

# Optimal Blocking for Three Treatments and BIBD Robustness

## Two Problems in Design Optimality

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### Abstract

Design optimality plays a central role in the area of statistical experimental design. In general, problems in design optimality are composed of two vital, but separable, components. One of these is determining conditions under which a design is optimal (such as criterion bounds, values of design parameters, or special structure in the information matrix). The other is construction of designs satisfying those conditions. Most papers deal with either optimality conditions, or design construction in accordance with desired combinatorial properties, but not both. This dissertation determines optimal designs for three treatments in the one-way and multi-way heterogeneity settings, first proving optimality through a series of bounding arguments, then applying combinatorial techniques for their construction. Among the results established are optimality with respect to the well known  $E$  and  $A$  criteria.  $A$ - and  $E$ -optimal block designs and row-column designs with three treatments are found, for any parameter set.  $E$ -optimal hyperrectangles with three treatments are also found, for any parameter set. Systems of distinct representatives theory is used for the construction of optimal designs. Efficiencies relative to optimal criterion values are used to determine robustness of block designs against loss of a small number of blocks. Nonisomorphic balanced incomplete block designs are ranked based on their robustness. A complete list of most robust BIBDs for  $v \leq 10$ ,  $r \leq 15$  is compiled.

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# Chapter 1

## Introduction

### 1.1 The Field of Experimental Design

The field of experimental design as a branch of statistics is said to have been introduced by Sir Ronald A. Fisher. In one of his most enduring works ([11]), Fisher discussed the experiment that probably is the most famous in statistics. A certain lady from Rothamsted Experiment Station claimed that she could distinguish between cups of tea and milk mixed in different ways. Whether or not she could, is not the purpose of an experiment designer; how to construct an experiment which would give us the most information about the lady's capabilities is. Even a simple question, as this one about tea tasting, requires some thinking, and the statistics involved is not trivial. For further discussion on this experiment see Hinkelmann and Kempthorne [14].

Another pioneer who set the foundations for this field, introducing many of the classical designs, is Frank Yates, also a British statistician, and a collaborator of Fisher's for many years. He was one of the first to apply statistical methods to experimental biology (see Yates [34]). Two more giants need to be mentioned here, whose far-reaching contributions are foundational not only for this research, but for entire areas in experimental design. R.C. Bose, starting at the Indian Statistical Institute in the late 1930's, published widely influential work in combinatorial mathematics and design of experiments spanning five decades. His

ideas in [4] for constructing balanced incomplete block designs are used today in every conceivable discrete design situation. For a survey of the relations between statistical design and combinatorics see Bose [6]. Jack Kiefer developed the fundamental ideas of optimal design, ideas upon which most of the work in this dissertation is based ([16], [17], and [18] are three of his major papers). His model-based optimality approach has been criticized over the years, and rightly so in situations where models change depending on experimental results. However, in the area of block designs for discrete treatments (as opposed to regression designs or response surface designs for continuous variables), the regular additive model (1.1) is used in most situations, and there are no major concerns about the validity of the assumed model.

Over the years, the field of experimental design has continually grown because of the new problems brought to the fore by researchers in domains varying from agriculture to jet-engine construction.

## 1.2 Block Designs

Block designs originated in agricultural experiments. Suppose a study on the effects of different nutrients on turf grass is conducted on a hill with a certain slope. A safe assumption would be that turf plots grown at the top of the hill are more like each other and less like the plots at the bottom of the hill. A large study on the efficacy of different gasoline additives can require sampling cars in more than one city. Due to traffic and environmental similarities, performances of cars in the same city are likely to be more homogeneous than the entire group.

In such cases, experimental units are naturally divided into a few sets with systematic variation from set to set. This fact must be taken into account when analyzing the experiment, of course, but also before running the experiment, that is, when designing it. If ignored, this systematic variation can lead to an inability to detect differences among treatments, or in the best case reduce the precision with which the treatment effects are estimated. The groups

of homogeneous units are called blocks. In the gasoline additive example, the cities from which cars are sampled would represent the blocks. In the turf grass example, one should consider the hill gradient as a blocking factor; if ignored, large variability in response due to the slope of the hill could prevent the experimenter from detecting differences in nutrients.

In general, the experimenter should only use blocking if the groups are more homogeneous than the entire collection of experimental units. Otherwise, tests for comparisons of treatment effects will be less powerful, due to an over-parameterized model.

### 1.3 Model and Estimation

Let there be  $v$  treatments to be compared in  $b$  blocks of  $k$  experimental units each, hence having a total number of  $n = bk$  units. The model for the response will depend on the way the treatments are assigned to the experimental units in the various blocks, in other words the design  $d$ . The design is incorporated into the model through the design matrix  $A_d$ , which is an  $n \times v$  plot-treatment incidence matrix specifying the assignment of treatments to each experimental unit. Given  $A_d$ , the usual model is

$$Y = \mu\mathbf{1} + A_d\tau + L\beta + \varepsilon, \quad (1.1)$$

where  $Y$  is the  $n \times 1$  vector of yields,  $\mathbf{1}$  is a vector of ones,  $L$  is the  $n \times b$  plot-block incidence matrix, and  $\varepsilon$  is a vector of uncorrelated random errors with zero means and equal variances. Randomization theory says that in reality the errors of observations from the same block are correlated; however, the result of the least-squares equations are the same under the assumption of uncorrelated errors (see [14]). More general models might include a variance matrix for the errors, blocks with not all their sizes being equal, or more than one blocking factor.

The overall mean response,  $\mu$ , the vector of treatment effects,  $\tau$ , and the vector of block effects,  $\beta$ , are the unknown parameters in the model. The interest is in estimating treatment contrasts of the form  $c'\tau$ , where  $c$  is a  $v \times 1$  vector such that  $c'\mathbf{1} = 0$ . Let the  $i$ th treatment

be replicated  $r_{di}$  times in the design, and occur  $n_{dij}$  times in block  $j$ . The matrix  $N_d = (n_{dij})$  of order  $v \times b$  is called the treatment-block incidence matrix and plays an important role in the analysis of designs; its elements  $n_{dij}$  are called *block-wise replication numbers*. If  $\hat{\tau}$  is the estimate of the treatment effects vector, the normal equations for  $\hat{\tau}$  are given by:

$$C_d \hat{\tau} = Q_d, \quad (1.2)$$

where

$$Q_d = (A'_d - \frac{1}{k} N_d L') Y, \quad (1.3)$$

and

$$C_d = \text{diag} [r_{d1}, r_{d2}, \dots, r_{dv}] - \frac{1}{k} N_d N'_d. \quad (1.4)$$

The matrix  $C_d$  defined in (1.4) is in fact the information matrix, and is commonly called the  $C$ -matrix of the design. The contrast  $c'\tau$  is estimated by  $c'\hat{\tau}$ , where

$$\hat{\tau} = C_d^- Q_d \quad (1.5)$$

and  $C_d^-$  is any generalized inverse of the  $C_d$ -matrix. The variance of this estimate is:

$$\text{Var}_d(c'\hat{\tau}) = \sigma^2 c' C_d^- c, \quad (1.6)$$

where  $\sigma^2$  is the constant variance of the observations. Clearly this is a function of the design  $d$  because of  $C_d$ 's dependence on  $A_d$ .

In order to ease notation, the subscript  $d$  (for the  $C$ -matrix, the replication numbers, etc.) will be dropped when the design is clear.

## 1.4 Optimality of Block Designs

The main purpose of any block design is to estimate treatment contrasts of the form  $c'\tau$ , as discussed in the previous section. A design which can estimate all such contrasts is said to be connected. Thus, connectedness is the first requirement of any design, and disconnected

designs will not be evaluated in terms of optimality criteria here. That is not to say that there are no cases in which disconnected designs are used. There are situations when treatment structure can make disconnected designs advantageous, such as designs with certain treatment interactions confounded with block effects. However, in this dissertation we deal with problems where all treatment contrasts are of interest, which certainly is true for most experiments with unstructured treatments, and for many with factorial structure.

Consider a  $(v - 1) \times v$  matrix  $P$  whose rows are orthonormal and orthogonal to constant vectors; then  $P\tau$  consists of  $v - 1$  linearly independent contrasts which can be estimated, and any other contrast  $c'\tau$  can be written as a linear combination of contrasts belonging to  $P$ . Note that for a connected design  $C_d$  has rank  $v - 1$  because it has zero row and column sums. It follows from (1.6) that the variance-covariance matrix of the least squares estimators of  $P\tau$  is  $\sigma^2 PC_d^- P' = \sigma^2 (PC_d P')^{-1}$ . Thus, it is natural to specify some optimality criteria as functions  $\psi$  on the  $(v - 1) \times (v - 1)$  covariance matrices, and to pose the problem:

$$\text{Find } d \text{ to minimize } \psi((PC_d P')^{-1}). \quad (1.7)$$

A design solving this problem is said to be  $\psi$ -optimal. Moreover, if  $\psi$  is orthogonal invariant (i.e.  $\psi(AX) = \psi(X)$  for any orthogonal matrix  $A$ ), the solution has the desirable advantage of not depending on the choice of  $P$ . In fact, functions  $\psi$  which are orthogonal invariant are most common when designing practical experiments. For a more in depth discussion on the foundations of optimality and classes of optimality functions, see [16] and [18].

When  $\psi$  is orthogonal invariant, the optimality criterion can be written as a real function  $\Phi$  of the vector of  $v - 1$  nonzero eigenvalues of  $C_d$ :

$$z_d = (z_{d1}, \dots, z_{d(v-1)}), \quad \text{where } z_{d1} \geq z_{d2} \geq \dots \geq z_{d(v-1)} > z_{dv} = 0.$$

**Definition 1.1** (Kiefer, 1975). A design  $d^* \in \mathcal{D}$  is *universally optimal* in the class  $\mathcal{D}$  if its information matrix  $C_{d^*}$  minimizes every function  $\Phi(C_d)$  satisfying:

- (a)  $\Phi(C_d) = \Phi(P'C_dP)$ , where  $P$  is any  $v \times v$  permutation matrix,
- (b)  $\Phi$  is a convex function,
- (c)  $\Phi(bC_d)$  is nonincreasing in the scalar  $b > 0$ .

There are other classes of functions which encompass a large number of criteria, but the universal optimality paradigm is well known, and induces one of the larger such classes. Another important, closely related class consists of sums of non-decreasing, convex functions of the eigenvalues. To work with this class, the following definition is needed.

**Definition 1.2.** Let  $x, y \in \mathcal{R}^v$  be two  $v$ -dimensional vectors with coordinates written in decreasing order. Then  $x$  is weakly majorized by  $y$  (written as  $x \prec^w y$ ) if:

$$\sum_{i=1}^l x_{v+1-i} \geq \sum_{i=1}^l y_{v+1-i}$$

for each  $l = 1, 2, \dots, v$ .

Weak majorization and affiliated, other concepts of majorization are very useful and powerful tools in the study of inequalities. Many applications in mathematics and statistics are given in Marshall and Olkin [20].

**Definition 1.3.** A design  $d^*$  is said to be *Majorization-optimal* (in short, *M-optimal*) in a class  $\mathcal{D}$  if  $\Phi(C_d)$  is minimal among all designs  $d \in \mathcal{D}$ , for every  $\Phi : C_d \rightarrow \sum_{i=1}^{v-1} \phi(z_{di})$  for convex, decreasing  $\phi$ .

The relationship of this optimality concept with weak majorization is provided by the next result, proof for which can be found in [20].

**Theorem 1.1.**  $x \prec^w y$  if and only if  $\sum_{i=1}^{v-1} f(x) \leq \sum_{i=1}^{v-1} f(y)$  for every convex, decreasing function  $f : \mathcal{R} \rightarrow \mathcal{R}$

We will often use the simpler term “majorization” to mean “weak majorization,” for it is the only form of majorization considered here. In certain optimality problems, the notion of

majorization is useful in proving that one design is better than another. Suppose  $\mu_1$  and  $\mu_2$  are the vectors containing the eigenvalues of designs  $d_1$  and  $d_2$  respectively. Then,  $\mu_1 \prec^w \mu_2$  implies  $\Phi(\mu_1) \leq \Phi(\mu_2)$  for every  $\Phi$  as specified in Definition 1.3. Any such  $\Phi$  we call a *majorization criterion*, and we say that  $d_1$  is *M-better* than  $d_2$ .

Next we introduce some individual optimality criteria. The most widely used criteria are E-, A-, and D- optimality, which all satisfy the conditions of definitions 1.1 and 1.3.

**Definition 1.4.** A design  $d^* \in \mathcal{D}$  is *E-optimal* in the class  $\mathcal{D}$  if  $\frac{1}{z_{d^*(v-1)}} \leq \frac{1}{z_{d(v-1)}}$  for any design  $d \in \mathcal{D}$ .

This is a mini-max criterion, because it minimizes the maximum eigenvalue of the variance-covariance matrix  $(PC_dP')^{-1}$ , which is equivalent to maximizing the smallest nonzero eigenvalue of the *C*-matrix. The *E* criterion is statistically meaningful because an *E*-optimal design minimizes the maximum variance over all normalized contrasts.

**Definition 1.5.** A design  $d^* \in \mathcal{D}$  is *A-optimal* in the class  $\mathcal{D}$  if  $\sum_{i=1}^{v-1} \frac{1}{z_{d^*_i}} \leq \sum_{i=1}^{v-1} \frac{1}{z_{d_i}}$  for any design  $d \in \mathcal{D}$ .

Designs which are *A*-optimal minimize the trace of the variance-covariance matrix for estimating  $P\tau$ . Thus, *A*-optimal designs minimize the average variance for a set of  $v - 1$  normalized and linearly independent contrasts. *A*-optimality is also equivalent to minimizing the average of the variances of the  $\binom{v}{2}$  elementary treatment contrasts  $\widehat{\tau_i - \tau_{i'}}$ .

**Definition 1.6.** A design  $d^* \in \mathcal{D}$  is *D-optimal* in the class  $\mathcal{D}$  if  $\prod_{i=1}^{v-1} \frac{1}{z_{d^*_i}} \leq \prod_{i=1}^{v-1} \frac{1}{z_{d_i}}$  for any design  $d \in \mathcal{D}$ .

Designs which are *D*-optimal minimize the determinant of the variance-covariance matrix  $(PC_dP')^{-1}$  for estimating the complete set of orthonormal contrasts  $P\tau$ . *D*-optimal designs also minimize the volume of the confidence hyper-disc for estimating  $P\tau$ .

It is not unusual to find that there is more than one optimal design with respect to a specific criterion. In such cases, one may wish to determine the “best of the best,” that is, find the

$\psi_2$ -best design amongst all  $\psi_1$ -optimal designs for selected primary and secondary criteria  $\psi_1$  and  $\psi_2$ . Such a design would be said to be  $\psi_1$ - $\psi_2$ -optimal. We will encounter a variant of this in Chapter 4.

## 1.5 Some Classes of Block Designs

In this section, classical block designs most commonly used in practice are introduced. For an extensive review of the construction and analysis of these designs, see [14] and [28].

The simplest block design is the *randomized complete block design* (RCBD), where the block size  $k$  is equal to the number of treatments  $v$ . Within each block the  $v$  treatments are randomly assigned to the experimental units. Thus each treatment is replicated  $r_i = b$  times, where  $b$  is the number of blocks in the design.

An extension of the RCBD is the *generalized randomized block design* (GRBD), where the block size is a multiple of the number of treatments (i.e.  $k = sv$ ). Each treatment is replicated  $r_i = bs$  times, this being a random assignment to  $s$  experimental units in each block.

Incomplete block designs are designs where the number of treatments is larger than the block size. One such design is the *balanced incomplete block design* (BIBD), which satisfies the following conditions:

- (a) Each treatment occurs at most once in each block.
- (b) Each treatment occurs in exactly  $r$  blocks.
- (c) Each pair of treatments occurs together in  $\lambda$  blocks.

The parameters of the BIBD are  $v$ ,  $b$ ,  $r$ ,  $k$ , and  $\lambda$  and satisfy:

$$\begin{aligned} vr &= bk \\ \lambda(v-1) &= r(k-1) \end{aligned} \tag{1.8}$$

A BIBD with  $v = b$ , and thus  $r = k$  is called a symmetrical BIBD. A special property of a symmetrical BIBD is that any two blocks intersect in  $\lambda$  common treatments. Important early contributions to balanced incomplete block designs were made by Yates [33], Fisher [12], and Bose [4]. Experimental design texts with good accountings of BIBDs from a combinatorial perspective, and containing many references, are Raghavarao [28] and Street and Street [31].

An extension of the BIBD is the *balanced block design* (BBD), which is not necessarily incomplete, and satisfies the following incidence matrix conditions:

- (a) Replication numbers are equal:  $r_i = \sum_j n_{ij}$  constant.
- (b)  $\lambda_{ih} = \sum_j n_{ij}n_{hj}$  is constant for any  $i \neq h$ .
- (c)  $|n_{ij} - k/v| < 1$  for any  $i, j$ .

Note that an incomplete block design is a BIBD if it satisfies the above conditions. The last condition can be described as “all  $n_{ij}$  as nearly equal as possible.” As discussed in Chapter 2, a design which satisfies this condition will be called generalized binary. Further properties of BBDs and their  $C$ -matrices will be discussed in later chapters.

In some cases, designs for the elimination of two-way heterogeneity, where two blocking factors enter the model, are needed. These are called *row-column designs*, where the rows and columns represent the two blocking factors. The model for such a design is similar to the one given in (1.1):

$$Y = \mu 1 + A_d \tau + R\rho + L\gamma + \varepsilon, \quad (1.9)$$

where  $\rho$  and  $\gamma$  are the vectors of row and column effects respectively. A very useful design in this class is the *Latin square design* (LSD), which has the following property: The  $v$  treatments are arranged in a  $v \times v$  square such that every treatment occurs exactly once in each row and in each column. If in two Latin squares of the same order, when superimposed on one another, every ordered pair of symbols occurs exactly once, the two Latin squares are said to be orthogonal, and their superimposition is called a Graeco-Latin square. A set

of Latin squares where any two are orthogonal, is called a set of mutually orthogonal Latin squares (MOLS). For a given order  $v$ , the set of MOLS contains at most  $v - 1$  elements, and their superimposition is called a Hyper-Graeco-Latin square. MOLS are useful in the elimination of multi-way heterogeneity (i.e. more than two blocking factors). An interesting fact about MOLS is that Euler conjectured in 1782 that when  $v \equiv 2 \pmod{4}$  two orthogonal Latin squares cannot be constructed. After decades of effort with no counterexamples to this conjecture, it turned out to be false. Bose, Shrikande and Parker [5] presented methods of constructing MOLS that disprove Euler's conjecture for every  $v > 6$ .

