

E-optimal Designs for Three Treatments

Valentin Parvu and J. P. Morgan

Virginia Tech

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Abstract: E-optimality is studied for three treatments in an arbitrary n -way heterogeneity setting. In some cases maximal trace designs cannot be E-optimal. When there is more than one E-optimal design for a given setting, the best with respect to all reasonable criteria is determined.

Key words and phrases: design optimality, multi-way heterogeneity, row-column design

1 Introduction

Of the many settings with multiple blocking factors, by far the most common are those where the arrangement of experimental units can be taken as an n -dimensional hyperrectangle for some $n \geq 2$. If b_j is the number of levels of the j th blocking factor, then $b_1 \times b_2 \times \dots \times b_n$ is the size of the hyperrectangle, and there is no loss of generality in taking $b_1 \leq b_2 \leq \dots \leq b_n$. Each cell corresponds to a single experimental unit, to be assigned one of v treatments. Denoting the total number of experimental units by $m = b_1 b_2 \dots b_n$, the size of each block of factor j , that is, the block size in direction j , is mb_j^{-1} . The standard linear model is:

$$y = \mu 1 + A_d \tau + \sum_{j=1}^n L_j \beta_j + \varepsilon, \quad (1)$$

where y is the $m \times 1$ vector of yields, 1 is a vector of ones, L_j is the $m \times b_j$ plot-block incidence matrix in direction j of the hyperrectangle with corresponding $b_j \times 1$ block effects vector β_j , and ε is a vector of uncorrelated random errors with zero means and equal variances. The design problem

is to optimize comparisons of members of the $v \times 1$ treatment effects vector τ , and the precision with which these comparisons are made is controlled by the assignment pattern of treatments to units, that is, by the choice of the $m \times v$ design matrix A_d .

Morgan and Bailey (2000) recently took a broad look at optimal allocations for multiple blocking factors, allowing for various combinations of nesting, crossing, and other relationships in the block factors structure. Readers are referred there for citations to past work as well as examples of such designs in practice. Like virtually all available theory, Morgan and Bailey's (2000) optimality results for the hyperrectangle described above place restrictions as a function of v on the collection of numbers (b_1, \dots, b_n) that can be quite severe. The same is seen, of course, in any design text: if you wish to compare 5 treatments, say, with two crossed blocking factors, neither texts nor the general literature will offer you much advice unless at least one of b_1 and b_2 is a multiple of 5. A consequence is that many experiments get "forced" into a standard design category, changing v and/or the b_i 's according to the limited options available. Statistical theory does not serve science well in these instances.

This paper takes a step towards resolving this situation, and in doing so helps illuminate the considerable technical difficulties involved. The E-optimality question is attacked, and solved, for $v = 3$ treatments and any (b_1, \dots, b_n) . Sonnemann (1985) has previously solved the optimality question for $v = 2$ in two-way heterogeneity settings, and those results are easily extended to n -way. Here the extension is not simple.

2 Information matrix and other preliminaries

Comparisons of competing designs are made through the $v \times v$ information matrix, also referred to as the C -matrix. Computation of the C -matrix for hyperrectangle block structure is simple using Morgan and Bailey's (2000) projection method. A mechanical derivation and explicit expression can be found in Cheng (1978), who deals specifically with this structure. The notation adopted here is also taken from Cheng (1978).

Let $N_j = (n_{ijl})$ be the $v \times b_j$ incidence matrix between the v treatments and the b_j levels of factor

j . By Theorem 2.1 in Cheng (1978), the C -matrix for design d is

$$C_d = D_r - \frac{1}{m} \sum_{j=1}^n b_j N_j N_j' + \frac{n-1}{m} D_r 11' D_r', \quad (2)$$

where $D_r = \text{diag}(r_1, \dots, r_v)$ is the diagonal matrix of replication numbers for the treatments. It follows that the i th diagonal element of C_d is

$$c_i = r_i - \frac{1}{m} \sum_{j=1}^n (b_j \sum_{l=1}^{b_j} n_{ijl}^2) + \frac{n-1}{m} r_i^2 \quad (3)$$

where n_{ijl} is the number of times treatment i occurs in block l of factor j . Each of r_i and n_{ijl} , and of course c_i , is a function of the design choice d through A_d ; this is taken to be understood, so that the notational complexity can be eased by not subscripting these quantities with d . A useful convention is to label the treatments so that the r_i 's are in nonincreasing order: $r_1 \geq r_2 \geq \dots$. This ordering will be maintained throughout this paper.

Any C -matrix is symmetric, non-negative definite, and has row and column sums of zero. Consequently, the C -matrix for a design with three treatments can be written solely in terms of its diagonal elements:

$$C_d = \begin{pmatrix} c_1 & \frac{1}{2}(-c_1 - c_2 + c_3) & \frac{1}{2}(-c_1 + c_2 - c_3) \\ \frac{1}{2}(-c_1 - c_2 + c_3) & c_2 & \frac{1}{2}(c_1 - c_2 - c_3) \\ \frac{1}{2}(-c_1 + c_2 - c_3) & \frac{1}{2}(c_1 - c_2 - c_3) & c_3 \end{pmatrix}, \quad (4)$$

where c_1 , c_2 , and c_3 correspond to treatments 1, 2, and 3, and are given in (3). The two non-zero eigenvalues of the matrix given in (4) are $\frac{1}{2} \left[\sum c_i \pm \sqrt{2 \sum_{i < j} (c_i - c_j)^2} \right]$. E-optimal designs maximize the quantity Z_d , the smaller of the two eigenvalues:

$$Z_d = \frac{1}{2} \left[\sum c_i - \sqrt{2 \sum_{i < j} (c_i - c_j)^2} \right]. \quad (5)$$

The expression for Z_d simplifies when some of the c_i 's are equal. These will be used often:

$$c_1 = c_2 \geq c_3 \Rightarrow Z_d = \frac{3}{2} c_3 \quad (6)$$

$$c_1 \geq c_2 = c_3 \Rightarrow Z_d = c_2 + c_3 - \frac{1}{2} c_1 \quad (7)$$

In some cases there are multiple designs which are E-optimal. With three treatments, the weak majorization order can always discriminate among them.

Definition 2.1. A design for three treatments is said to be E-M-optimal if (i) it is E-optimal, and (ii) it maximizes the largest eigenvalue of C_d amongst all E-optimal designs.

An E-M-optimal design is, for instance, A-best of all E-optimal designs. Indeed, it is best (amongst all E-optimal designs) with respect to every criterion expressed as the sum of a decreasing function of the eigenvalues. The “M” is chosen in accord with the usage by Bagchi and Bagchi (2001), as weak majorization is implied.

Next stated are two useful, well-known bounds for the smallest eigenvalue of a C -matrix. These bounds can be derived by the averaging technique described by Constantine (1981), or by other methods as given by Jacroux (1980).

Lemma 2.1. For a design d with information matrix $C_d = (c_{ii'})$, the minimum non-zero eigenvalue Z_d satisfies

$$Z_d \leq \frac{v}{v-1} \min_i (c_{ii}).$$

Lemma 2.2. For a design d with information matrix $C_d = (c_{ii'})$, the minimum non-zero eigenvalue Z_d satisfies

$$Z_d \leq \min_{i \neq i'} \frac{c_{ii} + c_{i'i'} - 2c_{ii'}}{2}.$$

One more concept is integral to the optimality arguments to follow.

