $C_B = C_{BV;G}$, $B \in \mathcal{B}$.

We note that in each of the above settings, $\mathbf{X}'_B 1_n = (n/s_B)1_{s_B}, \forall B \in \mathcal{B}$. Hence

$$C_B = N_B - (1/s_B)\mathbf{r}1'_{s_B} \text{ and so } 1'_v C_B = 0. \tag{4.3}$$

Lemma 4.1. *In the multi-way settings of the three types described in Notation 4.1 the C-matrix of a design d is as given below.*

(a) If the setting is of type 1 or type 2, then the C-matrix is

$$C_d = C_0 - \frac{1}{s} \sum_{B \in \mathcal{B}} C_B C'_B + \frac{p}{su} S_{\mathcal{B}} S'_{\mathcal{B}}, \text{ where } p = -1 \text{ for Type 1 }, u = s + mp, \text{ and } S_{\mathcal{B}} = \sum_{B \in \mathcal{B}} C_B.$$

(b) The C-matrix for a design in a setting is of type 3 is as given below.

$$C_d = C_0 - \frac{1}{s} \sum_{B \in \mathcal{B}} C_B C'_B + \frac{1}{su} \tilde{S}_{\mathcal{B}} \tilde{S}_{\mathcal{B}}',$$

where $u = s + (m-1)$ and $\tilde{S}_{\mathcal{B}} = \sum_{B \in \tilde{\mathcal{B}}} C_B$, $\tilde{\mathcal{B}}$ as in Notation 4.1 (c).

Proof : Taking $T = \mathcal{F} \setminus G$ in (2.3) we get the following system of reduced normal equations (written in compact form).

$$C_{\mathcal{B};G}\widehat{\alpha^{\mathcal{B}}} + C_{\mathcal{B}V;G}\widehat{\alpha^V} = Q_{\mathcal{B};G} \tag{4.4}$$

$$\text{and } C_{V\mathcal{B};G}\widehat{\alpha^{\mathcal{B}}} + C_0\widehat{\alpha^V} = Q_{V;G}. \tag{4.5}$$

Here $C_{\mathcal{B};G} = ((C_{AB;G}))_{A,B\in\mathcal{B}}$, $C_{\mathcal{B}V;G}$ is the $ms \times v$ matrix $= [C_{BV;G} : B \in \mathcal{B}]'$ and $C_{V\mathcal{B};G}$ is the transpose of $C_{\mathcal{B}V;G}$.

Note that (4.4) consists of m equations, a typical one of which is

$$C_{BB;G}\widehat{\alpha^B} + \sum_{B'\neq B} C_{BB';G}\widehat{\alpha^{B'}} + C_{BV;G}\widehat{\alpha^V} = Q_{B;G}. \tag{4.6}$$

For an integer t let K_t denote the symmetric idempotent matrix $I_t - (1/t)J_t$. $\qquad$ (4.7)

Proof of (a): By the hypothesis, we find that the individual C-matrices involving only the blocking factors are as follows.

$$C_{BB';G} = \begin{cases} (p+s)K_s & \text{if } B' = B, \\ pK_s & \text{otherwise} \end{cases}, \quad B, B' \in \mathcal{B}, \tag{4.8}$$

Here $p = -1$ for the type 1 setting.

For a fixed B, we eliminate all $\widehat{\alpha^{B'}}, B' \neq B$ from (4.6) by using (4.7) and (4.8). Then we get an equation involving only $\widehat{\alpha^B}$ and $\widehat{\alpha^V}$. We use this equation to eliminate all $\widehat{\alpha^B}$'s from (4.12). Then we get the reduced normal equation for $\widehat{\alpha^V}$, which is $C_d\widehat{\alpha^V} = Q$, where C_d is as in the statement.

Proof of (b): Let $\tilde{\mathcal{B}} = \mathcal{B} \setminus \{E\}$.

By the hypothesis, the individual C-matrices are as follows.

$$C_{BB';G} = \begin{cases} (s+1)K_s & \text{if } B' = B, \\ K_s & \text{otherwise} \end{cases}, \quad B, B' \in \tilde{\mathcal{B}}, \tag{4.9}$$

$$C_{BE;G} = \begin{cases} sK_{s+1} & \text{if } B = E, \\ 0 & \text{otherwise} \end{cases}, \quad B \in \mathcal{B}. \tag{4.10}$$

Following the same procedure as in Case (a) we get the C-matrix as in the statement. $\square$

5 Optimality of three multi-way designs

In this section we shall study a few multi-way designs, which are duals of main effect plans. So, we define what we mean by the dual of a main effect plan.

Definition 5.1. *Consider a main effect plan $\mathcal{P}$ for a $s_1 \times \cdots s_m$ experiment on n runs laid out on b blocks. By the dual $d(\mathcal{P})$ of $\mathcal{P}$ we mean the following design in a multi-way heterogeneity set up. $d(\mathcal{P})$ has b treatments, to be tested on n experimental units. The units are subjected to m heterogeneity directions (blocking factors), the ith one having s_i levels. A run $x = (x_1, \cdots x_n)'$ of $\mathcal{P}$ corresponds to the unit, say x, having x_i as the level of the ith blocking factor, $1 \leq i \leq m$. If x is in the jth block of $\mathcal{P}$, then $d(\mathcal{P})$ allocates treatment j is to x, $1 \leq j \leq b$.*

We proceed to the description of the multi-way designs of interest.

Notation 5.1. $s = ht + 1$ *is a prime power.* F *will denote the field of order* s. F^* *will denote the set of non-zero elements of* F.

(a) *For an integer* h, $I_h = \{0, 1, \cdots h - 1\}$.

Throughout this section addition in the suffix will be modulo h, *whenever the suffix is in* I_h.

(b) $C_i, i \in I_h$ *will denote the cosets of the subgroup* C_0 *of order* t *of* F^*. *The cosets are so ordered that* $C_i C_j = C_{i+j}$, $i, j \in I_h$. $\bar{C}_i = C_i \cup \{0\}$.

(c) $S_V = \{(x, i), x \in F, i \in I_h\}$ *will be the set of treatments for all the designs we discuss below. Thus,* $v = hs$.

(d) *All factors except* E *in Setting of type 3 have* F *as the set of levels, while for* E *it is* $F^+ = F \cup \{\infty\}$.

5.1 Optimality of d_1^* :

Corollary 2.3 of Morgan and Uddin (1996) has constructed an universally optimal main effect plan, say ρ_1, for a s^h experiment on hs blocks of size t each (here s, h and t are as in Notation 5.1). The dual of ρ_1 is an h-way design. In this section we shall study this multi-way design, named d_1^*, regarding its performance in terms of optimality. We present a description of d_1^* in terms of our notation. Before that we describe a class of matrices.