All the designs described above are *universally optimal*. Another class of designs, which are either universally optimal, or at least  $A-$ ,  $D-$ , and  $E-$  optimal, are the Youden type designs. A *Youden Design* (YD), is a  $p \times q$  row-column design, where the columns form a BIBD, and the rows form a RCBD. As an example, consider the following Youden design, with  $v = 5$ :

1	2	3	4	5
2	3	4	5	1
3	4	5	1	2
4	5	1	2	3

The *Generalized Youden Design* (GYD) is a  $p \times q$  row-column design, where the columns form a BBD, and the rows also form a BBD. Cheng [7] introduced a further extension of the Youden designs: the *Youden hyperrectangle* (YH), which is a generalization of the GYDs for elimination of  $n$ -way heterogeneity,  $n > 2$ . For optimality characteristics of Youden designs see Cheng [7] and Kiefer [18].

## 1.6 Scope and Structure of Dissertation

Over the years, mathematicians as well as statisticians have worked countless hours to construct designs which envelop a certain number of symmetries. Problems like finding complete sets of orthogonal Latin Squares have been attacked by numerous authors in the last decades. Multiple papers have been written on necessary or sufficient conditions for the existence of BIBDs and special subclasses such as quasi-symmetric designs (BIBDs with only two block

intersection numbers). Topics like these are so endearing to specialists in combinatorics, that they feel the fundamental question in design theory is: Given  $v, k, \lambda$ , does there exist a balanced block design with these parameters?

The experimental design literature is generally split into two camps: one finds designs with nice combinatorial properties (many mathematicians, but statisticians also), while the other studies optimality properties (chiefly statisticians). There is no doubt that the contribution of combinatorialists to the field of statistical design is crucial; compiling tables of classical designs is of major importance. It is also true that, when available, these elegant designs are used in practice. However, there is an area which needs more attention than it now receives. Further research is needed for finding designs that are useful in discriminating among treatments, or optimizing levels in a response surface setting, and where classical, elegant designs cannot be used due to economical or technical reasons. Optimal designs should be found for parameters which do not allow a BIBD, or a GYD, or even an equireplicated design.

Much of this work is left to statisticians, because of their closer relationship to the ideas of information matrix and statistical optimality. The work of Wald [32], Kiefer [18], and Cheng [7], proving optimality of classical designs, the work of Jacroux [15] and others, finding optimality bounds, must be continued.

Some of the work in this dissertation is to find optimal designs which do not necessarily have nice combinatorial properties. The problem is therefore stated: Can optimal block designs be found for *any* set of parameters  $(v, b, k)$ ? Part of this research will be on optimal designs for different blocking schemes, when the number of treatments is three. Robustness of designs when a small number of observations is lost will also be studied.

The dissertation is organized in the following fashion: Chapter 2 gives the set of optimality tools which will be needed in later chapters. Chapter 3 contains some results on the  $A$ -optimality of block designs with three treatments in one- and two-way heterogeneity settings. Chapter 4 studies the  $E$ -optimality of block designs with three treatments in one- and multi-way heterogeneity settings. Chapter 5 pertains to robustness of BIBDs to the loss of a small

number of observations, including constructing robust designs using the computer. Finally, Chapter 6 contains conclusions and an overview of a multitude of future research topics in optimal block design.

# Chapter 2

## Review of Optimality Tools

A few general definitions and general results will be presented in this chapter. Also, this chapter will review literature which is pertinent to the subjects treated in the chapters that follow.

### 2.1 Binariness and Uniformity of treatments

**Definition 2.1.** In a block design setting, the assignment of treatment  $i$  is *binary* if  $n_{ij} \in \{0, 1\}$  for all  $j$ . In general, the assignment of treatment  $i$  is *generalized binary*, if its block-wise replication numbers satisfy  $|n_{ij} - k/v| < 1$  for all  $j$ .

As a verbal shorthand, “treatment  $i$  is binary” will be used for “the assignment of treatment  $i$  is binary.” A block design is said to be *binary (generalized binary)* if all the treatments are *binary (generalized binary)*. The notion of *generalized binarity* can be extended to designs with multiple blocking factors. For instance, a treatment can be generalized binary in the rows of a  $p \times q$  row-column design, if it is generalized binary when rows are considered as blocks. Generalized binary designs maximize the trace of the  $C$ -matrix in the class of designs with one blocking factor:

$$\text{trace}(C_d) = bk - h(bk, b), \tag{2.1}$$

for any generalized binary design  $d$ , for function  $h$  defined below in (2.4).

**Definition 2.2.** In a block design, the assignment of treatment  $i$  is said to be *uniform* if  $|n_{ij} - n_{ij'}| \leq 1$  for any blocks  $j$  and  $j'$ .

As before, “treatment  $i$  is uniform” is shorthand for “the assignment of treatment  $i$  is uniform.” A design is said to be *uniform* if all the treatments are uniform. The above definition can be extended to designs with multiple blocking factors. Note that if treatment  $i$  is generalized binary, it is automatically uniform as well. Also, if treatment  $i$  is uniform with a replication number such that  $b[\text{int}(\frac{k}{v})] \leq r_i \leq b[\text{int}(\frac{k}{v}) + 1]$  and  $v \nmid k$ , treatment  $i$  is also generalized binary. When  $v|k$ , a uniform treatment  $i$  is generalized binary if and only if its replication is  $r_i = bk/v$ .

## 2.2 Information Matrix of Designs for Elimination of Multi-Way Heterogeneity

The material in this section, along with more detailed derivations of the results can be found in Cheng [7]. The notation is also taken from the same paper.

In settings with multiple blocking factors, the experimental units are arranged in an  $n$ -dimensional hyperrectangle ( $n \geq 2$ ) of size  $b_1 \times b_2 \times \dots \times b_n$ , where  $b_i$  is the number of levels of the  $i$ th factor, and  $b_1 \leq b_2 \leq \dots \leq b_n$ . The total number of experimental units to be assigned to treatments is  $m = b_1 b_2 \dots b_n$ . The size of each block in direction  $j$  is  $mb_j^{-1}$ . Let  $N_j$  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 [7], we have:

$$C_d = \text{diag}(r_1, \dots, r_v) - \frac{1}{m} \sum_{j=1}^n b_j N_j N_j' + \frac{n-1}{m} \mathbf{r} \mathbf{r}', \quad (2.2)$$

where  $\mathbf{r}$  is the  $v \times 1$  replication vector. From the above equation it follows that the  $i$ th diagonal element of  $C_d$  can be computed as:

$$c_i = r_i - \frac{1}{m} \sum_{j=1}^n (b_j \sum_{l=1}^{b_j} n_{ijl}^2) + \frac{n-1}{m} r_i^2, \quad (2.3)$$

where  $n_{ijl}$  is the number of times treatment  $i$  occurs in block  $l$  of factor  $j$ .

If  $\sum_{l=1}^{b_j} n_{ijl} = r_i$  is fixed, then  $\sum_{l=1}^{b_j} n_{ijl}^2$  is minimized when the  $n_{ijl}$ 's are as close to each other as possible (i.e. treatment  $i$  is *uniform* in direction  $j$ ). Thus, given that treatment  $i$  has replication  $r_i$ , the diagonal element  $c_i$  will be maximized if treatment  $i$  is uniform in all directions. Define the function

$$h(r, b) = r + (2r - b) \operatorname{int}\left(\frac{r}{b}\right) - b \left[ \operatorname{int}\left(\frac{r}{b}\right) \right]^2. \quad (2.4)$$

The function  $h(r, b)$  gives us the minimum of  $\sum_{j=1}^b a_j^2$  subject to  $\sum_{j=1}^b a_j = r$  and  $a_j$ 's nonnegative integers. For any design where treatment  $i$  is uniform in all directions, we'll have  $\sum_{l=1}^{b_j} n_{ijl}^2 = h(r_i, b_j)$  for each  $j$ , and

$$c_i = r_i - \frac{1}{m} \sum_{j=1}^n (b_j h(r_i, b_j)) + \frac{n-1}{m} r_i^2. \quad (2.5)$$

The nonuniformity of treatment  $i$  ( $NU_i$ ), is defined as the difference between the diagonal element of a uniform treatment with the same replication and its actual diagonal element:

$$NU_i = \frac{1}{m} \sum_{j=1}^n (b_j \sum_{l=1}^{b_j} n_{ijl}^2) - \frac{1}{m} \sum_{j=1}^n b_j h(r_i, b_j). \quad (2.6)$$

Another useful quantity defined in Morgan [23] is  $\Delta h$ , the difference between  $h(r+1, b)$  and  $h(r, b)$ . Simple manipulation of function  $h(r, b)$  gives:

$$\Delta h(r, b) = h(r+1, b) - h(r, b) = 1 + \frac{2}{b}(r - r_{(b)}), \quad (2.7)$$

where  $r_{(b)} = r \bmod b$ . If we let  $r$  be any positive real number,  $h(r, b)$  is continuous and an increasing function of  $r$ . It is also differentiable at all points, except  $r = sb$ , for integers  $s$ . It is easy to see that  $h$  is increasing and differentiable in any open interval  $(sb, (s+1)b)$ , where  $\operatorname{int}\left[\frac{r}{b}\right]$  is just a constant. To show continuity, the next identity may be checked:

$$\lim_{r \uparrow sb} h(r, b) = \lim_{r \downarrow sb} h(r, b) = s^2 b \quad (2.8)$$

Thus,  $c_i$  given in (2.5) is also a continuous function of  $r_i$ , differentiable at all points, except  $r_i = sb_j$ , for integers  $s$ , and  $b_j$ 's the dimensions of the hyperrectangle.

**Lemma 2.1.** *If  $r_i \leq \frac{m+n-1-\sum_{j=1}^n b_j}{2}$ , the function  $c_i(r_i)$  is an increasing function of  $r_i$ .*

*Proof.* Using (2.5) and (2.7), one gets:

$$\begin{aligned} m[c_i(r_i + 1) - c_i(r_i)] &= m - \sum_{j=1}^n (b_j \Delta h(r_i, b_j)) + (n-1)(2r_i + 1) \\ &= m + n - 1 - 2r_i - \sum_{j=1}^n b_j + 2 \sum_{j=1}^n (r_i)_{(b_j)} \end{aligned}$$

□

For regular block designs, if  $r_i \leq \frac{b(k-1)}{2}$ , then  $c_i$  is an increasing function of  $r_i$ .

## 2.3 On Completely Symmetric Designs and Averaging of Information Matrices

An important class of designs is the class of completely symmetric designs, also referred to as variance balanced designs. The  $C$ -matrix of these designs can be written as  $\alpha(I_v - \frac{1}{v}J_v)$ , where  $\alpha$  is a constant, and  $J$  is a matrix of ones. The following result is Proposition 1 from Kiefer [18], and it is useful in proving optimality of many designs in this class.

**Theorem 2.1** (Kiefer 1975). *Suppose a design  $d^*$  in the class  $\mathcal{D}$  of designs has information matrix  $C_{d^*}$  for which*

(a)  $C_{d^*}$  is completely symmetrical

(b)  $\text{tr } C_{d^*} = \max_{d \in \mathcal{D}} \text{tr } C_d$ .

*Then  $d^*$  is universally optimal in  $\mathcal{D}$ .*

A useful technique for finding optimality bounds was introduced by Constantine [9]. This technique involves averaging the information matrix using permutations. We present this result below.

Let  $C$  be the  $v \times v$  information matrix of a design with eigenvalues  $z_1 \geq z_2 \geq \dots \geq z_{v-1} > z_v = 0$ . Define  $\bar{C}$  as:

$$\bar{C} = \frac{1}{s} \sum_{i=1}^s P_i' C P_i, \quad (2.9)$$

where the  $P_i$ 's are a collection of  $s \leq v!$  permutation matrices. The eigenvalues of  $\bar{C}$  are  $\bar{z}_1 \geq \bar{z}_2 \geq \dots \geq \bar{z}_{v-1} > \bar{z}_v = 0$ .

Note that the trace of  $C$  is equal to the trace of  $\bar{C}$ . Also any matrix  $P_i' C P_i$  has the same eigenvalues as  $C$ . By 9.G.1 in Marshall and Olkin [20] the eigenvalues of  $C$  majorize the eigenvalues of  $\bar{C}$ . So for any  $\Phi$  specified in Definition 1.3:

$$\Phi(\bar{C}) \leq \Phi(C). \quad (2.10)$$

That is,  $\bar{d}$  is  $M$ -better than  $d$ .

One implication of this averaging technique is  $\bar{z}_{v-1} \geq z_{v-1}$ , and thus  $C$  is  $E$ -inferior, or at best  $E$ -equal, to  $\bar{C}$ . A common use of the technique is to average (or symmetrize) the  $C$ -matrix over a subset of  $p$  treatments. To do this use the  $p!$  permutation matrices that operate on treatments  $1, 2, \dots, p$ .

# Chapter 3

## Some $A$ -optimal Designs with Three Treatments

### 3.1 Eigenvalues of a $3 \times 3$ Information Matrix

In general, the  $C$ -matrix for block designs in one-way, as well as in multi-way heterogeneity settings, is a symmetric, non-negative definite matrix. It also has the property that each row and column sum to zero. Thus, the  $C$ -matrix of a design with three treatments can be written in terms of its diagonal elements:

$$C_d = \begin{pmatrix} c_1 & \frac{1}{2}(-c_1 - c_2 + c_3) & \frac{1}{2}(-c_1 + c_2 - c_3) \\ \frac{1}{2}(-c_1 - c_2 + c_3) & c_2 & \frac{1}{2}(c_1 - c_2 - c_3) \\ \frac{1}{2}(-c_1 + c_2 - c_3) & \frac{1}{2}(c_1 - c_2 - c_3) & c_3 \end{pmatrix}, \quad (3.1)$$

where  $c_1$ ,  $c_2$ , and  $c_3$  correspond to treatments 1, 2, and 3. The eigenvalues of the matrix given in (3.1) are the roots of the following equation:

$$\det(C_d - \lambda I_3) = 0, \quad (3.2)$$

where  $I_3$  is the  $3 \times 3$  identity matrix. Simple algebra gives:

$$\begin{aligned} \det(C_d - \lambda I_3) &= \frac{1}{4}\lambda(3c_1^2 + 3c_2^2 + 3c_3^2 - 6c_1c_2 - 6c_2c_3 - 6c_1c_3 + 4c_1\lambda + 4c_2\lambda + 4c_3\lambda - 4\lambda^2), \\ \text{with roots } z_1 &= \frac{1}{2} \left[ \sum c_i + \sqrt{2 \sum_{i<j} (c_i - c_j)^2} \right], \\ z_2 &= \frac{1}{2} \left[ \sum c_i - \sqrt{2 \sum_{i<j} (c_i - c_j)^2} \right], \text{ and } z_3 = 0. \end{aligned} \quad (3.3)$$

## 3.2 The $A$ -value of a $3 \times 3$ Information Matrix

An  $A$ -optimal design minimizes the quantity  $\frac{1}{z_1} + \frac{1}{z_2}$ , where  $z_1$  and  $z_2$  are given in (3.3).

Thus, a design  $d^* \in \mathcal{D}$  must be found to minimize:

$$A\text{-value} = \frac{1}{z_1} + \frac{1}{z_2} = \frac{4}{3} \left( c_1 + c_2 + c_3 - 2 \frac{c_1^2 + c_2^2 + c_3^2}{c_1 + c_2 + c_3} \right)^{-1}, \quad (3.4)$$

which is equivalent to maximizing the quantity  $A$  given below:

$$A = c_1 + c_2 + c_3 - 2 \frac{c_1^2 + c_2^2 + c_3^2}{c_1 + c_2 + c_3}. \quad (3.5)$$

To find such designs, several lemmas are needed. In this section  $d(x, y, z)$  will denote a design whose  $C$ -matrix has diagonal elements  $c_1 = x$ ,  $c_2 = y$ , and  $c_3 = z$ . Note that  $x$ ,  $y$ , and  $z$  are non-negative numbers, because the  $C$ -matrix of any design is non-negative definite.

**Lemma 3.1.** *Given a design  $d^*(x^*, y^*, z^*)$ , consider a competitor  $d(x, y, z)$ . If*

$$(a) \quad x^* + y^* + z^* \geq x + y + z, \text{ and}$$

$$(b) \quad x^{*2} + y^{*2} + z^{*2} < x^2 + y^2 + z^2$$

*then  $d^*$  is  $A$ -superior to  $d$ .*

The above lemma follows directly from (3.5).

**Lemma 3.2.** *If  $x \geq y \geq z$ , then  $A$  increases as  $x$  increases if and only if  $x < -(y + z) + 2\sqrt{y^2 + yz + z^2}$ . A sufficient condition for this is  $x < (\sqrt{3} - 1)(y + z)$ . Also,  $A$  is an increasing function of  $y$  and  $z$  for  $x \geq y \geq z$ ,*

*Proof.* The partial derivative of  $A$  with respect to  $x$  is:

$$\frac{\partial A}{\partial x} = 1 - 2 \frac{2x(x + y + z) - x^2 - y^2 - z^2}{(x + y + z)^2} = \frac{4y^2 + 4z^2 + 4yz - (x + y + z)^2}{(x + y + z)^2}. \quad (3.6)$$

The partial derivative is positive if and only if the numerator is positive, which is equivalent to:

$$\begin{aligned} 4y^2 + 4z^2 + 4yz &> (x + y + z)^2 && \Leftrightarrow \\ x + y + z &< 2\sqrt{y^2 + yz + z^2} && \Leftrightarrow \\ x &< -(y + z) + 2\sqrt{y^2 + yz + z^2}. && (3.7) \end{aligned}$$

Since  $y^2 + yz + z^2 \geq \frac{3}{4}(y + z)^2$ , with equality when  $y = z$ , a sufficient condition for the numerator to be positive is  $x < (\sqrt{3} - 1)(y + z)$ .

Next, consider the partial derivative of  $A$  with respect to  $y$ :

$$\frac{\partial A}{\partial y} = \frac{4x^2 + 4z^2 + 4xz - (x + y + z)^2}{(x + y + z)^2}. \quad (3.8)$$

The numerator can be rewritten as:  $(x^2 - y^2) + 2x(x - y) + 2z(x - y) + 3z^2$ , which is obviously positive because  $x \geq y$ . Therefore  $A$  is an increasing function of  $y$ ; similarly, it can be checked that  $A$  is an increasing function of  $z$ .  $\square$

**Lemma 3.3.** *Given a uniform design  $d^*(x^* \geq y^* \geq z^*)$ , consider a nonuniform design  $d(x, y, z)$  with the same treatment replications as  $d^*$ . If  $x^* < (\sqrt{3} - 1)(y^* + z^*)$ , then  $d$  is  $A$ -inferior to  $d^*$ .*

*Proof.* Since uniform designs maximize the diagonal elements of the  $C$ -matrix among designs with same replications, we have  $x^* \geq x$ ,  $y^* \geq y$ , and  $z^* \geq z$ , with strict inequality for at least one element. The result follows immediately from lemma 3.2.  $\square$

**Lemma 3.4.** *Given a design  $d^*(x^*, y^*, y^*)$  with  $x^* > y^*$ , consider a competitor  $d(x, y, y)$ . If*

$$(a) \quad x^* < 2(\sqrt{3} - 1)y^*,$$

$$(b) \quad x + 2y \leq x^* + 2y^*, \text{ and}$$

$$(c) \quad y < y^*$$

then  $d$  is  $A$ -inferior to  $d^*$ .