Definition 2.2. In a design with multiple blocking factors, the assignment of treatment i is said to be *uniform in direction j* , if $|n_{ijl} - n_{ijl'}| \leq 1$ for all l and l' . The assignment of treatment i is *uniform* if it is uniform in all directions. The design is said to be *uniform* if all treatments are assigned uniformly in all directions.

“Treatment i is uniform” will be shorthand for “the assignment of treatment i is uniform.” If treatment i is uniform in direction j , then $\sum_l n_{ijl}^2$ is minimized for a given replication r_i , and can be written in terms of r_i and b_j as:

$$h(r_i, b_j) = r_i + (2r_i - b_j) \text{int}\left(\frac{r_i}{b_j}\right) - b_j \left[\text{int}\left(\frac{r_i}{b_j}\right)\right]^2. \quad (8)$$

In general, if treatment i is uniform in the entire design, then (3) becomes:

$$c_i = r_i - \frac{1}{m} \sum_{j=1}^n (b_j h(r_i, b_j)) + \frac{n-1}{m} r_i^2. \quad (9)$$

It is important to realize that neither uniformity of a treatment, nor of the entire design, demands any particular values for the replication numbers r_i . Obviously, if treatments i and i' have the same replication but i is uniform while i' is not, then $c_{i'} < c_i$. For three treatments, the maximum replication is $r = \text{int}(\frac{m}{3})$. A design is as close as possible to having equal replication if $r_1 \leq r_3 + 1$.

Simple manipulation of function $h(r, b)$ defined in (8) gives

$$\Delta h(r, b) = h(r + 1, b) - h(r, b) = 1 + \frac{2}{b}(r - r_{(b)}), \quad (10)$$

where $r_{(b)} = r \bmod b$ (compare Morgan, 1997). For any design with treatment i uniform in direction j , $\sum_{l=1}^{b_j} n_{ijl}^2 = h(r_i, b_j)$. The *nonuniformity of treatment i in direction j* is

$$NU_{i(j)} = \frac{b_j}{m} \left[\sum_{l=1}^{b_j} n_{ijl}^2 - h(r_i, b_j) \right] \quad (11)$$

The total nonuniformity of treatment i is $NU_i = \sum_{j=1}^n NU_{i(j)}$, which is zero if i is uniform.

Suppose that the number of experimental units is $m \equiv 0 \pmod{3}$; this only occurs if at least one of the b_j is a multiple of three. For this setting, $r = \frac{m}{3}$ and one can easily construct a uniform design d^0 with $r_1 = r_2 = r_3 = r$. For this design the information matrix C_{d^0} is completely symmetric, and $Z_{d^0} = \frac{3c_i^0}{2}$. Any design d with either $r_3 < r$, or with nonuniformity in some treatment, will have C_d with at least one diagonal element $c_i < c_i^0$. Then by lemma 2.1, $Z_d < \frac{3c_i^0}{2} = Z_{d^0}$, and d is E-inferior to d^0 . In fact, d^0 is a *Youden hyperrectangle*, or YHR, which is universally optimal (see Corollary 3.1.2 in Cheng (1978)).

Open are the cases where equal replication is not possible, that is, the cases for which no b_j is a multiple of 3. Section 3 lays the groundwork for the general problem by determining E-optimal designs for an unstructured set of blocks ($n = 1$). Sections 4 and 5 solve the settings for $n \geq 2$ for $m \equiv 1 \pmod{3}$ and $m \equiv 2 \pmod{3}$, respectively. Concluding remarks are in section 6.

3 One blocking factor

In the one-way heterogeneity setting $\mathcal{D}(3, b, k)$, with three treatments to be compared in b blocks of k experimental units each, the total number of units is $m = bk$. Let treatment i have replication r_i ,

with block-wise replications n_{il} , $l = 1, 2, \dots, b$. For such a design d , the diagonal elements of C_d are $c_i = r_i - \frac{1}{k} \sum_{l=1}^b (n_{il})^2$. If treatment i is uniform, then $c_i^0 = r_i - \frac{1}{k} h(r_i, b)$, so that the nonuniformity of treatment i is $NU_i \equiv NU_{i(1)} = c_i^0 - c_i \geq 0$ as given by (11).

3.1 Block designs with $bk \equiv 1 \pmod{3}$

In this case the maximin replication is $r = \frac{bk-1}{3}$. Consider a uniform design d^0 , with replications $r_1 = r + 1$ and $r_2 = r_3 = r$. By (7) the E-value for this design is

$$Z_{d^0} = 2c_2^0 - \frac{c_1^0}{2} \quad (12)$$

It will be first shown that d^0 is E-superior to any design not as close as possible to equal replication.

Lemma 3.1. *Block designs with $r_3 \leq r - 1$ cannot be E-optimal for $bk \equiv 1 \pmod{3}$.*

Proof. It will be shown that $Z_{d^0} - \frac{3}{2}c_3 > 0$, where c_3 is the diagonal element of a uniform treatment with replication $r_3 = r - 1$. This implies $Z_{d^0} - \frac{3}{2}c_3 > 0$ for any $r_3 \leq r - 1$, and thus by Lemma 2.1 the result.

Computing the values of the diagonal elements of C_{d^0} gives

$$c_1^0 = r + 1 - \frac{1}{k} h(r + 1, b) = \begin{cases} \frac{2}{9k}(bk^2 - b + k - 1), & \text{when } b \equiv 1 \text{ and } k \equiv 1; \\ \frac{2}{9k}(bk^2 - b + k + 1), & \text{when } b \equiv 2 \text{ and } k \equiv 2; \end{cases} \quad (13)$$

$$c_2^0 = c_3^0 = r - \frac{1}{k} h(r, b) = \begin{cases} \frac{1}{9k}(2bk^2 - 2b - k + 1), & \text{when } b \equiv 1 \text{ and } k \equiv 1; \\ \frac{1}{9k}(2bk^2 - 2b - k - 1), & \text{when } b \equiv 2 \text{ and } k \equiv 2. \end{cases} \quad (14)$$

Suppose a design d has treatment 3 uniform with $r_3 = r - 1$. Then by (9):

$$c_3 = \begin{cases} \frac{2}{9k}(bk^2 - b - 2k + 2), & \text{when } b \equiv 1 \text{ and } k \equiv 1; \\ \frac{2}{9k}(bk^2 - b - 2k - 2), & \text{when } b \equiv 2 \text{ and } k \equiv 2, \end{cases}$$

from which

$$Z_{d^0} - \frac{3}{2}c_3 = 2c_2^0 - \frac{c_1^0}{2} - \frac{3}{2}c_3 = \begin{cases} \frac{k-1}{3k}, & \text{when } b \equiv 1 \text{ and } k \equiv 1; \\ \frac{k+1}{3k}, & \text{when } b \equiv 2 \text{ and } k \equiv 2, \end{cases}$$

and the proof is done. \square

So all the E-optimal designs must have the same replication numbers as d^0 . Now uniformity of the treatment assignment will be investigated. It will be seen that while treatments 2 and 3 must be uniform, E-optimality can demand that treatment 1 not be uniform. Before embarking on the proof, some relationships will be derived for designs uniform in treatments 2 and 3.

