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ON THE TYPE-1 OPTIMALITY OF NEARLY BALANCED INCOMPLETE BLOCK DESIGNS WITH SMALL CONCURRENCE RANGE

John P. Morgan and Sudesh K. Srivastav

Virginia Tech. and Tulane University

Abstract: The class of nearly balanced incomplete block designs with concurrence range l, or NBBD(l), is defined. This extends previous notions of "most balanced" designs to cover settings where off-diagonal entries of the concurrence matrix must differ by a positive integer $l \geq 2$. Sufficient conditions are found for optimality of NBBD(2)'s under type-1 criteria, then used to establish A- and D-optimality in settings where optimal designs were previously unknown. Some NBBD(3)'s are also found to be uniquely A- and D-optimal. Included is a study of settings where the necessary conditions for balanced incomplete block designs are satisfied, but no balanced design exists.

Key words and phrases: A-optimality, concurrence discrepancy, D-optimality, nearly balanced incomplete block design, semi-regular graph design.

1. Introduction

Consider the proper block design setting where v treatments are arranged in b blocks of size $k \leq v$. Let $D(v,b,k)$ denote the class of all block designs in such an experimental setting, and observe that each design $d \in D(v,b,k)$ corresponds to a $v \times b$ incidence matrix N_d whose entries n_{dij} are nonnegative integers indicating the number of times treatment i occurs in block j. The matrix N_dN_d' is referred to as the concurrence matrix of d, and its entries, the concurrence parameters, are denoted by λ_{dij}. The reduced normal equations for estimating treatment effects under the standard additive model, when the design d is used, are $C_d\hat{\tau} = T_d - \frac{1}{k}N_dB_d$, in which $C_d = diag(r_{d1},\ldots,r_{dv}) - \frac{1}{k}N_dN_d'$, B_d denotes the $b \times 1$ vector of block totals in d, T_d is the $v \times 1$ vector of treatment totals, r_{di} represents the number of times treatment i is replicated by d, and diag$(r_{d1},\ldots,r_{dv})$ is a $v \times v$ diagonal matrix. The information matrix or C-matrix of the design, C_d, is positive semi-definite for all $d \in D(v,b,k)$.

A treatment contrast is any linear combination $l'\tau = \sum l_i\tau_i$ of the treatment effects, where $\sum l_i = 0$. A block design in which all treatment contrasts are estimable is said to be connected, and all competing designs in this paper are assumed to have this property, so $D(v,b,k)$ is further defined to contain only connected designs. It is known that a block design is connected if and only if its C-matrix has rank $v-1$.

A design d is binary if all its blocks consist of distinct varieties, i.e., $n_{dij}=0$ or 1 for all i and j. For any given setting $D(v,b,k)$, define $M(v,b,k)$ as the binary subclass of $D(v,b,k)$, r as the greatest integer not exceeding bk/v, λ as the greatest integer not exceeding $r(k-1)/(v-1)$, $p=bk-vr$, and $\mu=r(k-1)-\lambda(v-1)$, as needed throughout. If $\mathrm{tr}(A)$ denotes the trace of a given square matrix A, then $M(v,b,k)$ is the subclass of designs in $D(v,b,k)$ with maximal $\mathrm{tr}(C_d)$.

A binary design d in which each treatment occurs in either r or $r+1$ blocks, and each pair of treatments is contained in either λ or $\lambda+1$ blocks, is called a semi-regular graph design (SRGD) (Jacroux (1985)), and is also a type of nearly balanced incomplete block design (NBBD) (Cheng and Wu (1981)). These notions generalize John and Mitchell's (1977) definition of a regular graph design (RGD), to which they reduce when bk/v is an integer. If d is an RGD and its concurrence matrix additionally has all its off diagonal elements equal, then d is called a balanced incomplete block design, or BIBD.

Let $z_{d0}=0<z_{d1}\le\cdots\le z_{dv-1}$ denote the eigenvalues of C_d. Let f be a nonincreasing, convex, real-valued function. A design $d\in D(v,b,k)$ is said to be ϕ_f-optimal provided $\phi_f(C_d)=\sum_{i=1}^{v-1}f(z_{di})$ is minimal over all designs in $D(v,b,k)$. The book by Shah and Sinha (1989) provides an excellent overview of the various criteria ϕ_f typically employed. This paper focuses on those f which Cheng (1978) included in the family of *type*-1 criteria.

Definition 1.1. $\phi_f(C_d)=\sum_{i=1}^{v-1}f(z_{di})$ is a type-1 criterion if f is a convex, real-valued function for which

(i) f is continously differentiable on $(0,\ max_{d\in D(v,b,k)}\ \mathrm{tr}(C_d))$ with $f'<0$, $f''>0$, and $f'''<0$ on this range, and

(ii) f is continous at 0 or $lim_{x\to 0}\ f(x)=f(0)=\infty$.

For instance, the well known A-, D-, and Φ_p-criteria are type-1 criteria: take $f(x)=1/x$, - log x, and x^{-p} in the above definition, respectively. Unless explicitly stated otherwise, any criterion used in this paper is assumed to be a type-1 criterion. The phrase "type-1 optimality" will be used for optimality with respect to an unspecified type-1 criterion ϕ_f.

A number of results are already known for type-1 optimality of block designs in $D(v,b,k)$, primarily for members of the classes of designs defined above. One example is the celebrated result that a BIBD is optimal under all type-1 criteria (Kiefer (1975)). Various types of block designs which are not BIBDs have also been shown to be optimal under different type-1 criteria in a number of classes and subclasses of $D(v,b,k)$ (e.g. Conniffe and Stone (1975); Shah, Ragavarao and

Khatri (1976); William, Patterson and John (1977); Cheng (1978, 1979); Jacroux (1985, 1989, 1991); and Yeh (1988)). However, those designs which are type-1 optimal in many cases remain unkown, and the primary goal here is to extend the reach of optimality arguments to settings where the strict combinatorial conditions previously studied cannot hold.

In Section 2 the class of nearly balanced incomplete block designs with concurrence range l, or NBBD(l), is defined. This class generalizes the SRGDs to cases where off-diagonal entries of the concurrence matrix differ by at most the positive integer l. The nonexistence of NBBD(1)'s is explored and an upper bound for the minimum eigenvalue z_{d1} is derived. These results are used in Section 3 to derive sufficient conditions for type-1 optimality of NBBD(2)'s in $D(v, b, k)$, then applied in Section 4 to establish A- and D-optimality of families of NBBD(2)'s. In some instances, NBBD(3)'s are found to be optimal. Not all of the problems are analytically tractable; in some cases theory reduces the optimality argument to a computationally feasible form. Concluding remarks are made in Section 5.

2. Preliminary Results

Definition 2.1. A nearly balanced incomplete block design d with concurrence range l, or NBBD(l), with v varieties and b blocks of size k is an incomplete block design satisfying the following conditions:

(i) each $n_{dij} = 0$ or 1,
(ii) each $r_{di} = r$ or $r + 1$,
(iii) $\max_{i \neq i', j \neq j'} |\lambda_{dii'} - \lambda_{djj'}| = l$,
(iv) d minimizes $\mathrm{tr}(C_d^2)$ over all designs satisfying $(i) - (iii)$.

The definition of a NBBD(l) generalizes those given by John and Mitchell (1977) for a RGD and by Jacroux (1985) for a SRGD. It reduces to the definition of a BIBD if bk/v is an integer and $l = 0$, to an RGD if bk/v is an integer and $l = 1$, and to that of a SRGD if $l = 1$. Closely related when $l = 1$ is the definition of a NBBD given by Cheng and Wu (1981), who require that (i) and (ii) of Definition 2.1 hold, and that for each fixed i, the $v - 1$ concurrences λ_{dij} for $j \neq i$ have range at most 1. For certain settings this allows treatments i replicated $r + 1$ times to have λ_{dij} values of $\lambda + 1$ and $\lambda + 2$, thus falling under our definition of a NBBD(2).

The need to extend the "nearly balanced" notion as in Definition 2.1 arises in settings where neither BIBD's nor NBBD(1)'s exist. These settings may be classified into two broad categories. In *category one*, for any binary d the combinatorics force $\lambda_{dij} \leq \lambda - 1$ for at least one treatment pair (i, j). That condition implies that $\lambda_{dij} \geq \lambda + 1$ for some treatment pair (i, j), and the nonexistence of NBBD(l)'s with $l \leq 1$ follows. That condition also typically forces a sharper bound on z_{d1} than can usually be obtained, as shown in Lemma 2.2. In *category two*, any d satisfying (i) and (ii) of Definition 2.1 with $\lambda_{dij} \geq \lambda$ for all (i, j) must have $\lambda_{dij} \geq \lambda + 2$ for some (i, j). Though this partially overlaps the settings studied by Cheng and Wu (1981) (in their notation, this occurs when $n < k-1$), we will offer optimal category two designs that do not satisfy their definition of a NBBD. We know of no previously published work addressing category one, though designs that fit into this framework have appeared, as shall be seen.

Lemma 2.2. *A binary block design $d \in D(v, b, k)$ with $k \geq 3$ for which either $r_{di} < r$ for some i, or $\lambda_{dij} \leq \lambda - 1$ for some $i \neq j$ with $r_{di} = r_{dj} = r$, satisfies*

$$z_{d1} \leq \frac{(k-1)r + \lambda - 1}{k}. \tag{1}$$

Proof. Suppose some treatment is replicated $r_{dp} < r$ times. Then by Theorem 3.1 of Jacroux (1980a) and regardless of binarity,

$$z_{d1} \leq \frac{v(k-1)r_{dp}}{k(v-1)} \leq \frac{v(k-1)(r-1)}{k(v-1)} \leq \frac{(k-1)r + \lambda - 1}{k},$$

the last inequality because $\lambda \geq \frac{r(k-1)-(v-2)}{v-1}$. The result for $\lambda_{dij} \leq \lambda - 1$ follows from Proposition 2.1(b) of Jacroux (1982).

A rich series of settings falling into category one and meeting the conditions of Lemma 2.2 is identified by Lemma 2.3. There are surely many others. Existence of d such that $\lambda_{dij} \geq \lambda$ for all $i \neq j$ depends not just on arithmetic relationships among the parameters v, b, and k, but on what assignments are combinatorially achievable. For instance, if the necessary parameter conditions for existence of a BIBD hold, but no BIBD exists, then the setting belongs to category one and again the conditions for (1) are met Lemma 2.3, with Lemma 2.2, generalizes Lemma 2 of Morgan and Uddin (1995).