*Proof.* If  $x \leq y^*$ , then  $d(x, y, y)$  is  $A$ -inferior to  $d(y^*, y^*, y^*)$  because the latter is completely symmetrical and of higher trace by (c). Also, by (a) and lemma 3.2,  $d(y^*, y^*, y^*)$  is  $A$ -inferior to  $d^*$ .

If  $y^* < x \leq x^*$ , then by (c) and lemma 3.2  $d(x, y, y)$  is  $A$ -inferior to  $d(x, y^*, y^*)$ , which is  $A$ -inferior to  $d^*$ .

If  $x > x^*$ , write  $x = x^* + a$ , and  $y = y^* - \frac{b}{2}$ . From (b) and (c) it follows that  $b \geq a > 0$ . We need to show that  $A^* - A > 0$ , where  $A^*$  and  $A$  are computed as in (3.5) for designs  $d^*(x^*, y^*, y^*)$  and  $d(x, y, y)$ :

$$\begin{aligned} A^* - A &= (x^* + 2y^*) - \frac{2(x^{*2} + 2y^{*2})}{x^* + 2y^*} - (x^* + 2y^* + a - b) + \frac{2[(x^* + a)^2 + 2(y^* - b/2)^2]}{x^* + 2y^* + a - b} \\ &= b - a - \frac{2(x^{*2} + 2y^{*2})}{x^* + 2y^*} + \frac{2(x^{*2} + 2y^{*2} + 2x^*a - 2y^*b + a^2 + b^2/2)}{x^* + 2y^* + a - b} \\ &= \frac{x^{*2}(a + 3b) - 8y^{*2}a + 4x^*y^*a + x^*(a^2 + 2ab) + y^*(2a^2 + 4ab)}{(x^* + 2y^*)(x^* + 2y^* + a - b)} \end{aligned}$$

Note that the denominator is positive. Since  $b > a > 0$  and  $x^* > y^*$ , it follows that  $x^{*2}(a + 3b) > 4ay^{*2}$  and  $4x^*y^*a > 4ay^{*2}$ , and thus:

$$A^* - A > \frac{x^*(a^2 + 2ab) + y^*(2a^2 + 4ab)}{(x^* + 2y^*)(x^* + 2y^* + a - b)} > 0$$

□

**Lemma 3.5.** *Given a design  $d^*(x^*, x^*, y^*)$  with  $x^* > y^*$ , consider a competitor  $d(x, x, y)$ . If*

(a)  $2x + y \leq 2x^* + y^*$ , and

(b)  $y < y^*$

then  $d$  is  $A$ -inferior to  $d^*$ .

*Proof.* First note that  $x < -(x+y) + 2\sqrt{x^2 + xy + y^2}$  for any  $x$  and  $y$ . Thus, if  $x \leq x^*$ , then by lemma 3.2,  $d(x, x, y)$  is  $A$ -inferior to  $d(x^*, x^*, y)$ , which by (b) and lemma 3.2 is  $A$ -inferior to  $d^*$ .

If  $x > x^*$ , then write  $x = x^* + \frac{a}{2}$ , and  $y = y^* - b$ . By (a) and (b), we have  $b \geq a > 0$ .

Similarly to the proof of lemma 3.4,  $A^* - A$  will be shown to be positive:

$$\begin{aligned} A^* - A &= b - a - \frac{2(2x^{*2} + y^{*2})}{2x^* + y^*} + \frac{2(2x^{*2} + y^{*2} + 2x^*a - 2y^*b + b^2 + a^2/2)}{2x^* + y^* + a - b} \\ &= \frac{8bx^{*2} - (3a + b)y^{*2} - 4bx^*y^* + x^*(2b^2 + 4ab) + y^*(b^2 + 2ab)}{(2x^* + y^*)(2x^* + y^* + a - b)} \end{aligned}$$

Since  $b > a > 0$  and  $x^* > y^*$ , it follows that  $(3a + b)y^{*2} < 4bx^{*2}$  and  $4bx^*y^* < 4bx^{*2}$ , and thus:

$$A^* - A > \frac{x^*(2b^2 + 4ab) + y^*(b^2 + 2ab)}{(2x^* + y^*)(2x^* + y^* + a - b)} > 0$$

□

### 3.3 $A$ -optimal Designs with One Blocking Factor

This section will find  $A$ -optimal designs in the regular  $(v, b, k)$  setting, where the number of treatments is  $v = 3$ , for any number of blocks  $b$ , and any block size  $k$ . We make the general assumption  $r_1 \geq r_2 \geq r_3$ . The diagonal elements of the  $C$ -matrix can be written as:

$$c_i = r_i - \frac{1}{k} \sum_{j=1}^b n_{ij}^2, \quad (3.9)$$

and if treatment  $i$  is uniform,

$$c_i = r_i - \frac{1}{k} h(r_i, b), \quad (3.10)$$

where  $h$  is defined in (2.4). The problem will be divided into three cases, depending on the value of  $bk \pmod 3$ . The main result of this section is stated below.

**Theorem 3.1.** *A block design with three treatments is  $A$ -optimal in the class  $\mathcal{D}(3, b, k)$  if and only if it is generalized binary and has the following replication numbers:*

- (a)  $r_1 = r_2 = r_3 = \frac{bk}{3}$  when  $bk \equiv 0 \pmod 3$ ,
- (b)  $r_1 = \frac{bk+2}{3}$ , and  $r_2 = r_3 = \frac{bk-1}{3}$  when  $bk \equiv 1 \pmod 3$ ,
- (c)  $r_1 = r_2 = \frac{bk+1}{3}$ , and  $r_3 = \frac{bk-2}{3}$  when  $bk \equiv 2 \pmod 3$ .

### 3.3.1 Case 1: $bk \equiv 0 \pmod 3$

For this setting we can create a generalized binary balanced design (BBD), which is universally optimum by Theorem 2.1. The  $C$ -matrix of this type of design is given by:

$$C_{BBD} = \frac{3}{2}[r - h(r, b)]I_3 - \frac{1}{2}[r - h(r, b)]J_3, \quad (3.11)$$

where  $r = bk/3$ . To eliminate other competitors, note that  $C_{BBD}$  is completely symmetric and of maximum trace in the class  $\mathcal{D}(3, b, k)$ . Since universal optimality implies maximal trace, any design that is not generalized binary cannot be universally optimal. Likewise a generalized binary design with unequal replications cannot have complete symmetry of its information matrix, so does not have equality of its nonzero eigenvalues, implying (by majorization) that it is not universally optimal.

### 3.3.2 Case 2: $bk \equiv 2 \pmod 3$

First consider a generalized binary design  $d^0(c_1^0, c_1^0, c_3^0)$ , with replications  $r_1 = r_2 = r + 1$ , and  $r_3 = r$ , where  $r = \frac{bk-2}{3}$ . It will be shown that  $d^0$  is  $A$ -optimal.

Consider a design  $d(c_1, c_2, c_3)$  with  $r_3 < r$ . Symmetrize  $d$  on treatments 1 and 2 as in (2.9) to produce  $\bar{d}(\bar{c}_1, \bar{c}_1, c_3)$ , where  $\bar{c}_1 = \frac{c_1+c_2}{2}$ . Since  $tr(C_d) = tr(C_{\bar{d}})$  and  $c_1^2 + c_2^2 \geq 2\bar{c}_1^2$ , it follows

from lemma 3.1 that  $A_d \leq A_{\bar{d}}$ . Treatment 3 is generalized binary and has higher replication in  $d^0$  than in  $d$ , so  $c_3^0 > c_3$ . Also,  $C_{d^0}$  has maximum trace, so the conditions of lemma 3.5 are satisfied. Therefore  $d^0$  is  $A$ -superior to  $\bar{d}$ , which is  $A$ -superior to  $d$ .

Since designs with  $r_3 < r$  are  $A$ -inferior to  $d^0$ , the only candidates left are designs with replications  $r_1 = r + 2$  and  $r_2 = r_3 = r$ , or  $r_1 = r_2 = r + 1$  and  $r_3 = r$ . Note that for generalized binary designs with these replications,  $c_1$  is maximum when  $r_1 = r + 2$  and  $c_2 + c_3$  is minimum when  $r_2 = r_3 = r$ . Hence, if we can show that  $c_1 < 2(\sqrt{3} - 1)c_2$  for a generalized binary design with replications  $r_1 = r + 2$  and  $r_2 = r_3 = r$ , then by lemma 3.3 the nonbinary competitors are eliminated. Using (3.10) we obtain:

$$c_1 = \frac{bk+4}{3} - \frac{1}{k}h\left(\frac{bk+4}{3}, b\right) = \begin{cases} \frac{2(k-1)(bk+b+2)}{9k} & \text{if } k \equiv 1 \pmod{3} \\ \frac{2(k+1)(bk-b+2)}{9k} & \text{if } k \equiv 2 \pmod{3} \end{cases} \quad \text{and}$$

$$c_2 = c_3 = \frac{bk-2}{3} - \frac{1}{k}h\left(\frac{bk-2}{3}, b\right) = \begin{cases} \frac{2(k-1)(bk+b-1)}{9k} & \text{if } k \equiv 1 \pmod{3} \\ \frac{2(k+1)(bk-b-1)}{9k} & \text{if } k \equiv 2 \pmod{3} \end{cases}.$$

So  $c_1 < 2(\sqrt{3} - 1)c_2$  if and only if  $\frac{c_1}{c_2} < 2(\sqrt{3} - 1)$ , which can be easily checked. Therefore, by lemma 3.3, the only two designs left to consider are  $d^0$  and a generalized binary design  $d'$  with replications  $r_1 = r + 2$  and  $r_2 = r_3 = r$ . These designs have equal trace, so by (3.5) the better design is the one which minimizes  $\sum_i c_i^2 = \frac{1}{3}[(\sum_i c_i)^2 + \sum_{i < j} (c_i - c_j)^2]$ . For  $d^0$  we have  $\sum_{i < j} (c_i - c_j)^2 = 2(c_1^0 - c_3^0)^2$ , and for  $d'$  we have  $\sum_{i < j} (c_i - c_j)^2 = 2(c'_1 - c'_2)^2$ . Since  $c'_2 = c_3^0 < c_1^0 < c'_1$ , it follows that  $d^0$  minimizes  $\sum_i c_i^2$ .

In conclusion,  $d^0$  is  $A$ -optimal in the class  $\mathcal{D}(3, b, k)$ , with  $bk \equiv 2 \pmod{3}$ . Also, it has been shown that other designs (i.e. with different replications, or nonbinary) are strictly  $A$ -inferior to  $d^0$ .

### 3.3.3 Case 3: $bk \equiv 1 \pmod{3}$

The arguments of this case are similar to the ones in the previous case. We start off with a generalized binary design  $d^0(c_1^0, c_2^0, c_2^0)$  with replications  $r_1 = r + 1$  and  $r_2 = r_3 = r$ , where  $r = \frac{bk-1}{3}$ . It will be shown that  $d^0$  is  $A$ -optimal.

First we eliminate designs with  $r_1 > r + 1$ . Consider a competitor design  $d(c_1, c_2, c_3)$  with replications  $(r_1 > r + 1, r_2, r_3)$ . Symmetrize  $d$  over treatments 2 and 3 to obtain  $\bar{d}(\bar{c}_1, \bar{c}_2, \bar{c}_2)$ , where  $\bar{c}_1 = c_1$  and  $\bar{c}_2 = \frac{c_2 + c_3}{2}$ . As discussed in Section 2.3,  $\bar{d}$  is  $A$ -superior to  $d$ . To show that  $d^0$  is  $A$ -superior to  $\bar{d}$ , we verify the three conditions of Lemma 3.4.

The first condition requires  $2(\sqrt{3} - 1)c_2^0 - c_1^0 > 0$ . Using (3.10), we get:

$$2(\sqrt{3}-1)c_2^0 - c_1^0 = \begin{cases} \frac{2}{9k}(k-1)[b(k+1)(2\sqrt{3}-3) - \sqrt{3}], & \text{if } b \equiv k \equiv 1 \pmod{3}; \\ \frac{2}{9k}(k+1)[b(k-1)(2\sqrt{3}-3) - \sqrt{3}], & \text{if } b \equiv k \equiv 2 \pmod{3}. \end{cases} \quad (3.12)$$

Both expressions are positive for any  $b \geq 2$ ,  $k \geq 2$ , except  $b = k = 2$ . There is only one connected design with  $v = 3$ ,  $b = k = 2$ , and that design is  $d^0$ . The second condition of Lemma 3.4 is satisfied, since  $d^0$  is generalized binary, and thus of maximal trace. To verify the third condition, we need  $c_2^0 > \bar{c}_2$ . So,

$$\begin{aligned} 2\bar{c}_2 &= bk - r_1 - \frac{1}{k} \sum_{j=1}^b (n_{2j}^2 + n_{3j}^2) \leq bk - r_1 - \frac{1}{k} h(bk - r_1, 2b), \\ 2c_2^0 &= bk - r_1^0 - \frac{1}{k} \sum_{j=1}^b [(n_{2j}^0)^2 + (n_{3j}^0)^2] = bk - r_1^0 - \frac{1}{k} h(bk - r_1^0, 2b), \end{aligned}$$

the latter being true since  $d^0$  is generalized binary with  $r_2^0 = r_3^0 = r$ , and  $2h(r, b) = h(2r, 2b)$ .

These expressions have the form of the diagonal element of an information matrix for a uniform treatment with replications  $bk - r_1$  and  $bk - r_1^0$  times, respectively, in a block design with  $b' = 2b$ ,  $k' = k$ . Note that  $bk - r_1 < bk - r_1^0 \leq b(k-1) = \frac{b'(k'-1)}{2}$  for any  $k \geq 3$ , and thus by Lemma 2.1,  $2\bar{c}_2 < 2c_2^0$  for any  $k \geq 3$ . If  $k = 2$ :

$$2c_2^0 - 2\bar{c}_2 \geq r_1 - r_1^0 + \frac{1}{2} h(2b - r_1, 2b) - \frac{1}{2} h(2b - r_1^0, 2b) = \frac{r_1 - r_1^0}{2} > 0$$

and so all designs with  $r_1 > r + 1$  are eliminated by Lemma 3.4.

The remaining competitors must have either  $r_1 = r_2 = r + 1$ ,  $r_3 = r - 2$ , or  $r_1 = r + 1$ ,  $r_2 = r_3 = r$ . Nonuniform designs with these replications are eliminated using Lemma 3.3 and after averaging over treatments 2 and 3 for the former case, (3.12). Comparing the uniform design  $d'$  with  $r_1 = r_2 = r + 1$ ,  $r_3 = r - 2$  versus  $d^0$ , we get:

$$A_{d^0} - A_{d'} = \begin{cases} \frac{2}{3bk(k+1)}(k-1), & \text{if } b \equiv k \equiv 1 \pmod{3}; \\ \frac{2}{3bk(k-1)}(k+1), & \text{if } b \equiv k \equiv 2 \pmod{3}. \end{cases}$$

Both expressions are positive for any  $b \geq 2$ ,  $k \geq 2$ , and so  $d^0$  is  $A$ -superior to  $d'$ .

### 3.4 $A$ -optimal Row-Column Designs

Designs with two blocking factors are called row-column designs. The parameters of these designs are  $p$ , the number of rows in the design,  $q$ , the number of columns in the design, and  $v$ , the number of treatments. In our case  $v = 3$ , and it will be assumed without loss of generality that  $p \leq q$ . The model for such a design is given in (1.9). The information matrix can be found as the special case of (2.2) with  $n = 2$ :

$$C_d = \text{diag}(r_1, \dots, r_v) - \frac{1}{p}N_dN'_d - \frac{1}{q}M_dM'_d + \frac{1}{pq}\mathbf{r}\mathbf{r}', \quad (3.13)$$

where  $N_d$  and  $M_d$  are the column-treatment and row-treatment incidence matrices, respectively. The diagonal element of  $C_d$  corresponding to a uniform treatment  $i$  can be written as:

$$c_{ii} = r_i - \frac{1}{p}h(r_i, q) - \frac{1}{q}h(r_i, p) + \frac{r_i^2}{pq}, \quad (3.14)$$

where  $h(r_i, q)$  is as defined in (2.4). For given  $p$  and  $q$ , the function  $c_i(r_i)$  is a continuous function of  $r_i$ . The function is not differentiable at  $r_i = sp$  or  $r_i = sq$  for positive integers  $s$ ; at these points the values of  $\text{int}[\frac{r_i}{p}]$  and  $\text{int}[\frac{r_i}{q}]$  in the component functions  $h$  change. In the following sections, the quantity  $A$  defined in (3.5) will be differentiated with respect to  $r_i$  and the derivative will take several forms depending on  $\text{int}[\frac{r_i}{p}]$  and  $\text{int}[\frac{r_i}{q}]$ . The integer values at boundary cases when  $r_i = sp$  or  $r_i = sq$ , will be treated the same as when  $(s-1)p \leq r_i < sp$  or  $(s-1)q \leq r_i < sq$ , respectively, since  $c_i(r_i)$  is continuous.

Note that the matrix  $X = \frac{1}{q}M_dM'_d - \frac{1}{pq}\mathbf{r}\mathbf{r}'$  is a non-negative definite matrix. When the rows in the design are permutations of each other,  $X$  is the null matrix. Further, if the design is generalized binary in columns, then trace of  $C_d$  is maximum. In fact, for any design  $d$

$$\Phi(\text{diag}(r_1, \dots, r_v) - \frac{1}{p}N_dN'_d) \leq \Phi(C_d), \quad (3.15)$$

for any majorization preserving function  $\Phi$  of the eigenvalues of  $C_d$ . The eigenvalues of the information matrix for the column component design majorize the eigenvalues of the

information matrix for the row-column design. This makes sense, because eliminating only one blocking factor results in more information available for estimating the treatment effects. Similar to the previous section, the task of finding  $A$ -optimal row-column designs can be divided into several parts based on the values of  $p \pmod 3$  and  $q \pmod 3$ .  $A$ -optimal designs maximize the quantity  $A$  defined in (3.5).

### 3.4.1 Case 1: $pq \equiv 0 \pmod 3$

When the number of experimental units in the row-column design is a multiple of  $v$  with  $v$  prime, a Generalized Youden Design (GYD) is universally optimal (see Cheng [7]). When  $v = 3$  and  $3|pq$ , a GYD can always be constructed. The information matrix of such a design is completely symmetrical and of maximum trace. In our case, assume without loss of generality that  $3|p$ .  $C_d$  can be written as the information matrix of a balanced block design with  $b = q$  and  $k = p$ :

$$C_{GYD} = \frac{3}{2}[r - h(r, q)]I_3 - \frac{1}{2}[r - h(r, q)]J_3, \quad (3.16)$$

where  $r = \frac{pq}{3}$ .