Notation 5.2. *For* $i \in I_h$, L_i *will denote the following* $s \times s$ *matrix with rows and columns indexed by* F.

$$L_i(x, y) = \begin{cases} 1 & \text{if } y - x \in C_i, \\ 0 & \text{otherwise} \end{cases}$$

L *will denote the following partitioned matrix of order* $v \times v$.

$$L = ((L_{i-j}))_{i,j \in I_h}.$$

The set up of d_1^*: The set of units is $U = F^* \times F$. The set $\mathcal{B}$ of block factors is of size h; the members of $\mathcal{B}$ are as follows. Fix $P = \{p_i : i \in I_h\} \subset F^*$, such that $p_i \in C_i, i \in I_h$. $\mathcal{B} = P$. The levels of p_i's in different units are as follows.

$$\text{the level of } p_i \text{ on the unit } (a, b) \in F^* \times F \text{ is given by } \eta_2((a, b), p_i) = ap_i + b. \qquad (5.1)$$

Let us compute the $p_i \times p_j$ incidence matrix M_{ij}, $i \neq j$ in the above set up. Fix $x, y \in F$. From (5.1) we see that the only possible unit $u = (a, b)$ such that $\eta_2(u, p_i) = x$ and $\eta_2(u, p_j) = y$ is given by

$$a = \frac{x - y}{p_i - p_j}, b = \frac{p_i y - p_j x}{p_i - p_j}.$$

This is a unit only if $x \neq y$. Thus, $M_{ij} = J_s - I_s$, for $i \neq j \in I_h$ and therefore this is a setting of type 1 with $m = h$.

The design d_1^* : We describe the allocation of treatments to the units of the above set up [recall Notation 5.1 (c)].

$$\text{For } u = (a, b) \in U = F^* \times F, \quad \eta_1(u) = (b, i), \text{ if } a \in C_i. \qquad (5.2)$$

[Recall that any $a \in F^*$ is in a unique $C_j, \; j \in I_h$].

Computation of the treatment-versus-p_i incidence matrix N_i of d_1^* : Fix $i \in h, (x,j) \in F \times I_h, \; y \in F$. $N_i((x,j),y)$ is the number of $u \in F^* \times F$ satisfying

$$\eta_1(u) = (x,j), \quad \eta_2(u, p_i) = y. \tag{5.3}$$

By (5.1) and (5.2), the only possible unit $u = (a,b)$ satisfying (5.3) is given by

$$a = (y-x)p_i^{-1}, \; b = x, \; \text{provided } (y-x)p_i^{-1} \in C_j.$$

So, $N_i((x,j),y) = 1$ if $y - x \in C_{i+j}$ and 0 otherwise.

$$\text{Thus, } N_i = \begin{bmatrix} L_i \\ L_{i+1} \\ \vdots \\ L_{i+h-1} \end{bmatrix}, \text{where } L_i\text{'s are as in Notation 5.2.} \tag{5.4}$$

We see that d_1^* is equireplicate with replication number $r = t$.

Lemma 5.1. d_1^* *satisfies the following properties.*
  (a) $C_{d_1^*} = rK_v - (1/s)LL' - 1/(s(s-h))J_h \otimes K_s + (hr^2/s^2)J_v$.
  (b) The spectrum of $C_{d_1^*}$ is $r^{h-1}(r - \frac{1}{s-h})^{s-1}(r-1)^{(h-1)(s-1)}0^1$.

  Proof : The proof of (a) follows from Lemma 4.1 (a) in view of (5.4). Proof of (b) is in the Appendix.

  Let d be an equireplicate competing design in the setting of d_1^*. We define $H = H_d$ by

$$H = \sum_{B \in \mathcal{B}} N_B. \tag{5.5}$$

Definition 5.2. *An m-way design is said to be* **totally binary** *if the entries of H are 0 or 1. The class of all equireplicate and totally binary m-way designs in the setting of d_1^* will be denoted by $\mathcal{D}_r^B$.*

We note that any design in $\mathcal{D}_r^B$ shares the following property with d_1^*.

Lemma 5.2. *For a design $d \in \mathcal{D}_r^B$, the following hold.*
  (a) $tr(C_d) = tr(C_{d_1^*})$.
  (b) By permuting the rows and columns if necessary, H_d can be reduced to $H_d = 1_h \otimes (J_s - I_s)$.
  (c) The spectrum of $S_{\mathcal{B}}S_{\mathcal{B}}'$ is $0^{v-s+1} \; h^{s-1}$. [Here $S_{\mathcal{B}}$ is as in Lemma 4.1 (a)].

  Proof : (a) follows from the definition of $\mathcal{D}_r^B$. To prove (b) we see that for a totally binary design, the entries of each N_B are 0 or 1, $\; B \in \mathcal{B}$, as the entries of each N_B are non-negative. Let $\bar{H} = J_{hs \times s} - H_d$. Since $d \in \mathcal{D}_r^B$, $\bar{H}$ is a $0,1$ matrix with exactly one entry 1 in every row and exactly h entries 1 in every column. So, $\bar{H} = 1_h \otimes I_s$ upto permutation of the rows and columns. Hence (b) follows.

9

By the definition of $S_\mathcal{B}$, the above relation imply that

$$S_\mathcal{B} S'_\mathcal{B} = HH' - ((s-1)^2/s)J_v = J_h \otimes K_s. \tag{5.6}$$

Now, (c) is immediate. $\square$

Remark 5.1: Now onwards we shall assume that for every deign d in $\mathcal{D}_r^B$, the rows and columns of each N_B is permuted (if necessary) in accordance with the permutation (if any) used in Lemma 5.2.

We proceed towards studying the performance of d_1^*.

Theorem 5.1. d_1^* is M-optimal in $\mathcal{D}_r^B$, the class of all equireplicate and totally binary designs in the Setting of d_1^*.

Towards the proof of this theorem, we fix a design $d \in \mathcal{D}_r^B$ and study certain properties of the matrices in the expression for C_d.

We shall use the following compact notations. Let N and $C_\mathcal{B}$ be the following $v \times sh$ matrices

$$N = [N_B : B \in \mathcal{B}], \text{ and } C_\mathcal{B} = [C_B : B \in \mathcal{B}].$$

The following relation hold.

$$C_\mathcal{B} C'_\mathcal{B} = NN' - (hr^2/s)J_v. \tag{5.7}$$

Lemma 5.3. The sum of $s-1$ smallest positive eigen values of $C_\mathcal{B} C'_\mathcal{B}$ is $\leq s-1$.