To begin, suppose $b \equiv k \equiv 1 \pmod{3}$. With treatments 2 and 3 uniform, their block-wise replications are $n_{2l}, n_{3l} \in \{int(\frac{r}{b}), int(\frac{r}{b}) + 1\}$, where $int(\frac{r}{b}) = \frac{bk-1}{3k} = \frac{k-1}{3}$. Treatment 1 will be nonuniform in block l if and only if $n_{2l} = n_{3l} = \frac{k+2}{3}$ which would make $n_{1l} = \frac{k-4}{3}$. Thus (see (11)) the nonuniformity NU_1 of treatment 1 is $\frac{2}{k}x$, where x is the number of blocks in which $n_{1l} = \frac{k-4}{3}$.

Similarly, when $b \equiv k \equiv 2 \pmod{3}$ and treatments 2 and 3 are uniform, the nonuniformity NU_1 of treatment 1 is $\frac{2}{k}x$, where x is the number of blocks in which $n_{1l} = \frac{k+4}{3}$.

Then for any design uniform in treatments 2 and 3, $c_1 = c_1^0 - NU_1$. Establishing E-optimality will require knowledge of the maximum nonuniformity of treatment 1, that is, the largest possible value of NU_1 , given that treatments 2 and 3 are constrained to be uniform. This maximum is obtained with the following block assignments:

$b \equiv 1$ and $k \equiv 1$				$b \equiv 2$ and $k \equiv 2$			
n_{1j}	n_{2j}	n_{3j}	no. of blocks	n_{1j}	n_{2j}	n_{3j}	no. of blocks
$\frac{k+2}{3}$	$\frac{k-1}{3}$	$\frac{k-1}{3}$	$\frac{2b+1}{3}$	$\frac{k-2}{3}$	$\frac{k+1}{3}$	$\frac{k+1}{3}$	$\frac{2b-1}{3}$
$\frac{k-4}{3}$	$\frac{k+2}{3}$	$\frac{k+2}{3}$	$\frac{b-1}{3} = xmax$	$\frac{k+4}{3}$	$\frac{k-2}{3}$	$\frac{k-2}{3}$	$\frac{b+1}{3} = xmax$

(15)

where $xmax$ denotes the maximum number of blocks in which treatment 1 is nonuniform.

Let D denote the difference between the diagonal elements of d^0 :

$$D = c_1^0 - c_2^0 = \begin{cases} \frac{k-1}{3k}, & \text{when } b \equiv k \equiv 1; \\ \frac{k+1}{3k}, & \text{when } b \equiv k \equiv 2 \end{cases}. \quad (16)$$

The idea is to maintain uniformity in treatments 2 and 3, but to make treatment 1 nonuniform in such a way that c_1 is as close as possible to c_2^0 . Consider a design d^* uniform in treatments 2 and 3 and with treatment 1 nonuniform in $x^* = \min \left[xmax, int(\frac{D}{2/k}) \right]$ blocks. Note that

$$int\left(\frac{D}{2/k}\right) = \begin{cases} int\left(\frac{k-1}{6}\right), & \text{when } b \equiv k \equiv 1; \\ int\left(\frac{k+1}{6}\right), & \text{when } b \equiv k \equiv 2. \end{cases} \quad (17)$$

Theorem 3.1. *In $\mathcal{D}(3, b, k)$ with $bk \equiv 1 \pmod{3}$, design d^* is E-M-optimal.*

Proof. By (7), the E-value of d^* is

$$Z_{d^*} = 2c_2^0 - \frac{1}{2}c_1^* = \frac{3}{2}c_2^0 - \frac{1}{2}(D - \frac{2}{k}x^*). \quad (18)$$

First, consider settings where $xmax \geq \text{int}(\frac{D}{2/k})$ and so $x^* = \text{int}(\frac{D}{2/k})$. Designs which are nonuniform in treatments 2 and 3 will be eliminated first, followed by designs which are nonuniform in treatment 1 in a different number of blocks than d^* .

By (16), $D - \frac{2}{k}x^* \leq \frac{1}{k}$, and so

$$Z_{d^*} \geq \frac{3}{2}c_2^0 - \frac{1}{2k}. \quad (19)$$

Any design d nonuniform in treatment 2 will have $c_2 \leq c_2^0 - \frac{2}{k}$, and by Lemma 2.1, $Z_d \leq \frac{3}{2}c_2 < Z_{d^*}$. Therefore, any design nonuniform in treatment 2 will be E-inferior to d^* . By symmetry, the same result holds for designs nonuniform in treatment 3.

Any design d uniform in treatments 2 and 3 and with treatment 1 nonuniform in less than x^* blocks will have $c_1 > c_1^*$. So by (7) and (19), $Z_d = 2c_2^0 - \frac{c_1}{2} < Z_{d^*}$. Any design d uniform in treatments 2 and 3 with treatment 1 nonuniform in more than $x^* = \text{int}(\frac{D}{2/k})$ blocks will have $c_1 \leq c_2^0 - \frac{1}{k}$ (see (16)). Then (6) and (19) $\Rightarrow Z_d = \frac{3}{2}c_3 < Z_{d^*}$.

Now consider settings where $xmax < \text{int}(\frac{D}{2/k})$, so $x^* = xmax$. Using (12), (13), and (14),

$$Z_{d^*} = 2c_2^0 - \frac{1}{2}(c_1^0 - xmax \frac{2}{k}) = Z_{d^0} + \frac{xmax}{k} = \frac{bk - 1}{3}.$$

By (4) and Lemma 2.2, it is known that for any d , an upper bound for Z_d is $ub_d = c_2 + c_3 - \frac{c_1}{2}$. As usual, let n_{il} denote the number of times treatment i appears in block l . Now write $n_{1l} = n_1 + e_l$, where $n_1 = \text{int}(\frac{r_1}{b}) = \text{int}(\frac{bk+2}{3b})$, and $\sum_{l=1}^b e_l = r_1 - bn_1 = r + 1 - bn_1$. The e_l 's are the deviations from equal block-wise replications for treatment 1. For a given set of e_l 's, ub_d is maximized when $c_2 + c_3 = 2r - \frac{1}{k} \sum_{l=1}^b (n_{2l}^2 + n_{3l}^2)$ is maximized. Thus the assignment pattern for the n_{2l} 's and n_{3l} 's that maximizes $c_2 + c_3$ for given assignment of treatment 1 (and thus c_1) is

$$n_{2l} = n_{3l} = \frac{k - n_{1l}}{2} = \frac{1}{2}(k - n_1 - e_l).$$

Note that when $x^* = xmax$, d^* is a special case of this assignment pattern (as shown by the block-wise replications (15) for d^*). In general, call this assignment pattern \bar{d} . Although a design with

these block-wise replications does not exist if $k - n_1 - e_l$ is odd for some l , the bound $ub_{\bar{d}} \equiv \overline{ub}$ will be useful in showing the optimality of d^* . $C_{\bar{d}}$ has diagonal elements $c_1 = r + 1 - \frac{1}{k} \sum_{l=1}^b (n_1 + e_l)^2$ and $c_2 = c_3 = r - \frac{1}{4k} \sum_{l=1}^b (k - n_1 - e_l)^2$ so that

$$\begin{aligned} \overline{ub} &= 2c_2 - \frac{c_1}{2} = \frac{3}{2}r - \frac{1}{2} - \frac{1}{2k} \sum_{j=1}^b [(k - n_1 - e_j)^2 - (n_1 + e_j)^2] \\ &= \frac{3}{2}r - \frac{1}{2} - \frac{1}{2} \sum_{j=1}^b (k - 2n_1 - 2e_j) = \frac{3}{2}r - \frac{1}{2} - \frac{1}{2} [bk - 2(r+1)] \\ &= r = \frac{bk - 1}{3}. \end{aligned}$$

A key observation is that the upper limit \overline{ub} does not depend on the values of the e_l 's!

