MBMUDs: A combinatorial extension of BIBDs showing good optimality behaviour

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Abstract

The construction of a Balanced Incomplete Block Design (BIBD) is formulated in terms of combinatorial optimization by defining a cost function that reaches its lower bound on all and only those configurations corresponding to a BIBD. This cost function is a linear combination of distribution measures for each of the properties of a block design (number of plots, uniformity of rows, uniformity of columns, and balance). The approach generalizes naturally to a super-class including BIBDs, which we call Maximally Balanced Maximally Uniform Designs (MBMUDs), that allow *two* consecutive values for their design parameters $[r, r+1; k, k+1; \lambda, \lambda+1]$. In terms of combinatorial balance, MBMUDs are the closest possible approximation to BIBDs for all experimental settings where no set of admissible parameters exists. Thus, other design classes previously proposed with the same approximation aim –such as RDGs, SRDGs and NBIBDs of type I– can be viewed as particular cases of MBMUDs. Interestingly, experimental results show that the proposed combinatorial cost function has a monotonic relation with A- and D- statistical optimality in the space of designs with uniform rows and columns, while its computational cost is much lower.

Keywords: block design, maximally balanced design, distribution measure, cost function

1 Introduction

Block designs are used in experimental planning with the purpose of maximising the information extracted from a given number of experiments.

In statistical terms, Balanced Incomplete Block Designs (BIBDs) are known to be optimal according to the usual A, D, and E criteria [16], as well as universally optimal [7], under some simple mathematical models applied to analyse the data, such as the linear model without block effects and the two-way additive model with fixed block effects, although not so for the more elaborate mixed effects model with variable blocksize [9].

Even restraining ourselves to the two simpler models mentioned, BIBDs are of little use in most experimental situations. This is because the parameters of a particular situation often do not satisfy the admissibility conditions of a BIBD. Therefore, a method for constructing efficient block designs for arbitrary parameter values is needed in practice.

Let us be more specific. Consider an experimental setting with v varieties or treatments, b blocks and u experimental units or plots. The *admissibility* conditions of a BIBD restrict the range of allowed parameter sets to those yielding integer values for the design descriptors: $r = \frac{u}{v}$, $k = \frac{u}{b}$, $\lambda = \frac{u(u-b)}{bv(v-1)}$. Several extensions of BIBDs have been proposed for the cases where one or two of these conditions do not hold. Regular Graph Designs (RGDs) [6,17] require strictly uniform rows (r) and columns (k), and allow two consecutive concurrence values (λ , $\lambda + 1$). Semi-Regular Graph Designs (SRGDs) [5] and Nearly Balanced Incomplete Block Designs (NBIBDs) of Type I [3] extend this idea to the unequally replicated case by allowing also two consecutive replication values (r , $r + 1$).

In this paper we go one step further and consider the cases where neither of the three admissibility conditions hold. Thus, we define Maximally Balanced Maximally Uniform Designs (MBMUDs), which permit also two consecutive block sizes (k , $k + 1$).

The idea underlying all these extensions is to choose designs that are as balanced as possible. Therefore, they can be generated by minimizing a *combinatorial* cost function that penalizes unbalance. We begin by defining a family of cost functions whose global minima coincide with BIBDs in the case of admissible parameters (Section 2). The structure of such functions permits deriving the optimal cost analytically, which provides an a priori bound for the minimization. When these functions are applied to *arbitrary* (v, b, u) , the configurations satisfying the derived combinatorial optimal cost, when existing, take at most two consecutive values for each descriptor $[r, r + 1; k, k + 1; \lambda, \lambda + 1]$, i.e., they are precisely MBMUDs. This is proven in Section 3, where some properties and existence conditions for MBMUDs are also derived.

The *statistical* interest of these combinatorial extensions of BIBDs is addressed in Section 4. Through experimentation, we find that the proposed combinatorial cost function has a monotonic relation with A- and D-optimality, while its

computational cost is much lower. Thus, it can be used directly as an approximation of A- and D- efficiencies, or either serve to initialize any algorithm based on a statistical optimality criterion, in order to speed up the minimisation. Another side benefit resulting from the computer implementation is that, for parameter settings for which MBMUDs do not exist but NBIBDs of Type II do exist [3], the proposed procedure converges to this well-established class.

Only binary designs are addressed in this paper, although the work in [14] reveals large classes (v, b, k) where binary designs cannot be optimal with respect to numerous statistical criteria. However, there is no known example of a non binary design that is optimal for A or D. Thus, in focusing on A and D only we expect to be safe with the binarity restriction.

2 Combinatorial cost functions for the generation of BIBDs

Let $\mathcal{A} - v \times b$ be the set of all binary matrices $A \equiv [x_{ij}]$ with v rows and b columns. Let

$$o = \sum_{i=1}^v \sum_{j=1}^b x_{ij}, \quad (1)$$

$$r_i = \sum_{j=1}^b x_{ij}, \quad (2)$$

$$k_j = \sum_{i=1}^v x_{ij}, \quad \text{and} \quad (3)$$

$$\lambda_{ik} = \sum_{j=1}^b x_{ij} x_{kj}. \quad (4)$$

Definition 1 (BIBD) For fixed r , k and λ , with $k < v$ and $\lambda > 0$, we say that A is the incidence matrix of a BIBD with parameters (v, b, u) and descriptors $[r, k, \lambda]$ if and only if the following properties are fulfilled:

- i) **Right number of ones:** $o = u$ ¹.
- ii) **Strictly uniform rows:** $r_i = r$, $i = 1, \dots, v$.
- iii) **Strictly uniform columns:** $k_j = k$, $j = 1, \dots, b$.
- iv) **Strict balance:** $\lambda_{ik} = \lambda$, $i = 1, \dots, v-1, k = i+1, \dots, v$.

¹ Although it can easily be shown that statistically optimal designs must have $o = u$, the variable o is introduced here to allow for the evaluation of matrices with any number of ones, as required in our combinatorial optimization framework.