### 3.4.2 Case 2: $p \equiv 1 \pmod 3$ and $q \equiv 1 \pmod 3$

When equireplicated designs do not exist, as in this case, the general strategy for finding  $A$ -optimal designs is:

- (1) reduce the range of possible replication numbers to a small interval in the neighborhood of  $r = \text{int}[\frac{pq}{3}]$  by eliminating competitors outside of this given range,
- (2) eliminate nonuniform designs with replications in the given range,
- (3) find the uniform  $A$ -optimal design with replications in the given range.

Assume that  $q = p + 3m$ , for integer  $m \geq 0$ . Construct design  $d^*$  as follows. In a  $p \times p$  Latin square, replace all copies of  $\frac{p+2}{3}$  of the symbols with treatment 1, all copies of  $\frac{p-1}{3}$  of the

symbols with treatment 2, and all copies of the remaining  $\frac{p-1}{3}$  symbols with treatment 3. For  $m > 0$ , adjoin to this a  $p \times 3m$  generalized Youden design with three treatments. Thus the resulting design is generalized binary, and has replications:

$$r_1^* = \frac{p(q+2)}{3} \quad r_2^* = r_3^* = \frac{p(q-1)}{3}. \quad (3.17)$$

For  $d^*$ , rows are permutations of each other, and thus the matrix  $C_{d^*}$  can be written as the information matrix of a block design with  $v = 3, b = q$ , and  $k = p$ . Also, since  $d^*$  is generalized binary,  $C_{d^*}$  is of maximal trace both among row-column designs, and among block designs with  $v = 3, b = q$ , and  $k = p$ .

**Theorem 3.2.** *The design  $d^*$  is  $A$ -optimal.*

Let  $d$  be any competitor design with  $r_1 \geq r_2 \geq r_3$ . The proof of this result will be accomplished by adopting the general strategy outline above to eliminating all competitors in 4 steps:

- (1) Eliminate all designs with  $r_1 > \frac{p(q+2)}{3}$ ,
- (2) Eliminate all nonuniform designs with  $r_i \in [\frac{p(q-4)}{3}, \frac{p(q+2)}{3}]$ ,
- (3) Eliminate all designs with  $r_3 < \frac{p(q-1)}{3}$ ,
- (4) Show that among uniform designs with replications  $r_i \in [\frac{p(q-1)}{3}, \frac{p(q+2)}{3}]$ ,  $d^*$  is  $A$ -optimal.

**Step 1.** Let design  $d$  have replication  $r_1 > \frac{p(q+2)}{3}$ . Using the averaging technique described in Section 2.3, let  $\bar{c}_1, \bar{c}_2, \bar{c}_2$  be the diagonal elements of the information matrix for the column component design, after averaging on treatments 2 and 3. In order to show that design  $d^*$  is superior to  $d$ , we will use Lemma 3.4 for designs  $d^*(c_1^*, c_2^*, c_2^*)$  and  $\bar{d}(\bar{c}_1, \bar{c}_2, \bar{c}_2)$ . Note that averaging of information matrices with identical trace results in a matrix with the same trace. Since  $d^*$  is of maximal trace among column component designs, condition (b) of Lemma 3.4 is satisfied.

To verify part (c) of Lemma 3.4, we must show that  $c_2^* > \bar{c}_2$ . Note that  $\text{int}[\frac{p(q-1)}{3q}] = \frac{p-1}{3}$ , so

$$\begin{aligned}
2c_2^* &= \frac{2p(q-1)}{3} - \frac{2}{p}h\left(\frac{p(q-1)}{3}, q\right) \\
&\stackrel{(2.4)}{=} \frac{2p(q-1)}{3} - \frac{2}{p}\left[\frac{p(q-1)}{3} + \left(2\frac{p(q-1)}{3} - q\right)\frac{p-1}{3} - q\frac{(p-1)^2}{9}\right] \\
&= \frac{2(p-1)}{9p}[p(2q-1) + 2q] \tag{3.18} \\
2\bar{c}_2 &= pq - r_1 - \frac{1}{p}\sum_{j=1}^q(n_{2j}^2 + n_{3j}^2) \\
&\leq pq - r_1 - \frac{1}{p}h(pq - r_1, 2q)
\end{aligned}$$

The last quantity is the same as the diagonal element of a information matrix corresponding to a uniform treatment replicated  $pq - r_1$  times in a block design with  $b = 2q$  and  $k = p$ . Therefore, it is decreasing in  $r_1$  by lemma 2.1, and its maximum is achieved when  $r_1 = \frac{p(q+2)}{3} + 1$ . Thus,

$$\begin{aligned}
2\bar{c}_2 &\leq pq - \frac{p(q+2)}{3} - 1 - \frac{1}{p}h\left(pq - \frac{p(q+2)}{3} - 1, 2q\right) \\
&= \frac{2p(q-1)}{3} - 1 - \frac{1}{p}h\left(\frac{2p(q-1)}{3} - 1, 2q\right)
\end{aligned}$$

Note that  $\text{int}[\frac{2p(q-1)-3}{6q}] = \begin{cases} \frac{p-1}{3} & \text{if } p < q \\ \frac{p-4}{3} & \text{if } p = q \end{cases}$ . Using (2.4), for  $p = q$  we have:

$$\begin{aligned}
2\bar{c}_2 &\leq \frac{2p(p-1)}{3} - 1 - \frac{1}{p}\left[\frac{2p(p-1)}{3} - 1 + \left(\frac{4p(p-1)}{3} - 2 - 2p\right)\frac{p-4}{3} - 2p\frac{(p-4)^2}{9}\right] \\
&= \frac{4p^3 - 2p^2 - 5p - 15}{9p} \\
&< 2c_2^*,
\end{aligned}$$

since  $2c_2^* = \frac{4p^3 - 2p^2 - 2p}{9p}$  when  $p = q$ . If  $p < q$ :

$$\begin{aligned}
2\bar{c}_2 &\leq \frac{2p(q-1)}{3} - 1 - \frac{1}{p}\left[\frac{2p(q-1)}{3} - 1 + \left(\frac{4p(q-1)}{3} - 2 - 2q\right)\frac{p-1}{3} - 2q\frac{(p-1)^2}{9}\right] \\
&= \frac{2(p-1)}{9p}[p(2q-1) + 2q - \frac{3}{2}] \\
&< 2c_2^*.
\end{aligned}$$

Next we need to show part (a) of Lemma 3.4,  $c_1^* < 2(\sqrt{3} - 1)c_2^*$ . Note that  $\text{int}[\frac{r_1^*}{q}] =$

$$\text{int}[\frac{p(q+2)}{3q}] = \begin{cases} \frac{p+2}{3} & \text{if } p = q \\ \frac{p-1}{3} & \text{if } p < q \end{cases}. \text{ For } p = q \text{ we have:}$$

$$\begin{aligned} c_1^* &= \frac{p(p+2)}{3} - \frac{1}{p}h\left(\frac{p(p+2)}{3}, p\right) \\ &\stackrel{(2.4)}{=} \frac{p(p+2)}{3} - \frac{1}{p}\left[\frac{p(p+2)}{3} + \left(2\frac{p(p+2)}{3} - p\right)\frac{p+2}{3} - p\frac{(p+2)^2}{9}\right] \\ &= \frac{2(p-1)(p+2)}{9} \end{aligned}$$

Since  $2(\sqrt{3}-1)c_2^* \stackrel{(3.18)}{=} 2(\sqrt{3}-1)\frac{(p-1)(2p+1)}{9}$  if  $p = q$ , inequality (a) holds if  $(\sqrt{3}-1)(2p+1) > p+2$ . This is true for any  $p \geq 4$ . Now, if  $p < q$ :

$$\begin{aligned} c_1^* &= \frac{p(q+2)}{3} - \frac{1}{p}h\left(\frac{p(q+2)}{3}, q\right) \\ &\stackrel{(2.4)}{=} \frac{p(q+2)}{3} - \frac{1}{p}\left[\frac{p(q+2)}{3} + \left(2\frac{p(q+2)}{3} - q\right)\frac{p-1}{3} - q\frac{(p-1)^2}{9}\right] \\ &= \frac{2(p-1)(pq+p+q)}{9p} \end{aligned}$$

Using (3.18),  $2(\sqrt{3}-1)c_2^* > c_1^*$  if and only if  $(\sqrt{3}-1)(2pq-p+2q) > pq+p+q$ , or  $p[(2\sqrt{3}-3)q-\sqrt{3}] + q(2\sqrt{3}-3) > 0$ . This is true for any  $p \geq 4, q \geq 4$ .

We have shown parts (a), (b), and (c) of Lemma 3.4. So  $d^*$  is  $A$ -superior to  $\bar{d}$ , which is an averaged version of any design  $d$  with  $r_1 > \frac{p(q+2)}{3}$ . All remaining competitors must have  $r_1 \leq \frac{p(q+2)}{3}$ , which also implies  $r_3 \geq \frac{p(q-4)}{3}$ .

**Step 2.** In this step of the proof we eliminate all nonuniform designs with  $r_i \in [\frac{p(q-4)}{3}, \frac{p(q+2)}{3}]$ .

Using Lemma 3.3, we will show that  $(\sqrt{3}-1)(c_2+c_3) - c_1 \geq 0$ , for all uniform designs  $d(c_1, c_2, c_3)$  with replications in this range.

First, if  $r_3 \geq \frac{p(q-1)}{3}$ ,  $c_i$  is an increasing function of  $r_i$ , for by (3.14), (2.7), and in this range  $\Delta h(r, q) = \frac{2p+1}{3}$ ,  $\Delta h(r, p) = \frac{2q+1}{3}$ ,

$$c[r+1] - c[r] = \frac{1}{3pq}(6r - pq - p - q + 3) \geq \frac{(p-1)(q-3)}{3pq} > 0.$$

Therefore, when  $r_3 \geq \frac{p(q-1)}{3}$ , for uniform designs we must have  $c_1 \leq c_1^*$ ,  $c_2 \geq c_2^*$ , and  $c_3 \geq c_3^*$ , since  $r_1 \leq r_1^*$ ,  $r_2 \geq r_2^*$ , and  $r_3 \geq r_3^*$ . Thus:

$$(\sqrt{3}-1)(c_2+c_3)-c_1 \geq (\sqrt{3}-1)(c_2^*+c_3^*)-c_1^* > 0,$$

as shown in the previous step of the proof.

Next we eliminate all nonuniform designs with  $\frac{p(q-4)}{3} \leq r_3 < \frac{p(q-1)}{3}$ . Let  $r_3 = \frac{p(q-1)}{3} - x$  for some  $0 < x \leq p$  and  $r_2 = pq - r_1 - r_3$ , where  $r_1 \in [\frac{2pq+p+3x}{6}, \frac{p(q+2)}{3}]$ , since  $r_2 \leq r_1$ . The values of  $\text{int}[\frac{r_i}{p}]$  and  $\text{int}[\frac{r_i}{q}]$  are:

$$\begin{aligned} \text{int}[\frac{r_1}{p}] = \text{int}[\frac{r_2}{p}] = \frac{q-1}{3}, \quad \text{int}[\frac{r_1}{q}] = \text{int}[\frac{r_2}{q}] = \frac{p-1}{3} \\ \text{int}[\frac{r_3}{p}] = \frac{q-4}{3}, \quad \text{int}[\frac{r_3}{q}] = \begin{cases} \frac{p-1}{3} & \text{if } x \leq \frac{q-p}{3} \\ \frac{p-4}{3} & \text{if } x > \frac{q-p}{3} \end{cases}. \end{aligned} \quad (3.19)$$

Note that when  $r_1 = \frac{p(q+2)}{3}$  we actually have  $\text{int}[\frac{r_1}{p}] = \frac{q+2}{3}$ . However, since the function  $h$  defined in (2.4) is continuous in  $r$ , we do not need to use a different value for  $\text{int}[\frac{r_1}{p}]$  at the boundary point  $r_1 = \frac{p(q+2)}{3}$  (i.e. in (2.4),  $h(\frac{p(q+2)}{3}, p)$  yields the same result whether we set  $\text{int}[\frac{p(q+2)}{3p}] = \frac{q+2}{3}$  or  $\text{int}[\frac{p(q+2)}{3p}] = \frac{q-1}{3}$ ). This is our first example illustrating the general discussion following (3.14). From now on, when looking at  $c_i(r_i)$  on an interval with  $sp \leq r_i \leq (s+1)p$  for some positive integer  $s$ , we will consider  $\text{int}[\frac{r_i}{p}] = s$  for the entire interval for computational purposes. This will eliminate the need for special consideration of boundary points where  $\text{int}[\frac{r_i}{p}]$  (or  $\text{int}[\frac{r_i}{q}]$ ) changes value.

We now return to step 2 of the proof. We will show that  $(\sqrt{3}-1)(c_2+c_3)-c_1 \geq 0$  separately for  $x \leq \frac{q-p}{3}$  and  $x > \frac{q-p}{3}$ . First, if  $0 < x \leq \frac{q-p}{3}$ :

$$\begin{aligned} 9pq[(\sqrt{3}-1)(c_2+c_3)-c_1] \stackrel{(3.14)}{=} 18(\sqrt{3}-1)x^2 - [18r_1(\sqrt{3}-1) - 6pq(\sqrt{3}-1) + 6p(\sqrt{3}-1)]x \\ + 9r_1^2(\sqrt{3}-2) - 3pqr_1(3\sqrt{3}-4) + 3\sqrt{3}qr_1 - 3pr_1(\sqrt{3}-2) \\ + [4 - 2\sqrt{3} + (\sqrt{3}-2)q + (6\sqrt{3}-8)q^2]p^2 - \sqrt{3}pq^2 - (4\sqrt{3}-6)q^2 \end{aligned} \quad (3.20)$$

The above expression is a quadratic in  $x$ , with positive coefficient for  $x^2$ . We will show that  $s_2^2 - 4s_1s_3 < 0$ , where  $s_1$ ,  $s_2$ , and  $s_3$  are the coefficients of  $x^2$ ,  $x^1$ , and  $x^0$  respectively, thus

forcing the entire expression to be positive.

$$\begin{aligned} \frac{1}{72}(s_2^2 - 4s_1s_3) &= 9(2\sqrt{3} - 3)r_1^2 + 3[p(q+1)(9 - 5\sqrt{3}) - q(3 - \sqrt{3})]r_1 \\ &+ p^2[12 - 7\sqrt{3} + (5\sqrt{3} - 9)q + (13\sqrt{3} - 24)q^2] - pq^2(\sqrt{3} - 3) - 10\sqrt{3}q^2 + 18q^2 \end{aligned}$$

The above expression is an increasing function of  $r_1$  for any positive  $r_1$ , and  $p \geq 4$ . We will show that it is negative at the largest value of  $r_1$ , thus forcing the expression to be negative in the entire range. Setting  $r_1 = \frac{p(q+2)}{3}$ :

$$\frac{1}{72}s_2^2 - 4s_1s_3 = 2pq(\sqrt{3} - 3) + 2q^2(9 - 5\sqrt{3}) + p^2[2q^2(5\sqrt{3} - 9) - 2q(\sqrt{3} - 3) - 9(\sqrt{3} - 2)].$$

The coefficients of  $p$  and  $p^2$  are negative for all  $q \geq 7$ , and since  $0 < x \leq \frac{q-p}{3}$ , we must have  $q \geq 7$ . The above expression is thus decreasing in  $p$ . Setting  $p = 4$  we obtain a quadratic in  $q$ , negative for all  $q \geq 7$ . Hence,  $s_2^2 - 4s_1s_3 < 0$ , which in turn implies  $(\sqrt{3} - 1)(c_2 + c_3) - c_1 > 0$ .

Next we show that the inequality holds when  $x > \frac{q-p}{3}$ , using a similar strategy as before. In this case the value of  $c_3$  changes, and:

$$\begin{aligned} 9pq[(\sqrt{3} - 1)(c_2 + c_3) - c_1] &\stackrel{(3.14)}{=} 18(\sqrt{3} - 1)x^2 - [18r_1(\sqrt{3} - 1) - 6pq(\sqrt{3} - 1) + 6p(\sqrt{3} - 1) \\ &+ 18q(\sqrt{3} - 1)]x + 9r_1^2(\sqrt{3} - 2) - 3pqr_1(3\sqrt{3} - 4) + 3\sqrt{3}qr_1 - 3pr_1(\sqrt{3} - 2) \\ &+ [4 - 2\sqrt{3} + (\sqrt{3} - 2)q + (6\sqrt{3} - 8)q^2]p^2 - \sqrt{3}pq^2 + 2\sqrt{3}q^2 - 6pq(\sqrt{3} - 1). \end{aligned} \quad (3.21)$$

Again, the expression is a quadratic in  $x$ , with a positive coefficient for  $x^2$ .

$$\begin{aligned} \frac{1}{72}(s_2^2 - 4s_1s_3) &= 9(2\sqrt{3} - 3)r_1^2 - 3(pq + p + q)(5\sqrt{3} - 9)r_1 + pq^2(5\sqrt{3} - 9) - (7\sqrt{3} - 12)q^2 \\ &+ p^2[12 - 7\sqrt{3} + (5\sqrt{3} - 9)q + (13\sqrt{3} - 24)q^2] - (18\sqrt{3} - 36)pq \end{aligned}$$

The above expression is increasing in  $r_1$ , because  $r_1 \geq 0$  and the coefficients of  $r_1^2$  and  $r_1$  are both positive. Setting  $r_1 = \frac{p(q+2)}{3}$ :

$$f(p, q) = \frac{1}{72}(s_2^2 - 4s_1s_3) = -2pq(14\sqrt{3} - 27) - q^2(7\sqrt{3} - 12) + p^2[2q^2(5\sqrt{3} - 9) - 2q(\sqrt{3} - 3) - 9(\sqrt{3} - 2)].$$

The function  $f$  is decreasing in  $q$  because in:

$$\frac{1}{2} \frac{\partial f}{\partial q} = [27 - 14\sqrt{3} + p(3 - \sqrt{3}) + 2pq(5\sqrt{3} - 9)]p + [12 - 7\sqrt{3}]q,$$

both terms in square brackets are negative for  $p \geq 4$  and  $q \geq 4$ . Now, setting  $q = 7$ ,

$$\frac{s_2^2}{2} - 2s_1s_3 = 588 - 343\sqrt{3} + (378 - 196\sqrt{3})p + (467\sqrt{3} - 822)p^2 < 0, \text{ when } p \geq 4.$$

We have thus shown that when  $q \geq 7$  and  $p \geq 4$ ,  $s_2^2 - 4s_1s_3 < 0$ , which in turn forces  $(\sqrt{3} - 1)(c_2 + c_3) - c_1 > 0$ . When  $p = q = 4$ , it can be shown that  $d^*$  is indeed the  $A$ -optimal design by enumerating all possible competitors.

Step 2 of the proof is finished. We have so far eliminated all designs with  $r_i \notin [\frac{p(q-4)}{3}, \frac{p(q+2)}{3}]$  and all nonuniform designs with replications in the above range.