Now $Z_{d^*} = \overline{ub}$, which means that d^* is E-optimal. The only question remaining is whether there are other E-optimal designs. Again, $Z_d \leq ub_d \leq \overline{ub}$, and ub_d does not attain \overline{ub} for most designs. For a given assignment of treatment 1, if $n_{2l} \neq n_{3l}$ for some l , then $ub < \overline{ub}$. But $n_{2l} = n_{3l}$ for all $l \Rightarrow c_2 = c_3$. If $c_1 < c_2 = c_3$, then (6) gives $Z_d = \frac{3c_1}{2} < \overline{ub}$. Therefore, for $xmax < int(\frac{diff}{2/k})$, a design can be E-optimal only if $n_{2l} = n_{3l}$ for all l , and $c_1 \geq c_2$.

If $xmax < int(\frac{diff}{2/k})$ and other E-optimal designs exist, d^* is E-M-optimal because it has higher trace, and C_d has only two non-zero eigenvalues. \square

Example 3.1. As a simple example of a design, other than d^* , which is E-optimal, consider two blocks of size 50. Here are the block assignments for designs d^* and d' , both E-optimal with minimum eigenvalue $Z_{d^*} = Z_{d'} = r = 33$. These designs are E-superior to the uniform design d^0 which places treatment 1 on 17 units in each block.

d^* :	<table border="1" style="border: none;"> <thead> <tr> <th style="border: none;">j</th> <th style="border: none;">n_{1j}</th> <th style="border: none;">n_{2j}</th> <th style="border: none;">n_{3j}</th> </tr> </thead> <tbody> <tr> <td style="border: none;">1</td> <td style="border: none;">16</td> <td style="border: none;">17</td> <td style="border: none;">17</td> </tr> <tr> <td style="border: none;">2</td> <td style="border: none;">18</td> <td style="border: none;">16</td> <td style="border: none;">16</td> </tr> </tbody> </table>	j	n_{1j}	n_{2j}	n_{3j}	1	16	17	17	2	18	16	16
j	n_{1j}	n_{2j}	n_{3j}										
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2	18	16	16										

d' :	<table border="1" style="border: none;"> <thead> <tr> <th style="border: none;">j</th> <th style="border: none;">n_{1j}</th> <th style="border: none;">n_{2j}</th> <th style="border: none;">n_{3j}</th> </tr> </thead> <tbody> <tr> <td style="border: none;">1</td> <td style="border: none;">14</td> <td style="border: none;">18</td> <td style="border: none;">18</td> </tr> <tr> <td style="border: none;">2</td> <td style="border: none;">20</td> <td style="border: none;">15</td> <td style="border: none;">15</td> </tr> </tbody> </table>	j	n_{1j}	n_{2j}	n_{3j}	1	14	18	18	2	20	15	15
j	n_{1j}	n_{2j}	n_{3j}										
1	14	18	18										
2	20	15	15										

3.2 Block designs with $bk \equiv 2 \pmod{3}$

Theorem 3.2. *In $\mathcal{D}(3, b, k)$ with $bk \equiv 2 \pmod{3}$, the E-M-optimal designs are uniform with replications $r_1 = r_2 = \frac{bk+1}{3}$, and $r_3 = \frac{bk-2}{3}$.*

Proof. Here the maximin replication is $r = \frac{bk-2}{3}$. Consider a uniform design d^0 with $r_1 = r_2 = r+1$, and $r_3 = r$. Then $c_1^0 = c_2^0 > c_3^0$, and the E-value for d^0 is $Z_{d^0} = \frac{3}{2}c_3^0$ by (6).

Any design d with $r_3 \leq r$ will have $c_3 \leq c_3^0$, and therefore $Z_d \leq Z_{d^0}$, by Lemma 2.1. By the same argument, any other design with $r_i = r$ and not uniform in treatment i is E-inferior to d^0 . Therefore d^0 is E-optimal.

Since d^0 is uniform, C_{d^0} has maximum trace amongst all block designs. Since C_d has only two non-zero eigenvalues, d^0 is E-M-optimal. Any nonuniform design will have smaller trace, so no nonuniform design can be E-M-optimal.

Uniform designs with $r_i < r$ are E-inferior to d^0 by lemma 2.1, leaving only one possible competitor. A uniform design d with $r_1 = r+2$, and $r_2 = r_3 = r$ has $c_1 > c_3^0$ and $c_2 = c_3 = c_3^0$. For these values (7) gives $Z_d = 2c_3^0 - \frac{1}{2}c_1 < Z_{d^0}$. \square

4 Experiment size $m \equiv 1 \pmod{3}$

For this setting the maximin replication is $r = \frac{m-1}{3}$. Consider a uniform design d^0 with $r_1 = r+1$ and $r_2 = r_3 = r$, call it d^0 . By (7) the E-value for this design

$$Z_{d^0} = 2c_2^0 - \frac{c_1^0}{2} \tag{20}$$

Similar to lemma 3.1, it will be shown that d^0 is E-superior to any design with $r_3 \leq r-1$, reducing the class of E-competitors.

Lemma 4.1. *Designs for which $r_3 \leq r-1$ cannot be E-optimal for $m \equiv 1 \pmod{3}$ if $n > 2$, or if $n = 2$ and $(b_1, b_2) \neq (4, 4)$.*

Proof. It will be shown that $Z_{d^0} - \frac{3}{2}c_3 \geq 0$, where c_3 is the diagonal element of a uniform treatment

with replication $r_3 = r - 1$ and Z_{d^0} is given by (20). This implies that $Z_{d^0} - \frac{3}{2}c_3 \geq 0$ for any $r_3 \leq r - 1$, and thus by Lemma 2.1, d^0 is E-superior to any design which has $r_3 \leq r - 1$.