Parameters and descriptors are related by the following *admissibility* conditions,

$$r = u/v \tag{5}$$

$$k = u/b \tag{6}$$

$$\lambda = \frac{r(k-1)}{v-1} = \frac{u(u-b)}{bv(v-1)}, \tag{7}$$

where r , k and λ must be *integers*. Therefore the range of *admissible* parameter sets is restricted. Equations (5) and (6) are trivial and condition 1-i is redundant, but it is explicitly defined for presentation purposes. Condition 1-ii can also be derived from 1-iii and 1-iv.

Notice that BIBDs are defined in terms of the *uniform* distribution of ones over the incidence matrix (see Definition 3 below).

Definition 2 (Cost functions for BIBDs) *Given a set (v, b, u) of admissible parameters, we say that $F : \mathcal{A} \rightarrow \mathcal{R}$ is a cost function for BIBD generation if there exists a lower bound F^* such that $F(A^*) = F^*$ if and only if there exists a (v, b, u) -BIBD with incidence matrix A^* .*

Observe that F^* may be calculated even if such a design does not exist. For all A corresponding to a non-BIBD configuration, then, it must hold that $F(A) > F^*$.

2.1 Combinatorial distribution measures for the properties of a BIBD

To illustrate the notion of *distribution measure*, let us consider the set $\mathcal{B}_w$ of all possible arrangements of w balls in p bins, and let b_j be the number of balls in bin j in a particular configuration $B \in \mathcal{B}_w$, with $w = \sum_j b_j$.

Definition 3 (Maximal or uniform distribution) *We say that w balls are maximally or uniformly distributed over p bins (we say that the number of balls per bin is maximally uniform) if, for a fixed d ,*

$$b_j = d \text{ or } b_j = d + 1, \quad j = 1, \dots, p. \tag{8}$$

In fact $d = \lfloor w/p \rfloor$, and there will be exactly $w \bmod p$ bins with $d + 1$ balls, and the remaining bins will have d balls. In particular, for (p, w) such that $p|w$ (*multiplicity condition*), it holds that $w \bmod p = 0$ and *all* bins will have exactly d balls. We say, in this case, that the distribution is *strictly* uniform.

Let us now consider the number of pairs that can be formed by taking balls belonging to the same bin in a given configuration $B \in \mathcal{B}_w$,

$$P(B) = \sum_j \binom{b_j}{2}. \quad (9)$$

This measure is quadratic on the b_j 's and, therefore, it is minimized for *all and only* those configurations that are uniformly distributed. We say that $P(B)$ is a *measure* of the *distribution* of w balls over p bins.

Extending the measure to any number of balls (i.e., for fixed p but arbitrary w), the *lower bound* on $P(B)$ may be written as a function of the number of balls w ,

$$P^{\min}(w) = p \binom{\lfloor w/p \rfloor}{2} + (w \bmod p) \lfloor w/p \rfloor, \quad (10)$$

and the *increment* of this lower bound is

$$\Delta P^{\min}(w) = P^{\min}(w+1) - P^{\min}(w) = \lfloor w/p \rfloor. \quad (11)$$

Notice that $\Delta P^{\min}(w)$ is a staircase-like function of w with a unit step at each multiple of p , and flat regions in between. Therefore, $P^{\min}(w)$ is a piece-wise linear non-decreasing convex function.

Going back to the case of block designs, and over the set $\mathcal{A} = v \times b$ of binary configurations, let us define the following combinatorial *measures*:

Number of ones:

$$U(A) = o = \sum_{i=1}^v \sum_{j=1}^b x_{ij} \quad (12)$$

Total pairs of ones:

$$P_t(A) = \binom{o}{2} = \sum_{i=1}^v \sum_{k=i}^v \sum_{j=1}^b \sum_{l=j}^b x_{ij} x_{kl} - U(A) \quad (13)$$

Horizontal pairs of ones:

$$P_h(A) = \sum_i \binom{r_i}{2} = \sum_{i=1}^v \sum_{j=1}^{b-1} \sum_{l=j+1}^b x_{ij} x_{il} \quad (14)$$

Vertical pairs of ones:

$$P_v(A) = \sum_j \binom{k_j}{2} = \sum_{j=1}^b \sum_{i=1}^{v-1} \sum_{k=i+1}^v x_{ij} x_{kj} \quad (15)$$

Quadruples of ones:

$$Q(A) = \sum_{i=1}^{v-1} \sum_{k=i+1}^v \binom{\lambda_{ik}}{2} = \sum_{i=1}^{v-1} \sum_{k=i+1}^v \sum_{j=1}^{b-1} \sum_{l=j+1}^b x_{ij} x_{il} x_{kj} x_{kl}. \quad (16)$$

The measures $U(A)$ and $P_t(A)$ are linear and quadratic, respectively, with the number of ones in A (independently from their distribution), and they will be used to account for the number of ones. $P_h(A)$ is a distribution measure of o ones over v rows, whereas $P_v(A)$ is a distribution measure of o ones over b columns. Thus, for $A' \in \mathcal{A}_o$ (the subset of all configurations with exactly o ones), $P_h(A') = P_h^{\min}(o)$ if and only if the rows in A' are *maximally* uniform, and $P_v(A') = P_v^{\min}(o)$ if and only if the columns in A' are *maximally* uniform. For $o = u$, since admissibility conditions (5)-(6) enforce multiplicities $(v|o$ and $b|o)$, these distributions are *strictly* uniform.

Likewise, let $p_v = P_v(A)$ be the number of vertical pairs in a given configuration A . Then, $Q(A)$ can be interpreted as a distribution measure of p_v

vertical pairs (“balls”) over $f = \binom{v}{2}$ *pairs of rows* (“bins”). In this sense, a

maximally distributed configuration is called *maximally balanced*, with lower bound $Q^{\min}(p_v)$. For (p_v, f) such that $f|p_v$ (multiplicity condition), a maximally balanced configuration is said to be *strictly* balanced. Yet, as long as p_v is the same, balance may equally be reached by a configuration with fewer ones unevenly distributed over columns, or by a configuration with more ones which are better distributed. Given a number o of ones, since $Q^{\min}(p_v)$ is non-decreasing, the lower bound on $Q(A)$ over $\mathcal{A}_o$, denoted $Q^{\min}(o)$, is

$$Q^{\min}(o) = Q^{\min}(P_v^{\min}(o)). \quad (17)$$

Since the complementary configuration of a (v, b, u) -BIBD is a $(v, b, vb - u)$ -BIBD, the number $\bar{Q}(A)$ of quadruples of *zeros* can also be used as a measure of balance, with $\bar{o} = vb - o$, $\bar{Q}(A) = Q(\bar{A})$ and $\bar{A} \equiv [\bar{x}_{ij}]^2$.