**Step 3.** In this step of the proof we further restrict the replication range, by eliminating all designs with  $r_3 < \frac{p(q-1)}{3}$ . The competitors being considered must be uniform with  $\frac{p(q-4)}{3} \leq r_3 < \frac{p(q-1)}{3}$ . The notation used here is the same as in the previous step, and the problem will be divided into two subparts, with  $r_3 = \frac{p(q-1)}{3} - x$ ,  $0 \leq x \leq \frac{q-p}{3}$  and  $\frac{q-p}{3} < x \leq p$ . The function  $A$  defined in (3.5) is a continuous function of  $x$ , and the only points where it is not differentiable are  $x = 0$ ,  $x = \frac{q-p}{3}$  and  $x = p$ . The strategy is to show that the derivative of  $A$  with respect to  $x$  is negative, thus forcing  $r_3 \geq \frac{p(q-1)}{3}$  for  $A$ -optimal designs.

$$\begin{aligned} \frac{\partial A}{\partial x} &= (c'_2 + c'_3) - 2 \frac{(2c_2c'_2 + 2c_3c'_3)(\sum c_i) - (c'_2 + c'_3)(\sum c_i^2)}{(\sum c_i)^2} \\ &\stackrel{\text{sign}}{=} \frac{81p^3q^3}{8} \{(c'_2 + c'_3)[(\sum c_i)^2 + 2 \sum c_i^2] - 4(c_2c'_2 + c_3c'_3)(\sum c_i)\}, \end{aligned} \quad (3.22)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ , and  $\frac{81p^3q^3}{8}$  is a multiplication constant which will make computations easier.

Note that  $c_1$  does not depend on  $x$ , and thus  $\frac{\partial c_1}{\partial x} = 0$ . We start with the case  $x > \frac{q-p}{3}$ . Using (2.4), (3.14), and (3.19) in *Mathematica*, (3.22) reduces to a quadratic function of  $x$ , which

can be written as  $s_2x^2 + s_1x + s_0$ , where:

$$\begin{aligned}
s_2 &= 9pq(p+q+4)[2p(q+1)+2q-3r_1], \\
s_1 &= -6\{p^4(4q^4+10q^3+7q^2-2q-4)-q(2q-3r_1)^2(q+3r_1) \\
&\quad -9pr_1[2q^3-5q^2r_1+3r_1^2+qr_1(3r_1-2)]+p^3q[-8+10q^3+q^2(8-18r_1)-6q(5r_1+2) \\
&\quad -15r_1]+p^2[9q^4+27r_1^2-2q^3(15r_1+1)+3qr_1(15r_1+4)+q^2(-16-9r_1+27r_1^2)]\}, \\
s_0 &= -p^5(4-6q-11q^2+7q^3+14q^4+4q^5)-3q(2q-3r_1)^2(q^2+4qr_1+3r_1^2) \\
&\quad +p[4q^5+36q^3r_1^2+27qr_1^3(2-3r_1)-81r_1^4+9q^2r_1^2(12r_1+1)-2q^4(27r_1+2)] \\
&\quad +p^4[-6q^5-12r_1+6q^4(5r_1-3)+3q^2(9r_1+4)-q(21r_1+4)+q^3(66r_1+7)] \\
&\quad +p^3[13q^5+27r_1^2-6qr_1(9r_1+2)+q^4(30r_1+7)-3q^2r_1(48r_1+7)+q^3(10+42r_1-81r_1^2)] \\
&\quad +3p^2[9q^5-11q^4r_1+18r_1^3+9qr_1^2(6r_1+1)-2q^3(15r_1^2+r_1+4)+2q^2r_1(18r_1^2-9r_1-4)].
\end{aligned}$$

Note that the coefficient of  $x^2$  is positive; by showing that the expression is negative at both the minimum and the maximum value of  $x$ , it will mean that it is negative in the entire range of  $x$ . To make computations easier, we reparameterize (3.22) by letting  $r_1 = u + \frac{q(2p+1)}{6}$ , where  $0 \leq u \leq \frac{4p-q}{6}$  since  $r_1 \geq \frac{pq-r_3}{2} \geq \frac{q(2p+1)}{6}$ . Note that  $\frac{q-p}{3} < x \leq 2u + \frac{q-p}{3}$ , since  $r_3 \geq pq - 2r_1 = \frac{p(q-1)}{3} - 2u - \frac{q-p}{3}$ . Setting  $x = \frac{q-p}{3}$ , expression (3.22) becomes a quartic polynomial in  $u$ , with the coefficients  $s_i$  for  $u^i$  given below:

$$\begin{aligned}
s_4 &= -81(pq+p+q), \quad s_3 = 0, \\
s_2 &= -\frac{9}{2}(6p^3q^3+8p^2q^3+8p^3q^2-8p^3q-3pq^3-18p^3-9q^3-9pq^2-2p^2q) \\
s_1 &= -3p^2(-pq^4+2p^2q^3+q^4-4pq^3+3p^2q^2+q^3-4pq^2+7q^2-9pq+4p^2) \\
s_0 &= -\frac{3}{16}(16p^4q^5+16p^5q^4-32p^5q^3+48p^4q^4+4p^3q^5-32p^3q^4-40p^2q^5-24p^4q^3-96p^5q^2 \\
&\quad -40p^2q^4-9pq^5-16p^3q^3+27pq^4+27q^5+20p^2q^3+116p^3q^2+32p^4q+64p^5)
\end{aligned}$$

All nonzero coefficients of powers of  $u$  are negative for all  $q \geq p \geq 4$ , except  $s_1$ , which is positive for some values of  $p$  and  $q$ . However, when we set  $u$  to its maximum value, which is  $\frac{4p-q}{6}$ , the expression  $s_0 + s_1u$  is still negative for any values of  $p \geq 4$  and  $q \geq 4$ . Hence, when  $x = \frac{q-p}{3}$  the expression is negative for any value of  $u$ . In general, the sign of coefficients was

found by checking numerically for a few values of  $p$  and  $q$ , and then using algebra to verify it for all values of  $p$  and  $q$ . The sign of a coefficient (if it has the same sign for all  $p$  and  $q$ ) is given away by the sign of the term of largest order in the  $(p, q)$  polynomial, where if there are several terms of largest order, among them choose the term with largest exponent in  $q$ .

Next, we set  $x = 2u + \frac{q-p}{3}$ , and obtain another quartic expression in  $u$  for (3.22), with the coefficients  $s_i$  for  $u^i$  given below:

$$\begin{aligned} s_4 &= 243(pq + p + q), & s_3 &= -162(2p + q)(pq + p + q), \\ s_2 &= \frac{27}{2}(pq + p + q)(6p^2q^2 + 2pq^2 + 2p^2q - 3q^2 + 8pq + 6p^2), \\ s_1 &= -\frac{9}{2}(6p^3q^4 + 12p^4q^3 + 10p^2q^4 + 12p^3q^3 + 18p^4q^2 - 3pq^4 - 18p^2q^3 - 8p^3q^2 \\ &\quad - 9q^4 - 15pq^3 - 36p^2q^2 - 6p^3q - 8p^4), \\ s_0 &= -\frac{3}{16}(16p^4q^5 + 16p^5q^4 + 4p^3q^5 + 48p^4q^4 - 32p^5q^3 - 40p^2q^5 - 32p^3q^4 - 24p^4q^3 - 96p^5q^2 \\ &\quad - 9pq^5 - 40p^2q^4 - 16p^3q^3 + 27q^5 + 27pq^4 + 20p^2q^3 + 116p^3q^2 + 32p^4q + 64p^5). \end{aligned}$$

Simple algebra can show that coefficients  $s_0$ ,  $s_1$  and  $s_3$  are negative, and coefficients  $s_2$  and  $s_4$  positive, for any  $q \geq p \geq 4$ . However,  $s_3 + s_4u < 0$ , and  $s_1 + s_2u < 0$ , for any  $0 \leq u \leq \frac{4p-q}{6}$ , making  $u^3(s_4u + s_3) + u(s_2u + s_1) + s_0$  negative. Hence, when  $x = 2u + \frac{q-p}{3}$  the expression (3.22) is negative for any value of  $u$ . Remember that  $\frac{\partial A}{\partial x}$  is a quadratic function of  $x$ , with a positive coefficient for  $x^2$ . We have shown that  $\frac{\partial A}{\partial x}$  is negative for all  $x > \frac{q-p}{3}$ , because it is always negative at both the largest, and the smallest value of  $x$ .

Now, moving on to the case  $0 < x \leq \frac{q-p}{3}$ , equation (3.22) reduces to another quadratic of the form  $s_2x^2 + s_1x + s_0$ , where:

$$\begin{aligned} s_2 &= 9pq(p-1)(2pq + 2p - 3r_1 - q), \\ s_1 &= -6\{p^4(-4 - 2q + 7q^2 + 10q^3 + 4q^4) - q(2q - 3r_1)(q + 3r_1)^2 + p[5q^4 + 9q^2r_1(1 - 3r_1) \\ &\quad - 27r_1^3 - 9qr_1^2(3r_1 + 2) + q^3(9r_1 + 4)] - p^3q[-2 + 6q^3 + 15r_1 + 6q^2(3r_1 + 1) \\ &\quad + 3q(10r_1 - 1)] + p^2[-q^4 + 27r_1^2 + 3qr_1(15r_1 - 1) + q^3(18r_1 - 7) + q^2(27r_1^2 + 12r_1 - 7)]\}, \end{aligned}$$

$$\begin{aligned}
s_0 = & -p^5(4 - 6q - 11q^2 + 7q^3 + 14q^4 + 4q^5) - 3qr_1(2q - 3r_1)(q + 3r_1)^2 + p[2q^5 - 81r_1^4 \\
& - 27qr_1^3(3r_1 + 2) - 18q^2r_1^2(6r_1 - 1) + 3q^3r_1(9r_1 + 4) + q^4(24r_1 + 1)] + p^4[6q^5 - 12r_1 \\
& + 6q^4(5r_1 + 2) + 3q^2(9r_1 - 1) - q(21r_1 + 2) + 2q^3(33r_1 + 1)] + p^2[-5q^5 + 54r_1^3 + 162qr_1^3 \\
& - 4q^4(3r_1 + 2) + 9q^2r_1(12r_1^2 + 8r_1 - 1) + q^3(81r_1^2 - 24r_1 - 2)] + p^3[q^5 + 4q^4(2 - 9r_1) \\
& + 3qr_1(1 - 18r_1) + 27r_1^2 + q^3(-81r_1^2 - 42r_1 + 5) - q^2(144r_1^2 + 5)].
\end{aligned}$$

Similar to the previous case, the coefficient of  $x^2$  is positive for any  $q \geq p \geq 4$  and  $r_1 \leq \frac{p(q+2)}{3}$ . We reparameterize, by letting  $r_1 = u + \frac{p(2q+1)}{6}$ , with  $0 \leq u \leq \frac{p}{2}$  since  $r_1 \geq \frac{pq-r_3}{2} \geq \frac{p(2q+1)}{6}$ . The minimum value of  $x$  is 0, and its maximum value is  $2u$ . We will show that (3.22) is negative at  $x = 0$  and  $x = 2u$ , thus making it negative in the entire range of  $x$ . Setting  $x = 0$ , expression (3.22) becomes a quartic polynomial in  $u$  with coefficients:

$$\begin{aligned}
s_4 &= -81(pq + p - q), & s_3 &= 0 \\
s_2 &= -\frac{9}{2}(6p^3q^3 - 6p^2q^3 + 8p^3q^2 - 6pq^3 - 4p^2q^2 - 3p^3q + 6q^3 - 4pq^2 + 3p^2q - 9p^3), \\
s_1 &= -3q^2(p - 1)^2(2pq^2 - p^2q + 2q^2 - pq + p^2), \\
s_0 &= -\frac{3}{16}p^2(16p^3q^4 - 16p^2q^4 + 4p^3q^3 - 16pq^4 - 4p^2q^3 - 40p^3q^2 + 16q^4 - 4pq^3 \\
&\quad + 8p^2q^2 - 9p^3q + 4q^3 + 32pq^2 + 9p^2q + 27p^3)
\end{aligned}$$

All coefficients are negative, for any  $p \geq 4$ ,  $q \geq 4$ . Next,  $q = p$  implies  $x = 0$ , so for  $x = 2u$  assume that  $q \geq p+3$ . Setting  $x = 2u$ , expression (3.22) becomes another quartic polynomial in  $u$  with coefficients:

$$\begin{aligned}
s_4 &= 243(pq + p - q), & s_3 &= -162p(pq + p - q), \\
s_2 &= \frac{27}{2}(pq + p - q)(6p^2q^2 + 2p^2q - 6q^2 - 2pq - 3p^2), \\
s_1 &= -\frac{9}{2}(-4p^3q^4 + 6p^4q^3 + 4p^2q^4 - 6p^3q^3 + 10p^4q^2 + 4pq^4 - 6p^2q^3 + 4p^3q^2 - 3p^4q \\
&\quad - 4q^4 + 6pq^3 - 14p^2q^2 + 3p^3q - 9p^4), \\
s_0 &= -\frac{3}{16}p^2(16p^3q^4 - 16p^2q^4 + 4p^3q^3 - 16pq^4 - 4p^2q^3 - 40p^3q^2 + 16q^4 - 4pq^3 \\
&\quad + 8p^2q^2 - 9p^3q + 4q^3 + 32pq^2 + 9p^2q + 27p^3).
\end{aligned}$$

The coefficients  $s_3$  and  $s_0$  are negative for any  $q > p \geq 4$ . Coefficient  $s_4$  is positive, but  $us_4 + s_3$  is negative since  $u \leq \frac{p}{2}$ . Coefficient  $s_2$  is also positive, but the remaining quadratic  $s_2u^2 + s_1u + s_0 < 0$  is negative at  $u = 0$  for any  $q > p \geq 4$ , and it is also negative at  $u = \frac{p}{2}$  for any  $q \geq 10$ . Therefore, the entire expression is negative for any  $u$  if  $q \geq 10$ . The only competitor designs left to consider are the uniform row-column designs with  $p = 4$  and  $q = 7$ , and replications  $r_3 = 7, r_2 = 10, r_1 = 11$  (call it  $d'$ ), or  $r_3 = 7, r_2 = 9, r_1 = 12$  (call it  $d''$ ). Both designs can be eliminated by the numerical computation of (3.5):

$$A_{d^*} = 5.75714, \quad A_{d'} = 5.65238, \quad A_{d''} = 5.65289.$$

With this we have concluded step 3 for the proof of Theorem 3.2. The only remaining competitors are uniform designs with  $r_i \in [\frac{p(q-1)}{3}, \frac{p(q+2)}{3}]$ .

**Step 4.** This step will be divided into two parts. First it will be shown that for a given  $r_3$ , the  $A$ -best design has  $r_2 = r_3$  and  $r_1 = \frac{pq-2r_3}{2}$ . Assuming  $r_2 = r_3$ , we will then show that  $A$  is a decreasing function of  $r_2$ . Note that when  $r_i \in [\frac{p(q-1)}{3}, \frac{p(q+2)}{3}]$ , we take (by the earlier discussion)  $\text{int}[\frac{r_i}{p}] = \frac{q-1}{3}$  and  $\text{int}[\frac{r_i}{q}] = \frac{p-1}{3}$ .

Let  $r_2 = r_3 + x$ , and  $r_1 = pq - r_2 - r_3 = pq - 2r_3 - x$ , where  $0 \leq x \leq \frac{pq-3r_3}{2}$  since  $r_1 \geq r_2 \geq r_3$ . Also,  $\frac{p(q-1)}{3} \leq r_3 \leq \frac{pq-1}{3}$ . The function  $A$  defined in (3.5) is differentiable in the entire interval, except at  $x = 0$ , when  $r_3 = \frac{p(q-1)}{3}$ . Just like in the previous step, we will show that the derivative of  $A$  with respect to  $x$  is negative. Analogous to step 3,

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} \frac{27p^3q^3}{8} \{(c'_1 + c'_2)[(\sum c_i)^2 + 2 \sum c_i^2] - 4(c_1c'_1 + c_2c'_2)(\sum c_i)\}, \quad (3.23)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ , and  $\frac{27p^3q^3}{8}$  is a multiplication constant which will simplify computations. Note that  $c_3$  does not depend on  $x$ , and thus  $\frac{\partial c_3}{\partial x} = 0$ . Using (2.4), and (3.14) in *Mathematica*, (3.23) reduced to a linear function of  $x$ , which can be written as  $s_1x + s_0$ , where:

$$\begin{aligned} s_1 &= -2[-2p^4 - 2p^3q + 5p^4q - 4p^2q^2 + 5p^3q^2 - p^4q^2 - 2pq^3 + 5p^2q^3 + 2p^3q^3 - 6p^4q^3 \\ &\quad - 2q^4 + 5pq^4 - p^2q^4 - 6p^3q^4 + 4p^4q^4 + 9r_3(-p^3 - p^2q + p^3q - pq^2 + 2p^3q^2 \\ &\quad - q^3 + pq^3 + 2p^2q^3 - 2p^3q^3) + 27r_3^2(-p^2q - pq^2 + p^2q^2) + 27r_3^3(p + q - pq)], \\ s_0 &= -\frac{pq - 3r_3}{2}s_1. \end{aligned}$$

At the maximum value of  $x$ , which is  $\frac{pq-3r_3}{2}$ , (3.23) reduces to 0. We next show that the expression is negative at the minimum value of  $x$ , which is 0. Rewriting  $r_3 = u + \frac{p(q-1)}{3}$  with  $0 \leq u \leq \frac{p-1}{3}$ , and setting  $x = 0$ , we get:

$$(3.23) = 81u^4(pq - p - q) - 108u^3p(pq - p - q) + 27u^2(pq - p - q)(p^2q^2 + p^2 - q^2) \\ - 6uq^2(p - 1)(-p^2q^2 + q^2 + 2p^3q - 2pq - 2p^3 - p^2) \\ - pq^2(p - 1)^2(2pq^2 + 2q^2 - p^2q - pq + p^2)$$

Now,  $81u^4(pq - p - q) - 108u^3p(pq - p - q) \leq 0$  for all  $0 \leq u \leq \frac{p-1}{3}$ . The remaining quadratic in  $u$  has a positive coefficient for  $u^2$ , but is negative at both  $u = 0$  and  $u = \frac{p-1}{3}$ , and thus negative in the entire range of  $u$ . We have thus shown that (3.23) is linear in  $x$  and negative at the maximum and the minimum of  $x$ , and therefore in the entire range of  $x$ . Hence  $A$  is a decreasing function of  $x$ .

Now consider designs with  $r_2 = r_3$ , and write  $r_2 = r_3 = \frac{p(q-1)}{3} + x$ ,  $r_1 = \frac{p(q+2)}{3} - 2x$ , for some  $0 \leq x \leq \frac{p-1}{3}$ . We will now show that  $A$  is a decreasing function of  $x$ , by showing that the derivative of  $A$  with respect to  $x$  is negative. Since  $c_2 = c_3$  we have:

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} \frac{27p^3q^3}{16} \{(c'_1 + 2c'_2)[(\sum c_i)^2 + 2 \sum c_i^2] - 4(c_1c'_1 + 2c_2c'_2)(\sum c_i)\}, \quad (3.24)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ , and  $\frac{27p^3q^3}{16}$  is a multiplication constant which will simplify computations.