To do this, the following identities are required:

$$r \bmod b_j = r_{(b_j)} = \begin{cases} \frac{b_j-1}{3} & \text{when } b_j \equiv 1 \pmod{3}; \\ \frac{2b_j-1}{3} & \text{when } b_j \equiv 2 \pmod{3}. \end{cases} \quad (21)$$

$$r-1 \bmod b_j = (r-1)_{(b_j)} = \begin{cases} \frac{b_j-4}{3} & \text{when } b_j \equiv 1 \pmod{3}; \\ \frac{2b_j-4}{3} & \text{when } b_j \equiv 2 \pmod{3}. \end{cases} \quad (22)$$

Note that $(r-1)_{(b_j)} = r_{(b_j)} - 1$, so

$$\begin{aligned} b_j[2h(r, b_j) - \frac{1}{2}h(r+1, b_j) - \frac{3}{2}h(r-1, b_j)] &= -b_j[\frac{1}{2}\Delta h(r, b_j) - \frac{3}{2}\Delta h(r-1, b_j)] \\ &= -b_j[\frac{1}{2} + \frac{1}{b_j}(r - r_{(b_j)}) - \frac{3}{2} - \frac{1}{b_j}(r-1 - (r-1)_{(b_j)})] \\ &= b_j + 2(r - r_{(b_j)}) \end{aligned} \quad (23)$$

Now using (20) and (9):

$$\begin{aligned} Z_{d^0} - \frac{3}{2}c_3 &= 2r - \frac{r+1}{2} - \frac{3(r-1)}{2} + \frac{n-1}{m}[2r^2 - \frac{1}{2}(r+1)^2 - \frac{3}{2}(r-1)^2] \\ &\quad - \frac{1}{m} \sum_{j=1}^n b_j[2h(r, b_j) - \frac{1}{2}h(r+1, b_j) - \frac{3}{2}h(r-1, b_j)] \\ &\stackrel{(23)}{=} 1 + \frac{2}{m}(n-1)(r-1) - \frac{1}{m} \sum_{j=1}^n (b_j + 2r - 2 - 2(r-1)_{(b_j)}) \\ &= \frac{1}{m}(m + 2(n-1)(r-1) - \sum b_j - 2nr + 2n + 2 \sum (r-1)_{(b_j)}) \\ &= \frac{1}{m}(m - 2r + 2 - \sum b_j + 2 \sum (r-1)_{(b_j)}) \\ &= \frac{1}{3m}(m + 8 - 3 \sum b_j + 6 \sum (r-1)_{(b_j)}), \end{aligned} \quad (24)$$

since $r = \frac{m-1}{3}$. Write $y = \prod b_j + 8 - 3 \sum b_j + 6 \sum (r-1)_{(b_j)}$; $y \geq 0$ will be shown by induction. For the first induction step, check inequality for $n = 2$, with the two cases:

1. $b_1 \equiv b_2 \equiv 1 \pmod{3} \Rightarrow y \stackrel{(22)}{=} (b_1 - 1)(b_2 - 1) - 9 \geq 0$ with equality if and only if $b_1 = b_2 = 4$.
2. $b_1 \equiv b_2 \equiv 2 \pmod{3} \Rightarrow y \stackrel{(22)}{=} (b_1 + 1)(b_2 + 1) - 9 \geq 0$ with equality if and only if $b_1 = b_2 = 2$ (in which case no connected design exists).

By (22), $(r-1)_{(b_j)} \geq \frac{b_j-4}{3}$, with equality when $b_j \equiv 1 \pmod{3}$, so $y \geq \prod b_j - \sum b_j - 8(n-1)$.

For the second induction step, assume for $n \geq 3$ that $y \geq 0$ for $n-1$ factors, that is, $\prod_{j=1}^{n-1} b_j \geq \sum_{j=1}^{n-1} b_j + 8(n-2)$. This implies that $\prod_{j=1}^n b_j \geq [\sum_{j=1}^{n-1} b_j + 8(n-2)]b_n > \sum_{j=1}^n b_j + 8(n-1)$. Therefore $y \geq 0$ for any $n \geq 2$, and $y = 0$ if and only if $n = 2$ and $b_1 = b_2 = 4$ or $b_1 = b_2 = 2$. \square

Lemma 4.1 leaves open the possibility of different replications for the 4×4 layout. This case is easily disposed of by complete enumeration, which shows there are two E-optimal designs:

$$d_1 : \begin{array}{|c|c|c|c|} \hline 1 & 2 & 3 & 1 \\ \hline 2 & 3 & 1 & 2 \\ \hline 3 & 1 & 2 & 3 \\ \hline 1 & 2 & 3 & 1 \\ \hline \end{array} \qquad d_2 : \begin{array}{|c|c|c|c|} \hline 3 & 2 & 1 & 1 \\ \hline 1 & 3 & 2 & 1 \\ \hline 2 & 1 & 3 & 2 \\ \hline 2 & 1 & 2 & 3 \\ \hline \end{array}$$

Both designs are uniform, with replication vectors $(6, 5, 5)$ and $(6, 6, 4)$, respectively.

Henceforth assume $r_1 = r + 1$, $r_2 = r_3 = r$. Now uniformity of the treatment assignment will be investigated. It will be seen that while treatments 2 and 3 must be uniform, E-optimality can demand that treatment 1 not be uniform. Before embarking on the proof, some relationships will be derived for the case of treatments 2 and 3 uniform.

To begin, suppose $b_j \equiv 1 \pmod{3}$, which means that $mb_j^{-1} \equiv 1 \pmod{3}$. Every block of factor j has mb_j^{-1} cells. With treatments 2 and 3 uniform, their block-wise replications are $n_{2jl}, n_{3jl} \in \{\text{int}(\frac{r}{b_j}), \text{int}(\frac{r}{b_j}) + 1\}$, and by (21) $\text{int}(\frac{r}{b_j}) = \frac{mb_j^{-1}-1}{3}$. Treatment 1 will be nonuniform in block l of factor j if and only if $n_{2jl} = n_{3jl} = \frac{mb_j^{-1}+2}{3}$ which would make $n_{1jl} = \frac{mb_j^{-1}-4}{3}$. Thus (see (11)) the nonuniformity $NU_{1(j)}$ of treatment 1 due to factor j is $\frac{2}{mb_j^{-1}}x_j$, where x_j is the number of blocks of factor j in which $n_{1jl} = \frac{mb_j^{-1}-4}{3}$. Then for any design uniform in treatments 2 and 3, $c_1 = c_1^0 - NU_1$.

Establishing E-optimality will require knowledge of the maximum nonuniformity of treatment 1 in factor j , that is, the largest possible value of $NU_{1(j)}$, given that treatments 2 and 3 are constrained to be uniform. This maximum is obtained with the following block assignments:

$$b_j \equiv 1 \pmod{3}$$

$$\begin{array}{cccc} n_{1jl} & n_{2jl} & n_{3jl} & \text{no. of blocks} \\ \frac{mb_j^{-1}+2}{3} & \frac{mb_j^{-1}-1}{3} & \frac{mb_j^{-1}-1}{3} & \frac{2b_j+1}{3} \\ \frac{mb_j^{-1}-4}{3} & \frac{mb_j^{-1}+2}{3} & \frac{mb_j^{-1}+2}{3} & \frac{b_j-1}{3} = xmax_j \end{array} \quad (25)$$

where $xmax_j$ is the maximum number of blocks in which treatment 1 can be nonuniform in factor j . Similarly, when $b_j \equiv 2 \pmod{3}$, $NU_{1(j)} = \frac{2}{mb_j^{-1}}x_j$, where x_j is the number of blocks of factor j in which $n_{1jl} = \frac{mb_j^{-1}-4}{3}$. This is obtained with these block assignments:

$$\begin{array}{cccc}
& b_j \equiv 2 \pmod{3} & & \\
n_{1jl} & n_{2jl} & n_{3jl} & \text{no. of blocks} \\
\frac{mb_j^{-1}-2}{3} & \frac{mb_j^{-1}+1}{3} & \frac{mb_j^{-1}+1}{3} & \frac{2b_j-1}{3} \\
\frac{mb_j^{-1}+4}{3} & \frac{mb_j^{-1}-2}{3} & \frac{mb_j^{-1}-2}{3} & \frac{b_j+1}{3} = xmax_j
\end{array} \tag{26}$$

where now $xmax_j = \frac{b_j+1}{3}$.