Lemma 2.3. *Any binary block design $d \in D(v, b, k)$, where $bk = vr + 1$, and $r(k-1)/(v-1) = \lambda$ is an integer, satisfies the conditions of Lemma 2.2. Thus no NBBD(1) exists for this setting, and (1) holds.*

Proof. If some treatment is replicated $r_{di} < r$ times, the result is immediate. So assume $r_{d1} = r_{d2} = \cdots = r_{d,v-1} = r$ and $r_{dv} = r + 1$. Since the design is binary there are $r + 1$ blocks containing the vth treatment, and the total number of ordered pairs of treatments containing the vth treatment is $(r + 1)(k - 1) = \lambda(v-1) + (k-1)$. This implies that there is at least one treatment, say i_0, which occurs exactly $(\lambda + l)$ times in these $r + 1$ blocks for some $1 \leq l \leq k - 1$. Thus there are $(\lambda + l)(k-2)$ ordered pairs in these $r + 1$ blocks, and $(r - \lambda - l)(k - 1)$

in the other blocks, involving treatment i_0 and treatments other than v. So the total number of ordered pairs with treatment i_0 but not with treatment v is $(\lambda+l)(k-2)+(r-\lambda-l)(k-1) \le r(k-1)-(\lambda+1) < \lambda(v-2)$. This clearly shows that there exists at least one pair (i, i_0) for some $i \in \{1, \ldots, v-1\}$, $i \neq i_0$, such that $\lambda_{dii_0} \le \lambda - 1$.

Sufficient conditions for a setting to fall into category two are stated in Lemma 2.4, with proof in Cheng and Wu (1981, pp. 494-495). Their NBBD's which overlap with our NBBD(2)'s occur in settings satisfying condition (i) of the lemma. The result under condition (ii) is a restatement of their Proposition 1.

Lemma 2.4. *Let $d \in M(v,b,k)$ have $r_{di} \ge r$ for all i, and $\lambda_{dij} \ge \lambda$ for all $i \neq j$. If* (i) *$\mu > v-k$, or* (ii) *$\mu \le v-k$ and $p(k-p) > (v-2p)\mu$, then $\lambda_{dij} \ge \lambda+2$ for some $i \neq j$.*

Section 3 will focus on optimality of NBBD(2)'s, and the chief tools will require minimizing $\mathrm{tr}(C_d^2) = \sum_i z_{di}^2$. This is a bit harder in settings where NBBD(1)'s do not exist than in those where they do. The final lemmas of this section state results which will aid in that task.

Lemma 2.5. *Let $y_1, \ldots, y_n$, $n \ge 3$, be integer-valued variables subject to the constraints $\sum_{i=1}^n y_i = c$ and $max_i\{y_i\} - min_i\{y_i\} = R$. Denote the minimum value of $\sum y_i^2$ by $Q(R,c)$. With $c_1 = int(c/n) = int(\bar{c})$,*

(i) *$Q(1,c) = -nc_1^2 + c_1(2c-n) + c$, provided $c_1 \neq \bar{c}$.*

(ii) *$Q(2,c) = -nc_1^2 + c_1(2c-n) + c + 2$.*

(iii) If *$c_1 \neq \bar{c}$, then* $Q(R+1,c) - Q(R,c) \ge \begin{cases} R & \text{for even } R \ge 2, \\ R+1 & \text{for odd } R \ge 1. \end{cases}$

(iv) If *$c_1 = \bar{c}$, then* $Q(R+1,c) - Q(R,c) \ge \begin{cases} R+2 & \text{for even } R \ge 2, \\ R-1 & \text{for odd } R \ge 3. \end{cases}$

Lemma 2.6. *Let $y_1, \ldots, y_n$, $n \ge 3$, be integer-valued variables subject to the constraints $\sum_{i=1}^n y_i = c$, $max_i\{y_i\} - min_i\{y_i\} = R$, and $\sum_{i=1}^n max\{0, c_1 - y_i\} = \delta$, where $c_1 = int(c/n)$. Here c and R are positive integers and δ is a nonnegative integer. Let $Q_\delta(R,c)$ denote the minimum value of $\sum y_i^2$ subject to these constraints, provided the constraints are consistent, in which case $Q_\delta(R,c)$ is said to exist. Fix $\delta_1 \in \{1, \ldots, \frac{n-(c-nc_1)}{2}\}$.*

(i) *$Q_{\delta_1}(2,c) = -nc_1^2 + c_1(2c-n) + c + 2\delta_1$, and $Q_\delta(2,c)$ does not exist for $\delta > \frac{n-(c-nc_1)}{2}$.*

(ii) *$Q_{\delta_1}(R,c)$ exists if and only if $2 \le R \le (c-nc_1) + 2\delta_1$, and for these $R \ge 3$, $Q_{\delta_1}(R,c) - Q_{\delta_1}(R-1,c) \ge 2$.*

(iii) *For every $\delta > \delta_1$ and $R \ge 3$ for which $Q_\delta(R,c)$ exists, at least one of $Q_\delta(R-1,c)$, $Q_{\delta-1}(R,c)$ and $Q_{\delta-1}(R-1,c)$ exists, and at least one of these* *inequalities holds:*

$$Q_\delta(R,c) - Q_\delta(R-1,c) \geq 2; Q_\delta(R,c) - Q_{\delta-1}(R,c) \geq 2;$$
$$Q_\delta(R,c) - Q_{\delta-1}(R-1,c) \geq 4.$$

The above inequalities are generally only sharp for small R, which is sufficient for our purposes.

3. Type-1 Optimality

This section uses results from Section 2 in adapting Jacroux's (1985) approach for optimality of NBBD(1)'s to encompass problems on type-1 optimality of category one NBBD(2)'s. Two lemmas needed from Jacroux (1985) on minimization of type-1 optimality functions are stated first. Let $n \geq 3$ be an integer and let C and D be fixed and positive constants such that $C^2 \geq D \geq C^2/n$. Let $f(x)$ be a convex, real-valued function satisfying the conditions of Definition 1.1. The problem is to find $x_1, \ldots, x_n$ which

$$\text{minimize} \quad \sum_{i=1}^{n} f(x_i) \tag{2}$$

subject to the constraints

$$\begin{array}{rl} \text{(i)} & x_i \geq 0 \ \text{ for } \ i = 1, \ldots, n, \\ \text{(ii)} & \sum_{i=1}^n x_i = C, \\ \text{(iii)} & \sum_{i=1}^n x_i^2 \geq D, \\ \text{(iv)} & x_1 \leq F \text{ for a number } F \text{ satisfying} \\ & \text{(a)} F \leq (C - [n/(n-1)]^{1/2} P)/n \text{ where } P = [D - (C^2/n)]^{1/2} \\ & \text{(b)} \ (C-F)^2 \geq D - F^2 \geq (C-F)^2/(n-1). \end{array} \tag{3}$$

The constraint (iv)(b) of (3) is solely to insure that a set of x_i's satisfying (i)-(iii) can be found with $x_1 = F$, for which it is both necessary and sufficient.

The following lemmas yield the solution to two related minimization problems. The proofs for both may be found in Jacroux (1985).

Lemma 3.1. *With* $P_F = [(D-F^2) - ((C-F)^2/(n-1))]^{1/2}$*, the solution to* (2) *subject to the constraints* (3) *occurs when* $x_1 = F$*,* $x_n = \{(C-F) + [(n-1)(n-2)]^{1/2} P_F\}/(n-1)$*, and* $x_i = \{(C-F) - [(n-1)/(n-2)]^{1/2} P_F\}/(n-1)$ *for* $i = 2, \ldots, n-1$*.*

Constraint (iv)(a) of (3) implies that the solution of Lemma 3.1 satisfies $x_1 \leq x_i$ for all i. Conversely, it can be shown that if $F \leq \{(C-F) - [(n-1)/(n-2)]^{1/2} P_F\}/(n-1)$ then (iv)(a) holds.

The solution in Lemma 3.1 is found at a set of x_i's for which $\sum_{i=1}^n x_i^2 = D$, that is, the quantity $\sum_{i=1}^n x_i^2$ is made as small as possible. As the bound D for $\sum_{i=1}^n x_i^2$ is made smaller, the solution for x_n moves to that of $x_2, \ldots, x_{n-1}$. When the constraint is dropped altogether, one gets $x_2 = x_3 = \cdots = x_n$, as found in Lemma 3.2.

Lemma 3.2. *The solution to* (2) *subject to constraints* (i), (iv) *of* (3) *and* $\sum_{i=1}^n x_i \leq C$, occurs when $x_1 = F$ *and* $x_i = (C - F)/(n-1)$ *for* $i = 2, \ldots, n$.

Lemmas 3.1 and 3.2 will be used in conjunction with bounds on z_{d1}, $\mathrm{tr}(C_d)$, and $\mathrm{tr}(C_d^2)$, to establish bounds on the ϕ_f-values of designs which are not NBBD(2)'s. For $\bar{d}$ any NBBD(2) in $D(v,b,k)$, define the quantities A and B_2 by $A = \mathrm{tr}(C_{\bar{d}})$ and $B_2 = \mathrm{tr}(C_{\bar{d}}^2) + \frac{4}{k^2}$. The main optimality result depends on B_2 being the minimum value of $\mathrm{tr}(C_d^2)$ among binary competitors of the NBBD(2)'s. The value of this quantity depends on the setting parameters and the *concurrence discrepancy* (shortly, *discrepancy*) of $\bar{d}$.

Definition 3.3. The concurrence discrepancy of design d, denoted δ_d, is the quantity $\delta_d = \sum\sum_{i<j} \max\{0, \lambda - \lambda_{dij}\}$. The minimum discrepancy δ is the minimum of δ_d over the binary class, ie., $\delta = \min_{d \in M} \delta_d$.

By Lemma 2.6, the value of $\mathrm{tr}(C_{\bar{d}}^2) = (\frac{k-1}{k})^2 \sum_{i=1}^v r_{\bar{d}i}^2 + \frac{2}{k^2} \sum\sum_{i<j} \lambda_{\bar{d}ij}^2$ in a category one setting is $\mathrm{tr}(C_{\bar{d}}^2) = (\frac{k-1}{k})^2(vr^2 + 2pr + p) + \frac{1}{k^2}[bk(k-1)(2\lambda+1) + 4\delta_{\bar{d}} - v(v-1)\lambda(\lambda+1)]$ and the NBBD(2) $\bar{d}$ minimizes $\mathrm{tr}(C_{\bar{d}}^2)$ over M if $\delta_{\bar{d}} = \delta$. Category one settings are exactly those for which $\delta > 0$.