2.2 Characterizing BIBDs in terms of the distribution measures: Combinatorially optimal values

The following theorem is a necessary and sufficient condition for the existence of a BIBD:

Theorem 4 *Given a set (v, b, u) of admissible parameters, a configuration $A^* \in \mathcal{A} - v \times b$ is the incidence matrix of a (v, b, u) -BIBD if and only if*

² For P_t , P_h and P_v , minimization in terms of ones is equivalent to minimization in terms of zeros, thus the corresponding complementary measures are not necessary. This is not so for measure Q , as discussed in Section 3.1.

$$U(A^*) = u \quad \text{and} \tag{18}$$

$$Q(A^*) = Q^{\min}(u). \tag{19}$$

Proof. Let A_1 be a configuration corresponding to a BIBD. Then, by definition, A_1 must have the right number of ones, must have strictly uniform columns and must be strictly balanced. The first fact simply states that $U(A_1) = u$. From this and the second fact it follows that the number of vertical pairs is given by $P_v(A_1) = P_v^{\min}(u)$. The third fact, balance, enforces maximal distribution of the available pairs $Q(A_1) = Q^{\min}(P_v(A_1)) = Q^{\min}(P_v^{\min}(u))$ which, by equation (17), leads to (19).

On the other hand, let A_1 be a configuration satisfying (18) and (19). The first equation states that A_1 has the right number of ones and, since $Q(A_1)$ reaches its lower bound for u ones, it follows that A_1 is maximally balanced. The number of vertical pairs involved must satisfy $P_v(A_1) \geq P_v^{\min}(u)$ but, by equation (17), only the equality is possible, otherwise $Q(A_1)$ would be higher than expressed in (19)³. Therefore, A_1 has maximally uniform columns. Since the parameter set is admissible, maximalities are satisfied in the strict sense; and, from strict balance, strictly uniform columns and the admissibility conditions it follows that rows are strictly uniform as well, thus completing the definition of BIBD. $\square$

A configuration A^* satisfying conditions (18) and (19) is said to be a *combinatorially optimal configuration*.

Expanded according to (12) and (16), Theorem 4 constitutes the *shortest* definition of a BIBD in terms of the variables x_{ij} .

In the following, the *assumption of optimality* denotes the assumption that conditions 1-i to 1-iv in Definition 1 hold, even if no configuration exists that satisfies them, and the term *optimal value* refers to the value of an expression under such assumption (i.e., the value that the expression *would* take on a BIBD, if any existed).

For $M \in \{U, P_t, P_v, P_h, Q, \bar{Q}\}$, let $M^{\min}(o)$ denote the lower bound of M over $\mathcal{A}_o$, and let $\Delta M^{\min}(o)$ denote its *increment*, as defined in (11). Under the assumption of optimality, *optimal values* M^* satisfy $M^* = \Delta M^{\min}(o)$, whereas *optimal increments* are defined as

$$\Delta^- M^* \equiv \Delta M^{\min}(u - 1) \tag{20}$$

³ This is only true for $\lambda > 0$, which is in accordance with the definition of BIBD. Otherwise, the number of quadruples can remain zero even after adding vertical pairs ($Q^{\min}(u) = 0, u = 0, \dots, f$).

Table 1

Given a set (v, b, u) of admissible parameters, optimal values and optimal increments for U , P_t , P_h , P_v , Q and $\bar{Q}$, expressed in terms of the descriptors of the design (with $\bar{k} = v - k$ and $\bar{\lambda} = b + \lambda - 2r$).

M	M^*	$\Delta^- M^*$	$\Delta^+ M^*$
U	u	1	1
P_t	$\binom{u}{2}$	$u - 1$	u
P_h	$v \binom{r}{2}$	$r - 1$	r
P_v	$b \binom{k}{2}$	$k - 1$	k
Q	$f \binom{\lambda}{2}$	$(k - 1)(\lambda - 1)$	$k\lambda$
$\bar{Q}$	$f \binom{\bar{\lambda}}{2}$	$-\bar{k}\bar{\lambda}$	$-(\bar{k} - 1)(\bar{\lambda} - 1)$

$$\Delta^+ M^* \equiv \Delta M^{\min}(u). \quad (21)$$

Under the assumption of optimality, admissibility conditions hold, thus enforcing multiplicities. In that case, for each of the above measures, the expressions for the lower bounds (from 10) and increments (from 11) are simple, as shown in Table 1.

2.3 The parametric cost function F

We are now in condition to define a generic combinatorial cost function for the generation of BIBDs. Let

$$F = \rho_u U + \rho_t P_t + \rho_h P_h + \rho_v P_v + \rho_q Q + \rho_{\bar{q}} \bar{Q}, \quad (22)$$

be a linear combination of the measures defined in Section 2.1 (the dependence on A is omitted hereafter for the sake of clarity). Then, a particular function is univocally specified by the set of its *composition coefficients*

$$F(\rho_u, \rho_t, \rho_h, \rho_v, \rho_q, \rho_{\bar{q}}). \quad (23)$$

Theorem 5 *Given a set (v, b, u) of admissible parameters, the measure F in equation (22) is a combinatorial cost function for the generation of BIBDs if*

$$\rho_q > 0 \quad (24)$$

$$\rho_t, \rho_h, \rho_v, \rho_{\bar{q}} \geq 0 \quad (25)$$

and ρ_u is such that

$$\Delta^- F^* < 0 \tag{26}$$

$$\Delta^+ F^* > 0. \tag{27}$$

Its global minimum is

$$\begin{aligned} F^* &= F^{\min}(u) = \\ &= \rho_u U^* + \rho_t P_t^* + \rho_h P_h^* + \rho_v P_v^* + \rho_q Q^* + \rho_{\bar{q}} \bar{Q}^*, \end{aligned} \tag{28}$$

with the optimal values given in Table 1.