Design d^0 was defined above as the uniform design with replications $r_1 = r + 1$, and $r_2 = r_3 = r$. Let D denote the difference between c_1^0 and c_2^0 .

$$\begin{aligned}
D = c_1^0 - c_2^0 &= 1 - \frac{1}{m} \sum_{j=1}^n b_j \Delta h(r, b_j) + \frac{n-1}{m} (2r+1) = \\
&= \frac{2mn + m + n - 1}{3m} - \frac{1}{m} \sum_{j=1}^n [b_j + 2(r - r(b_j))]
\end{aligned} \tag{27}$$

Now competitors to d^0 can be defined. The idea is to maintain uniformity in treatments 2 and 3, but to make treatment 1 nonuniform in such a way that c_1 is as close as possible to c_2^0 . Thus consider two designs, call them d^* and d_* , where for d^* , $c_1^* \geq c_2^0$, and for d_* , $c_{1*} \leq c_2^0$. To find the number of blocks x_j^* and x_{j*} of factor j in which treatment 1 should be made nonuniform, solve the following integer minimization/maximization problems:

$$\text{maximize } \frac{2}{m} \sum_{j=1}^n (b_j x_j^*), \quad \text{subject to } 0 \leq x_j^* \leq xmax_j \text{ and } \frac{2}{m} \sum_{j=1}^n (b_j x_j^*) \leq D \tag{28}$$

$$\text{minimize } \frac{2}{m} \sum_{j=1}^n (b_j x_{j*}), \quad \text{subject to } 0 \leq x_{j*} \leq xmax_j \text{ and } \frac{2}{m} \sum_{j=1}^n (b_j x_{j*}) \geq D \tag{29}$$

Note that (29) may not have a solution. This occurs exactly when $\frac{2}{m} \sum_{j=1}^n (b_j xmax_j) < D$.

Theorem 4.1. *For $m \equiv 1 \pmod{3}$, if $n > 2$, or if $n = 2$ and $(b_1, b_2) \neq (4, 4)$, E-M-optimal designs have the same block assignments as either d^* or d_* . Furthermore, d^* is E-M-optimal if and only if $\frac{1}{m} \sum_{j=1}^n b_j (3x_{j*} - x_j^*) \leq D$ or $\frac{2}{m} \sum_{j=1}^n (b_j xmax_j) < D$.*

When $n = 2$ and $b_1 = b_2 = 4$, an E-M-optimal design different from d^* and d_* exists, as discussed following lemma 4.1.

Proof. The E-values for the two proposed designs are

$$Z^* = 2c_2^0 - \frac{c_1^*}{2} \quad \text{and} \quad Z_* = \frac{3}{2}c_{1*} \quad (30)$$

where $c_1^* = c_2^0 + D - \frac{2}{m} \sum_{j=1}^n (b_j x_j^*)$, and $c_{1*} = c_2^0 + D - \frac{2}{m} \sum_{j=1}^n (b_j x_{j*})$. It can be easily seen that $Z^* \geq Z_*$ if and only if $D \geq \frac{1}{m} \sum_{j=1}^n b_j (3x_{j*} - x_j^*)$. In case of equality, design d^* is E-M better because $c_1^* > c_{1*}$.

By lemmas 2.1 and 2.2, the E-value of any design d with $c_2 = c_3 = c_2^0$ is $Z_d = \begin{cases} 2c_2^0 - \frac{c_1}{2} & \text{if } c_1 \geq c_2^0 \\ \frac{3}{2}c_1 & \text{if } c_1 < c_2^0 \end{cases}$.

The conditions on d^* and d_* imply $Z^* > 2c_2^0 - \frac{c_1}{2}$ if $c_1 \geq c_2^0$, and $Z_* > \frac{3}{2}c_1$ if $c_1 < c_2^0$. The goal is to show that any design nonuniform in treatments 2 or 3 cannot have a higher E-value than both d^* and d_* , so that E-M-optimal designs must have $c_2 = c_3 = c_2^0$.

First, note that by the definition of d^* , if $c_1^* - c_2^0 \geq \frac{2b_j}{m}$ then $x_j^* = \text{max}_j$, otherwise treatment 1 could have been made nonuniform in one more block of factor j . Also $c_1^* - c_2^0 \geq \frac{2b_j}{m}$ implies one of the following two statements are true:

1. $x_{j*} = 0$, for otherwise making treatment 1 nonuniform in $x_{j*} - 1$ blocks in direction j would bring c_1 closer to c_2^0 than at least one of c_1^* or c_{1*} ;
2. $x_j^* = \text{max}_j$ for all j and equation (29) has no solution.

In the latter situation, d^* will be shown to be E-M-optimal (see the last paragraph of this proof).

Now suppose

$$\begin{aligned} c_1^* - c_2^0 &\geq \frac{2b_j}{m} \text{ for all } j < s \\ c_1^* - c_2^0 &< \frac{2b_j}{m} \text{ for all } j \geq s \end{aligned} \quad (31)$$

for some $s \leq n$. It follows that

$$x_j^* = \text{max}_j \text{ and } x_{j*} = 0 \text{ for all } j < s. \quad (32)$$

This implies that $Z^* = 2c_2^0 - \frac{c_1^*}{2} > \frac{3}{2}c_2^0 - \frac{b_j}{m}$ for all $j \geq s$. Then any design which has treatment 2 nonuniform in any direction $j \geq s$ will have $c_2 \leq c_2^0 - \frac{2b_j}{m}$, and so by Lemma 2.1, (30) and (31), $Z_d \leq \frac{3}{2}c_2 \leq \frac{3}{2}c_2^0 - \frac{3b_j}{m} < Z^*$; this also applies for any design that has treatment 3 nonuniform in any direction $j \geq s$.