Let z_1 and $z_1^\star$ be nonnegative constants (they appear below as upper bounds for the minimum nonzero eigenvalues z_{d1} of designs in the subclasses of binary and nonbinary designs in $D(v,b,k)$, respectively) which satisfy

$$(A - z_1)^2 \geq B_2 - {z_1}^2 \geq \frac{(A-z_1)^2}{(v-2)} \quad \text{and} \quad (A - z_1^\star)^2 \geq B_2 - z_1^{\star 2} \geq \frac{(A-z_1^\star)^2}{(v-2)}.$$

Given z_1, and for $P_2 = [(B_2 - z_1^2) - ((A - z_1)^2/(v-2))]^{1/2}$, define z_2 and z_3 (cf. x_i and x_n of Lemma 3.1) by $z_2 = [(A - z_1) - (\frac{(v-2)}{(v-3)})^{1/2} P_2]/(v-2)$ and $z_3 = [(A-z_1) + ((v-2)(v-3))^{1/2} P_2]/(v-2)$. Given $z_1^\star$, let $z_4 = [A - (2/k) - z_1^\star]/(v-2)$ (cf. x_i of Lemma 3.2).

Theorem 3.4. *Let* $D(v,b,k)$ *be a setting with* $k \geq 3$ *and* $\delta > 0$. *Let* $\bar{d} \in D(v,b,k)$ *be a NBBD*(2) *with* $\delta_{\bar{d}} = \delta$ *and* C*-matrix* $C_{\bar{d}}$ *having nonzero eigenvalues* $z_{\bar{d}1} \leq z_{\bar{d}2} \leq \cdots \leq z_{\bar{d},v-1}$. *Let* $z_1 = \frac{r(k-1)+\lambda-1}{k}$ *and* $z_1^\star = \frac{r(k-1)v}{(v-1)k}$. *Then if* $z_1 \leq z_2$ *and*

$$\sum_{i=1}^{v-1} f(z_{\bar{d}i}) < f(z_1) + (v-3)f(z_2) + f(z_3), \tag{4}$$

a ϕ_f-optimal design in $M(v,b,k)$ must be an NBBD(2). If, moreover, $z_1^\star \leq z_4$ and

$$\sum_{i=1}^{v-1} f(z_{\bar{d}i}) < f(z_1^\star) + (v-2)f(z_4), \tag{5}$$

then a ϕ_f-optimal design in $D(v,b,k)$ must be an NBBD(2).

Proof. Let d be any design in $D(v,b,k)$. If $d \notin M(v,b,k)$ then N_d has $|n_{dil} - n_{djm}| > 1$ for some i, j and $l \neq m$, and consequently $\mathrm{tr}(C_d) \leq \mathrm{tr}(C_{\bar{d}}) - (2/k)$. Furthermore, such d must have $z_{d1} \leq z_1^*$ (Jacroux (1980a, Theorem 3.1)). Thus the z_{di} satisfy the constraints of Lemma 3.2 for the variables x_i with $n = v-1$, $C = A - 2/k$, $D = (A-2/k)^2/(v-1)$, and $F = z_1^*$, implying that $\sum_{i=1}^{v-1} f(z_{di}) \geq f(z_1^\star) + (v-2)f(z_4)$. So if the last statement of the theorem holds, a ϕ_f-optimal design in $D(v,b,k)$ must be in $M(v,b,k)$.

Now suppose d is in $M(v,b,k)$ but is not an NBBD(2). Since $\delta > 0$, no NBBD(1) exists, and it must be true that either (i) $|r_{di} - r_{dj}| > 1$ for some $i \neq j$; (ii) $|\lambda_{dij} - \lambda_{dkl}| > 2$ for some fixed values of i, j, k, and l, $i \neq j, k \neq l$; or (iii) d fails the last condition of Definition 2.1. It will be established that for each of these cases, $\mathrm{tr}(C_d^2) \geq B_2$.

Case (i). If $|r_{di} - r_{dj}| > 1$ for some $i \neq j$, then by Lemma 2.5, identifying the y_i's with the r_{di}'s for $n = v$ and $c = vr + p$,

$$\sum_{i=1}^{v} r_{di}^2 - \sum_{i=1}^{v} r_{\bar{d}i}^2 \geq \begin{cases} Q(2,c) - Q(1,c) \geq 2 & \text{if } p > 0, \\ Q(2,c) - Q(0,c) \geq 2 & \text{if } p = 0. \end{cases}$$

By Lemma 2.6, identifying the y_i's with the λ_{dij}'s for $i < j$ with $n = v(v-1)/2$ and $c = bk(k-1)/2$, for some $R \geq 2$ and some $\delta_d \geq \delta$, $2[\sum\sum_{i<j} \lambda_{dij}^2 - \sum\sum_{i<j} \lambda_{\bar{d}ij}^2] \geq 2[Q_{\delta_d}(R,c) - Q_\delta(2,c)] \geq 0$. Thus $\mathrm{tr}(C_d^2) - \mathrm{tr}(C_{\bar{d}}^2) \geq 2\left(\frac{k-1}{k}\right)^2 \geq \frac{4}{k^2}$ for $k \geq 3$.

Case (ii). If the λ_{dij} have a range exceeding 2, then by Lemma 2.6 for some $R \geq 3$,

$$\mathrm{tr}(C_d^2) - \mathrm{tr}(C_{\bar{d}}^2) \geq \frac{2}{k^2}[\sum_{i<j}\sum \lambda_{dij}^2 - \sum_{i<j}\sum \lambda_{\bar{d}ij}^2] \geq \frac{2}{k^2}[Q_{\delta_d}(R,c) - Q_\delta(2,c)] \geq \frac{4}{k^2}.$$

Case (iii) follows from yet one more application of Lemma 2.6 with the λ_{dij}'s as variables:

$$\mathrm{tr}(C_d^2) - \mathrm{tr}(C_{\bar{d}}^2) \geq \frac{2}{k^2}[\sum_{i<j}\sum \lambda_{dij}^2 - \sum_{i<j}\sum \lambda_{\bar{d}ij}^2] \geq \frac{2}{k^2}[Q_{\delta+1}(2,c) - Q_\delta(2,c)] \geq \frac{4}{k^2}.$$

Now invoking Lemma 2.2, the z_{di} are seen to satisfy (i) $z_{d1} > 0$, (ii) $\mathrm{tr}(C_d) = \sum_{i=1}^{v-1} z_{di} = A$, (iii) $A^2 \geq \mathrm{tr}(C_d^2) = \sum_{i=1}^{v-1} z_{di}^2 \geq B_2$, and (iv) $z_{d1} \leq z_1$. These restrictions on the z_{di} are the same as those given in Lemma 3.1 for the variables x_i with $n = v-1$, $C = A$, $D = B_2$, and $F = z_1$, and the condition $z_1 \leq z_2$ guarantees that (iv)(a) of (3) holds. Thus $\sum_{i=1}^{v-1} f(z_{di}) \geq f(z_1) + (v-3)f(z_2) + f(z_3) > \sum_{i=1}^{v-1} f(z_{\bar{d}i})$, eliminating all binary competitors to $\bar{d}$ outside of the NBBD(2) class. If any binary design is ϕ_f-better than $\bar{d}$, it must be some other NBBD(2).

An interesting feature of this theorem is that the upper bounds z_1 and z_1^* for z_{d1}, for members of $M(v,b,k)$ and $D(v,b,k)$ respectively, satisfy $z_1 < z_1^*$. That is, the possibility is allowed that a nonbinary design may be E-better than the best binary design. This indeed does occur in some cases (see Theorem 4.1). In other settings it is possible to sharpen the theorem with a corresponding sharpening of one or both of the bounds, which will be done when advantageous.

Given any setting where the minimum discrepancy δ must be positive, one can apply Theorem 3.4 after addressing the sometimes onerous combinatorial problem of determining the exact value of δ. Typically $\delta_d = \delta$ for some binary d in the subclass satisfying condition (ii) of Definition 2.1, and $\delta_d > \delta$ for all d not in that subclass; the difficulties arise in sorting through the possibilities for the "as equally replicated as possible" designs. Example 1 demonstrates some of these difficulties.

Example 1. Consider the design $\bar{d}$ having parameters $v = 9$, $b = 11$, and $k = 5$, whose blocks are the columns

$$\begin{array}{ccccccccccc}
1 & 1 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 3 & 3 \\
2 & 2 & 2 & 3 & 4 & 5 & 3 & 3 & 4 & 4 & 4 \\
3 & 4 & 5 & 6 & 7 & 6 & 5 & 6 & 5 & 5 & 5 \\
4 & 6 & 8 & 8 & 8 & 7 & 7 & 7 & 6 & 6 & 7 \\
5 & 7 & 9 & 9 & 9 & 9 & 9 & 8 & 8 & 9 & 8.
\end{array}$$

Then $A = \mathrm{tr}(C_{\bar{d}}) = 44$, $B_2 = \mathrm{tr}(C_{\bar{d}}^2) + .16 = 243.36109$, $-\sum_{i=1}^{v-1} \log(z_{\bar{d}i}) = -13.61922$ and $\sum_{i=1}^{v-1} z_{\bar{d}i}^{-1} = 1.46120$. Calculating z_1, $z_1^\star$, z_2, z_3, and z_4 as outlined in Theorem 3.4 and the preceding text gives $z_1 = 5.2$, $z_1^\star = 5.4$, $z_2 = 5.36977$, $z_3 = 6.58136$, $z_4 = 5.45714$. It is now an easy matter to check that (4) and (5) hold, so that A- and D-optimal designs in $D(9,11,5)$ must be NBBD(2)'s, *provided* $\bar{d}$ itself is an NBBD(2), that is, provided $\delta_{\bar{d}} = 3$ is the smallest achievable δ_d among binary designs with replicate range of 1 and concurrence range of 2, and *provided* that $\delta_{\bar{d}}$ is in fact δ, the latter value being determined over all of M.