Proof. Since all lower bounds are non-concave, the drawing of $F^{\min}(o)$ must have a single valley, and multiplicity conditions (derived from parameter admissibility) guarantee that the bottom of this valley is not flat. We can then apply (26)-(27) and use ρ_u to set its global minimum at the desired point ($o = u$). Condition (24) is necessary to guarantee that Theorem 4 can be applied. $\square$

The family of cost functions defined by the above theorem has been experimentally validated on the set of all BIBDs of size $vb \leq 1000$. This was a by-product of a study where the generation of BIBDs was used as a benchmark for comparing the performance of several optimization strategies based on neural networks [2]. We omit the details here, since the main objective of this work is the extension of these cost functions to the case of non-admissible parameters, which is undertaken in the next section.

3 A combinatorial extension of BIBDs: MBMUDs

The general criterion of *maximally uniform* distribution (Definition 3) is used here as a generalization of the *strictly* uniform criterion applied in the definition of BIBDs (Definition 1). In other words, the admissibility constraints (5-7) on the design parameters are relaxed, and a super-class including BIBDs is defined for *arbitrary* (v, b, u) . In terms of combinatorial balance, Maximally Balanced Maximally Uniform Designs (v, b, u) -MBMUDs are the closest possible approximation to BIBDs in cases where the parameter set is not admissible.

Definition 6 (MBMUD) We say that $A \in \mathcal{A} - v \times b$ is the incidence matrix of a *Maximally Balanced Maximally Uniform Design (MBMUD)* with parameters (v, b, u) and descriptors $[(r, k, \lambda), (v_0, b_0, f_0)]$, with $0 \leq u \leq vb$, if and only if the following properties are fulfilled:

i) **Right number of ones:** $o = u$.

A1, a (6,10,27)-MBMUD										A2, non uniform rows											
1		1	1	1	4	2	1	1	1	2		1	1	1	1	5	2	2	2	1	2
1	1			1	1	4	1	1	2	2		1	1	1		4	2	1	1	1	
1	1	1	1		1	5	2	2	2			1	1	1	1	4	1	1	2		
		1	1	1	1	4	1	2			1		1	1		4	2	2			
1		1	1	1	1	5	2				1	1			1	1	4	2			
		1			1	1	1	1	5			1	1		1	1	6				
2 3 3 3 2 2 3 3 3 3 27										3 2 3 3 3 3 3 3 2 2 3 27											

Fig. 1. Examples of $(6, 10, 27)$ -configurations (ones of the incidence matrix, row and column sizes, number of ones and triangular matrix of row concurrences). A1 is a $(6, 10, 27)$ -MBMUD with descriptors $[(4, 2, 1)(3, 7, 9)]$. In A2, although columns and concurrences are maximally uniform, the number of ones per row takes three different values.

- ii) **Maximally uniform rows:** *There are v_0 rows with $r + 1$ ones and the remaining rows have r ones.*
- iii) **Maximally uniform columns:** *There are b_0 columns with $k + 1$ ones and the remaining columns have k ones.*
- iv) **Maximum balance:** *There are f_0 pairs of rows with concurrence $\lambda + 1$ and the remaining pairs have concurrence $\lambda_{ik} = \lambda$.*

This time, property 6-ii can no longer be derived from 6-iii and 6-iv, as was the case for BIBDs. This fact is shown in Figure 1. According to the criterion of maximal distribution, parameters and descriptors are now related by

$$r = \lfloor u/v \rfloor \quad v_0 = u \bmod v \quad (29)$$

$$k = \lfloor u/b \rfloor \quad b_0 = u \bmod b \quad (30)$$

$$\lambda = \lfloor p_v^*/f \rfloor \quad f_0 = p_v^* \bmod f, \quad (31)$$

with $f = \binom{v}{2}$ the number of *pairs* of rows, and $p_v^* = b \binom{k}{2} + b_0 k$ the *optimal* number of vertical pairs. Notice that maximum balance can be reached by a configuration with non-uniform columns, as long as it has the optimal value of vertical pairs (Section 3.1).

For (v, b, u) such that *all* multiplicity conditions hold, all maximal distributions are achieved in the strict sense, the second set of descriptors (v_0, b_0, f_0) is $(0, 0, 0)$, and the corresponding configuration is a BIBD. For (v, b, u) such that $v|u$ and $b|u$, the corresponding configuration is a RGD [6,17]. When only $b|u$, the corresponding configuration is a SRDG [5], which coincides with a NBIBD of Type I [3].

The above definition is the natural consequence of applying cost function F (22) to a set of non-admissible parameters. In fact, if the coefficients of F satisfy some additional constraints (Section 3.2) then optima under F correspond to MBMUDs. In the next sections we use the generalized criterion of *maximally* uniform distribution to derive optimal values for the distribution

Table 2

Optimal values and increments for the measures U , P_t , P_h , P_v and Q , in terms of the descriptors $[(r, k, \lambda), (v_0, b_0, f_0)]$ of a MBMUD with parameters (v, b, u) . Measure $\bar{Q}$ has been omitted since it can no longer be used for MBMUD generation in the general case (see text).

M	M^*	$\Delta^- M^*$	$\Delta^+ M^*$
U	u	1	1
P_t	$\binom{u}{2}$	$u - 1$	u
P_h	$v \binom{r}{2} + v_0 r$	$\begin{cases} r - 1 & \text{if } v_0 = 0 \\ r & \text{if } v_0 \neq 0 \end{cases}$	r
P_v	$b \binom{k}{2} + b_0 k$	$\begin{cases} k - 1 & \text{if } b_0 = 0 \\ k & \text{if } b_0 \neq 0 \end{cases}$	k
Q	$f \binom{\lambda}{2} + f_0 \lambda$	$\begin{cases} (k-1)(\lambda-1) + f_0 & \text{if } b_0 = 0, f_0 < k-1 \\ (k-1)\lambda & \text{if } b_0 = 0, f_0 \geq k-1 \\ k(\lambda-1) + f_0 & \text{if } b_0 \neq 0, f_0 < k \\ k\lambda & \text{if } b_0 \neq 0, f_0 \geq k \end{cases}$	$\begin{cases} k\lambda & \text{if } f_0 \leq f - k \\ k(\lambda+1) - (f - f_0) & \text{if } f_0 > f - k \end{cases}$

measures of Section 2.1, and MBMUDs are characterized in terms of them.