Proof : Let $X = \{x_1, \cdots x_{s-1}\}$ be a set of orthonormal vectors in $\langle 1_s \rangle^\perp$. Let $Z = \{z_i = 1_h \otimes x_i, \; x_i \in X\}$. For a $z \in Z$, $Nz = Hx_i$ for some i, so that $Nz = -z$ and so $z'N'Nz = z'z$. Let $\tilde{\mu}_1 \leq \cdots \leq \tilde{\mu}_{s-1}$ be the smallest $s-1$ positive eigen values of NN'. Then, $\tilde{\mu}_1, \cdots, \tilde{\mu}_{s-1}$ are also the smallest $s-1$ positive eigen values of $N'N$. So,

$$\sum_{i=1}^{s-1} \tilde{\mu}_i \leq \sum_{i=1}^{s-1} (z_i' N'N z_i)/(z_i' z_i) = (s-1).$$

Since N is an incidence matrix, the largest eigenvalue of NN' corresponds to the eigenvector 1_v. Thus, the eigenvector e_i corresponding to $\tilde{\mu}_i$ can not be 1_v and therefore $e_i' 1_v = 0$, for each i. Hence the result follows from (5.7). $\square$

Let $\mathcal{N}(A)$ denote the null space of the matrix A and $\nu(A)$ the nullity of A.

Lemma 5.4. $\mu(C_d)$ satisfies the following.
    (0) $\mu_0(C_d) = 0$.
    (i) $\mu_{v-i}(C_d) = r$, $1 \leq i \leq h-1$.
    (ii) $\sum_{i=0}^{s-2} \mu_{v-h-i}(C) \geq (s-1)(r - \frac{1}{s-h})$.

Proof : By Lemma 4.1 (a)

$$C_d = C_0 - \frac{1}{s} C_\mathcal{B} C'_\mathcal{B} - \frac{1}{s(s-h)} S_\mathcal{B} S'_\mathcal{B}.$$

10

Using (4.3) we see that $1'vC_{\mathcal{B}} = 0 = 1'_v S_{\mathcal{B}}$. Thus, $C_d 1_v = 0$ and (0) is proved.

We now prove (i). Substituting for $C_{\mathcal{B}} C'_{\mathcal{B}}$ from (5.7) and $S_{\mathcal{B}} S'_{\mathcal{B}}$ from (5.6) we get the following expression for C_d.

$$C_d = rK_v - (NN' - \frac{r(s-1)}{s} J_v) - \frac{1}{s(s-h)}(HH' - \frac{(s-1)^2}{s} J_v).$$

By definition of $H = H_d$, $\mathcal{N}(NN') \subset \mathcal{N}(HH')$. Now, let $W = \langle 1_h \rangle^{\perp} \otimes 1_s$. Since d is equireplicate, $Nw = 0, \forall w \in W$. Therefore, $\nu(NN') = \nu(N'N) \geq |W| = h - 1$, implying $\nu(HH') \geq h - 1$. Let $x \in \mathcal{N}(NN')$. Since 1_v is the eigenvector of NN' corresponding to the largest eigenvalue, $x \neq 1_v$. Therefore, $x'1_v = 0$. So, using the expression of C_d above, (5.6)and (5.7) we see that $C_d x = r$. Hence (i) follows.

Next we proceed to prove (ii), which is about the next largest eigen values of C_d, Let $P = aC_{\mathcal{B}} C'_{\mathcal{B}} + bS_{\mathcal{B}} S'_{\mathcal{B}}$, $a, b > 0$. While proving (i), we have also proved that $\mu_i(P) = 0$, $0 \leq i \leq h - 1$. Let $\tilde{\mu}_1(T) \leq \cdots \leq \tilde{\mu}_{s-1}(T)$ be the smallest $s - 1$ positive eigen values of T, $T = P$ or $C_{\mathcal{B}} C'_{\mathcal{B}}$. Fix $i : 1 \leq i \leq s - 1$. By an well-known result [see Corollary III.2.2 of Bhatia (2013), for instance] we get

$$\tilde{\mu}_i(P) \leq a\tilde{\mu}_i(C_{\mathcal{B}} C'_{\mathcal{B}}) + b\mu_{v-1}(S_{\mathcal{B}} S'_{\mathcal{B}}),$$

which is $a\tilde{\mu}_i(C_{\mathcal{B}} C'_{\mathcal{B}}) + bh$, by Lemma 5.2 (c). So, by Lemma 5.3,

$$\sum_{i=1}^{s-1} \tilde{\mu}_i(P) \leq (s-1)(a + bh). \tag{5.8}$$

But P becomes $rK_v - C_d$, if we put $a = \frac{1}{s}, b = \frac{1}{s(s-h)}$. So, the result follows from (5.8).□

Proof of Theorem 5.1 : From Lemma 5.1 (b) the spectrum of $C_{d_1^*}$ is

$$r^{h-1}(r - \frac{1}{s-h})^{s-1}(r-1)^{(h-1)(s-1)}0^1.$$

Now let us take a pair of $v - h \times 1$ vectors x and y, where $y_i = \mu_i(C_d)$ and $x_i = \mu_i(C_{d_1^*})$, $1 \leq i \leq v - h$. Lemma 5.4 says that the other eigenvalues of C_d are equal to the corresponding ones of $C_{d_1^*}$. This, in view of Lemma 5.2 (a) , shows that Lemma 3.2 is applicable here. Applying that lemma and the results obtained in Lemma 5.4 to x and y we find that y is M-worse than x. Hence the proof is complete. □

5.2 Optimality of d_2^*

Among the universally optimal main effect plans constructed in Lemma 2.5 of Morgan and Uddin (1996) one is a plan, say ρ_2, for a s^t experiment on hs blocks of size $t + 1$ each (here s, h and t are as in Notation 5.1). We shall study the mutiway design, named d_2^*, which is the dual of ρ_2 We describe it using our notation.

The setting : The set of units $U = \{(a, b, j) : j \in I_h, b \in F, a \in \bar{C}_j\}$. The set of block factors is $\mathcal{B} = C_0$. The set of level of each block factor is F. Finally,

the level of $\alpha \in C_0$ on the unit $u = (a, b, j) \in U$ is given by $\eta_2(u, \alpha) = a\alpha + b$. (5.9)

11

Computation of the α -versus- β incidence matrix $M_{\alpha\beta}$: Fix $\alpha \neq \beta$, $\alpha,\beta \in C_0$. For $x,y \in F$, the only possible unit $u = (a,b,i)$ satisfying $\eta_2(u,\alpha) = x$, $\eta_2(u,\beta) = y$ is given by

$$a = \frac{x-y}{\alpha-\beta}, \; b = \frac{ay-bx}{\alpha-\beta} \text{ and } i \in I_h \text{ is such that } a \in \bar{C}_i.$$

Therefore, $m_{\alpha,\beta}(x,y) = 1$ if $x \neq y$ and h if $x = y$. Thus ,

$$M_{\alpha,\beta} = (h-1)I_s + J_s, \; \forall \alpha \neq \beta.$$

Hence, this setting is of type 1 with $m = t$.