Using (2.4), and (3.14) in *Mathematica*, (3.24) reduces to:

$$(3.24) = 81x^4(pq - p - q) - 108x^3p(pq - p - q) + 27x^2(pq - p - q)(p^2q^2 + p^2 - q^2) \\ - 6xq^2(p - 1)(-p^2q^2 + q^2 + 2p^3q - 2pq - 2p^3 - p^2) \\ - pq^2(p - 1)^2(2pq^2 + 2q^2 - p^2q - pq + p^2).$$

Interestingly enough, this is the same as the quartic function in  $u$  obtained when we set  $x = 0$  in (3.23). As shown in the previous paragraph, it is negative for any  $u \in [0, \frac{p-1}{3}]$ , which is the same as the range for  $x$  in (3.24). Therefore (3.24) is negative, and so  $A$  is a decreasing function of  $x$ ; the  $A$ -best design must have  $x = 0$ , and this is a characteristic of  $d^*$ .

This concludes the proof of Theorem 3.2. We have shown that when  $p \equiv q \equiv 1 \pmod{3}$ , the uniform design with replications  $r_1^* = \frac{p(q+2)}{3}$ ,  $r_2^* = r_3^* = \frac{p(q-1)}{3}$  is  $A$ -optimal.

### 3.4.3 Case 3: $p \equiv 2 \pmod{3}$ and $q \equiv 2 \pmod{3}$

Finding  $A$ -optimal designs in this case follows the strategy described in the  $p \equiv q \equiv 1 \pmod{3}$  case. However, the results differ from that case. The nearly equireplicated uniform design, and not the maximal trace design, will be shown to be  $A$ -optimal. Construct  $d^*$  as the uniform design with replications:

$$r_1^* = \frac{pq+2}{3}, \quad r_2^* = r_3^* = \frac{pq-1}{3}. \quad (3.25)$$

**Theorem 3.3.** *The design  $d^*$  is  $A$ -optimal.*

Let any competitor design  $d$  have replications  $r_1 \geq r_2 \geq r_3$ . The proof of this theorem will be divided into the following steps:

- (1) Eliminate all designs with  $r_3 < \frac{p(q-2)}{3}$ ,
- (2) Eliminate all nonuniform designs with  $r_i \in [\frac{p(q-2)}{3}, \frac{p(q+4)}{3}]$ ,
- (3) Eliminate all designs with  $r_1 > \frac{p(q+1)}{3}$ ,
- (4) Show that among uniform designs with replications  $r_i \in [\frac{p(q-2)}{3}, \frac{p(q+1)}{3}]$ ,  $d^*$  is  $A$ -optimal.

Before we get into the first step of the proof, we introduce an additional uniform design,  $d^0$  with the following replications:

$$r_1^0 = r_2^0 = \frac{p(q+1)}{3}, \quad r_3^0 = \frac{p(q-2)}{3}. \quad (3.26)$$

This design has maximal trace and will be used to eliminate some of the competitor designs. A special case which will be studied at the end is the  $p = 2$  case. This is studied separately because some of the inequalities in the proof do not hold for  $p = 2$ . From now on assume

$q \geq p \geq 5$ . The 4-step proof is similar in many ways to the one for the  $p \equiv q \equiv 1 \pmod{3}$  case, and some of the details will be left out.

**Step 1.** Consider a design  $d$  with  $r_3 < \frac{p(q-2)}{3}$ . Create the symmetrized design  $\bar{d}$  with  $\bar{c}_3 = c_3$  and  $\bar{c}_1 = \bar{c}_2 = \frac{c_1+c_2}{2}$ . Design  $\bar{d}$  is  $A$ -inferior to  $d^0$  by Lemma 3.5, since  $c_3 < c_3^0$  by Lemma 2.1, and  $d^0$  is of maximal trace. As discussed in Section 2.3 design  $d$  is  $A$ -inferior to  $\bar{d}$ . All remaining competitor designs must have  $r_i \in [\frac{p(q-2)}{3}, \frac{p(q+4)}{3}]$ .

**Step 2.** In this step we eliminate all nonuniform designs with replications in the remaining range. In order to use Lemma 3.3, we must show that  $(\sqrt{3}-1)(c_2+c_3)-c_1 \geq 0$  where the  $c_i$ 's are the diagonal elements of a uniform design. Write  $r_1 = \frac{p(q+4)}{3} - x$ , for some  $0 \leq x \leq \frac{4p-2}{3}$ ,  $r_3 = \frac{p(q-2)}{3} + u$ , for some  $0 \leq u \leq \frac{x}{2}$ . For these replications, there are three subcases for  $x$  depending on  $\text{int}[\frac{r_1}{q}]$  and  $\text{int}[\frac{r_1}{p}]$ .

$$\begin{aligned} \text{int}[\frac{r_1}{p}] &= \begin{cases} \frac{q+1}{3} & \text{if } 0 \leq x \leq p \\ \frac{q-2}{3} & \text{if } p < x \leq \frac{4p-2}{3} \end{cases}, \quad \text{int}[\frac{r_1}{q}] = \begin{cases} \frac{p+1}{3} & \text{if } 4p \geq q \text{ and } 0 \leq x \leq \frac{4p-q}{3} \\ \frac{p-2}{3} & \text{if } x > \min[0, \frac{4p-q}{3}] \end{cases} \\ \text{int}[\frac{r_2}{p}] &= \text{int}[\frac{r_3}{p}] = \frac{q-2}{3}, \quad \text{int}[\frac{r_2}{q}] = \text{int}[\frac{r_3}{q}] = \frac{p-2}{3} \end{aligned} \quad (3.27)$$

Suppose  $4p \geq q$  and  $0 \leq x \leq \frac{4p-q}{3}$ , making  $\text{int}[\frac{r_1}{q}] = \frac{p+1}{3}$  and  $\text{int}[\frac{r_1}{p}] = \frac{q+1}{3}$ . Using (3.14), in conjunction with the fact that  $\text{int}[\frac{r_2}{q}] = \text{int}[\frac{r_3}{q}] = \frac{p-2}{3}$  and  $\text{int}[\frac{r_2}{p}] = \text{int}[\frac{r_3}{p}] = \frac{q-2}{3}$ :

$$\begin{aligned} 9pq[(\sqrt{3}-1)(c_2+c_3)-c_1] &= 2(12pq - 2\sqrt{3}pq - 2\sqrt{3}p^2q - 2\sqrt{3}q^2 - 3p^2q^2 + 2\sqrt{3}p^2q^2 - 9u^2 \\ &\quad + 9\sqrt{3}u^2) + 3(6p - 3\sqrt{3}p - 6q + \sqrt{3}q + \sqrt{3}pq + 6u - 6\sqrt{3}u)x - 9(2 - \sqrt{3})x^2 \end{aligned} \quad (3.28)$$

The coefficient of  $x^2$  is negative. Setting  $x = 0$  we obtain an increasing function of  $q$ , which is positive for any  $q \geq 8$ . If  $p = q = 5$  nonuniform designs can be eliminated numerically, by noting that when  $c_1$  becomes nonuniform it decreases by at least  $\frac{2}{5}$ . Setting  $x = \frac{4p-2}{3}$  we obtain a quadratic expression in  $u$  with coefficients:

$$\begin{aligned} s_2 &= 18(\sqrt{3}-1), \quad s_1 = -12(\sqrt{3}-1)(2p-1), \\ s_0 &= -2(2-\sqrt{3})(p-2)(2p-1) - 2(\sqrt{3}p + \sqrt{3}-6)q + 2(2\sqrt{3}p^2 - 3p^2 - 2\sqrt{3})q^2. \end{aligned}$$

This is a decreasing function of  $u$  because  $2s_2u + s_1 \leq 0$  since  $u \leq \frac{x}{2} \leq \frac{4p-2}{6}$ . The intercept  $s_0$  is increasing in  $q$ , and is positive for any  $q \geq p \geq 5$ . In fact, it is positive even if  $p = 4$

and  $q \geq 5$ . This will be used in the future to show that other expressions are positive. In conclusion, (3.28) is positive for any  $x \in [0, \frac{4p-2}{3}]$ .

If  $\frac{4p-q}{3} < x \leq p$ , then:

$$9pq[(\sqrt{3}-1)(c_2+c_3)-c_1] = 2(-2\sqrt{3}pq - 2\sqrt{3}p^2q + 3q^2 - 2\sqrt{3}q^2 - 3p^2q^2 + 2\sqrt{3}p^2q^2 - 9u^2 + 9\sqrt{3}u^2) + 3(6p - 3\sqrt{3}p + \sqrt{3}q + \sqrt{3}pq + 6u - 6\sqrt{3}u)x - 9(2 - \sqrt{3})x^2. \quad (3.29)$$

Note that (3.29)–(3.28) =  $6q(-4p + q + 3x) > 0$ , for any  $x > \frac{4p-q}{3}$ . Thus (3.29) is also positive. Finally, suppose  $p < x \leq \frac{4p-2}{3}$ , which implies  $\text{int}[\frac{r_1}{q}] = \frac{p-2}{3}$ ,  $\text{int}[\frac{r_1}{p}] = \frac{q-2}{3}$ . Then:

$$9pq[(\sqrt{3}-1)(c_2+c_3)-c_1] = 2(-9p^2 - 2\sqrt{3}pq - 2\sqrt{3}p^2q + 3q^2 - 2\sqrt{3}q^2 - 3p^2q^2 + 2\sqrt{3}p^2q^2 - 9u^2 + 9\sqrt{3}u^2) + 3(12p - 3\sqrt{3}p + \sqrt{3}q + \sqrt{3}pq + 6u - 6\sqrt{3}u)x - 9(2 - \sqrt{3})x^2. \quad (3.30)$$

Note that (3.30)–(3.29) =  $18p(x-p) > 0$ , for any  $x > p$ . Therefore  $(\sqrt{3}-1)(c_2+c_3)-c_1 > 0$  for any replications  $r_i \in [\frac{p(q-2)}{3}, \frac{p(q+4)}{3}]$ , and so nonuniform designs are eliminated.

**Step 3.** In this step we further restrict the replication range from step 1, by eliminating all designs with  $r_1 > \frac{p(q+1)}{3}$ . For a fixed  $r_3 = \frac{p(q-2)}{3} + u$  with  $0 \leq u \leq \frac{p}{2}$  (since  $r_3 \leq \frac{pq-r_1}{2}$ ), write  $r_1 = \frac{p(q+1)}{3} + x$ , and  $r_2 = pq - r_1 - r_3 = \frac{p(q+1)}{3} - x - u$ . Note that  $0 \leq x \leq p - 2u$  since  $r_2 \geq r_3$ . The values of  $\text{int}[\frac{r_i}{p}]$  and  $\text{int}[\frac{r_i}{q}]$  are given below:

$$\begin{aligned} \text{int}[\frac{r_1}{p}] &= \frac{q+1}{3}, & \text{int}[\frac{r_1}{q}] &= \begin{cases} \frac{p-2}{3} & \text{if } x \leq \frac{q-p}{3} \\ \frac{p+1}{3} & \text{if } x > \frac{q-p}{3} \end{cases}, \\ \text{int}[\frac{r_2}{p}] &= \text{int}[\frac{r_3}{p}] = \frac{q-2}{3}, & \text{int}[\frac{r_2}{q}] &= \text{int}[\frac{r_3}{q}] = \frac{p-2}{3}. \end{aligned} \quad (3.31)$$

The function  $A$  defined in (3.5) is differentiable in  $x$  everywhere except at  $x = \frac{q-p}{3}$ . Just like in (3.23), we have:

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} \frac{27p^3q^3}{8} \{(c'_1 + c'_2)[(\sum c_i)^2 + 2 \sum c_i^2] - 4(c_1c'_1 + c_2c'_2)(\sum c_i)\}, \quad (3.32)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ . We will show that the partial derivative of  $A$  with respect to  $x$  is negative separately for  $x \leq \frac{q-p}{3}$  and  $x > \frac{q-p}{3}$ . First, if  $x \leq \frac{q-p}{3}$ , (3.32) is a quadratic function in  $x$

with coefficients:

$$\begin{aligned}
s_2 &= 3pq(p+1)(pq+q-3u) \\
s_1 &= -2q^2(p+1)^2[-p^2+2pq(p-1)+2q^2(p-1)]+18q(p+1)[pq-q^2 \\
&\quad +p^2(q^2-q+1)]u-18p[-3p+4q(p+1)]u^2+54[p(q-1)+q]u^3 \\
s_0 &= -pq^2(p+1)^2(p+q-pq)^2-q(p+1)\{-8pq^2-2q^3+p^2q(2q^2+5) \\
&\quad +p^3[9+q(8q-13)]\}u+3[-9p^3+12p^2q(p+1)-2pq^2(2p^2+p-1) \\
&\quad +3q^3(p-1)(p+1)^2]u^2-54p[p(q-1)+q]u^3+27[p(q-1)+q]u^4
\end{aligned}$$

The coefficient of  $x^2$  is positive. We will show that (3.32) is negative at the minimum and maximum values of  $x$ . If  $x = 0$ , (3.32) becomes a quartic polynomial in  $u$  with coefficients:

$$\begin{aligned}
s_4 &= 27(pq-p+q), & s_3 &= -2ps_4, \\
s_2 &= 3(-9p^3+12p^2q+12p^3q+2pq^2-2p^2q^2-4p^3q^2-3q^3-3pq^3+3p^2q^3+3p^3q^3), \\
s_1 &= -q(p+1)(9p^3+5p^2q-13p^3q-8pq^2+8p^3q^2-2q^3+2p^2q^2), \\
s_0 &= -pq^2(p+1)^2(pq-p-q)^2
\end{aligned}$$

Coefficients  $s_4$  and  $s_2$  are positive. However,  $s_4u^4+s_3u^3 \leq 0$  because  $u \leq \frac{p}{2}$ . The remaining quadratic is negative both at  $u = 0$  and  $u = \frac{p}{2}$ , and thus in the entire range of  $u$  since  $s_2 \geq 0$ . Setting  $x = p - 2u$  results in another quartic polynomial in  $u$  with coefficients:

$$\begin{aligned}
s_4 &= -81(pq-p+q), & s_3 &= -\frac{4}{3}ps_4, \\
s_2 &= -9(pq-p+q)(3p^2-pq-p^2q-3q^2+3p^2q^2), \\
s_1 &= 3q^2(p+1)(-p^2-7p^3-6pq+6p^3q-2q^2+2p^2q^2), \\
s_0 &= -pq^2(p+1)^2(-4p^2-2pq+2p^2q-3q^2+2pq^2+p^2q^2).
\end{aligned}$$

Coefficients  $s_4$ ,  $s_2$ , and  $s_0$  are negative, while the others are positive. Using the fact that  $u \leq \frac{p}{2}$ , some algebra will show that the quantities  $s_0+s_1u$  and  $s_2+s_3u$  are negative, making the entire quartic polynomial negative for any  $u \in [0, \frac{p}{2}]$ . In conclusion  $\frac{\partial A}{\partial x}$  is negative for

any  $x \leq \frac{q-p}{3}$ . If  $x > \frac{q-p}{3}$ , (3.32) becomes another quadratic function in  $x$  with coefficients:

$$\begin{aligned}
s_2 &= 3pq(p+q-4)(pq-2q-3u) \\
s_1 &= -2\{p^4q^2(2q-1) - q(q-3u)(2q+3u)^2 + p^2[2q^2(3q^2+q-2) + 9q^2u(q+3) \\
&\quad + 9u^2(4q-3)] - 9pu(2q+3u)[q(u+2) - u] + p^3q[-9u+q(-9qu+9u-4q^2+q-2)]\} \\
s_0 &= q^2\{-p^3[p(p+2)+4] + p^2q[p(2p^2+p-6)+4] - pq^2[p^3(p-4)+4] - q^3[p^2(p^2+2p-6) \\
&\quad + 4]\} - q\{9p^4 - p^2q[p(13p-1)+4] + 4pq^2[2p(p-2)(p+1)+9] + q^3(p-2)(2p^2+p \\
&\quad + 2)\}u + 3\{-9p^3 + 3p^2q(4p-3) - pq^2(4p^2-1) + q^3[p(p-2)(3p+2)+9]\}u^2 \\
&\quad - 54p[p(q-1) - q]u^3 + 27[p(q-1) - q]u^4
\end{aligned}$$

Again, the coefficient of  $x^2$  is positive, and we will show that the expression is negative at the minimum and maximum values of  $x$ . Setting  $x = \frac{q-p}{3}$ , (3.32) becomes a quartic polynomial in  $u$  with coefficients:

$$\begin{aligned}
s_4 &= 27(pq - p - q), \quad s_3 = -\frac{2}{3}(4p - q)s_4, \\
s_2 &= 3(-15p^3 - 11p^2q + 20p^3q + 15pq^2 - 12p^2q^2 - 4p^3q^2 + 3q^3 - 4p^2q^3 + 3p^3q^3) \\
s_1 &= -q(-4p^3 + 16p^4 + 28p^2q - 24p^3q - 19p^4q + 8pq^2 + p^2q^2 - 8p^3q^2 + 14p^4q^2 - 4q^3 + pq^3 \\
&\quad + 3p^2q^3 - 4p^3q^3) \\
s_0 &= -\frac{1}{3}q^2(p+1)(12p^3 + 4p^4 - 4p^2q + 4p^3q - 10p^4q + 12pq^2 - 6p^2q^2 - 3p^3q^2 \\
&\quad + 3p^4q^2 + 4q^3 - 2pq^3 - 5p^2q^3 + 3p^3q^3)
\end{aligned}$$

Here,  $s_4$  and  $s_2$  are positive. Note that  $x \geq \frac{q-p}{3}$  implies  $u \leq \frac{4p-q}{6}$  since  $x \leq p - 2u$ . For  $u$  in this range,  $s_4u^4 + s_3u^3$  is negative. The remaining quadratic in  $u$  is negative at both  $u = 0$  and  $u = \frac{4p-q}{6}$ . Hence the entire expression is negative at  $x = \frac{q-p}{3}$ . Next, we set  $x = p - 2u$ ,

and again obtain a quartic polynomial in  $u$  with coefficients:

$$\begin{aligned} s_4 &= -81(pq - p - q), & s_3 &= \frac{4}{3}(q - p)s_4, \\ s_2 &= -9(pq - p - q)(3p^2 - 14pq - p^2q + 3q^2 - pq^2 + 3p^2q^2), \\ s_1 &= 3q(12p^3 - 12p^2q - 7p^4q - 12pq^2 + 16p^2q^2 - 6p^3q^2 + 6p^4q^2 - 4q^3 + 9p^2q^3 - 6p^3q^3), \\ s_0 &= -q^2(-28p^3 + 16p^4 - 4p^5 - 4p^2q + 16p^3q - 2p^4q + 2p^5q - 4pq^2 + 12p^3q^2 - 12p^4q^2 \\ &\quad + p^5q^2 + 4q^3 - 6p^2q^3 + 2p^3q^3 + p^4q^3) \end{aligned}$$

Here all coefficients except  $s_1$  are negative for any  $q \geq p \geq 5$ . Also,  $s_1u + s_0 \leq 0$  for any  $u \leq \frac{4p-q}{6}$ . Thus (3.32) is negative at  $x = p - 2u$ , and as shown earlier at  $x = \frac{q-p}{3}$  as well, and in the entire  $[0, \frac{q-p}{3}]$  interval. Thus (3.32) is negative for any  $x$ . This implies that for any  $r_3$ ,  $x$  should be set to 0 to maximize  $A$ , which eliminates all designs with  $r_1 > \frac{p(q+1)}{3}$ .