3.1 The distribution measures applied to MBMUDs: Optimal values

In the case of MBMUDs, the assumption of optimality refers to Definition 6. Under such assumption, optimal values and optimal increments are listed in Table 2.

Theorem 7 *Given a set (v, b, u) of parameters, with $0 \leq u \leq vb$, a configuration $A^* \in \mathcal{A} - v \times b$ is the incidence matrix of a (v, b, u) -MBMUD if and only if*

$$U(A) = u, \tag{32}$$

$$P_h(A) = P_h^*, \tag{33}$$

$$P_v(A) = P_v^* \text{ and } \tag{34}$$

$$Q(A) = Q^*. \tag{35}$$

Proof. If A^* is a MBMUD, the above conditions follow. In the other sense of the implication, conditions (32) and (35) together enforce balance, but since λ is now unrestricted, the condition on P_v must also be fulfilled to enforce column uniformity (when $Q^* = 0$). Besides, since column-uniformity and balance no longer guarantee row-uniformity (Figure 1), the condition on P_h must also be

imposed in the general case. $\square$

For some parameter sets it is easy to show that no MBMUD can exist. One such situation is the case when

$$b_0 = 0, f_0 = 0, \text{ and } v_0 \neq 0. \quad (36)$$

If there exists a configuration satisfying the first two conditions then it must have *strictly* uniform rows, in contradiction with the fact that $v_0 \neq 0$ (multiplicity for rows is not satisfied). An example of this situation is the set (6,10,40) with descriptors [(6,4,4),(4,0,0)], which is particularly interesting since, as reported in Section 3.3, there *do* exist MBMUDs with the complementary parameters (6, 10, 20). Thus, given two sets of complementary parameters (v, b, u) and $(v, b, vb - u)$, the existence of a (v, b, u) -MBMUD does not imply that its complementary configuration is a $(v, b, vb - u)$ -MBMUD. In fact, it does not even imply that there exists any $(v, b, vb - u)$ -MBMUD.

Proposition 8 *Given a set (v, b, u) of parameters, if*

$$v_0 = 0 \text{ or } (f_0 = 0 \text{ and } (v_0 = 1 \text{ or } v_0 = v - 1)), \quad (37)$$

then, if there exists a (v, b, u) -MBMUD, its complementary configuration is also a MBMUD with parameters $(v, b, vb - u)$.

Proof. If condition (37) is satisfied, the casuistry for

$$\bar{\lambda}_{ik} = b + \lambda_{ik} - r_i - r_k \quad (38)$$

yields at most two different values. $\square$

Of course, admissible parameters for BIBDs satisfy (37).

For measures U, P_t, P_h and P_v it is easy to verify that optimality in a given configuration A implies optimality in its complementary configuration $\bar{A}$. Thus, from Theorem 7 and the above examples it follows that optimality on Q does *not* imply optimality on $\bar{Q}$ (i.e., $Q(A) = Q^* \not\Rightarrow Q(\bar{A}) = \bar{Q}^*$).

The next result states a relationship with the *dual* configuration space $\mathcal{A}' - b \times v$. The optimal lower bound on Q was derived by assuming column uniformity and balance, that is, by taking $Q^* = Q^{\min}(u) = Q^{\min}(P_v^{\min}(u))$. Let us call this bound the *balanced* lower bound on Q for balanced, column-uniform

configurations with u ones, and let us denote it by Q_b . Then (Table 2),

$$Q_b = f \binom{\lambda}{2} + f_0 \lambda. \quad (39)$$

Yet, using a *dual* point of view, the number of *quadruples* in a configuration A can also be interpreted as a distribution measure of the *horizontal* pairs (“balls”) in A over pairs of *columns* (“bins”). From this point of view, let μ_{jl} be the concurrence between columns j and l . Then, for any configuration A ,

$$Q(A) = \sum_j \sum_{l \neq j} \binom{\mu_{jl}}{2}. \quad (40)$$

We say that a configuration is *maximally linked* when concurrences between pairs of columns are maximally uniform. As usual, with p_h the number of horizontal pairs and $g = \binom{b}{2}$ the number of pairs of columns, we say that the configuration is *strictly linked* when the multiplicity $g|p_h$ holds. Then, proceeding as before, the *linked* lower bound on Q for linked, row-uniform configurations with u ones is

$$Q_l = g \binom{\mu}{2} + g_0 \mu, \quad (41)$$

with $\mu = \lfloor p_h^*/g \rfloor$, $g_0 = p_h^* \bmod g$, and $p_h^* = v \binom{r}{2} + v_0 r$ the *optimal* number of horizontal pairs.

Theorem 9 *A necessary condition for the existence of a (v, b, u) -MBMUD is that Q_b (39) and Q_l (41) satisfy*

$$Q_b \geq Q_l. \quad (42)$$

Proof. Since both Q_b and Q_l are lower bounds on Q , both underlying assumptions (i.e., maximum balance and maximum linkage) can only be fulfilled simultaneously when $Q_b = Q_l$. Then, since MBMUDs are defined in terms of balance, (42) must hold. $\square$

For instance, designs with parameters $(6, 10, 40)$, $(6, 10, 50)$ and $(6, 10, 51)$ do not exist (the first was already mentioned as an example of (36)).

The following statements are derived from the preceding theorem:

- The *dual* of a maximally balanced design is a maximally linked configuration.
- If there exists a MBMUD with $Q_b > Q_l$, its dual is *not* a MBMUD.
- If there exists a (v, b, u) -MBMUD with $Q_b = Q_l$, then it is a maximally linked MBMUD, and its dual is a (b, v, u) -MBMUD.

And it also holds that

- If a MBMUD is square ($v = b$), then $Q_b = Q_l$. But $Q_b = Q_l$ does *not* imply $v = b$.

As an existence condition, Theorem 9 is ineffective when $v = b$, it is hardly restrictive when $v < b$, but it is strongly restrictive for $v > b$. Fisher's condition, thus, seems to show up in a sort of relaxed way. For $b_0 = 0$ MBMUDs revert to type I NBIBDs. The reader is referred to [3] and [13] for further existence results.