The design d_2^* : $S_V = F \times I_h$. For $u = (a,b,j) \in U$, $\eta_1(u) = (b,j)$. Thus, for $\alpha \in C_0$, $(x,i) \in S_V$, the unit $u = (a,b,j)$ satisfies $\eta_1(u) = (x,i)$, $\eta_2(u,\alpha) = y$ only if $b = x, j = i, a = (y-x)\alpha^{-1}$ and a is in $\bar{C}_i$. It follows that for every $\alpha \in C_0$, the $((x,i),y)$th entry of the treatment-versus-α incidence matrix N_α is $N_\alpha((x,i),y) = 1$ if $y - x \in \bar{C}_i$ and 0 otherwise. Thus,

$$\text{For each } \alpha \in C_o, \; N_\alpha = \begin{bmatrix} L_0 + I \\ L_1 + I \\ \vdots \\ L_{h-1} + I \end{bmatrix}, \text{ where } L_i \text{ is as in Notation 5.2.} \qquad (5.10)$$

We present the following well-known result for ready reference.

Lemma 5.5. *If N is the incidence matrix of a BIBD with parameters (v,b,r,k,λ), then the spectrum of $N'N$ is is $0^{b-v}(r-\lambda)^{v-1}(rk)^1$.*

Lemma 5.6. *(a) The C-matrix of d_2^* is $C_{d_2^*} = rK_v - (t/u)(N_2'N_2 - ((t+1)^2/s)J_{v\times s})$, where N_2 is the incidence matrix of a BIBD with parameters $(v = s, b = hs, r = h(t+1), k = t+1, \lambda = t+1)$.*
(b) The spectrum of C_{d*_2} is $r^{(h-1)(s-1)}(r - (t/u)(t+1))^{s-1}0^1$.

Proof : From the description of d_2^*, one can see that d_2^* is a design in Setting 2 with $m = t, p = h - 1$. So, (a) follows from Lemma 4.1 (a) in view of (5.10)
(b) follows from (a) in view of Lemma 5.5. $\square$

We now proceed towards studying optimality aspects of d_2^*. We shall use a few well-known results, presented below.

Lemma 5.7. *Suppose $x_1, \cdots x_n$ are real numbers with $\sum_{i=1}^n x_i = T$. Then, the following hold.*
(a) $\sum_{i=1}^n x_i^2 \geq T^2/n$, " $=$ " when $x_i = T/n$, $\forall i$.
(b) In particular, if x_i's are integers, then $\sum_{i=1}^n x_i^2$ is minimum, when $x_i = [T/n]$ or $[T/n]+1$.

Lemma 5.8. *Consider an $m \times n$ matrix A having the $m \times 1$ vector b as the vector of row sums. Then, $AA' \geq bb'/n$.*

Proof : Fix an arbitrary $x \in R^m$, let $y = A'x$. Now, using Lemma 5.7 on the components of y, we get the result. $\square$

Lemma 5.9. *Consider $m \times n$ matrices $A_1, \cdots A_q$. Let $T = \sum_{i=1}^q A_i$. Then, the following hold.*
(a) $\sum_{i=1}^q A_i A_i' \geq (1/q)TT'$.
(b) $q \sum_{i=1}^q A_i A_i' - TT' = \sum_{i=1}^q \sum_{j<i} (A_i - A_j)(A_i - A_j)'$.

Proof of (a) : Fix an arbitrary $x \in R^m$. For $1 \leq i \leq q$, let us write $A'_i x$ as $y_i = [\begin{array}{ccc} y_{i1} & \cdots y_{in} \end{array}]'$. Then, $x' \sum_{i=1}^{q} A_i A'_i x = \sum_{i=1}^{q} y'_i y_i = \sum_{j=1}^{n} \sum_{i=1}^{q} y_{ij}^2$. Now, $\sum_{i=1}^{q} y_{ij} = \sum_{l=1}^{m} T(l,j) x_l = z_j$, say. Therefore, by Lemma 5.7, $\sum_{i=1}^{q} y_{ij}^2 \geq z_j^2/q$. Since z_j is the jth entry of $T'x$, the result follows.

(b) Follows by straightforward computation. $\square$

The next two results are not so well-known.

Lemma 5.10. *Suppose $H = \sum_{l=1}^{m} N_l$, where each N_l is an integer matrix of order $v \times b$. Suppose each N_l satisfies $\sum_{j=1}^{b} N_l(i,j) = r$, $i = 1, \cdots v$, where $r < b$. Then, $Tr(HH') \geq m^2 vr$.*

Proof : $Tr(HH') = \sum_{i=1}^{v} \sum_{j=1}^{b} (H(i,j))^2$. Again, $\sum_{i=1}^{v} \sum_{j=1}^{b} H(i,j) = mvr$. Therefore, by Lemma 5.7, $\sum_{i=1}^{v} \sum_{j=1}^{b} (H(i,j))^2$ is minimum, when the following hold. $H(i,j) = [rm/b]$ or $[rm/b]+ 1, 1 \leq i \leq v, 1 \leq j \leq b$. Since a sufficient condition for the above is $N_1 = N_2 = \cdots N_m$, and $N_1(i,j) = 0$ or 1, $1 \leq i \leq v, 1 \leq j \leq b$, the result follows. $\square$

Lemma 5.11. *Let A be an $n \times n$ n.n.d matrices each with row sum 0, rank $\leq \rho$ and trace $\geq T$. Let $C = dK_n - A$, where $d \geq T/\rho = a$ (say) and K_n is as in (4.7). Let $\gamma \in (\mathbb{R}^+)^n$ be the vector given by $\gamma_0 = 0, \gamma_i = d - a$ for $1 \leq i \leq \rho$, $\gamma_i = d$ for $\rho + 1 \leq i \leq n - 1$. Then, γ is M-better than $\mu(C)$.*

Proof : By definition of C, $\mu_0(C) = 0 = \gamma_0$, $\mu_i(C) = d - \mu_{n+1-i}(A)$ for $i > 0$. Therefore, $\sum_{i=1}^{\rho} \mu_i(C) = d\rho - tr(A) \leq \rho(d-a)$. Since $(1/l) \sum_{i=1}^{l} \mu_i(C)$ is increasing in l, it follows that $\sum_{i=1}^{l} \mu_i(C) \leq l(d-a)$, $1 \leq l \leq \rho$. Since $\mu_i(C) \leq d \,\forall i$, the result follows. $\square$

Theorem 5.2. *d_2^* is M-optimal in $\mathcal{D}_2$, the class of all equireplicate designs in the setting containing d_2^*.*