Thus, E-optimal designs have treatments 2 and 3 uniform in any direction $j \geq s$. Let $NU_{1(\geq s)}$ denote the nonuniformity of treatment 1 in directions $j \geq s$.

$$NU_{1(\geq s)} = \sum_{j=s}^n NU_{i(j)} = \frac{1}{m} \sum_{j=s}^n b_j \left[\sum_{l=1}^{b_j} n_{1jl}^2 - h(r+1, b_j) \right] \quad (33)$$

Similarly, define $NU_{1(< s)}$ as the nonuniformity of treatment 1 in directions $j < s$. Also let $NU_{1(\geq s)}^*$ and $NU_{1(\geq s^*)}$ represent treatment 1 nonuniformity in directions $j \geq s$ in designs d^* and d_* . By (28) and (29) there is no design d uniform in treatments 2 and 3 with $c_{1*} < c_{d1} < c_1^*$. Suppose there exists a design d' uniform in treatments 2 and 3 in directions $j \geq s$ which has $NU_{1(\geq s)}^* < NU_{1(\geq s)}' < NU_{1(\geq s^*)}$. It is claimed that this is not possible because it would contradict the preceding statement:

1. If $NU_{1(\geq s)}' \geq D$, arranging treatments 1, 2 and 3 uniformly in directions $j < s$ of d' , will result in $c_{1*} < c_1' \leq c_1^0 - D < c_1^*$ since $NU_{< s^*} = 0$ by (32).
2. If $D - \frac{2b_{s-1}}{m} < NU_{1(\geq s)}' < D$, arranging treatments 1, 2 and 3 uniformly in directions $j < s$ of d' , will result in $c_{1*} \leq c_1^0 - D < c_1' < c_1^*$, since by (31), $c_1^* - c_2^0 \geq \frac{2b_j}{m}$ for all $j < s$.
3. If $NU_{1(\geq s)}' \leq D - \frac{2b_{s-1}}{m}$ then $c_1' - c_2^0 \geq \frac{2b_j}{m}$ for all $j < s$ if all treatments of d' are uniform in all directions $j < s$. Note that $c_1^* - c_2^0 \geq \frac{2b_j}{m}$ for all $j < s$, as well. Now, keeping treatments 2 and 3 uniform in all directions, take $x_j' = x_{max_j} = x_j^*$ for all $j < s$, where treatment 1 of d' is nonuniform in x_j' blocks of direction $j < s$. Then $c_1' < c_1^0 - D$ by definition of c_1^* and the fact that $NU_{1(\geq s)}^* < NU_{1(\geq s)}'$, and so $c_1' < c_{1*}$ by definition of c_{1*} . Now decrease x_1' one unit at a time down to 0, then decrease x_2' one unit at a time down to 0, and so on, stopping as soon as $c_1' > c_1^0 - D$ is achieved. Due to the ordering on the b_j 's and consequently on the step sizes this procedure takes in changing c_1' , and since $NU_{1(\geq s)}^* < NU_{1(\geq s)}'$, the ending value must satisfy $c_1' < c_1^*$.

Each case says $c_{1*} < c_1' < c_1^*$ with a uniform arrangement of treatments 2 and 3 in d' , which contradicts (28) and (29). Hence, there is no competitor design, uniform in treatments 2 and

3 in directions $j \geq s$, which has $NU_{1(\geq s)}^* < NU_{1(\geq s)} < NU_{1(\geq s^*)}$. Also, any design which has $NU_{1(\geq s)} > NU_{1(\geq s^*)}$, will have $c_1 < c_1^*$ by (32), and thus $Z_d < Z_*$. Therefore any competitor must have treatments 2 and 3 uniform in directions $j \geq s$, and the nonuniformity of treatment 1 in directions $j \geq s$ must be $NU_{1(\geq s)} \leq NU_{1(\geq s)}^*$.

By lemma 2.2, any design d satisfies $Z_d \leq c_2 + c_3 - \frac{c_1}{2}$. Call this upper bound ub_d . Using (3) and (9), for the competitors remaining, the bound can be computed as:

$$\begin{aligned}
ub_d &= 2r - \frac{r+1}{2} + \frac{n-1}{m} \left(2r^2 - \frac{(r+1)^2}{2} \right) - \frac{1}{m} \sum_{j=1}^n [b_j \sum_{l=1}^{b_j} (n_{2jl}^2 + n_{3jl}^2 - \frac{n_{1jl}^2}{2})] \\
&= const_1 - \frac{1}{m} \sum_{j=1}^{s-1} [b_j \sum_{l=1}^{b_j} (n_{2jl}^2 + n_{3jl}^2 - \frac{n_{1jl}^2}{2})] \\
&\quad - \frac{1}{m} \sum_{j=s}^n [2b_j h(r, b_j) - b_j \frac{h(r+1, b_j)}{2}] + \frac{1}{2} NU_{1(\geq s)} \\
&= const_2 - \frac{1}{m} \sum_{j=1}^{s-1} [b_j \sum_{l=1}^{b_j} (n_{2jl}^2 + n_{3jl}^2 - \frac{n_{1jl}^2}{2})] + \frac{1}{2} NU_{1(\geq s)} \tag{34}
\end{aligned}$$

where $const_1$ and $const_2$ are constants, depending only on s and the dimensions of the hyperrectangle. Expression (34) depends on the nonuniformity of treatment 1 in every direction, and of treatments 2 and 3 in directions $j < s$. Note that d^* reaches its bound since $Z^* = 2c_2^0 - \frac{c_1^*}{2} = ub^*$.

Next it is shown that ub_d for any other design uniform in treatments 2 and 3 in directions $j \geq s$, and with $NU_{1(\geq s)} \leq NU_{1(\geq s)}^*$, cannot be higher than ub^* . Since $NU_{1(\geq s)} \leq NU_{1(\geq s)}^*$, it is sufficient to show that d^* minimizes the sum $\sum_{l=1}^{b_j} (n_{2jl}^2 + n_{3jl}^2 - \frac{n_{1jl}^2}{2})$ for each $j \leq s-1$. Given a set of block assignments for treatment 1, $(n_{1j1}, n_{1j2}, \dots, n_{1jb_j})$, this sum is minimized by setting $n_{2jl} = n_{3jl} = \frac{1}{2}(mb_j^{-1} - n_{1jl})$ for all l , with value

$$\sum_{l=1}^{b_j} (n_{2jl}^2 + n_{3jl}^2 - \frac{n_{1jl}^2}{2}) = \sum_{l=1}^{b_j} \frac{1}{2} [(mb_j^{-1} - n_{1jl})^2 - n_{1jl}^2] = \frac{m^2}{2b_j} - mb_j^{-1} \sum_{l=1}^{b_j} n_{1jl} = \frac{m^2}{2b_j} - mb_j^{-1}(r+1)$$

This value is the same for any $(n_{1j1}, n_{1j2}, \dots, n_{1jb_j})$, as long as $n_{2jl} = n_{3jl} = \frac{1}{2}(mb_j^{-1} - n_{1jl})$ for all l . For d^* this is achieved (see (32) and the block assignments in direction j when $x_j^* = xmax_j$ given by (25) and (26)). Thus ub is maximized by d^* .

This also proves that d^* is E-optimal when (29) has no solution (i.e. when $x_j^* = xmax_j$ for all j). In this case d^* reaches the absolute maximum of (34) because $n_{2jl}^* = n_{3jl}^*$ for any j and l . \square

In some cases, E-optimal designs other than d^* or d_* might exist, having treatments 2 and 3 nonuniform. However, C_{d^*} or C_{d_*} will have higher trace, meaning these competitors are inferior with respect to every criterion depending on both eigenvalues.

For a given hyperrectangle of size $b_1 \times b_2 \times \cdots \times b_n$, equations (28) and (29) must be solved numerically. A *Mathematica* program that computes x_j^* and x_{j*} for all j , and decides whether d^* or d_* is E-M-optimal, is available from the first author.