3.2 Cost function F for MBMUDs

The constraints on the coefficients of the cost function F when applied to MBMUDs depend on the descriptors (v_0, b_0, f_0) . In order to get a valid cost function for *any* MBMUD, we now consider the worst-case.

Theorem 10 *Given a set (v, b, u) of parameters, with $0 \leq u \leq vb$, the measure $F(\rho_u, \rho_t, \rho_h, \rho_v, \rho_q, \rho_{\bar{q}})$ is a combinatorial cost function for the generation of MBMUDs if*

$$\rho_t, \rho_h, \rho_v, \rho_q > 0 \tag{43}$$

$$\rho_{\bar{q}} = 0, \tag{44}$$

and ρ_u is such that

$$\Delta^- F^* < 0 \tag{45}$$

$$\Delta^+ F^* > 0. \tag{46}$$

Its global minimum is

$$\begin{aligned} F^* &= F^{\min}(u) = \\ &= \rho_u U^* + \rho_t P_t^* + \rho_h P_h^* + \rho_v P_v^* + \rho_q Q^*, \end{aligned} \tag{47}$$

with the optimal values given in Table 2.

Fig. 2. Optimal distribution of zeros for a configuration with parameters (6,10,52). All other alternatives are isomorphic. No other distribution preserves the uniformity of rows and columns, but concurrences are not balanced. Therefore, no (6,10,52)-MBMUD can exist.

Proof. From Theorem 7, the terms on Q , P_v and P_h must be present in a general-case cost function for MBMUDs, and the term on $\bar{Q}$ must be discarded, as discussed in relation to the complementary configuration. The worst case occurs for (v, b, u) such that none of the multiplicity conditions holds. In this case, in order to avoid that $\Delta F^{\min}$ be flat in the desired region, P_t must be explicitly included, since it has a *monotonically* increasing increment. Then, since the resulting lower bound is convex, the minimum is set by adjusting ρ_u so that (45)-(46) are satisfied. $\square$

3.3 Experimental validation

All MBMUDs in this section were generated using $F(\alpha_u, 1, 9, 3, 7, 0)$ and Simulated Annealing [8] as optimization technique. The dual search spaces $\mathcal{A} - 6 \times 10$ and $\mathcal{A}' - 10 \times 6$ were thoroughly analysed in order to check the properties discussed, and results are summarized in Table 3.

A “pathological” situation was detected when the desired number of ones u is close to the size vb of the incidence matrix. If both row and column uniformities are to be preserved, the $vb - u$ zeros of the design should all be in different rows *and* columns, but then concurrences between rows would take three different values. This happens when

$$\bar{u} \leq \max(v, b) \quad \text{and} \quad 1 < v_0 < v - 1. \quad (48)$$

As an example, the case (6,10,52) is shown in Figure 2. Besides these, and the non-existing cases derived from Theorem 9 and from equation (36), the only unsolved case was (6,10,41). Although the size vb was the same for them all, notice the differences in cost to the first solution obtained from problem to problem.

Finally, 30 other problems were tried with sizes similar to those of BIBDs ($vb < 300$). From 23 cases with $v \leq b$, 19 problems were solved, whereas from

Table 3

Exploration of the search space $\mathcal{A} - 6 \times 10$ (left), and its dual $\mathcal{A}' - 10 \times 6$ (right). With u and $\bar{u}$ all possible number of ones are covered. In each case, $\hat{E}(\mathbf{z})$ is the estimated cost to the first solution (in iterations), and “Exists?” describes existence results. Non-existence is signaled with $\star$ for Theorem 9, $\circ$ for equation (36) and $\diamond$ for equation (48) (see text).

		$\mathcal{A} - 6 \times 10$				$\mathcal{A}' - 10 \times 6$			
		DME(v, b, u)		DME($v, b, \bar{u}$)		DME(v, b, u)		DME($v, b, \bar{u}$)	
u	$\bar{u}$	$\hat{E}(\mathbf{z})$	Exists?	$\hat{E}(\mathbf{z})$	Exists?	$\hat{E}(\mathbf{z})$	Exists?	$\hat{E}(\mathbf{z})$	Exists?
0	60	1.0		1.0		1.0		1.0	
1	59	1.0		1.0		1.0		1.0	
2	58	2.0		-	no $[\diamond]$	1.9		-	no $[\diamond]$
3	57	2.0		-	no $[\diamond]$	2.0		-	no $[\diamond]$
4	56	2.0		-	no $[\diamond]$	2.0		-	no $[\diamond, \star]$
5	55	2.0		2.0		2.0		-	no $[\diamond, \star]$
6	54	24.6		2.8		2.7		-	no $[\diamond, \star]$
7	53	291.5		2.6		2.7		-	no $[\diamond, \star]$
8	52	93.3		-	no $[\diamond]$	2.2		-	no $[\diamond]$
9	51	39.1		-	no $[\star]$	2.6		2.4	
10	50	3.0		-	no $[\star]$	8.3		4.1	
11	49	4.4		3.2		133.3		-	no $[\star]$
12	48	9.5		7.4		15.6		-	no $[\star]$
13	47	13.9		4.0		3.1		-	no $[\star]$
14	46	6.5		75.5		2.7		-	no $[\star]$
15	45	3.7		113.9		2.7		-	no $[\star]$
16	44	2.6		123.6		2.6		-	no $[\star]$
17	43	2.7		2520.2		2.4		-	no $[\star]$
18	42	16.7		154.2		2.5		-	no $[\star]$
19	41	171.5		-		30.0		-	no $[\star]$
20	40	6.3		-	no $[\circ, \star]$	8.6		246.8	
21	39	66.2		1556.9		83.4		2487.5	
22	38	27.1		80.6		133.8		-	no $[\star]$
23	37	38.7		180.0		-	no $[\star]$	-	no $[\star]$
24	36	10.8		18.6		-	no $[\star]$	-	no $[\circ, \star]$
25	35	22.3		67.3		-	no $[\star]$	-	no $[\star]$
26	34	21.9		46.2		-	no $[\star]$	-	no $[\star]$
27	33	18.3		86.6		-	no $[\star]$	-	no $[\star]$
28	32	23.5		91.1		-	no $[\star]$	-	no $[\star]$
29	31	595.6		274.6		-	no $[\star]$	-	no $[\star]$
30		24.7				4060.6			

7 cases with $v > b$ only 3 problems were solved. Results are detailed in [1]. In all, MBMUD problems proved to be about as difficult as BIBDs.