Proof : Let $d \in \mathcal{D}_2$. Then, C_d is as given in (a) of Lemma 4.1 with $m = t, p = h - 1$. So, using Lemma 5.9 (b) on the set of matrices $\{C_B, B \in B \in \mathcal{B}\}$, we get

$$C_d = C_0 - (1/u) \sum_{B \in \mathcal{B}} C_B C'_B - (h-1)/(su) \sum_{B' \neq B} D_{BB'}, \ u = s + (h-1)t,$$

where $D_{BB'} = (C_B - C_{B'})(C_B - C_{B'})'$, $B' \neq B \in \mathcal{B}$. Since d is equireplicate, $C_0 = rK_v$. Now, applying Lemma 5.9 (a) on the set of matrices $\{D_{BB'}, B, B' \in \mathcal{B}\}$ we get $C_d \leq C_1 = rK_v - (1/u) \sum_{B \in \mathcal{B}} C_B$. Again, by Lemma 5.9 (a) on the set of matrices $\{C_B, B \in \mathcal{B}\}$ we get $C_1 \leq C_2$, where $C_2 = rK_v - (1/(tu)S_{\mathcal{B}} S'_{\mathcal{B}}$. Here $S_{\mathcal{B}}$ is as in Lemma 4.1 (a). Now, C_2 is of the form of C in Lemma 5.11 with $n = hs, d = r, A = (1/tu)S_{\mathcal{B}} S'_{\mathcal{B}}, \rho = s - 1$. Also, $T = (h-1)(s-1)(t+1)t/u$ by Lemma 5.10. In view of (4.3) the row sum of A is 0. So, $a = (h-1)(t+1)t/u$. By Lemma 5.11, $\mu(C_2)$ is M-worse than γ. But from Lemma 5.6 we see that $\gamma = \mu(C_{d_2^*})$. Since $C_d \leq C_2$, the result follows from Lemma 3.1. $\square$

5.3 Construction and Optimality of d_3^*

In this section we construct a multi-way design d_3^* and prove its optimality property. In this section we assume that $s \equiv 3 \pmod 4$. We follow Notation 5.1 with the extra assumption

that $h = 2$. So, here C_0 (respectively C_1) is the set of non-zero squares (respectively non-zero non-squares). Moreover, $t = (s-1)/2$.

The following result lies at the foundation of the construction of d_3^*.

Lemma 5.12. *Let $s \equiv 3 \pmod 4$ be a prime power. Then there is a subset W of C_0 and a function $f : W \to C_1$ satisfying the following.*

(a) $|W| = (s-3)/4$.

(b) For every $\xi \in W$, $(\xi - 1)(f(\xi) - 1) \in C_0$.

(c) For $\xi \neq \xi' \in W$, $(\xi - \xi')(f(\xi) - f(\xi')) \in C_0$.

Proof : Let $W = \{x \in C_0 : 1 - x^2 \in C_0\}$, $\tilde{W} = \{x \in C_1 : 1 - x^2 \in C_1\}$. Note that $x \to -x$ is a bijection from W onto $(C_1 \setminus \tilde{W}) \setminus \{-1\}$. Therefore, $|W| = |C_1 \setminus \tilde{W}| - 1 = (s-3)/2 - |\tilde{W}|$. Thus, $|W| + |\tilde{W}| = (s-3)/2$. Also, $x \to -1/x$ is a bijection from W onto $\tilde{W}$. Thus, $|W| = |\tilde{W}|$, which proves (a).

Let $f : W \to \tilde{W}$ be defined by $f(x) = -1/x$, $x \in W$. Then, for $\xi \in W$, $1 - \xi^2 \in C_0$, so that $(1 - \xi)(1 - f(\xi)) = \xi^{-1}(1 - \xi^2)$ which is in C_0. This proves (b).

Again, for $\xi \neq \xi' \in W$, $(f(\xi) - f(\xi'))(\xi - \xi') = (\xi\xi')^{-1}(\xi - \xi')^2 \in C_0$, which implies (c). $\square$

We shall now construct the design d_3^*. Let $w = |W|$. So, $w = (t-1)/2$.

The set up : $U = \{(a, b, i) : a \in \bar{C}_0, b \in F, i = 0, 1\}$. $\mathcal{B} = W \cup \{\infty\}$, where W is as in Lemma 5.12. The set of levels of factor ∞ is $F^+ = F \cup \{\infty\}$, while the set of levels of the factor ξ is F, for each $\xi \in W$. The levels of different factors in the units are as follows. [Here f is as in the proof of Lemma 5.12].

For $u = (a, b, i) \in U$, $\xi \in W$,

$$\eta_2(u, \xi) = \begin{cases} b + a\xi & \text{if } i = 0, \\ b - af(\xi) & \text{if } i = 1 \end{cases} \quad \text{and} \tag{5.11}$$

$$\eta_2(u, \infty) = \begin{cases} a + b & \text{if } a \in \bar{C}_0, \ i = 0, \\ b - a & \text{if } a \in C_0, \ i = 1, \\ \infty & \text{if } a = 0, \ i = 1 \end{cases} \tag{5.12}$$

Fix $\xi \in W$. For $x \in F$, $y \in F^+$. We count the number of $u = (a, b, i) \in U$ such that

$$\eta_2(u, \xi) = x \text{ and } \eta_2(u, \infty) = y. \tag{5.13}$$

If $y = \infty$, then by the equation next to (5.11), $u = (0, x, 1)$ is the only unit satisfying (5.13).

Now, let $y \in F$. If $y = x$, then $u = (0, x, 0)$ is the only unit satisfying (5.13).

So, let $y \neq x, x, y \in F$. Using (5.11) and the equation next to it we find that the only unit u satisfying (5.13) is

$$u = \begin{cases} (\frac{y-x}{1-\xi}, \frac{x-y\xi}{1-\xi}, 0) & \text{if } (1-\xi)(y-x) \in C_0 \\ (\frac{y-x}{f(\xi)-1}, \frac{yf(\xi)-x}{f(\xi)-1}, 1) & \text{if } (f(\xi)-1)(y-x) \in C_0. \end{cases}$$

Moreover, by Lemma 5.12 (b), exactly one of $1 - \xi$ and $f(\xi) - 1$ is in C_0. Thus for a given pair $x \neq y$, exactly one of the two cases occur. Hence $M_{\xi\infty} = J_{s \times s+1}$.