For convenience, some E-M-optimal assignments for 2 and 3 blocking factors are given in Table 1 and Table 2, respectively. The 4-tuples in Table 1 are $(b_1, b_2; x_1, x_2)$ for a $b_1 \times b_2$ row-column design with x_1 units of nonuniformity in rows and x_2 in columns, $b_1 \leq b_2 \leq 20$. For example, a 5×8 E-M-optimal row-column design has treatment 1 nonuniform in 0 rows and 1 column. Here is one such design, with treatment 1 nonuniform in the first column:

1	2	3	1	2	3	1	2
3	1	2	3	1	2	3	1
2	3	1	2	3	1	2	3
1	2	3	1	2	3	1	2
1	3	2	3	1	2	3	1

Similarly, Table 2 contains 6-tuples $(b_1, b_2, b_3; x_1, x_2, x_3)$ for 3-dimensional hyperrectangles and $b_1 \leq b_2 \leq b_3 \leq 10$, where x_j is the number of blocks of factor j where treatment 1 is nonuniform.

At least for two blocking factors, achievement of the required nonuniformity is usually accomplished quickly by trial and error. The construction problem has been solved in its full generality, for any number n of factors, in Parvu (2004).

5 Experiment size $m \equiv 2 \pmod{3}$

For this setting the maximin replication is $r = \frac{m-2}{3}$. Create a uniform design d^0 with $r_1 = r_2 = r+1$, and $r_3 = r$. Then (6) says $Z_{d^0} = \frac{3}{2}c_3^0$. Any design d must have some $r_i \leq r$, implying $c_i \leq c_3^0$ and hence $Z_d \leq \frac{3}{2}c_i \leq Z_{d^0}$. Therefore d^0 is E-optimal, and since uniformity implies maximal trace of the information matrix, it is E-M optimal. The main result of this section says that there are no

other E-M-optimal designs. There are, however, other E-optimal designs.

Theorem 5.1. *For $m \equiv 2 \pmod{3}$, E-M-optimal designs are uniform with replications $r_1 = r_2 = \frac{m+1}{3}$, $r_3 = \frac{m-2}{3}$.*

Proof. Competitors with $r_3 < r$ have $c_3 < c_3^0$, and hence by lemma 2.1, $Z_d < Z_{d^0}$. For $r_3 \geq r$, the only replication numbers different from those of d^0 are $r_1 = r + 2$, $r_2 = r_3 = r$. For such a design d , if either treatment 2 or treatment 3 is nonuniform, then again lemma 2.1 says $Z_d < Z_{d^0}$. Thus d must have $c_2 = c_3$ and so (7) $\Rightarrow Z_d = c_2 + c_3 - \frac{1}{2}c_1 = 2c_3^0 - \frac{1}{2}c_1 \leq \frac{3}{2}c_3^0$ with equality if and only if $c_1 = c_2 = c_3 = c_3^0$. But if this condition for E-optimality is met, trace of C_d is not maximal. \square

The proof says E-optimal (but not E-M-optimal) designs can be constructed whenever for replications $(r+2, r, r)$ and treatments 2 and 3 both uniform, treatment 1 can be made nonuniform in such a way that $c_1 = c_2 = c_3$; this is only sometimes possible. E-optimality without trace maximization can also be achieved with replications $(r+1, r+1, r)$, as follows. First, as already shown, treatment 3 must be uniform and so $c_3 = c_3^0$. Now for fixed $c_1 + c_2$ and c_3 , it is easy to show that Z_d in (5) is decreasing in $|c_1 - c_2|$. So by (6), $Z_d \leq \frac{3}{2}c_3^0$ with equality if and only if $c_1 = c_2 \geq c_3$. Consequently this d is E-optimal if and only if $NU_1 = NU_2$ and $c_1 - c_3 \geq 0$.

6 Discussion

The E-optimality problem has been solved for three treatments and arbitrary numbers of levels (b_1, \dots, b_n) of crossed blocking factors. The surprising results are those for settings with one more experimental unit than needed for equal replication, for example, 5×5 or 7×7 row-column layouts. While in all cases the best strategy is to replicate as equally as possible, in these cases the assignment of the treatment with largest replication is made nonuniformly. In effect, E-efficiency increases as trace of the information matrix decreases to the extent allowed by (28) and (29).

In results to be reported elsewhere, we have solved the A-problem for three treatments in row-column layouts. The two criteria sometimes agree, and sometimes disagree, on what design is best. The assignment conditions for A-optimality depend more crucially on the particular values of b_1 and b_2 , and not just on the mod 3 value of their product. Common to the A- and E-problems is that

maximal trace need not produce the best design. This phenomenon, now definitively established for $v = 3$, is a chief reason that optimality theory for general v is difficult for row-column designs.

The statistical literature is sorely lacking in design results for settings where equal replication is not possible. This work is a step towards addressing that shortcoming, so that design theory can move closer to having a complete, flexible catalog of optimal designs available for experimenters. Though as seen here, optimality investigations without “nice” divisibility conditions on the design parameters can be both challenging and counterintuitive, progress can and should be made.

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Table 1: E-M-optimal assignments for 2 blocking factors

(2,2;0,0)	(2,5;1,0)	(2,8;1,0)	(2,11;1,0)	(2,14;1,0)	(2,17;1,0)	(2,20;1,0)
(4,4;0,0)	(4,7;0,0)	(4,10;1,0)	(4,13;1,0)	(4,16;1,0)	(4,19;1,0)	(5,5;0,1)
(5,8;0,1)	(5,11;0,1)	(5,14;0,1)	(5,17;0,1)	(5,20;0,1)	(7,7;0,1)	(7,10;1,0)
(7,13;0,1)	(7,16;2,0)	(7,19;0,1)	(8,8;0,1)	(8,11;2,0)	(8,14;1,1)	(8,17;1,1)
(8,20;1,1)	(10,10;0,1)	(10,13;0,1)	(10,16;2,0)	(10,19;1,1)	(11,11;0,2)	(11,14;0,2)
(11,17;0,2)	(11,20;2,1)	(13,13;0,2)	(13,16;1,1)	(13,19;1,1)	(14,14;0,2)	(14,17;2,1)
(14,20;2,1)	(16,16;0,2)	(16,19;0,2)	(17,17;0,3)	(17,20;0,3)	(19,19;0,3)	(20,20;0,3)

Table 2: E-M-optimal assignments for 3 blocking factors

(2,2,4;0,1,0)	(2,2,7;1,1,0)	(2,2,10;1,1,0)	(2,4,5;1,0,1)	(2,4,8;0,1,1)	(2,5,7;0,1,1)	(2,5,10;0,1,1)
(2,7,8;1,0,2)	(2,8,10;0,2,1)	(4,4,4;0,1,1)	(4,4,7;1,1,1)	(4,4,10;0,1,2)	(4,5,5;0,1,2)	(4,5,8;1,0,3)
(4,7,7;0,2,2)	(4,7,10;0,2,3)	(4,8,8;1,2,3)	(4,10,10;0,3,3)	(5,5,7;1,2,2)	(5,5,10;0,2,3)	(5,7,8;2,2,3)
(5,8,10;2,3,3)	(7,7,7;2,2,2)	(7,7,10;2,2,3)	(7,8,8;2,3,3)	(7,10,10;2,3,3)	(8,8,10;3,3,3)	(10,10,10;3,3,3)