4 MBMUDs and statistical optimality: some experimental results

4.1 Optimality measures, optimization procedure and experimental set

The *statistical* optimality criteria for block designs are usually defined in terms of the information matrix (or C -matrix). The generalized inverse of this matrix is proportional to the variance-covariance matrix for estimating the treatment effects.

For an arbitrary design with incidence matrix A , the C -matrix is given by [16]:

$$C = R - AK^{-1}A^T, \quad (49)$$

where R and K are diagonal matrices with the number of ones per row and column, respectively.

Let μ_i be the non-zero eigenvalues of C , then the A- and D-optimality measures Φ_A and Φ_D are derived as follows:

$$\Phi_A(A) = \sum 1/\mu_i, \quad (50)$$

$$\Phi_D(A) = 1/\prod \mu_i. \quad (51)$$

In the experiments, we will be using these two statistically optimality measures to assess how informative is the proposed combinatorial cost function.

It is also important to define precisely the domain in which the optimization will be carried out. Let $\mathcal{A}(v, b, u)$ be the set of $v \times b$ configurations with exactly u ones, uniform rows and uniform columns. The search strategy of our optimization algorithm explores only configurations in $\mathcal{A}(v, b, u)$, by updating at each step square-wise arrangements of units from (10,01) to (01,10) [10]. In this way, the first subgoals of our cost function (number of ones, ones per row and ones per column) are guaranteed by construction, and the only term that needs to be minimized is the number of quadruples. Combinatorially optimal designs over $\mathcal{A}(v, b, u)$ according to this criterion will be hereafter called Q-optimal designs.

For the interested reader, the source code and executable version of our algorithm are available at [4].

The set of designs selected to perform our experiments is based on the set explored in [3], extended with several non-NBIBD MBMUDs. The list of designs considered appears in Table 4, classified as BIBDs, RGDs, type-I NBIBDs (or SRGDs), type-II NBIBDs, non-existing NBIBDs, and non-NBIBD MBMUDs.

4.2 Optimality behaviour of the proposed combinatorial cost function

The first set of experiments was aimed at determining the relation of the proposed combinatorial cost function with the Φ_A - and Φ_D - statistical optimality measures. For all designs, the space $\mathcal{A}(v, b, u)$ was sampled with a uniform distribution and the values of the three measures were recorded for each configuration. As an example of the results, Figure 3 plots the $\Phi_A(A)$ values as a function of the $Q(A)$ values obtained for a particular design. An almost identical plot was obtained for $\Phi_D(A)$ versus $Q(A)$, and similar graphs came out for the other designs as well. The discrete nature of the Q function versus the continuous nature of the statistical optimality measures is apparent. For every value of Q there are several values of $\Phi_A(A)$ (i.e., there exist several non-isomorphic configurations with the same Q), but the overall tendency of the plot is clearly *monotonic*. Some of the strides overlap, meaning that it is sometimes possible to minimize Q while actually increasing Φ_A , but only for Q values larger than Q^* . In fact, for *all* the designs tested (including the non-

Fig. 3. Plot of $\Phi_A(A)$ vs $Q(A)$ for uniform configurations with parameters (6,11,30).

existing ones), the leftmost strides didn't overlap, and had the lowest values. In the case of BIBDs, since they are Q-, A- and D-optimal, the leftmost stride reduces to a single point.

In general terms, thus, combinatorial optimality was found to be a necessary but not sufficient condition for statistical optimality. For small u this leads to complete enumeration of competing concurrence patterns to determine statistical optimality as in [12], while for larger u it tells us that statistical optimality is generally much harder to establish than combinatorial optimality.

The next set of experiments consisted of performing 30 descents of the optimization procedure on each of the three landscapes, i.e., using measures $Q(A)$, $\Phi_A(A)$ and $\Phi_D(A)$, respectively. The average values of Φ_A attained in the descents on $Q(A)$ and $\Phi_A(A)$ are recorded in the second and third columns of Table 4, while the average values of Φ_D attained in the descents on $Q(A)$ and $\Phi_D(A)$ are recorded in the fifth and sixth columns of the same table.

At first glance one sees that the values of Φ_A obtained by descending on the Q - and Φ_A -landscapes are very similar. And the same observation holds for the Φ_D values. Hence, the proposed cost function has minima close to those of the usual A- and D- statistical optimality measures. More precisely, we observe that there is a perfect match in the cases of BIBDs and type-II NBIBDs, and in several of the RGDs and type-I NBIBDs as well. As should be expected, for designs coincident with those listed in Table 1 of [3], the values of Φ_A and Φ_D are concordant with the efficiency bounds recorded there.

Some other observations are worth mentioning. The number of Q-optimal designs obtained was high for the three landscapes (around 98% of the descents). Type-II NBIBD settings were of course not Q-optimal, but in this case our procedure actually converged to Type-II NBIBD. On the contrary, non-existing NBIBDs converged to configurations with 3 different concurrence values for the same row. Yet, best Q s are only 2 or 3 steps away from Q^* .

$Q(A)$ showed a consistently much lower computational cost (with savings ranging from 50% to 90%) for two reasons. On the one hand, the computational complexity of each function evaluation is much lower, as compared with the statistical optimality measures, which require a singular value decomposition per evaluation. In fact, $Q(A)$ is computed incrementally by considering the joint effect of a $(10, 01) \rightarrow (01, 10)$ transformation (the gradient has an explicit closed form, which permits avoiding to really "evaluate" the function each time). On the other hand, and as an experimental observation, the number of iterations per descent was almost always smaller in the case of $Q(A)$, while reaching minima that were similar in quality.