14

Now, fix $\xi' \neq \xi \in W$. We fix a pair $x, y \in F$ and count the number of $u = (a, b, i) \in U$ such that

$$\eta_2(u, \xi) = x \text{ and } \eta_2(u, \xi') = y. \tag{5.14}$$

If $y = x$, then $u_1 = (0, x, 0)$ and $u_2 = (0, x, 1)$ are the only units satisfying (5.14). Let $y \neq x$. From (5.11) we find that the only unit u satisfying (5.14) is

$$u = \begin{cases} (\frac{x-y}{\xi-\xi'}, \frac{y\xi - x\xi'}{\xi-\xi'}, 0) & \text{if } (\xi - \xi')(x - y) \in C_0 \\ (\frac{x-y}{f(\xi')-f(\xi)}, \frac{yf(\xi)-xf(\xi')}{f(\xi')-f(\xi)}, 1) & \text{if}(f(\xi') - f(\xi))(x - y) \in C_0. \end{cases}$$

By by Lemma 5.12 (c) exactly one of $\xi - \xi'$ and $f(\xi') - f(\xi)$ is in C_0, so that for any given pair $x \neq y$, exactly one of these two cases occur.

Hence $M_{\xi\xi'} = I_s + J_s$ and the setting is a setting of type 3 with $m = (s + 1)/4 = (t + 1)/2$.

The design d_3^* : d_3^* has $v = 2s$ treatments ; $S_V = \{(x, i) : x \in F, \ i = 0, 1\}$. The treatments are assigned to the units by the rule that for $u = (a, b, i)$

$$\eta_1(u) = (b, i). \tag{5.15}$$

Theorem 5.3. *d_3^* is a design in a setting of Type 3 with $(s + 1)/4$ blocking factors, satisfying the following properties.*

(a) d_3^* is equireplicate with replication number $r = t + 1 = (s + 1)/2$.

(b) The treatment-versus-blocking factor incidence matrices are as follows. [The set of blocking factors is indexed by $W \cup \{\infty\}$, where W is as in Lemma 5.12]

(i) For all $\xi \in W, N_\xi'$ is the incidence matrix of a BIBD, (independent of ξ) with parameters $(v = s, b = 2s, r = s + 1, k = t + 1, \lambda = t + 1)$.

(ii) N_∞' is the incidence matrix of a BIBD with parameters $(v = s + 1, b = 2s, r = s, k = t + 1, \lambda = t)$.

(c) For every $\xi \in W$, ξ and ∞ are adjusted orthogonal with respect to the treatment factor.

(d) The spectrum of $C_{d_3^*}$ is $(\frac{rs}{s+w})^{s-1}(\frac{r(s-1)}{s})^s 0^1$.

Proof : By the description of d_3^*, we see that there are $w = (s-3)/4$ s-level and one $s+1$-level blocking factors. (a) follows from the allocation of treatments [see (5.15)]. We proceed to prove (b). Fix $\xi \in W$. For a fixed $(x, i) \in S_V$ and $y \in F$, $N_\xi((x, i), y))$ is the number of units u such that

$$\eta_1(u) = (x, i) \text{ and } \eta_2(u, \xi) = y. \tag{5.16}$$

Using (5.11) and (5.15) we see that (5.16) has a solution only when $y - x \in \bar{C}_0$. In that case the only unit u satisfying (5.16) is

$$u = \begin{cases} ((y - x)/\xi, x, 0) \text{ if } i = 0 \\ ((x - y)/f(\xi), x, 1) \text{ if } i = 1. \end{cases}$$

Since ξ and $-f(\xi)$ are in C_0, the first entry of u is in $\bar{C}_0$, as required. Therefore,

$$N_\xi = \begin{bmatrix} L_0 + I \\ L_0 + I \end{bmatrix}, \ \xi \in W. \tag{5.17}$$

15

where L_0 is as in Notation 5.2 with $h = 2$. Thus, (b) (i) is proved.

Towards proving (b) (ii), we fix $(x, i) \in S_V$ and $y \in F^+$. $N_\infty((x, i), y)$ is the number of units u such that

$$\eta_1(u) = (x, i) \text{ and } \eta_2(u, \infty) = y. \tag{5.18}$$

Clearly if $y = \infty$, then $u = (0, x, 1)$ is the only unit satisfying (5.18) when $i = 1$ and there is no such unit when $i = 0$.

Next, let $y \in F$. $y = x \implies$ that the only unit satisfying (5.18) is $u = (0, x, 0)$. Let $y \neq x$. From the equation next to (5.11) and (5.15) we see that if $y = x$, then the only unit satisfying (5.18) is

$$u = \begin{cases} (y - x, x, 0) \text{ if } y - x \in C_0 \\ (x - y, x, 1) \text{ if } y - x \in C_1. \end{cases}$$

It follows that

$$N_\infty = \begin{bmatrix} L_0 + I & 0_{s \times 1} \\ L_1 & 1_s \end{bmatrix}, \tag{5.19}$$

where L_0 and L_1 are as in Notation 5.2 with $h = 2$. Hence (b) (ii) is proved.

Now we prove (c). By definition of L_0 and L_1 given in Notation 5.2, $(L_0 + I)1_s = (t + 1)1_s$ and $L_0 + I + L_1 = J_s$. So, from (5.17) and (5.19) we see that $N'_\xi N_\infty = (L_0 + I)' J_{s \times s+1} = (t + 1)J_{s \times s+1} = rM_{\xi\infty}$ for every $\xi \in W$. Now (c) follows from Definition 2.3.

Finally, we prove (d). By Lemma 4.1 (b), Lemma 5.9 (b) and the information on d_3^* we have got so far, we see that

$$C_{d*3} = rK_v - \frac{w}{s + w} C_\xi C'_\xi - \frac{1}{s} C_\infty C'_\infty, \tag{5.20}$$

where C_B is as in (4.3), $B \in W \cup \{\infty\}$. So, $C_\xi C'_\xi = N_\xi N'_\xi - \frac{r^2}{s} J_v$ and $C_\infty C'_\infty = N_\infty (N_\infty)' - \frac{r^2}{s+1} J_v$. Here N_ξ is as in (5.17) and N_∞ is as in (5.19). By part (b) and Lemma 5.5 we find that the spectrum of $C_\xi C'_\xi$ is $r^{s-1} 0^{v-s+1}$ and the spectrum of $C_\infty C'_\infty$ is $r^s 0^{v-s}$. Now (d) follows from (5.20), in view of Lemma 2.1. $\square$

Theorem 5.4. d_3^* is M-optimal in $\mathcal{D}_3$, the class of all equireplicate designs in the setting of d_3^*.