So consider any binary d. If $r_{di} < 6$ for some i, then $\sum_{j\neq i} \lambda_{dij} \leq 20$ and so $\delta_d \geq \lambda(v-1) - \sum_{j\neq i} \lambda_{dij} \geq 4$, eliminating designs with replicate range greater than 1. Thus assume that $r_{d1} = 7$ and $r_{di} = 6$ for $i > 1$. If $\lambda_{d1i} \geq x$ for some i, then $\delta_d \geq \lambda(v-2) - \sum_{j\neq 1,i} \lambda_{dij} \geq \lambda(v-2) - (24-x) = x-3$. So d for which some $\lambda_{d1i} \geq 6$ need not be considered further, and the last inequality also shows in short order that d with two or more i for which $\lambda_{d1i} = 5$ has $\delta_d \geq 4$. Hence $\delta_d < 3$ requires either $\lambda_{d1i} \leq 4$ for all i (implying four i with $\lambda_{d1i} = 4$ and four with $\lambda_{d1i} = 3$, as with $\bar{d}$ above), or $\lambda_{d12} = 5$ and $3 \leq \lambda_{d1i} \leq 4$ for $i > 2$. We have enumerated all possibilities with all $\lambda_{d1i} \leq 4$, and found in every case that $\delta_d \geq 3$, proving that $\bar{d}$ is a NBBD(2) (since if $\lambda_{d12} = 5$, the concurrence range must be 3). Furthermore, there is exactly one other, nonisomorphic NBBD(2) $\tilde{d}$, which is

$$\begin{array}{ccccccccccc}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 2 & 2 & 3 & 3 \\
2 & 2 & 2 & 2 & 3 & 3 & 4 & 4 & 5 & 4 & 5 \\
6 & 4 & 3 & 3 & 4 & 6 & 5 & 6 & 7 & 6 & 6 \\
7 & 5 & 4 & 5 & 5 & 7 & 8 & 7 & 8 & 8 & 7 \\
9 & 6 & 9 & 8 & 7 & 8 & 9 & 8 & 9 & 9 & 9.
\end{array}$$

The design $\tilde{d}$ is inferior to $\bar{d}$ in terms of the A- and D-criteria, but cannot be said to be uniformly inferior; it is better, for instance, in terms of the MV-criterion. For the $\lambda_{d12} = 5$ situation, we were surprised to find a design d^*. It is the unique NBBD(3), and establishes that $\delta = 2$ for $D(9, 11, 5)$:

$$\begin{array}{ccccccccccc}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 2 & 3 & 3 & 4 \\
2 & 2 & 2 & 2 & 2 & 3 & 3 & 5 & 5 & 4 & 5 \\
7 & 3 & 3 & 4 & 4 & 4 & 4 & 6 & 6 & 7 & 6 \\
8 & 5 & 6 & 5 & 6 & 6 & 5 & 7 & 7 & 8 & 8 \\
9 & 9 & 8 & 7 & 9 & 7 & 8 & 8 & 9 & 9 & 9.
\end{array}$$

Existence of d^* means that Theorem 3.4 does not directly apply, but it is still useful. Since d^* is the unique design achieving the minimum discrepancy $\delta = \delta_{\bar{d}} - 1$, it is the only design not ruled out by Theorem 3.4. Calculating $-\sum_{i=1}^{v-1} \log(z_{d^*i}) = -13.61974$ and $\sum_{i=1}^{v-1} z_{d^*i}^{-1} = 1.46093$ thus proves that d^* is A- and D-optimal in $D(9, 11, 5)$.

Example 1 shows there is no guarantee that a NBBD(2) in a category one setting will minimize δ_d; nonetheless Theorem 3.4 is still a key component of the optimality proof. And Theorem 3.4 does not assure that a given NBBD(2) $\bar{d}$ satisfying its conditions is actually ϕ_f-optimal. Rather, it says that a ϕ_f-optimal design must then be some NBBD(2). In those settings where there are nonisomorphic NBBD(2)'s, the best design still must be determined within the NBBD(2) class.

Before closing this section, a theorem due to Cheng (1978, Theorem 2.3) will be restated in a form suited to the current endeavor. Theorem 3.5 will be used in proving optimality of some NBBD(2)'s in category two.

Theorem 3.5. *If there is a design $\bar{d} \in M(v, b, k)$ such that*

(i) $C_{\bar{d}}$ *has two distinct eigenvalues* $z_{\bar{d}1} = z_{\bar{d}2} = \cdots = z_{\bar{d},v-2} \leq z_{\bar{d},v-1}$, *and*
(ii) $\bar{d}$ *minimizes* $\sum_{i=1}^{v-1} z_{di}^2$ *over* M,
then $\bar{d}$ *is* ϕ_f*-optimal in* M *for all type* I *criteria with* $\lim_{x\to 0^+} f(x) = \infty$.

4. Applications

4.1. Two infinite series

This section is devoted to applications of the results of Section 3. Optimality will be studied for some interesting individual designs, and for several infinite series of designs. There are many more possibilities than shown here.

Consider the setting $D(3t+2, 3t^2+3t+1, 3)$ for $t \geq 1$, in which $r = 3t+1$ and $\lambda = 2$. Then $bk = vr+1$ and $r(k-1)/(v-1)$ is the integer λ, so by virtue of Lemma 2.3, NBBD(1)'s do not exist and binary members d of this class satisfy both $\delta_d \geq 1$ and (1). Morgan and Uddin (1995) have constructed nonbinary E-optimal designs for each $t \geq 1$, and their E-value is the bound z_1^* of Theorem 3.4.

For given t, let $\tilde{d}$ be the E-optimal design of Morgan and Uddin (1995). It contains one nonbinary block of the form $(1,1,2)$, and has completely symmetric information matrix with $\lambda_{\tilde{d}ij} = \lambda$ for all $i \neq j$. Construct a binary design $\bar{d}$ from $\tilde{d}$ by replacing this nonbinary block with the block $(1,2,3)$. Then $\bar{d}$ satisfies (i) and (ii) of Definition 2.1, with 3 being the sole treatment replicated $r+1$ times. The concurrence parameters of $\bar{d}$ are the same as those of $\tilde{d}$, with the exception of those among 1, 2, and 3: $\lambda_{\bar{d}12} = \lambda - 1$ and $\lambda_{\bar{d}13} = \lambda_{\bar{d}23} = \lambda + 1$. This establishes that $\delta_{\bar{d}} = 1$ is the achievable value of δ for this class, and thus by Lemma 2.6, that $\bar{d}$ satisfies (iii) and (iv) of Definition 2.1 with $l = 2$. That is, $\bar{d}$ is a NBBD(2). Moreover, up to treatment labeling, $\bar{d}$ is the unique NBBD(2), for such a design must have two treatment pairs $i < j$ with $\lambda_{dij} = \lambda + 1$, and both must involve the treatment replicated $r+1$ times.

Theorem 4.1. *The NBBD*(2) $\bar{d} \in D(3t+2, 3t^2+3t+1, 3)$ *is A- and D-optimal.*

Proof. The C-matrix of $\bar{d}$ has nonzero eigenvalues $2t+1$, $2t+\frac{4}{3}$, and $2t+\frac{7}{3}$, with multiplicities of 1, $(3t-1)$, and 1, respectively, and gives $A = \mathrm{tr}(C_{\bar{d}}) = 6t^2+6t+2$ and $B_2 = \mathrm{tr}(C_{\bar{d}}^2) + 4/k^2 = 12t^3 + 20t^2 + \frac{40t}{3} + \frac{46}{9}$. So $z_1 = 2t+1$, $z_1^\star = 2t + \frac{4}{3}$, $z_2 = 2t+\frac{4}{3}+\frac{1}{3t}-\frac{1}{3t}((13t-3)/(9t-3))^{1/2}$, $z_3 = 2t+\frac{4}{3}+\frac{1}{3t}+\frac{1}{3t}((13t-3)(3t-1)/3)^{1/2}$, and $z_4 = 2t + \frac{4}{3}$. As might be expected from these values, some quite messy algebra is involved in checking the conditions of Theorem 3.4. The main lines of argument are sketched below. Readers may find, as we did, that checking some of the steps is eased by use of an algebraic manipulator such as Maple.

For A-optimality, consider $f(x) = 1/x$ in Theorem 3.4. Since $z_1 \leq z_2$, $z_1^\star \leq z_4$, and $\sum_{i=1}^{v-1} f(z_{\bar{d}i}) < \frac{(9t+3)}{(6t+4)} = f(z_1^\star) + (v-2)f(z_4)$ is trivial, it remains to show that (4) holds. That is, that

$$\frac{1}{2t+\frac{7}{3}} - \frac{1}{2t+\frac{4}{3}+\frac{1}{3t}+\frac{1}{3t}((13t-3)(3t-1)/3)^{1/2}}$$
$$< \frac{3t-1}{2t+\frac{4}{3}+\frac{1}{3t}-\frac{1}{3t}((13t-3)/(9t-3))^{1/2}} - \frac{3t-1}{2t+\frac{4}{3}}.$$

Label the denominators in this inequality as $y_1,\ldots,y_4$ so that it is

$$\frac{1}{y_1}-\frac{1}{y_2} < (3t-1)\left(\frac{1}{y_3}-\frac{1}{y_4}\right) \iff 1 < \left[\frac{(3t-1)(y_4-y_3)}{(y_2-y_1)}\right]\left(\frac{y_1}{y_4}\right)\left(\frac{y_2}{y_3}\right).$$

Since the term in brackets is 1, this is just

$$1 < (1+\frac{1}{2t+\frac{4}{3}})\left[1+\frac{\frac{1}{3t}((13t-3)(3t-1)/3)^{1/2}+\frac{1}{3t}((13t-3)/(9t-3))^{1/2}}{2t+\frac{4}{3}+\frac{1}{3t}-\frac{1}{3t}\sqrt{(13t-3)/(9t-3)}}\right].$$

The last inequality is clearly true for all $t \geq 1$ and hence $\bar{d}$ is A-optimal.