Most A- and D-local minima were also Q-local minima but not the other way around. This fact suggested a third set of experiments. Local minima of

Table 4

Average values of Φ_A (respectively, Φ_D) attained in the following three situations: after 30 descents on the Φ_A -landscape (resp. Φ_D -landscape), after 30 descents on the Q -landscape, and by minimizing Φ_A (resp. Φ_D) after the descents on Q .

(v, b, u)	Φ_A values			10000 * Φ_D values		
	Φ_A -landscape	Q -landscape	Q -initialization	Φ_D -landscape	Q -landscape	Q -initialization
BIBDs						
(6,10,30)	1.2500	1.2500	1.2500	9.7656	9.7656	9.7656
(6,15,60)	0.5556	0.5556	0.5556	0.1694	0.1694	0.1694
RGDs						
(6,3,12)	2.8333	2.8333	2.8333	555.5556	555.5556	555.5556
(6,4,12)	0.0030	0.0032	0.0030	1.0404	1.0547	1.0404
(6,6,18)	2.1250	2.1250	2.1250	131.5566	131.8359	131.5566
(6,6,24)	1.3987	1.3988	1.3987	16.8310	16.8327	16.8298
(6,8,24)	1.5871	1.5871	1.5871	30.9917	30.9917	30.9917
(6,9,36)	0.9286	0.9288	0.9286	2.1939	2.1947	2.1939
(6,12,36)	1.0490	1.0491	1.0490	3.9941	3.9945	3.9942
(6,12,48)	0.6952	0.6952	0.6952	0.5183	0.5183	0.5183
Type-I NBIBDs						
(6,3,9)	0.0051	0.0054	0.0054	6.3333	7.5000	6.3333
(6,7,21)	1.8533	1.8556	1.8464	63.7996	63.9943	63.5616
(6,9,27)	1.4184	1.4178	1.4113	17.4072	17.3980	17.1213
(6,11,33)	1.1500	1.1500	1.1500	6.2500	6.2500	6.2500
(6,14,56)	0.5972	0.5972	0.5972	0.2411	0.2411	0.2411
(6,16,64)	0.5222	0.5222	0.5222	0.1235	0.1235	0.1235
Type-II NBIBDs						
(6,2,8)	0.0052	0.0052	0.0052	6.6667	6.6667	6.6667
(6,13,52)	0.6438	0.6438	0.6438	0.3501	0.3501	0.3501
Non-existing NBIBDs						
(6,4,16)	2.2038	2.2139	2.2029	143.9496	144.9410	143.7103
(6,5,15)	2.7049	2.7272	2.7045	380.6391	385.6167	381.7127
(6,5,20)	1.7167	1.7228	1.7166	44.4444	44.7197	44.4387
(6,7,28)	1.2125	1.2131	1.2125	8.0058	8.0127	8.0053
(6,8,32)	1.0549	1.0554	1.0549	4.0537	4.0564	4.0539
(6,10,40)	0.8404	0.8406	0.8404	1.3135	1.3138	1.3135
(6,11,44)	0.7623	0.7625	0.7623	0.8112	0.8116	0.8113
Non-NBIBD MBMUDs						
(6,6,22)	1.6031	1.6048	1.6031	31.7618	31.8115	31.7676
(6,7,23)	1.5928	1.5954	1.5924	31.2000	31.3085	31.2487
(6,8,23)	1.7116	1.7157	1.7088	43.9096	44.1675	43.7948
(6,11,30)	1.3197	1.3276	1.3179	12.7065	12.9025	12.6774
(6,14,63)	0.5115	0.5116	0.5115	0.1113	0.1114	0.1113

descents with Q were used as starting points for subsequent descents with Φ_A and Φ_D . The results are recorded in the fourth and seventh columns of Table 4. Concerning the Φ_A values, in most cases the same result obtained with the direct minimization of Φ_A is reached, but note that in eight cases, this Q -initialization leads to a lower value and only in the case (6,3,9) the resulting value is slightly higher. For the Φ_D values, the general trend is very similar, although the magnitude of the differences looks larger because the absolute values are larger. The success of the Q -initialization seems to suggest that the minima of Q are located in areas containing "good" local minima of Φ_A and Φ_D . By "good" we mean that they are lower than the average local minima in the entire Φ_A - and Φ_D -landscapes. This use of the Q function as initialization deserves further consideration, since it might lead to better quality results at a reduced computational cost.

As a final comment let us mention that, besides the special behaviour of BIBDs, no other differences were observed between the different classes of designs. This somehow supports the validity of the MBMUD generalization.

5 Conclusions

This paper has discussed the generation of block designs as a combinatorial optimization problem, by defining a family of combinatorial cost functions that enforce the *maximal distribution* of ones in the incidence matrix of the design, for rows, columns and balance. Parameter admissibility on the independent (v, b, u) parameters enforces single distinct values for the $[r, k, \lambda]$ design descriptors, leading to *strictly* uniform distributions, in all senses, i.e., leading to BIBDs.

The combinatorial optimization approach was then extended to arbitrary (v, b, u) , leading to the definition of Maximally Balanced Maximally Uniform Designs (v, b, u) -MBMUDs that, being *maximally* distributed, allow two distinct consecutive values for each of their descriptors $[r, r + 1; k, k + 1; \lambda, \lambda + 1]$.

From a practical point of view, using (v, b, u) as independent parameters makes sense since v is the number of treatments under study, b is the number of uniform blocks available, and u , the number of plots, is a measure of the resources that are necessary to perform the experiment (assume, for instance, a constant cost per trial). For *arbitrary* (v, b, u) , and in terms of combinatorial balance, MBMUDs are as similar as possible to BIBDs and, unlike pseudo-solutions, they have a well-defined structure.

Through experimentation, we found that combinatorial optimality is apparently a necessary but not sufficient condition for statistical optimality. This

is consistent with what has been known for binary designs in the restricted combinatorial class allowing just equisized blocks, as summarized in conjecture (3) of [15], page 60. We also found that the proposed combinatorial cost function has a monotonic relation with A- and D- statistical optimality, while its computational cost is much lower. Thus, it can be used directly as an approximation of A- and D-efficiencies, or either serve to initialize any algorithm based on a statistical optimality criterion in order to speed up the minimization. Preliminary results suggest that, by using this initialization, local optimization procedures based on a statistical criterion may reach more efficient designs.

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