Proof : Let $d \in \mathcal{D}_3$. From Lemma 4.1 (b) we get C_d is as given below.

$$C_d = C_0 - \frac{1}{s} \sum_{\xi \in W^*} C_\xi C'_\xi + \frac{1}{su} \tilde{S}_W \tilde{S}'_W,$$

where $u = s + w$, $W^* = W \cup \{\infty\}$ and $\tilde{S}_W$ is defined in the same way as in Lemma 4.1 (b). By arguments similar to those used in Theorem 5.2 we see that $C_d \leq C_1$, where

$$C_1 = rK_v - (1/u) \sum_{\xi \in W} C_\xi C'_\xi - (1/s) C_\infty C'_\infty.$$

Again by similar arguments we find that $C_1 \leq C_2$, where

$$C_2 = rK_v - (1/wu) \tilde{S}_W \tilde{S}'_W.$$

16

We see that C_2 is of the form of C in Lemma 5.11 with $n = 2s, A = (wu)^{-1}\tilde{S}_W\tilde{S}'_W, d = r, \rho = s - 1, T = wr(s - 1)/u$. So, $a = wr/u$. Therefore, by the same lemma, $\mu(C_2)$ is M-worse than γ. As $C_1 \leq C_2$, $\mu(C_1)$ is M-worse than γ. In particular,

$$\sum_{j=1}^{l} \mu_j(C_1) \leq l(r - a), 1 \leq l \leq s - 1.$$

Again, one can check that $Tr(C_1) \leq (s - 1)(r - a) + r(s - 1)$. Let δ be a $v - 1 \times 1$ vector such that $\delta_i = r - a$ if $1 \leq i \leq s - 1$ and $r(s - 1)/s$ if $s \leq i \leq v - 1$. It follows that $\mu(C_1)$ is M-worse than δ. But, by Theorem 5.3 (d) $\delta = \mu(C_{d_3^*})$. Since $C_d \leq C_1$ the result follows. $\square$

Remark 5.2: Theorem 5.4 is an extension of the result of Bagchi and Shah (1989). The design analogous to d_3^* in a row-column set up exists for every prime power s. [See Preece, Wallis and Yucas (2005) and Nilson and Cameron (2017) for more details].

Remark 5.3: In Bagchi and Bagchi (2020) an MEP $\mathcal{P}^*$ is constructed for an $s^t(s + 1)$ experiment on $2s$ blocks of size $t + 1$ each. Let d_4 denote the dual of ρ^*, which is a multi-way design with $t + 1$ blocking factors, one having $s + 1$ levels and others having s levels. Although d_4 satisfies properties similar to those of d_3^* given in Theorem 5.3, it does not satisfy condition (c). As a result, we are unable to prove M-optimality of d_4. Whether d_4 satisfies any specific optimality property remains to be seen.

6 Appendix

Consider $C_{d_1^*}$ of Section 5.1. We prove the following result.

Theorem 6.1. *The spectrum of $C_{d_1^*}$ is $r^{h-1}(r - (1/(s - h))^{s-1}(r - 1)^{(h-1)(s-1)}$.*

To prove this, we need a number of tools.

Notation 6.1. *(0) $s = p^m = ht + 1$, where p is a prime, m, t, h are integers, $m \geq 1, h, t \geq 2$. F_p and F_s are finite fields of orders p and s respectively. [In this section we use the notation F_s (rather than F like in the other sections) so as to distinguish it from the field of order p].*

(i) Addition and subtraction in $I_h = \{0.1, \cdots h - 1\}$ will always be modulo h.

The rows and columns of every $s \times s$ (respectively $h \times h$) matrix will be indexed by F_s (respectively I_h). Moreover, the rows and columns of every $hs \times hs$ matrix will be indexed by $I_h \otimes X$.

(ii) η and ω are primitive hth and pth roots of unity.

(iii) Consider the function trace $: F_s \to F_p$ defined as follows. $trace(x) = \sum_{i=1}^{m} x^{p^i}, x \in F_s$. [This is F_p-linear and into F_p since $x \to x^p$ is an automorphism of F_s and its fixed field is F_p].

(iv) U and V are unitary matrices of orders h and s respectively, given as follows.

$$U(i, j) = (1/\sqrt{h})\eta^{ij}, i, j \in I_h \text{ and } V(x, y) = (1/\sqrt{s})\omega^{trace(xy)}, x, y \in F_s.$$

(iv) Consider the sums g_i given by $g_i = \sum_{x \in C_i} \omega^{trace(x)}, i \in I_h$.

(v) As in Notation 5.2, L will denote the $hs \times hs$ matrix $((L_{i-j}))_{i,j \in I_h}$, where for $i \in I_h, L_i$ will denote the $s \times s$ matrix $L_i(x, y) = \begin{cases} 1 & \text{if } y - x \in C_i, \\ 0 & \text{otherwise} \end{cases}$

(vi) For $k \in I_h$, G_k is the $h \times h$ matrix given by $G_k(i,j) = g_{i-j+k}$, $i,j \in I_h$.
(vii) For $k \in I_h$, E_k is the $s \times s$ diagonal matrix given by

$$E_k(x,x) = \begin{cases} -t & \text{if } x = 0 \\ 1 & \text{if } x \in C_k \\ 0 & \text{otherwise} \end{cases}$$

Here C_k is as in Notation 5.1.

We study the behaviour of L under the actions of U and V.

Lemma 6.1. $(I_h \otimes V)^* L (I_h \otimes V) = \sum\limits_{k \in I_h} G_k \otimes E_k$.

Proof : By definition of L, the left hand side of the statement is $((V^* M_{i-j} V))_{i,j \in I_h}$.

Claim ! $V^* M_i V = Diag(\lambda_i(x),\ x \in F_s) = \sum\limits_{k \in I_h} g_{i+k} E_k$. Here $\lambda_i(x) = \begin{cases} & \text{if } x = 0 \\ g_{i_k} & \text{if } x \in C_k. \end{cases}$

The equality can be verified by computation. Now,

$$\sum_{k \in I_h} g_{i+k} = \sum_{k \in I_h} g_k = \sum_{x \in F_s^*} \omega^{trace(x)} = -1 \text{ as } \sum_{x \in F_s} \omega^{trace(x)} = 0.$$

So, by definition of E_k, $\mathcal{V}_2(1,1) = t$ and for $x \in C_j$, $\mathcal{V}_2(x,x) = \sum\limits_{k \in I_h} g_{i+k} \delta_{jk} = g_{i+j}$. Thus, the claim is proved and the second equality follows.

Now, the result follows from the definition of G_k.

Notation 6.2. *(a) W will denote the $hs \times hs$ unitary matrix $U \otimes V$.*
(b) T is the $h \times h$ diagonal matrix with the entries : $T(l,l) = \eta^l$, $l \in I_h$.