**Step 4.** The remaining competitors must be uniform and have replications  $r_i \in [\frac{p(q-2)}{3}, \frac{p(q+1)}{3}]$ . In this range  $\text{int}[\frac{r_i}{p}] = \frac{q-2}{3}$  and  $\text{int}[\frac{r_i}{q}] = \frac{p-2}{3}$  (except at boundary points). Similar to step 4 of the  $p \equiv q \equiv 1 \pmod{3}$  case, we will divide the problem into two parts. First it will be shown that for any  $r_1$ , the best design has  $r_2 = r_3$ . Assuming  $r_2 = r_3$ , it will then be shown (unlike the previous case) that  $A$  is a decreasing function of  $r_1$ , thus making  $d^*$  the  $A$ -optimal design.

Suppose that  $r_1 = \frac{p(q+1)}{3} - u$  for some  $u \in [0, \frac{p-2}{3}]$  since  $r_1 \geq \frac{pq+2}{3}$ . Also let  $r_2 = \frac{pq-r_1}{2} + \frac{x}{2} = \frac{p(2q-1)}{6} + \frac{u+x}{2}$  and  $r_3 = \frac{pq-r_1}{2} - \frac{x}{2} = \frac{p(2q-1)}{6} + \frac{u-x}{2}$ , where  $0 \leq x \leq p - 3u$  since  $r_1 \geq r_2 \geq r_3$ .

We will show that  $A$  is a decreasing function of  $x$ . Just like in (3.22):

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} \frac{27p^3q^3}{4} \{(c'_2 + c'_3)[(\sum c_i)^2 + 2 \sum c_i^2] - 4(c_2c'_2 + c_3c'_3)(\sum c_i)\}, \quad (3.33)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ . Using (3.14), we obtain:

$$\begin{aligned} (3.33) &= x[-q^2(p+1)^2(-p^2 + pq - p^2q - 2q^2 + 2pq^2) - 9q^2(p-1)(p+1)(pq + p + q)u \\ &\quad + 27p(pq + p + q)u^2 - 27(pq + p + q)u^3] \end{aligned} \quad (3.34)$$

The linear coefficient of  $x$  is negative for any  $u \in [0, \frac{p-2}{3}]$ . Therefore,  $A$  is a decreasing function of  $x$ , and for a given  $r_1$ , the  $A$ -best design must have  $x = 0$ , that is,  $r_2 = r_3 = \frac{pq-r_1}{2}$ .

Now, in order to show that for designs with  $r_2 = r_3$ ,  $A$  is decreasing in  $r_1$ , let  $r_1 = \frac{p(q+1)}{3} - x$ , where  $x \in [0, \frac{p-2}{3}]$ , and  $r_2 = r_3 = \frac{pq-r_1}{2}$ . We will show that  $A$  is increasing in  $x$ . Just like in (3.24), we have:

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} 54p^3q^3\{(c'_1 + 2c'_2)[(\sum c_i)^2 + 2\sum c_i^2] - 4(c_1c'_1 + 2c_2c'_2)(\sum c_i)\} = f(x), \quad (3.35)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ . Using (3.14),  $f(x)$  becomes a quartic polynomial in  $x$  with coefficients:

$$\begin{aligned} s_4 &= 81(pq + p + q), & s_3 &= -\frac{4}{3}ps_4 \\ s_2 &= 54(pq + p + q)(2p^2q^2 - 2q^2 - p^2), \\ s_1 &= -12(-9p^4 - 9p^3q - 9p^4q - 14p^2q^2 - 4p^3q^2 + 10p^4q^2 - 10pq^3 - 10p^2q^3 + 10p^3q^3 \\ &\quad + 10p^4q^3 - 4q^4 - 4pq^4 + 4p^2q^4 + 4p^3q^4), \\ s_0 &= p[-27p^4 - 27q(p^3 + p^4) + 4q^2(-11p^2 - 4p^3 + 7p^4) + 28q^3(-p - p^2 + p^3 + p^4) \\ &\quad + 16q^4(-1 - p + p^2 + p^3)]. \end{aligned}$$

For  $0 \leq x \leq \frac{p-2}{3}$ , we have  $f''(x) > 0$  and thus  $f'(x)$  is increasing in  $x$ . At  $x = \frac{p-2}{3}$  we have

$$f'(\frac{p-2}{3}) = -48(p+1)(q+1)(2p-2p^2-p^3+2q-2pq-p^2q-2q^2-pq^2+2p^2q^2+p^3q^2-q^3+p^2q^3) < 0,$$

for any  $q \geq p \geq 5$ . Hence  $f'(x)$  is negative in the entire range of  $x$ , and thus  $f(x)$  is minimum at  $x = \frac{p-2}{3}$ . Since  $f(\frac{p-2}{3}) > 0$ , it follows that  $A$  is increasing in  $x$ , and  $d^*$  is  $A$ -optimal because it has  $x = \frac{p-2}{3}$  and  $r_2 = r_3$ .

To end the proof of Theorem 3.3, we must analyze the special case  $p = 2$ , for which  $q \geq 5$  since there is no connected  $2 \times 2$  design. Step 1 above works for  $p = 2$  if we can show that  $c_i$  defined in (3.14) is an increasing function of  $r_i$ , for  $r_i < \frac{2(q-2)}{3}$ . Indeed, when  $r_i < \frac{2(q-2)}{3}$ :

$$c_i[r_i] = r_i + \frac{r_i^2}{2q} - \frac{1}{2}h(r_i, q) - \frac{1}{q}h(r_i, 2) = \begin{cases} \frac{r_i}{2} & \text{if } r_i \text{ is even} \\ \frac{r_i}{2} - \frac{1}{2q} & \text{if } r_i \text{ is odd} \end{cases}. \quad (3.36)$$

Both are increasing functions of  $r_i$ , and so designs with  $r_3 < \frac{2(q-2)}{3}$  need not be considered. Also,  $r_1 > \frac{2(q+1)}{3}$  implies  $r_3 \leq \frac{2(q-2)}{3}$ , and again Lemma 3.5 can be used to eliminate such designs. The only replication numbers left to consider are  $(r_1 = r_2 = \frac{2(q+1)}{3}, r_3 = \frac{2(q-2)}{3})$ ,

which are the replications for  $d^0$ , and  $(r_1 = \frac{2(q+1)}{3}, r_2 = r_3 = \frac{2q-1}{3})$ , which are the replications for  $d^*$ . Nonuniform designs with these replications can be eliminated with Lemma 3.3. Finally, to show that  $d^*$  is  $A$ -superior to  $d^0$ , use (3.5) and (3.14) to get:

$$A_{d^*} - A_{d^0} = \frac{2(q-2)}{3q(q-1)} > 0. \quad (3.37)$$

Thus,  $d^*$  is  $A$ -optimal for  $p = 2$ . With this we conclude the proof of Theorem 3.3.

### 3.4.4 Case 4: $p \equiv 1 \pmod{3}$ and $q \equiv 2 \pmod{3}$

Remember that the overall assumption in this section is that  $p \leq q$ . Therefore the cases ( $p \equiv 1 \pmod{3}$ ,  $q \equiv 2 \pmod{3}$ ) and ( $p \equiv 2 \pmod{3}$ ,  $q \equiv 1 \pmod{3}$ ) must be analyzed separately. The strategy used for finding  $A$ -optimal designs is the same here as in cases 2 and 3.

If  $q \geq 2p$ , let  $d^*$  denote a uniform design with replications:

$$r_1 = r_2 = \frac{p(q+1)}{3}, \quad r_3 = \frac{p(q-2)}{3}. \quad (3.38)$$

If  $q < 2p$ , let  $d^*$  denote a uniform design with replications:

$$\begin{aligned} r_1 = r_2 = \frac{q(2p+1)}{6}, \quad r_3 = \frac{q(p-1)}{3}, \quad \text{if } q \text{ is even,} \\ r_1 = \frac{q(2p+1)+3}{6}, \quad r_2 = \frac{q(2p+1)-3}{6}, \quad r_3 = \frac{q(p-1)}{3}, \quad \text{if } q \text{ is odd.} \end{aligned} \quad (3.39)$$

**Theorem 3.4.** *The design  $d^*$  is  $A$ -optimal.*

The proof of this result will be divided into two parts, depending on the ratio  $\frac{q}{p}$ , and each part will be further divided into several steps, similar to previous cases.

**Part I.** Assume  $q \geq 2p$ . Note that in this case  $d^*$  is of maximal trace (i.e. rows are permutations of each other, and the design is generalized binary in columns). Let any competitor design  $d$  have replications  $r_1 \geq r_2 \geq r_3$ . In this part, the steps are the same as in the  $p \equiv q \equiv 2 \pmod{3}$  case:

- (1) Eliminate all designs with  $r_3 < \frac{p(q-2)}{3}$ ,

- (2) Eliminate all nonuniform designs with  $r_i \in [\frac{p(q-2)}{3}, \frac{p(q+4)}{3}]$ ,
- (3) Eliminate all designs with  $r_1 > \frac{p(q+1)}{3}$ ,
- (4) Show that among uniform designs with replications  $r_i \in [\frac{p(q-2)}{3}, \frac{p(q+1)}{3}]$ ,  $d^*$  is  $A$ -optimal.

**Step 1.** Consider a design  $d$  with  $r_3 < \frac{p(q-2)}{3}$ , and  $c_1, c_2, c_3$  the diagonal elements for the column component design's information matrix. Create the symmetrized design  $\bar{d}$  with  $\bar{c}_3 = c_3$  and  $\bar{c}_1 = \bar{c}_2 = \frac{c_1+c_2}{2}$ . Design  $\bar{d}$  is  $A$ -inferior to  $d^*$  by Lemma 3.5, since  $c_3 < c_3^*$  by Lemma 2.1, and  $d^*$  is of maximal trace. As discussed in Section 2.3 design  $d$  is  $A$ -inferior to  $\bar{d}$ . All remaining competitor designs must have  $r_i \in [\frac{p(q-2)}{3}, \frac{p(q+4)}{3}]$ . Note that in this step it is not necessary to have  $q \geq 2p$ .

**Step 2.** In this step we eliminate all nonuniform designs with replications in the above range. In order to use Lemma 3.3, we must show that  $(\sqrt{3}-1)(c_2+c_3)-c_1 \geq 0$  where the  $c_i$ 's are the diagonal elements of a uniform design. Write  $r_1 = \frac{p(q+4)}{3} - x$ , for some  $0 \leq x \leq \frac{4p-1}{3}$ ,  $r_3 = \frac{p(q-2)}{3} + u$ , for some  $0 \leq u \leq \frac{x}{2}$ , and  $r_2 = \frac{p(q-2)}{3} + x - u$ . Depending on  $\text{int}[\frac{r_1}{p}]$ , the problem will be divided into two cases. For these replications, note also that  $x \leq p + \frac{u}{2}$  and

$$\begin{aligned} \text{int}[\frac{r_1}{q}] &= \frac{p-1}{3}, & \text{int}[\frac{r_1}{p}] &= \begin{cases} \frac{q+1}{3} & \text{if } 0 \leq x \leq p \\ \frac{q-2}{3} & \text{if } p < x \leq \frac{4p-1}{3} \end{cases}, \\ \text{int}[\frac{r_2}{q}] &= \text{int}[\frac{r_3}{q}] = \frac{p-1}{3}, & \text{int}[\frac{r_2}{p}] &= \text{int}[\frac{r_3}{p}] = \frac{q-2}{3}. \end{aligned}$$

except at boundary points. First, assume that  $0 \leq x \leq p$ . Using (3.14):

$$\begin{aligned} 9pq[(\sqrt{3}-1)(c_2+c_3)-c_1] &= 2(2\sqrt{3}pq - 2\sqrt{3}p^2q + 3q^2 - 2\sqrt{3}q^2 - 3p^2q^2 + 2\sqrt{3}p^2q^2 - 9u^2 \\ &\quad + 9\sqrt{3}u^2) + 3(6p - 3\sqrt{3}p - \sqrt{3}q + \sqrt{3}pq + 6u - 6\sqrt{3}u)x - 9(2 - \sqrt{3})x^2. \end{aligned} \quad (3.40)$$

This expression is similar to (3.28), which was shown to be positive for any  $0 \leq x \leq \frac{4p-2}{3}$  and  $q \geq 2p \geq 8$ . In fact,

$$(3.40) - (3.28) = 2q(-12p + 4\sqrt{3}p + 3q + 9x - 3\sqrt{3}x) > 0, \quad (3.41)$$

since  $x \geq 0$  and  $q \geq 2p$ . Hence 3.40 is also positive for any  $x \in [0, \frac{4p-1}{3}]$  since (3.41) is increasing in  $x$ . Next, assume that  $x > p$ . In this case:

$$9pq[(\sqrt{3}-1)(c_2+c_3)-c_1] = 2(-9p^2+2\sqrt{3}pq-2\sqrt{3}p^2q+3q^2-2\sqrt{3}q^2-3p^2q^2+2\sqrt{3}p^2q^2-9u^2+9\sqrt{3}u^2)+3(12p-3\sqrt{3}p-\sqrt{3}q+\sqrt{3}pq+6u-6\sqrt{3}u)x-9(2-\sqrt{3})x^2. \quad (3.42)$$

It is easy to see that (3.42)-(3.40) =  $18p(x-p) > 0$  since  $x > p$ . Thus, (3.42) is also positive, and so all nonuniform designs are eliminated.

**Step 3.** In this step we further restrict the replication range from step 1, by eliminating all designs with  $r_1 > \frac{p(q+1)}{3}$ . For a fixed  $r_3 = \frac{p(q-2)}{3} + u$  with  $0 \leq u \leq \frac{p}{2}$  (since  $r_3 \leq \frac{pq-r_1}{2}$ ), write  $r_1 = \frac{p(q+1)}{3} + x$ , and  $r_2 = pq - r_1 - r_3 = \frac{p(q+1)}{3} - x - u$ . Note that  $0 \leq x \leq p - 2u$  since  $r_2 \geq r_3$ . The function  $A$  defined in (3.5) is differentiable in  $x$  everywhere. Just like in (3.32), we have:

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} \frac{27p^3q^3}{8} \{(c'_1 + c'_2)[(\sum c_i)^2 + 2 \sum c_i^2] - 4(c_1c'_1 + c_2c'_2)(\sum c_i)\}, \quad (3.43)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ . We will show that the partial derivative of  $A$  with respect to  $x$  is negative. The values of  $\text{int}[\frac{r_i}{p}]$  and  $\text{int}[\frac{r_i}{q}]$  are:

$$\text{int}[\frac{r_1}{p}] = \frac{q+1}{3}, \quad \text{int}[\frac{r_2}{p}] = \text{int}[\frac{r_3}{p}] = \frac{q-2}{3}, \quad \text{int}[\frac{r_1}{q}] = \text{int}[\frac{r_2}{q}] = \text{int}[\frac{r_3}{q}] = \frac{p-1}{3},$$

except at the boundary point  $r_1 = \frac{p(q+4)}{3}$ . Using (3.14), (3.43) becomes a quadratic function in  $x$  with coefficients:

$$\begin{aligned} s_2 &= 3pq(p-1)(pq-q-3u), \\ s_1 &= -2q^2(p-1)^2[-p^2+2pq(p+1)-2q^2(p+1)] + 18q(p-1)[p^2-pq(p+1)+q^2(p^2-1)]u \\ &\quad -18p[-3p+4q(p-1)]u^2 + 54(pq-p-q)u^3, \\ s_0 &= -pq^2(p-1)^2(pq-p+q)^2 + q(p-1)[8pq^2-2q^3+p^3(-9+13q-8q^2)+p^2q(2q^2+5)]u \\ &\quad +3[-9p^3+12p^2q(p-1)-2pq^2(p-1)(2p+1)+3q^3(p+1)(p-1)^2]u^2 \\ &\quad -54p(pq-p-q)u^3 + 27(pq-p-q)u^4. \end{aligned}$$

Coefficients  $s_2$  and  $s_1$  are positive for any  $0 \leq u \leq \frac{p}{2}$  and  $q \geq 2p \geq 8$ . Thus the derivative of this quadratic is an increasing function of  $x$ . Setting  $x$  at its maximum value, which is  $p - 2u$ , we obtain a quartic polynomial in  $u$  with coefficients:

$$\begin{aligned} s_4 &= -81(pq - p - q), & s_3 &= -\frac{4}{3}ps_4, & s_2 &= \frac{1}{9}(3p^2q^2 - 3q^2 - p^2q + pq + 3p^2)s_4, \\ s_1 &= 3q^2(p-1)(p^2 - 7p^3 - 6pq + 6p^3q + 2q^2 - 2p^2q^2) \\ s_0 &= -pq^2(p-1)^2(-4p^2 + 2pq + 2p^2q - 3q^2 - 2pq^2 + p^2q^2) \end{aligned}$$

Note that coefficients  $s_0$ ,  $s_2$ , and  $s_4$  are negative for any  $q \geq 2p \geq 8$ . Also,  $s_2 + s_3u < 0$  and  $s_0 + s_1u < 0$  since  $u \leq \frac{p}{2}$ . Therefore, the derivative of  $A$  with respect to  $x$  is negative, and thus designs with  $x = 0$  (i.e.  $r_1 = \frac{p(q+1)}{3}$ ) are  $A$ -better than designs with  $x > 0$ . The remaining competitor designs are uniform and have  $r_i \in [\frac{p(q-2)}{3}, \frac{p(q+1)}{3}]$ .