To show $\bar{d}$ is also D-optimal it is sufficient to establish (4) with $f(x) = -\log(x)$, for again (5) is trivial. This can be checked directly for small t, so the remainder of the proof will assume $t \geq 5$. Now $\sum_{i=1}^{v-1} f(z_{\bar{d}i})$ is $-\log[(2t+\frac{7}{3})(2t+1)(2t+\frac{4}{3})^{3t-1}]$ and $f(z_1)+(v-3)f(z_2)+f(z_3)$ is

$$-\log\{(2t+1)[2t+\frac{4}{3}+\frac{1}{3t}-\frac{1}{3t}((13t-3)/(9t-3))^{1/2}]^{3t-1}[2t+\frac{4}{3}$$
$$+\frac{1}{3t}+\frac{1}{3t}((13t-3)(3t-1)/3)^{1/2}]\}.$$

With a bit of manipulation the inequality (4) is

$$\log\left\{1-\frac{\frac{1}{3t}[((13t-3)(3t-1)/3)^{1/2}+1-3t]}{2t+\frac{4}{3}+\frac{1}{3t}+\frac{1}{3t}((13t-3)(3t-1)/3)^{1/2}}\right\}$$
$$-(3t-1)\log\left\{1-\frac{\frac{1}{3t}[((13t-3)/(9t-3))^{1/2}-1]}{2t+\frac{4}{3}}\right\} > 0.$$

Write this inequality as

$$\log(1-w(t))-(3t-1)\log(1-u(t)) > 0 \tag{6}$$

where $u(t) = \frac{\frac{1}{3t}[((13t-3)/(9t-3))^{1/2}-1]}{2t+\frac{4}{3}}$ and $w(t) = \frac{\frac{1}{3t}[((13t-3)(3t-1)/3)^{1/2}+1-3t]}{2t+\frac{4}{3}+\frac{1}{3t}+\frac{1}{3t}((13t-3)(3t-1)/3)^{1/2}}$. Observe that $0 < u(t) < 1$ and $0 < w(t) < 1$ for all $t \geq 1$. Thus for (6) it is sufficient that $h(t) = \log(1-w^\star(t))-(3t-1)\log(1-u^\star(t)) > 0$ for some $u^\star(t) < u(t)$ and $w^\star(t) > w(t)$. Let $u^\star(t) = \frac{a}{2t(3t+2)}$ where a is the constant $(13/9)^{1/2}-1$, and $w^\star(t) = (3t-1.5)u^\star(t)$. Calculations for showing $u^\star(t) < u(t)$

and $w^\star(t) > w(t)$ for $t \geq 5$ are straightforward, and (6) follows if $\lim_{t\to\infty} h(t) = 0$, and if $\partial h(t)/\partial t < 0$ for all $t \geq 5$. The limit is easy. The derivative is

$$\begin{aligned}
\frac{\partial}{\partial t}h(t) &= \frac{-1}{1-w^*(t)}\frac{\partial}{\partial t}w^*(t) + \frac{(3t-1)}{1-u^*(t)}\frac{\partial}{\partial t}u^*(t) - 3\log(1-u^*(t)) \\
&= \frac{a(18t^2-18t-6)}{(6t^2+4t)[6t^2+4t-a(3t-1.5)]} - \frac{a(3t-1)(12t+4)}{(6t^2+4t-a)(6t^2+4t)} - 3\log(1-u^*(t)) \\
&= -3u^*(t) - \frac{a[(36-54a)t^3+(36+99a)t^2+(8-12a-9a^2)t-(12a-4.5a^2)]}{(6t^2+4t)[36t^4+(48-18a)t^3+(16-9a)t^2+(2a+3a^2)t-1.5a^2]} \\
&\quad -3\log(1-u^*(t)).
\end{aligned}$$

Now $0 < u^*(t) < 1$, so $-3[u^*(t) + \log(1-u^*(t))] = -3(u^*(t) - \sum_{j=1}^{\infty}\frac{[u^*(t)]^j}{j}) \leq \frac{3}{2}\sum_{j=2}^{\infty}[u^*(t)]^j = \frac{3u^{*2}(t)}{2(1-u^*(t))} = \frac{3a^2}{2(6t^2+4t)(6t^2+4t-a)}$. Putting this bound in the derivative above, collecting terms over a common denominator, and then dropping all terms from the numerator involving a with a negative coefficient gives

$$\begin{aligned}
&\frac{\partial}{\partial t}h(t) \\
&\leq \frac{-(432-648a)t^5-720t^4-384t^3-(64-360a-189a^2)t^2+112at+4.5a^3}{2(6t^2+4t)(6t^2+4t-a)[36t^4+(48-18a)t^3+(16-9a)t^2+(2a+3a^2)t-1.5a^2]}.
\end{aligned}$$

This is clearly negative for $t \geq 5$.

Example 2. As a consequence of Theorem 4.1, this NBBD(2) is uniquely A- and D-optimal in $D(8, 19, 3)$. Interestingly, it is Φ_p-inferior to Morgan and Uddin's (1995) design for all $p \geq 17$.

1	1	1	1	1	1	1	2	2	2	2	2	2	3	3	3	4	4	5
2	3	3	4	5	6	6	3	3	4	4	5	6	4	5	7	5	6	7
3	4	5	8	7	7	8	6	7	5	7	8	8	8	6	8	6	7	8

Closely related to the designs of Theorem 4.1 are members of a series whose optimality will follow from Theorem 3.5. The setting for any $t \geq 1$ is $D(3t + 2, 6t^2 + 6t + 2, 3)$, in which $r = 6t + 2$ and $\lambda = 4$. This is a category two setting, and Lemma 2.4 implies the nonexistence of NBBD(1)'s for this class.

The proposed design is constructed from two copies of the previously discussed design $\tilde{d}$ with $v = 3t+2,\ b = 3t^2 + 3t + 1$, and $k = 3$, due to Morgan and Uddin (1995). Again, $\tilde{d}$ contains a single nonbinary block $(1, 1, 2)$. In the first copy of $\tilde{d}$, replace this block with $(1, 2, 3)$. In the second copy of $\tilde{d}$, first permute the first three treatment labels $1, 2, 3$ by $1 \to 2,\ 2 \to 3,\ 3 \to 1$. Then replace the block $(2, 2, 3)$ with $(1, 2, 3)$. The resulting design $\bar{d} \in D(3t + 2, 6t^2 + 6t + 2, 3)$ is binary and has $r_{\bar{d}1} = r+1$, $\lambda_{\bar{d}13} = \lambda+2$, all other $r_{\bar{d}i} = r$, and all other $\lambda_{\bar{d}ij} = \lambda$. If $\bar{d}$ satisfies (iv) of Definition 2.1, it is a NBBD(2).

Theorem 4.2. *The NBBD*(2) $\bar{d} \in D(3t+2, 6t^2+6t+2, 3)$ *is* ϕ_f*-optimal amongst all binary competitors for all type I criteria* ϕ_f *with* $\lim_{x\to 0^+} f(x) = \infty$. *Putting* $z_1^* = 4t + \frac{8}{3}$ *and* $z_4 = 4t + \frac{8}{3} + \frac{2}{9t}$, *the optimality holds over the entire class D for all these* ϕ_f *for which* (5) *is satisfied. In particular,* $\bar{d}$ *is A-, D-, and E-optimal.*

Proof. In Lemma 2.5, put $n = \frac{v(v-1)}{2} = \frac{9t^2+9t+2}{2}$ and $c = \frac{bk(k-1)}{2} = 18t^2+18t+6$, and so $c_1 = 4$. Since there is no NBBD(1), any $d \in M(v,b,k)$ must have $\sum\sum_{i<j} \lambda_{dij}^2 \geq Q(2,c) = 72t^2 + 72t + 36 = \sum\sum_{i<j} \lambda_{\bar{d}ij}^2$. Hence $\bar{d}$ is a NBBD(2) which minimizes $\mathrm{tr}(C_d^2)$ over M. The eigenvalues of $C_{\bar{d}}$ are $4t + \frac{8}{3}$ and $4t+4$, with multiplicities of $3t$ and 1 respectively. Theorem 3.5 now gives the result for the binary class.

Nonbinary competitors are eliminated with the same inequality used in Theorem 3.4; this follows from Lemma 3.1 just as in the proof of that theorem. The bound z_1^* given there is applicable here, and simplifies along with the corresponding z_4 to the stated values. E-optimality is immediate, and the calculations to show that (5) holds for the A- and D-criteria are trivial.

4.2. BIBD settings

Another interesting class of applications is found in settings where the necessary conditions for existence of a balanced incomplete block design are fulfilled, but a BIBD does not exist. Say that $D(v,b,k)$ is a *BIBD setting* if $r = \frac{bk}{v}$ and $\lambda = \frac{r(k-1)}{v-1}$. Nonexistence of a BIBD (i.e. of a NBBD(0)) in a BIBD setting implies that the conditions of Lemma 2.2 are fulfilled, opening the possibility of optimal, category one NBBD(2)'s. To exploit Theorem 3.4 in such a setting, a preliminary result on the discrepancy values δ_d is needed.

Lemma 4.3. *Let d be a binary, equireplicate design in the BIBD setting* $D(v,b,k)$. *Then* $\delta_d \geq 2\max_{i,j} |\lambda_{dij} - \lambda|$.

Proof. Suppose $\lambda_{d12} = \lambda + \alpha$ for some $\alpha > 0$. Then $\delta_d \geq \sum_{i>1} \max\{0, \lambda - \lambda_{d1i}\} + \sum_{i>2} \max\{0, \lambda - \lambda_{d2i}\} \geq 2\alpha$.

Suppose $\lambda_{d12} = \lambda + \alpha$ for some $\alpha < 0$. Binarity and equireplication implies that $\sum_{i\neq j} \lambda_{dij} = \lambda(v-1)$ for each j, so $\sum_{i>2} \max\{0, \lambda_{d1i} - \lambda\} + \sum_{i>2} \max\{0, \lambda_{d2i} - \lambda\} \geq 2\alpha$. Thus $2\delta_d = \sum\sum_{i\neq j} \max\{0, \lambda - \lambda_{dij}\} = \sum\sum_{i\neq j} \max\{0, \lambda_{dij} - \lambda\} \geq 2\sum_{i>2} \max\{0, \lambda_{d1i} - \lambda\} + 2\sum_{i>2} \max\{0, \lambda_{d2i} - \lambda\} \geq 4\alpha$.

Theorem 4.4. *Let* $D(v,b,k)$ *be a BIBD setting in which a BIBD does not exist. Let* $\bar{d} \in D$ *be a NBBD*(2) *with* $\delta_{\bar{d}} \leq 4$. *Taking* $z_1 = z_1^* = \frac{\lambda v - 1}{k}$, *if* (4) *and* (5) *of Theorem* 3.4 *hold, then a* ϕ_f*-optimal design must be a NBBD*(2).

Proof. The bounds $z_1 = z_1^*$ for z_{d1} follow from the proof of Lemma 2.2 for unequally replicated d, and from Propositions 3.1 and 3.2 of Jacroux (1980b) for equireplicated d. The relations $z_1 \leq z_2$ and $z_1^* \leq z_4$ are easy to check. The result follows from Theorem 3.4 if it can be shown that $\delta_d \geq 4$ for any binary d with replication range > 0 or concurrence range > 2. If d is not equireplicate, then $r_{di} \leq r - 1$ for some i, implying $\sum_{j \neq i} \lambda_{dij} \leq (r-1)(k-1) = \lambda(v-1) - (k-1)$ and thus $\delta_d \geq k - 1 \geq 4$, since nonexistence of the BIBD implies $k \geq 5$. If d is equireplicate, but $\max\{\lambda_{dij}\} - \min\{\lambda_{dij}\} > 2$, then Lemma 4.3 gives the result.