Lemma 6.2. *$W^* LW$ is a diagonal matrix with the following entries. For $i \in I_h, x \in F_s$, the (i,x)th diagonal entry of $W^* LW$ is*

$$\delta(i,x) = \begin{cases} s-1 & \text{if } i = 0, x = 0 \\ 0 & \text{if } i \neq 0, x = 0 \\ \eta^{ik} \sum\limits_{j \in I_h} g_j \eta^{-ij} & \text{if } x \in C_k. \end{cases}$$

Proof : Since $W = (I \otimes v)(U \otimes I)$, by Lemma 6.1, $W^* LW = (U \otimes I)^* (\sum\limits_{k \in I_h} G_k \otimes E_k)(U \otimes I) = \sum\limits_{k \in I_h} (U^* G_k U) \otimes E_k$. One can verify that

$$U^* G_k U = \sum_{j \in I_h} g_{k-j} T^j,\ k \in I_h.$$

So, $W^* LW = \sum\limits_{k \in I_h} \sum\limits_{j \in I_h} g_{k-j} T^j \otimes E_k$. Now, the formulae for T and E_k imply the result. $\square$

We are to obtain $W^* L(L)' W = (W^* LW)^2$. So, we need to find a simpler expression for $|\sum\limits_{j \in I_h} \eta^{-ij}|^2$. For that we need the following.

18

Notation 6.3. *(a)* Ω_h *is the multiplicative group of all hth roots of unity.*
(b) For $i \in I_h$, $\chi_i : F_s^* \to \Omega_h$ is defined by $\chi_i(x) = \eta^{-ij}$, if $x \in C_j, j \in I_h$.

Lemma 6.3. $|\sum\limits_{j \in I_h} g_i \eta^{-ij}|^2 = \begin{cases} 1 & \text{if } i = 0, \\ s & \text{if } 0 < i < h \end{cases}$

Proof : Since $C_j C_k = C_{j+k}$ (where the addition in the suffix is modulo h), χ_i is a group homomorphism (character) on F_s^*. From the definition of g_j's we have

$$\sum_{j \in I_h} g_j \eta^{-ij} = \sum_{j \in I_h} \sum_{x \in C_j} \omega^{trace(x)} \chi_i(x) = \sum_{x \in F_s} \omega^{trace(x)} = g(\chi_i),$$

which is the Gauss sum attached to the character χ_i. But $|g(\chi_i)|^2 = \begin{cases} 1 & \text{if } i = 0, \\ s & \text{if } i \neq 0 \end{cases}$, by a classical result on such Gauss sums [see, for instance Chapter 10 of Ireland and Rosen (1982)]. Hence the result. $\square$

Putting the information from Lemmas 6.2 and 6.3 together, we get the spectrum of $L(L)'$.

Lemma 6.4. $W^* L(L)' W = D$, *where the diagonal entries of the diagonal matrix D are as follows.*

$$|\delta(i,x)|^2 = \begin{cases} (s-1)^2 & \text{if } i = 0, x = 0 \\ 0 & \text{if } i \neq 0, x = 0 \\ 1 & \text{if } i = 0, x \neq 0, \\ s & \text{if } i \neq 0, x \neq 0. \end{cases}$$

In order to get the spectrum of $C_{d_1^*}$ we need the spectrum of HH'.

Lemma 6.5. $W^* HH'W$ *is a diagonal matrix with the (i,x)th entry* $= \begin{cases} h(s-1)^2 & \text{if } i = 0, x = 0 \\ h & \text{if } i \neq 0, x \neq 0 \\ 0 & \text{if } i \neq 0. \end{cases}$

Proof : Let $\triangle_h$ denote the $h \times h$ matrix having the $(0,0)$th entry 1 and all other entries 0. $\triangle_s$ is defined in a similar manner. It is easy to verify that

$$U^* J_h U = h \triangle_h \text{ and } V^* J_s V = s \triangle_s.$$

Since $H = 1_h \otimes (J_s - I_s)$, [recall Lemma 5.2], we see that

$$W^* HH'W = h \triangle_h \otimes (s \triangle_s - I_s)^2,$$

which is a diagonal matrix with the entries as in the statement. $\square$

Proof of Theorem 6.1 : Lemmas 6.4 and 6.5 imply the result in view of the expression for $C_{d_1^*}$ in Lemma 5.1. $\square$

7 Reference

1. Bagchi, B. and Bagchi, S. (2001). Optimality of partial geometric designs. Ann. Stat., vol. 29, p : 577 - 594.

2. Bagchi, S. and Bagchi, B. (2020). Aspects of optimality of plans orthogonal through other factors. Submitted.

3. Bagchi, S. and Mukhopadhyay, A.C. (1989) Optimality in the presence of two-factor interactions among the nuisance factors. Comm. Stat. Theory. Method. vol. 18, p : 1139-1152.

4. Bagchi, S. and Shah, K.R. (1989). On the optimality of a class of row-column designs. Jour. Stat. Plan. Inf., vol. 23, p : 397-402.

5. Bhatia. R. (2013) Matrix Analysis. Graduate texts in Mathematics, Springer.

6. Eccleston, J.A. and Russell, K.G. (1977). Adjusted orthogonality in nonorthogonal designs. Biometrika, vol. 64, p : 339-345.

7. Ireland, K. and Rosen, M (1982). A classical introduction to modern number theory, Springer Verlag.

8. Kiefer, J. (1975). Construction and optimality of generalized Youden designs. In: Srivastava JN (ed) A survey of statistical design and linear models. North-Holland, Amsterdam, p : 333 - 353

9. Marshall, A.W, Olkin, I, Arnold, B.C. (2011) Inequalities: theory of majorization and its applications. Springer series in statistics, 2nd edn. Springer, New York.

10. Morgan, J.P. (1997). Optimal design for interacting blocks with OAVS incidence. Metrika, 45, p : 67-83.

11. Morgan, J.P. and Uddin, N. (1996). Optimal blocked main effect plans with nested rows and columns and related designs. Ann. Stat. vol. 24, p: 1185-1208.

12. Mukerjee, R., Dey, A. and Chatterjee, K. (2001). Optimal main effect plans with non-orthogonal blocking. Biometrika, 89, p: 225-229.

13. Mukhopadhyay, A.C. and Mukhopadhyay, S. (1984). Optimality in a balanced multi-way heterogeneity set up. In Proceedings of the Indian Statistical Institute Golden Jubilee International conference on Statistics : Applications and new directions., p : 466-477.

14. Nilson, T. and Cameron, P.J. (2017) Triple arrays from difference sets. Jour. Combin Designs. 2017, 25, p : 494 - 506.

15. Preece, D. A., Wallis, W. D. and Yucas, J. L. (2005). Paley triple arrays. Australas J. Combin., 33, p: 237 - 246.

16. Shah, K.R. and Eccleston, J.A. (1986). On some aspects of row-column designs. Jour. Stat. Plan. Inf. 15, p : 87-95.

17. Shah KR, Sinha BK (1989) Theory of optimal designs.Lecture notes in statistics, vol 54. Springer. Berlin

* Foot note : Both the authors are retired from Indian Statistical Institute, Bangalore Center

On behalf of all authors, the corresponding author states that there is no conflict of interest.