Corollary 4.5. *Let $D(v, b, k)$ be a BIBD setting in which $r \leq 41$ and in which a BIBD does not exist. If there exists a design $\bar{d}$ satisfying the first three conditions of Definition* 2.1 *with $l = 2$ and $\delta_{\bar{d}} \leq 4$, then an A-optimal design must be a $NBBD(2)$, and a D-optimal design must be a $NBBD(2)$.*

Proof. It is obvious from the proofs of Theorems 3.4 and 4.4 that any d not satisfying the conditions required of $\bar{d}$ will have $\mathrm{tr}(C_d^2) \geq B_2 = \mathrm{tr}(C_{\bar{d}}^2) + \frac{4}{k^2}$. Hence the corollary amounts to saying that (4) and (5) hold for all equireplicate, binary designs $\bar{d}$ with $\delta_{\bar{d}} \leq 4$ and concurrence range 2 in all of the BIBD settings mentioned. Given any such $\bar{d}$, let $v_{\bar{d}}$ be the number of treatments i for which $\lambda_{\bar{d}ij} < \lambda$ for some j. With appropriate labeling these are the first $v_{\bar{d}}$ members of the treatment set, and certainly $v_{\bar{d}} \leq 8$. Hence the conceivable information matrices $C_{\bar{d}}$ whose eigenvalues must be examined are determined by the symmetric matrices of order $v_{\bar{d}} \leq 8$ for which (a) all off-diagonal elements are in the set $\{\lambda - 1, \lambda, \lambda + 1\}$, ($b$) the sum of the off-diagonal elements in each row is $(v_{\bar{d}} - 1)\lambda$, and (c) the number of elements above the diagonal which equal $\lambda - 1$ is no more than 4. There are eleven such *discrepancy matrices*, listed in Table 1 with, for compactness, the variable λ replaced by 0. Their diagonal values are irrelevant, since the diagonal of $C_{\bar{d}}$ is fixed by the first two conditions of Definition 2.1.

A list of the settings $D(v, b, k)$ with $r \leq 41$ for which either a BIBD does not exist, or for which existence is not known, may be found in Mathon and Rosa (1996); there are 497 cases when complements are included. It is then a simple exercise to write a computer routine to check the conditions (4) and (5) for each case and for each of the eleven conceivable information matrices $C_{\bar{d}}$. We have done this and found that the conditions indeed do always hold in this range. Alternatively, one could analytically derive the eigenvalues from each of the nine concurrence patterns shown in Table 1, and likely prove with nine repetitions of some extremely messy algebra akin to that sketched in the proof of Theorem 4.1 that the result of the corollary holds for any r. We have not done that, preferring the much quicker and more compact computational approach in applying the theorem, which has covered essentially all of the cases of practical interest.

Table 1. Discrepancy matrices of order 8 and lower with $\delta \leq 4$.

$$\begin{matrix} x & -1 & 1 & 0 \\ -1 & x & 0 & 1 \\ 1 & 0 & x & -1 \\ 0 & 1 & -1 & x \end{matrix} \qquad \begin{matrix} x & -1 & -1 & 1 & 1 \\ -1 & x & 1 & 0 & 0 \\ -1 & 1 & x & 0 & 0 \\ 1 & 0 & 0 & x & -1 \\ 1 & 0 & 0 & -1 & x \end{matrix} \qquad \begin{matrix} x & -1 & 1 & 0 & 0 & 0 \\ -1 & x & 0 & 0 & 1 & 0 \\ 1 & 0 & x & -1 & 0 & 0 \\ 0 & 0 & -1 & x & 0 & 1 \\ 0 & 1 & 0 & 0 & x & -1 \\ 0 & 0 & 0 & 1 & -1 & x \end{matrix}$$

$$\begin{matrix} x & -1 & -1 & 1 & 1 & 0 \\ -1 & x & 0 & 0 & 0 & 1 \\ -1 & 0 & x & 0 & 0 & 1 \\ 1 & 0 & 0 & x & 0 & -1 \\ 1 & 0 & 0 & 0 & x & -1 \\ 0 & 1 & 1 & -1 & -1 & x \end{matrix} \qquad \begin{matrix} x & -1 & -1 & 1 & 1 & 0 \\ -1 & x & 0 & 1 & 0 & 0 \\ -1 & 0 & x & 0 & 0 & 1 \\ 1 & 1 & 0 & x & -1 & -1 \\ 1 & 0 & 0 & -1 & x & 0 \\ 0 & 0 & 1 & -1 & 0 & x \end{matrix}$$

$$\begin{matrix} x & -1 & -1 & 1 & 1 & 0 \\ -1 & x & 1 & -1 & 0 & 1 \\ -1 & 1 & x & 0 & 0 & 0 \\ 1 & -1 & 0 & x & 0 & 0 \\ 1 & 0 & 0 & 0 & x & -1 \\ 0 & 1 & 0 & 0 & -1 & x \end{matrix} \qquad \begin{matrix} x & -1 & -1 & 1 & 1 & 0 & 0 \\ -1 & x & 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & x & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & x & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & x & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & x & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 & x \end{matrix}$$

$$\begin{matrix} x & -1 & -1 & 1 & 1 & 0 & 0 \\ -1 & x & 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & x & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & x & -1 & 0 & 0 \\ 1 & 0 & 0 & -1 & x & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & x & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 & x \end{matrix} \qquad \begin{matrix} x & -1 & -1 & 1 & 1 & 0 & 0 \\ -1 & x & 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & x & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & x & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & x & 0 & -1 \\ 0 & 1 & 0 & -1 & 0 & x & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & x \end{matrix}$$

$$\begin{matrix} x & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & x & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & x & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & x & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & x & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & x & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & x & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & x \end{matrix} \qquad \begin{matrix} x & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & x & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & x & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & x & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & x & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & x & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & x & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & x \end{matrix}$$

What is known of NBBD(2)'s in BIBD settings like those considered here? Unfortunately very little, and the general combinatorial problem of determining the achievable lower bound δ for the discrepancy values δ_d appears to be quite difficult. A pair of recent papers by Hedayat, Stufken and Zhang (1995a,b) have begun the combinatorial study of the design possibilities, and their *virtually balanced incomplete block designs* will be NBBD(2)'s whenever they have minimum discrepancy δ. They display a few of these designs, but do not address what we term as the minimum discrepancy problem. Of relevance here is their design for $D(22, 33, 8)$ with discrepancy 4. Existence of a BIBD for this setting is not yet determined, so Corollary 4.5 tells us that if there is no BIBD, then the A-optimal and D-optimal designs are NBBD(2)'s.

The smallest BIBD setting, in terms of either r or k, for which a BIBD does not exist, is $D(15, 21, 5)$, for which Zhang (1994) gives a design with concurrence range 2 and discrepancy 6. Example 3 displays the discrepancy matrix for that design, along with a discrepancy matrix for a NBBD(3) which, should the design exist, is A- and D-better than the discrepancy 6 design. This illustrates the pitfalls in trying to extend Corollary 4.5 to include values $\delta_d > 4$, and gives a hint at the richness of the combinatorial difficulties in the optimal design problem for these settings. We conjecture that optimal designs for BIBD settings will always be found within the NBBD(l) classes for $l \leq 3$ and, based on the results above, suggest that the attack on the combinatorial existence/construction problems should now generally focus on the minimum discrepancy problem, and specifically on equireplicate, binary designs with discrepancy no more than 4. The concept of *treatment deficiency* as defined by Hedayat, Stufken and Zhang (1995a, b) will certainly be useful in this endeavor.

Example 3. Discrepancy matrices for a known design and a potentially better competitor in $D(15, 21, 5)$.

$$\begin{array}{ccccccccc}
x & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\
0 & x & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\
0 & 0 & x & 0 & 0 & 0 & 0 & -1 & 1 \\
0 & 0 & 0 & x & 0 & 0 & -1 & 0 & 1 \\
0 & 0 & 0 & 0 & x & 0 & -1 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & x & 0 & 1 & -1 \\
1 & 1 & 0 & -1 & -1 & 0 & x & 0 & 0 \\
-1 & 0 & -1 & 0 & 1 & 1 & 0 & x & 0 \\
0 & -1 & 1 & 1 & 0 & -1 & 0 & 0 & x
\end{array}
\qquad
\begin{array}{cccccc}
x & 2 & -1 & -1 & 0 & 0 \\
2 & x & 0 & 0 & -1 & -1 \\
-1 & 0 & x & 1 & 0 & 0 \\
-1 & 0 & 1 & x & 0 & 0 \\
0 & -1 & 0 & 0 & x & 1 \\
0 & -1 & 0 & 0 & 1 & x
\end{array}$$

4.3. A series with four blocks

The final class to be discussed finds either NBBD(2)'s or NBBD(3)'s to be optimal, depending on the value of k in the series

$$v = 2k - 1, \quad b = 4, \quad k, \quad r = 2, \quad \lambda = 1 \tag{7}$$

with $k \geq 4$. The first job is to establish the value of δ.

Lemma 4.6. *For $d \in M(v, b, k)$ with parameters in the series (7),*

$$\delta = \begin{cases} k(k-3)/3, & \text{if } k \equiv 0 \ (mod\ 3), \\ (k-1)(k-2)/3, & \textit{otherwise.} \end{cases}$$

Proof. Let d be binary and suppose that d has $r_{di} = 1$ for some i, say $r_{dv} = n_{d1v} = 1$. Then either (a) some treatment, say 1, has $r_{d1} = 4$ (since d is binary, 4 is the maximum replication); or (b) at least three treatments, say 1,2,3, occur three times each. In case (a), form d' from d by changing 1 to v in block 2; since 1 and v have exactly the same concurrences in block 1, it follows easily that $\delta_d \geq \delta_{d'}$. For case (b), if any of λ_{d1v}, λ_{d2v}, λ_{d3v}, say λ_{d1v}, is greater than 0, then form d' by changing 1 to v in a block not containing v; as in (a), $\delta_d \geq \delta_{d'}$, and this process can be repeated until $r_{di} \geq 2$ for all i. If none of λ_{d1v}, λ_{d2v}, λ_{d3v} is nonzero, then the four blocks $B_1, \ldots, B_4$ have the form of the following four columns

$$\begin{array}{cccc} B_1 & B_2 & B_3 & B_4 \\ v & 1 & 1 & 1 \\ 4 & 2 & 2 & 2 \\ 5 & 3 & 3 & 3 \\ 6 & ? & ? & ? \\ \vdots & \vdots & \vdots & \vdots \\ k{+}2 & ? & ? & ? \end{array}$$

where the lower $(k-3) \times 3$ does not contain v. Let S_1 denote the treatments in block 1 other than v; let S_2 denote all other treatments other than 1, 2, 3, and v; and for $j > 1$, let B_j^* denote the treatments in block j not found in the others of blocks 2, 3, and 4. Let $g_j = |S_2 \cap B_j|$, $d_j = |B_j^*|$, and $r_2 = \sum_{i \in S_2} r_{di}$. The goal is still to change one copy of 1 to v without increasing the number of zero concurrences. This can be done in block j unless $d_j - g_j - 2 \geq 1$; if the change cannot be made in any of the blocks, then $\sum_{j=2}^{4}(d_j - g_j) \geq 9$. Since the $3(k-3)$ plots in the lower $(k-3) \times 3$ contain only treatments from the $2k-5$ treatments in $S_1 \cup S_2$, the maximum value of $\sum_{j=2}^{4} d_j$ can be written as a function of r_2 thusly:

$$\sum_{j=2}^{4} d_j \leq \begin{cases} [k-4-int(\frac{r_2-(k-4)+1}{2})] + [3(k-3)-r_2], & \text{if } 3(k-3)-r_2 \leq k-1 \\ [k-4-int(\frac{r_2-(k-4)+1}{2})] + [r_2-k+7], & \text{if } 3(k-3)-r_2 > k-1 \end{cases},$$

(in each line the two terms in brackets are the maximum contributions of S_2 and S_1, respectively). It follows that $\sum_{j=2}^{4}(d_j - g_j) = \sum_{j=2}^{4} d_j - r_2 \leq 3$, the maximum occurring when r_2 takes its minimum value of $k-4$, so that the desired change can be made.

Thus to determine δ, it is sufficient to consider only binary designs d in which $r_{di} \geq 2$ for all i, that is, only designs satisfying (i) and (ii) of Definition 2.1. Such designs contain exactly two treatments, say 1 and 2, replicated thrice, all others being replicated twice, and λ_{d12} is either two or three. Assuming that the first two blocks contain both 1 and 2, and letting e denote the number of other treatments common to both B_1 and B_2, there are two cases d_{1e} and d_{2e} to be considered:

d_{1e}

B_1	B_2	B_3	B_4
1	1	1	2
2	2	$2k-e-1$	$2k-e-1$
3	3	$2k-e$	$2k-e$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$e+2$	$e+2$	v	v
$e+3$	$k+1$	?	?
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$k-1$	$2k-e-3$	?	?
k	$2k-e-2$	?	?

d_{2e}

B_1	B_2	B_3	B_4
1	1	1	?
2	2	2	?
3	3	$2k-e-1$	$2k-e-1$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$e+2$	$e+2$	$v-1$	$v-1$
$e+3$	$k+1$	v	v
$\vdots$	$\vdots$	?	?
$k-1$	$2k-e-3$	$\vdots$	$\vdots$
k	$2k-e-2$	?	?

In either case, the ? plots must be filled by using each treatment from $S_e = \{e+3, e+4, \ldots, 2k-e-2\}$ exactly once. These must be placed so that, for given e, the number of zero concurrences among treatments in S_e is minimized. This number of zero concurrences can then be minimized as a function of e. For fixed e the desired placement is not difficult; in rough terms, "half" of the set $S_e \cap B_1$ is placed into B_3 along with "half" of the treatments in $S_e \cap B_2$; the complementary "halves" are placed in B_4. The exact manner in which this is done depends on whether or not $k-e-2$ is even, and also on the two displayed cases. Writing $h = |(B_1 \cap B_3) - \{1,2\}|$, the minimized values are as stated in the lemma, and occur in d_{2e} with $e = h = (k-3)/3$ when $k \equiv 0(mod\ 3)$; in d_{1e} with $e = (k-4)/3$ and $h = e+1$, and in d_{2e} with $e = h = (k-4)/3$, when $k \equiv 1(mod\ 3)$; and in d_{1e} with $e = h = (k-2)/3$, and in d_{2e} with $e = (k-2)/3$ and $h = e-1$, when $k \equiv 2(mod\ 3)$.

Given the results of the preceding two sections, one may suspect that with Lemma 4.6 in hand optimality could be established in very short order. However a number of details must be attended to before arriving at the optimality result in Theorem 4.8 below.

The designs d_{1e} and d_{2e} determined in the proof to minimize δ_d are NBBD(2)'s and NBBD(3)'s, respectively, and several observations follow. First, if $k \equiv 0(mod\ 3)$, the lower bound for δ_d is not achieved by a NBBD(2). The best NBBD(2) in this situation (also $e = h = (k-3)/3$) has $\delta_d = \delta + 1$, and has $\mathrm{tr}(C_d^2)$ equal to that of the NBBD(3). Second, for $k \not\equiv 0(mod\ 3)$, both types of designs attain the bound; in this case the NBBD(3) must have $\mathrm{tr}(C_d^2) \geq B_2$ (see Lemma 2.6 (iii)), so that the NBBD(2)'s are expected to be best. Thus there are four series of designs from which the best is expected to be found: the unique NBBD(2) and the unique NBBD(3) when $k \equiv 0(mod\ 3)$, and the unique NBBD(2)'s when $k \equiv 1(mod\ 3)$ and when $k \equiv 2(mod\ 3)$.

The messy eigenvalue structure of these designs, an unavoidable situation for any reasonably efficient design in this setting given the small amount of experimental material relative to v, precludes a direct application of Theorem 3.4. For instance, the inequality (4) is never satisfied. Theorem 3.4 is best suited for designs that are "closer to balance" than those encountered here.

These problems will be resolved through a 3-step approach. First, all binary d with some $r_{di} < r$ will be eliminated by an inequality akin to (4). Second, most binary d with all $r_{di} \geq r$ will be eliminated using bounds on the z_{di}'s. Finally, the few remaining binary designs can be sorted out computationally. The problem of nonbinarity will be briefly discussed at the end of the section. Use $\bar{d}$ to denote a NBBD with $\delta_{\bar{d}} = \delta$.

So first let binary d have some $r_{di} < r$. It is established in the proof of Theorem 3.4 that $\mathrm{tr}(C_d^2) \geq \mathrm{tr}(C_{\bar{d}}^2) + 2\left(\frac{k-1}{k}\right)^2 = B_2$, say. Taking this value for B_2 and $z_1 = \frac{(k-1)v}{(v-1)k}$ to calculate z_2 and z_3, d will be eliminated if the inequality displayed in (4) holds.

Next, let binary d have all $|r_{di} - r_{di'}| \leq 1$. Then d is a member of one of the two series d_{1e} and d_{2e} discussed in the proof of Lemma 4.6. These designs are indexed by the parameters e and h defined in the proof, and for convenience also define $g = |B_1 - B_2| = k - e - 2$. Using e, g, and h, the information matrices may be displayed in partitioned form as shown in Tables 3 and 4 in the appendix ($J_{x,y}$ denotes an $x \times y$ matrix of 1's). Here $0 \leq e \leq k-2$ and $0 \leq h \leq int(\frac{g}{2})$ for members of d_{1e}. For d_{2e}, $0 \leq h \leq e \leq k-4$, and $h \leq int(\frac{g-1}{2})$ if $e = \frac{k-3}{3}$, while $h \leq int(\frac{g-2}{2})$ otherwise. The upper bounds on h are to avoid repetition of designs having information matrices which are identical up to row/column permutation. Such repetition is also found from the pairs (e, h) and $(e^*, h^*) = (k-3-e-h, h)$.

Exact eigenvalues for the matrices in Tables 3 and 4 are extremely messy, if not analytically intractable, as functions of e and h. Since the large number of cases makes exact computation of all of the eigenvalues for all e and h over a reasonable range of v infeasible, an intermediate approach is needed, to wit, bounds for the z_{di}'s will be established. These bounds can then be used in the next lemma.

Lemma 4.7. *Let $d \in M(v,b,k)$ have information matrix C_d with nonzero eigenvalues $z_{d1} \le z_{d2} \le \cdots \le z_{d,v-1}$ which satisfy $z_{di} \le w_i$ for $i \le s_1$, and $z_{di} \ge w_i$ for $i \ge s_2$, where $w_1 \le w_2 \le \cdots \le w_{v-1}$, $\sum_i w_i = \sum_i z_{di}$, and $w_{s_1+1} = w_{s_1+2} = \cdots = w_{s_2-1}$. Then $\sum_i f(z_{di}) \ge \sum_i f(w_i)$ for any type-1 criterion f.*

Lemma 4.7 is a simple consequence of the convexity of f. Bounds w_i for members of the two series d_{1e} and d_{2e} are shown in Table 2; the respective values of (s_1, s_2) are $(v-3, v-1)$ and $(v-5, v-2)$. The unspecified values w_{v-2} for d_{1e}, and $w_{v-4} = w_{v-3}$ for d_{2e}, are chosen to make the w_i's sum to $\mathrm{tr}(C_d) = 4(k-1)$. The method of derivation is explained in the appendix.

Table 2. Eigenvalue bounds w_i as functions of e, g, h, and $a = \max\{e+1, h+1, g-h\}$.

Series	w_1	w_2	w_3	$w_i,\ 4 \le i \le s_1$	w_{v-2}	w_{v-1}
d_{1e}	w_{01}	w_{02}	w_{03}	2	w_{v-2}	$3-\frac{1}{k}$
d_{2e}	$\min_{i\ge 1}\{w_{i1}\}$	$\min_{i\ge 1}\{w_{i2}\}$	$\min_{i\ge 1}\{w_{i3}\}$	2	$\frac{5k-6-2a+((k-6)^2+4a(k+a-4))^{1/2}}{2k}$	3

i	$w_{i1} \le w_{i2} \le w_{i3}$ are the ordered values of
0	$2-\frac{2e+g+1}{k}+\frac{(g^2+1)^{1/2}}{k},\ 2-\frac{2(g-h)}{k},\ 2-\frac{2h}{k}$
1	$2-\frac{2e+g}{k}+\frac{((g-1)^2+1)^{1/2}}{k},\ 2-\frac{2(g-h-1)}{k},\ 2-\frac{2h}{k}$
2	$2-\frac{2g+e-h-1}{k}+\frac{((e+h)^2+1)^{1/2}}{k},\ 2-\frac{2e}{k},\ 2-\frac{2h}{k}$
3	$2-\frac{e+g+h}{k}+\frac{((e+g-h-1)^2+1)^{1/2}}{k},\ 2-\frac{2(g-h-1)}{k},\ 2-\frac{2e}{k}$

These bounds do *not* lend themselves to a nice analytic proof that $\bar{d}$ is optimal; rather, they allow a simple computation to eliminate *most* of the competitors in d_{1e} and d_{2e}. To get a sense of the magnitudes of the numbers involved, a few of the triples (v, number of competitors, number of competitors eliminated by the bounds) when simultaneously examining the A and D criteria are $(25, 56, 51)$, $(51, 225, 213)$, $(101, 867, 844)$, and $(201, 3400, 3357)$. So, for $v = 101$, for instance, after verifying the inequality based on (4) mentioned above, we calculate two simple functions of known lists of numbers for 867 cases, then need only calculate the eigenvalues of 23 matrices of order 101. The time-heavy alternative would be to calculate the eigenvalues of 867 matrices of order 101. The bounding approach allows us to extend the computational proof of the final result much further than would otherwise be possible.

The only competitors not covered by the discusion so far are those with $r_1 = 4$ and all other $r_{di} = 2$; call this family d_{3e}. A general member of this family can be found from d_{1e} by changing the 2 in B_4 to 1. The information matrix, displayed in Table 5, has generalized group divisible structure (Srivastav and Morgan (1998)) with eigenvalues of 2 with frequency $v-5$, and one each of $\frac{4v}{v+1}$, $2-\frac{2(e+1)}{k}$, $2-\frac{2h}{k}$, and $2-\frac{2(g-h)}{k}$. The Schur-optimal member of d_{3e} is found at the values of (e,g,h) for which all possible values of the last three eigenvalues are majorized. Subject to the constraints $g-h \le h \le e+1$ (to avoid isomorphic repetition), the optimizing triples are $(\frac{k-3}{3}, \frac{2k-3}{3}, \frac{k}{3})$ for $k \equiv 0(mod\ 3)$, $(\frac{k-4}{3}, \frac{2k-2}{3}, \frac{k-1}{3})$ for $k \equiv 1(mod\ 3)$, and $(\frac{k-2}{3}, \frac{2k-4}{3}, \frac{k-2}{3})$ for $k \equiv 2(mod\ 3)$. For any given v and concurrent with the computations above, the resulting unique optimality criteria values for this family can be directly compared to those for $\bar{d}$.

Theorem 4.8. *The NBBD $\bar{d} \in D(2k-1,4,k)$ with $\delta_{\bar{d}} = \delta$ as given in Lemma* 4.6 *is uniquely A- and D-optimal over $M(2k-1,4,k)$ for $4 \le k \le 101$.*

Thus in every case with $k \equiv 0(mod\ 3)$, the NBBD(3) is best and is A- and D-superior to the NBBD(2). As expected, for $k \not\equiv 0(mod\ 3)$, the NBBD(2)'s are best and are superior to the NBBD(3)'s which also have minimum discrepancy. Curiously, the Schur-best member of d_{3e}, identified just prior to Theorem 4.8, is E- and MV-better than the A- and D-best NBBD(2) whenever $k \equiv 1(mod\ 3)$, though not otherwise.

We have not tackled the larger problem of optimality over the full class $D(2k-1,4,k)$. Though there seems little doubt that A- and D-optimality of the NBBDs will still hold, we have found no reasonably compact method to sift through the greater variety of structures for C_d allowed by nonbinarity. This problem remains open.

From a larger perspective, the difficulties dealt with for $D(2k-1,4,k)$ are typical of problems that design theory has as yet to adequately address. Arguments based on concepts of "near symmetry" of the information matrix are not effective for settings where that condition cannot be even approximately met. The tack taken here, blending theory and computation, and deriving bounds for multiple eigenvalues, provides an approach that is likely to prove fruitful elsewhere. If further significant progress is to be made on the block design optimality problem, slowed in recent years, such a blend will be needed.

5. Concluding Comments

In embarking on this study we had entertained thoughts of debunking this conjecture from Shah and Sinha (1989, p.60): "Binary (or generalized binary) designs form an essentially complete class." The results of Morgan and Uddin (1995) establishing that E- and MV-optimal designs in some settings must lie in the nonbinary class suggested that perhaps a similar result would hold with respect to criteria that focus less on extreme behavior, such as A and D (compare

Example 2). We are now fairly firmly convinced otherwise. All of our results give conditions for optimality of binary designs, including some in settings explored by Morgan and Uddin (1995), and we are now inclined to support the conjecture for the A-optimality problem.

We have not encountered any setting where the A-optimal design lies outside of the NBBD(l) classes for $l \leq 3$. Another interesting observation is that whenever designs with different discrepancies δ_d but the same minimum value $\mathrm{tr}(C_d^2)$ have been encountered, the smaller discrepancy has proven superior for the A and D criteria.

The main thrust of this paper, the first systematic study to do so, has been to explore optimality in block design settings where the "near balance" studied by other authors cannot hold. When complete symmetry of the information matrix can still be fairly closely approximated, earlier used tools adopt fairly well, as seen in Sections 3, 4.1, and 4.2. When that approximation is not close, such as in Section 4.3, other tools are needed, and increased reliance on computational methodology is inevitable.

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Appendix. Eigenvalue Bounds for the d_{1e} and d_{2e} Series

For both series, bounds can be established by using a Sturmian separation theorem (see Rao (1973, p.64)). Consider first d_{1e}. If the first two rows and columns of the information matrix as displyed in Table 3 are deleted, the ordered eigenvalues of the resulting order $v-2$ matrix are upper bounds for the $v-2$ smallest eigenvalues of the information matrix. Deriving eigenvalues for the order $v-2$ matrix is straightforward; the smallest is $2-\frac{2e+g+1}{k}-\frac{(g^2+1)^{1/2}}{k}$ and the other $v-3$ are $w_1,\ldots,w_{v-3}$ as shown in Table 2. The largest eigenvalue of the upper left-most 2×2 of C_{d1e} is $3-\frac{1}{k}$, which is a lower bound w_{v-1} for the largest eigenvalue of C_{d1e}.

For d_{2e}, deleting the first two rows and columns of the information matrix as done for d_{1e} leaves an order $v-2$ matrix which, while appearing to be only slightly more complicated than that found with d_{1e}, does not admit tractable expressions for its four smallest eigenvalues. Simple expressions (which, since in any case the bounds will not eliminate all competitors, are preferred) can be found by deleting two more rows/columns to get an order $v-4$ matrix in the same form as the order $v-2$ matrix used with d_{1e}. There are $\binom{3}{2}$ ways to do this, since the deletion must reduce by one the order of two of the three diagonal blocks of orders $e+1$, $h+1$, and $g-h$; the key is that the result will have two pairs of identically sized diagonal blocks, making the eigenvalue computation analytically tractable. The ith of these three distinct sets of deletions yields w_{i1}, w_{i2}, w_{i3} in Table 2.

To derive w_{v-1} and w_{v-2} for d_{2e}, let $a = \max\{e+1, h+1, g-h\}$. Delete all rows and columns from C_{d2e} except the first two and those corresponding to a diagonal block of order a. The two largest eigenvalues of the resulting order $a+2$ matrix are w_{v-1} and w_{v-2}.

Table 3. Partitioned information matrix for series d_{1e}.

$$\left(\begin{array}{c|c|c|c|c|c|c}
\begin{matrix} 3-\frac{3}{k} & -\frac{2}{k} \\ -\frac{2}{k} & 3-\frac{3}{k} \end{matrix} & -\frac{2}{k}J_{2,e} & -\frac{1}{k}J_{2,e+1} & \begin{matrix} -\frac{2}{k}J_{1,h} \\ -\frac{1}{k}J_{1,h} \end{matrix} & \begin{matrix} -\frac{1}{k}J_{1,h} \\ -\frac{2}{k}J_{1,h} \end{matrix} & \begin{matrix} -\frac{1}{k}J_{1,g-h} \\ -\frac{2}{k}J_{1,g-h} \end{matrix} & \begin{matrix} -\frac{2}{k}J_{1,g-h} \\ -\frac{1}{k}J_{1,g-h} \end{matrix} \\ \hline
 & 2I-\frac{2}{k}J & 0 & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & 2I-\frac{2}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & & 2I-\frac{2}{k}J & 0 & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & & & 2I-\frac{2}{k}J & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & & & & 2I-\frac{2}{k}J & 0 \\ \hline
 & & & & & & 2I-\frac{2}{k}J
\end{array}\right)$$

Table 4. Partitioned information matrix for series d_{2e}.

$$\left(\begin{array}{c|c|c|c|c|c|c}
\begin{matrix} 3-\frac{3}{k} & -\frac{3}{k} \\ -\frac{3}{k} & 3-\frac{3}{k} \end{matrix} & -\frac{2}{k}J_{2,e} & -\frac{1}{k}J_{2,e+1} & -\frac{2}{k}J_{2,h} & -\frac{1}{k}J_{2,h+1} & -\frac{1}{k}J_{2,g-h} & -\frac{2}{k}J_{2,g-h-1} \\ \hline
 & 2I-\frac{2}{k}J & 0 & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & 2I-\frac{2}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & & 2I-\frac{2}{k}J & 0 & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & & & 2I-\frac{2}{k}J & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & & & & 2I-\frac{2}{k}J & 0 \\ \hline
 & & & & & & 2I-\frac{2}{k}J
\end{array}\right)$$

Table 5. Partitioned information matrix for series d_{3e}.

$$\left(\begin{array}{c|c|c|c|c|c|c}
4-\frac{4}{k} & -\frac{2}{k}J_{2,e+1} & -\frac{2}{k}J_{2,e+1} & -\frac{2}{k}J_{2,h} & -\frac{2}{k}J_{2,h} & -\frac{2}{k}J_{2,g-h} & -\frac{2}{k}J_{2,g-h} \\ \hline
 & 2I-\frac{2}{k}J & 0 & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & 2I-\frac{2}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & & 2I-\frac{2}{k}J & 0 & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & & & 2I-\frac{2}{k}J & -\frac{1}{k}J & -\frac{1}{k}J \\ \hline
 & & & & & 2I-\frac{2}{k}J & 0 \\ \hline
 & & & & & & 2I-\frac{2}{k}J
\end{array}\right)$$

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Department of Statistics, Virginia Tech., Blacksburg, Virginia 24061-0439, U.S.A.
E-mail: jpmorgan@vt.edu

Department of Biostatistics, Tulane University, New Orleans, Louisiana 70112-2699, U.S.A.
E-mail: ssrivas@mailhost.tcs.tulane.edu

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