**Step 4.** Now we must show that among uniform design with replications in the above range,  $d^*$  is  $A$ -optimal. This final step of part I of the proof will be handled in two stages. First, for a fixed  $r_1 = \frac{p(q+1)}{3} - u$  with  $0 \leq u \leq \frac{p-1}{3}$ , let  $r_3 = \frac{p(q-2)}{3} + x$  and so  $r_2 = \frac{p(q+1)}{3} + u - x$  with  $2u \leq x \leq \frac{p+u}{2}$ , since  $r_1 \geq r_2 \geq r_3$ . We will show that  $A$  is a decreasing function of  $x$ . Note that when  $\frac{p(q-2)}{3} \leq r_i < \frac{p(q+1)}{3}$ , we have  $\text{int}[\frac{r_i}{p}] = \frac{q-2}{3}$  and  $\text{int}[\frac{r_i}{q}] = \frac{p-1}{3}$ . Similar to (3.33), we have:

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} \frac{27p^3q^3}{8} \{ (c'_2 + c'_3) [(\sum c_i)^2 + 2 \sum c_i^2] - 4(c_2c'_2 + c_3c'_3)(\sum c_i) \}, \quad (3.44)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ . Using (3.14), the above equation becomes a linear function of  $x$ , which can be written as  $(p + u - 2x)S$ , where  $S$  is a cubic polynomial in  $u$  with coefficients:

$$\begin{aligned} s_3 &= 27(pq + p - q), & s_2 &= -ps_3, & s_1 &= \frac{1}{3}q^2(p-1)(p+1)s_3, \\ s_0 &= -q^2(p-1)^2(2pq^2 + 2q^2 + p^2q + pq + p^2). \end{aligned}$$

Simple algebra can show that  $s_0 + s_1u$  and  $s_2 + s_3u$  are negative for any  $u \in [0, \frac{p-1}{3}]$ . Thus  $S$  is negative, and since  $p + u - 2x \geq 0$ , (3.44) is negative for any  $x$ . This means that  $A$  is a decreasing function of  $x$ , and so the  $A$ -best designs, for a fixed  $r_1$ , have  $x = 2u$ , and so  $r_1 = r_2 = \frac{p(q+1)}{3} - u$ ,  $r_3 = \frac{p(q-2)}{3} + 2u$ .

The next stage is to show that among all such designs, the best one is  $d^*$ , which has  $u = 0$ . However, simply taking the derivative of  $A$  with respect to  $u$  does not yield the result because  $\frac{\partial A}{\partial u}$  changes sign for some values of  $p$  and  $q$  inside the interval  $u \in [0, \frac{p-1}{3}]$ . The strategy is to show that the second derivative of  $A$  with respect to  $u$  is positive, thus making  $A$  a convex function of  $u$  in the given interval. Then it will be shown that  $A$  is larger at  $u = 0$  than at  $u = \frac{p-1}{3}$ . Similar to (3.35), we have

$$\frac{\partial A}{\partial u} \stackrel{\text{sign}}{=} \frac{9}{32} p^3 q^3 \{ (2c'_1 + c'_3) [(\sum c_i)^2 + 2 \sum c_i^2] - 4(2c_1 c'_1 + c_3 c'_3) (\sum c_i) \} = f(u), \quad (3.45)$$

where  $c'_i = \frac{\partial c_i}{\partial u}$ . Using (3.14),

$$\begin{aligned} f(u) = & -\frac{27}{2}(pq + p - q)u^4 + 18p(pq + p - q)u^3 - \frac{9}{2}(p^2q^2 + p^2 - q^2)(pq + p - q)u^2 + q^2(p^2 + 2p^3 \\ & - 2pq + 2p^3q - q^2 + p^2q^2)(p - 1)u - \frac{1}{6}pq^2(p - 1)^2(p^2 + pq + p^2q + 2q^2 + 2pq^2) \end{aligned} \quad (3.46)$$

Taking the derivative of  $f$  with respect to  $u$ , we get a cubic polynomial in  $u$  with coefficients:

$$\begin{aligned} s_3 &= -54(pq + p - q), \quad s_2 = -ps_3, \quad s_1 = \frac{1}{6}(p^2q^2 + p^2 - q^2)s_3, \\ s_0 &= q^2(p - 1)(p^2q^2 - q^2 + 2p^3q - 2pq + 2p^3 + p^2). \end{aligned}$$

Note that  $s_0 + s_1u$  and  $s_2 + s_3u$  are positive for any  $0 \leq u \leq \frac{p-1}{3}$ . Therefore (3.46) is positive, which means that  $A$  is a convex function of  $u$ . Next, let  $A^*$  and  $A'$  denote the function  $A$  at  $u = 0$ , and at  $u = \frac{p-1}{3}$ , respectively. By (3.5) and (3.14):

$$A^* - A' = \frac{4(p-1)(pq - p + q)}{9pq(p+1)(q-1)} > 0. \quad (3.47)$$

Since  $A$  is convex inside  $[0, \frac{p-1}{3}]$ , its maximum is achieved at one of the endpoints; as shown above  $A^* > A'$ , so  $A$  is maximum at  $u = 0$ . Hence, the design  $d^*$  with replications  $r_1 = r_2 = \frac{p(q+1)}{3}$  and  $r_3 = \frac{p(q-2)}{3}$  is  $A$ -optimal. With this we conclude part I of the proof.

**Part II.** Assume  $p < q < 2p$ . In fact, it must be that  $p+1 \leq q \leq 2p-3$  because  $p \equiv 1$  and  $q \equiv 2 \pmod{3}$ . In order to eliminate some of the competitor designs, we introduce a uniform design  $d^0$  with replications:

$$r_1^0 = \frac{q(p+2)}{3}, \quad r_2^0 = r_3^0 = \frac{q(p-1)}{3}, \quad (3.48)$$

and  $c_1^0, c_2^0, c_3^0 = c_2^0$  the diagonal elements of its information matrix. Note that  $C_{d^0}$  is the same as the row component information matrix since in  $d^0$  columns are permutations of each other. Let any competitor design  $d$  have replications  $r_1 \geq r_2 \geq r_3$ . From step 1 of part I, we know that  $r_i \in [\frac{p(q-2)}{3}, \frac{p(q+4)}{3}]$ . This part of the proof will be again divided into the following steps, similar to the case  $p \equiv q \equiv 1 \pmod{3}$ .

- (1) Eliminate all designs with  $r_1 > \frac{q(p+2)}{3}$ ,
- (2) Eliminate all nonuniform designs with  $r_i \in [\frac{p(q-2)}{3}, \frac{q(p+2)}{3}]$ ,
- (3) Eliminate all designs with  $r_3 < \frac{q(p-1)}{3}$ ,
- (4) Show that among uniform designs with replications  $r_i \in [\frac{q(p-1)}{3}, \frac{q(p+2)}{3}]$ ,  $d^*$  is  $A$ -optimal.

**Step 1.** Consider a design  $d$  with replication  $r_1 > \frac{q(p+2)}{3}$ , and  $c_1, c_2, c_3$  the diagonal elements of the row component design's information matrix. Create the symmetrized design  $\bar{d}$  with  $\bar{c}_1 = c_1$  and  $\bar{c}_2 = \bar{c}_3 = \frac{c_2+c_3}{2}$ . We know that  $d$  is  $A$ -inferior to  $\bar{d}$  since  $\bar{d}$  is an averaged version of  $d$ . We will show that  $\bar{d}$  is  $A$ -inferior to  $d^0$  using Lemma 3.4.

First, to show part (a) of Lemma 3.4, compute:

$$2(\sqrt{3}-1)c_2^0 - c_1^0 = -\frac{2}{9}(\sqrt{3}q + \sqrt{3} - 6) + \frac{2p[(2\sqrt{3}-3)q^2 - 2\sqrt{3}]}{9q}. \quad (3.49)$$

This is positive for any  $q > p \geq 4$ . To show part (b) of Lemma 3.4, we need  $\text{trace}[C_{d^0}] \geq \text{trace}[C_{\bar{d}}] = c_1 + c_2 + c_3$ . By (3.9):

$$\begin{aligned} c_1 + c_2 + c_3 &= pq - \frac{1}{q} \sum_{j=1}^p (n_{d1j}^2 + n_{d2j}^2 + n_{d3j}^2), \\ c_1^0 + 2c_2^0 &= pq - \frac{1}{q} \sum_{j=1}^p (n_{d^01j}^2 + n_{d^02j}^2 + n_{d^03j}^2), \end{aligned}$$

where  $n_{ij}$  is the number of times treatment  $i$  occurs in row  $j$ . To maximize  $\text{trace}[C_{\bar{d}}]$ , assume  $d$  is uniform in rows. Since  $r_1 \in [\frac{q(p+2)}{3} + 1, \frac{p(q+4)}{3}]$ , we have  $n_{d1j} \in \{\frac{q+1}{3}, \frac{q+4}{3}\}$ . Also, since  $r_i \geq \frac{p(q-2)}{3}$ , we must have  $r_3 \leq r_2 \leq \frac{p(q+1)}{3}$ , and thus  $n_{dij} \in \{\frac{q-2}{3}, \frac{q+1}{3}\}$  for  $i = 2, 3$ . Similar,

for  $d^0$  we have  $n_{d^0 1j} \in \{\frac{q+1}{3}, \frac{q+4}{3}\}$  and  $n_{d^0 ij} \in \{\frac{q-2}{3}, \frac{q+1}{3}\}$  for  $i = 2, 3$ . In a generalized binary design in rows,  $n_{ij} \in \{\frac{q-2}{3}, \frac{q+1}{3}\}$  and  $\sum_{j=1}^p \sum_{i=1}^3 n_{ij}^2 = p[h(q, 3)]$ . For designs  $d$  and  $d^0$ :

$$\begin{aligned} \sum_{j=1}^p \sum_{i=1}^3 n_{dij}^2 &= p[h(q, 3)] + 2(r_1 - \frac{p(q+1)}{3}), \\ \sum_{j=1}^p \sum_{i=1}^3 n_{d^0 ij}^2 &= p[h(q, 3)] + 2(r_1^0 - \frac{p(q+1)}{3}). \end{aligned}$$

This implies  $c_1 + c_2 + c_3 < c_1^0 + 2c_2^0$  because  $r_1 > r_1^0$ .

Condition (c) of Lemma 3.4 requires  $c_2^0 > \bar{c}_2$ . The quantity  $2\bar{c}_2 = c_2 + c_3$  is maximized if  $d$  is uniform in rows, and then

$$c_2 + c_3 = pq - r_1 - \frac{1}{q} \sum_{i=1}^2 \sum_{j=1}^p n_{dij}^2 \leq pq - r_1 - \frac{2}{q} p \left( \frac{pq - r_1}{2p} \right)^2 = \frac{pq}{2} - \frac{r_1^2}{2pq}.$$

If  $r_1 \geq r_1^0 + 2$ , then

$$2c_2^0 - 2\bar{c}_2 \geq \frac{2[(q+3)^2 + 2pq - 2p^2]}{9pq} > 0.$$

If  $r_1 = r_1^0 + 1$ , then

$$2c_2^0 - 2\bar{c}_2 \geq 2c_2^0 - (pq - r_1^0 - 1) + \frac{1}{q} h[pq - r_1^0 - 1, 2p] = \frac{q+1}{3q} > 0.$$

Thus, all conditions of Lemma 3.4 are met, so all designs with  $r_1 > \frac{q(p+2)}{3}$  are eliminated.

**Step 2.** The remaining competitor designs must have  $r_i \in [\frac{p(q-2)}{3}, \frac{q(p+2)}{3}]$ . In this step we eliminate all nonuniform designs with replications in the above range. In order to use Lemma 3.3, we need to show that for any uniform design  $d$ ,  $(\sqrt{3}-1)(c_2+c_3)-c_1 > 0$ . First, note that when  $r_i \leq \frac{q(p-1)}{3}$ , then  $c_i$  is an increasing function of  $r_i$  by Lemma 2.1. If  $\frac{q(p-1)}{3} \leq r_i \leq \frac{q(p+2)}{3}$ , then  $c_i$  is still an increasing function of  $r_i$  as shown below. Using (3.14):

$$c_i(r_i + 1) - c_i(r_i) = \begin{cases} \frac{1}{3pq}(6r_i - pq - q + p + 3) & \text{if } \frac{q(p-1)}{3} \leq r_i < \frac{p(q+1)}{3} \\ \frac{1}{3pq}(6r_i - pq - q - 5p + 3) & \text{if } \frac{p(q+1)}{3} \leq r_i < \frac{q(p+2)}{3} \end{cases}.$$

Both expressions are positive, and so  $c_i$  is an increasing function of  $r_i$  in the entire interval

$[\frac{p(q-2)}{3}, \frac{q(p+2)}{3}]$ . Thus,  $c_2 \geq c_3 \geq c_i[\frac{p(q-2)}{3}]$  and  $c_1 \leq c_i[\frac{q(p+2)}{3}]$ . Using (3.14) again:

$$2(\sqrt{3}-1)c_i[\frac{p(q-2)}{3}] - c_i[\frac{q(p+2)}{3}] = -\frac{2}{9}(-15 + 10\sqrt{3} - 2p + 2\sqrt{3}p) - \frac{4p}{9q} + \frac{2q(-4 + 4\sqrt{3} - p - 3p^2 + 2\sqrt{3}p^2)}{9p}.$$

This is an increasing function of  $q$ . It is positive if  $q \geq p + 4$  or if  $p \geq 7$ . The only  $(p, q)$  pair that does not yield a positive number is  $p = 4$  and  $q = 5$ . However, in this case all nonuniform designs can be eliminated numerically.

**Step 3.** In this step we further lower the number of competitors, by eliminating all designs with  $r_3 < \frac{q(p-1)}{3}$ . For a given  $r_1 = \frac{q(p+2)}{3} - u$  with  $0 \leq u \leq \frac{q}{2}$ , write  $r_3 = \frac{q(p-1)}{3} - x$  and  $r_2 = pq - r_1 - r_3 = \frac{q(p-1)}{3} + x + u$  with  $0 \leq x \leq \min[q - 2u, \frac{2p-q}{3}]$ , where the restrictions for  $u$  and  $x$  follow directly from  $r_1 \geq r_2 \geq r_3 \geq \frac{p(q-2)}{3}$ . Similar to previous cases, we will show that the derivative of the function  $A$  defined in (3.5) with respect to  $x$  is negative.

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} \frac{27p^3q^3}{8} \{(c'_2 + c'_3)[(\sum c_i)^2 + 2 \sum c_i^2] - 4(c_2c'_2 + c_3c'_3)(\sum c_i)\}, \quad (3.50)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ . Depending on the value of  $\text{int}[\frac{r_1}{p}]$ , there are two forms that (3.50) can take. If  $r_1 \geq \frac{p(q+1)}{3}$ , which is true when  $u \leq \frac{2q-p}{3}$ , then (3.50) is a quadratic function of  $x$  with coefficients:

$$\begin{aligned} s_2 &= 3pq(q+1)(pq+p+3u), \\ s_1 &= -2\{p^2[-q^2(q-5)^2 - 2pq(q^3 - 4q^2 + 4q - 9) + p^2(q-2)(2q^2 + q + 2)] \\ &\quad + 3p[-9p^2 + 2pq(2p+13) - q^2(2p^2 + 16p + 15) + 3q^3(p^2 + p + 1)]u \\ &\quad + 9[pq(9-4q) - 3q^2 + p^2(5q-6)]u^2 + 27(pq-p+q)u^3\}, \\ s_0 &= -p^2q(pq^2 + q^2 - 5q + 2p)^2 - p\{-4p^3 + 48p^2q - pq^2(3p^2 + 14p + 112) + q^3[45 + 2p(p^2 \\ &\quad + 10p + 23)] - q^4(8p^2 + 13p + 9)\}u - 3\{-9p^3 + 4p^2q(p+12) - pq^2(2p^2 + 26p + 45) \\ &\quad + q^3[9 + p(3p^2 + 4p + 12)]\}u^2 - 9[-6p^2 + pq(5p+13) - 6q^2(p+1)]u^3 - 27(pq-p+q)u^4. \end{aligned}$$

The coefficient of  $x^2$  is positive. We will show that (3.50) is negative both at  $x = 0$  and at

$x = q - 2u$ . First, if  $x = 0$ , then (3.50) becomes a quartic polynomial in  $u$  with coefficients:

$$\begin{aligned} s_4 &= -27(pq - p + q), \quad s_3 = 9(6pq^2 + 6q^2 - 5p^2q - 13pq + 6p^2), \\ s_2 &= -3(3p^3q^3 + 4p^2q^3 + 12pq^3 + 9q^3 - 2p^3q^2 - 26p^2q^2 - 45pq^2 + 4p^3q + 48p^2q - 9p^3), \\ s_1 &= -p[-4p^3 + 48p^2q - (112p + 14p^2 + 3p^3)q^2 + (45 + 46p + 20p^2 + 2p^3)q^3 - (9 + 13p + 8p^2)q^4], \\ s_0 &= -p^2q(pq^2 + q^2 - 5q + 2p)^2. \end{aligned}$$

Coefficients  $s_4$ ,  $s_2$ , and  $s_0$  are negative. Furthermore,  $s_2 + s_3u$  and  $s_0 + s_1u$  are also negative at the maximum value of  $u$ , which is  $\frac{2q-p}{3}$ . Hence, (3.50) is negative at  $x = 0$  for any  $r_1 \geq \frac{p(q+1)}{3}$ .

Setting  $x = q - 2u$ , (3.50) becomes another quartic polynomial in  $u$  with coefficients:

$$\begin{aligned} s_4 &= 81(pq - p + q), \quad s_3 = -27(4pq^2 + 4q^2 - 5p^2q - 11pq + 6p^2), \\ s_2 &= 9(3p^3q^3 + 4p^2q^3 + 4pq^3 + 3q^3 - 2p^3q^2 - 20p^2q^2 - 27pq^2 + 4p^3q + 32p^2q - 9p^3), \\ s_1 &= -3p(6p^2q^4 + 7pq^4 - 2p^3q^3 - 8p^2q^3 - 22pq^3 - 18q^3 + 3p^3q^2 + 14p^2q^2 + 52pq^2 - 26p^2q + 4p^3), \\ s_0 &= -p^2q(p^2q^4 - 2pq^4 - 4q^4 + 4p^2q^3 + 6pq^3 + 4q^3 - 2p^2q^2 - 12pq^2 - 28q^2 + 16pq - 4p^2). \end{aligned}$$

Note that  $s_4$  is positive, and also  $s_2 + 3s_3u > 0$  since  $0 \leq u \leq \frac{2q-p}{3}$ . Thus, the second derivative of the above polynomial is positive. Also, the polynomial is negative both at  $u = 0$  and  $u = \frac{2q-p}{3}$ . Thus, if  $r_1 \geq \frac{p(q+1)}{3}$ , then  $A$  is decreasing in  $x$ , so  $A$ -best designs have  $r_3 \geq \frac{q(p-1)}{3}$ .

Next, if  $r_1 < \frac{p(q+1)}{3}$ , then (3.50) becomes another quadratic function of  $x$  with coefficients:

$$\begin{aligned} s_2 &= 3pq(q+1)(pq + p + 3u), \\ s_1 &= -2\{p^2(q+1)^2[2(p^2 - pq)(q-1) - q^2] + 9p(q+1)[pq(q-1) + q^2 + p^2(q^2 - 1)]u \\ &\quad - 9q[3q + 4p(q+1)]u^2 + 27(pq + p + q)u^3\}, \\ s_0 &= -27q(q-u)^2u^2 - p^4(q-1)(q+1)^2[q(q-1) + 2u] - p^2q(q+1)(q-u)(q^2 + q + 6u \\ &\quad - 12qu) + 9pu(q+1)(q-u)(q^2 - 3qu + 3u^2) - p^3(q-1)(q+1)^2(2q^2 - 8qu + 9u^2). \end{aligned}$$

Again, the coefficient of  $x^2$  is positive, and it will be shown that the quadratic is negative

both at  $x = 0$  and  $x = q - 2u$ . At  $x = 0$ , we obtain a quartic polynomial in  $u$  with coefficients:

$$\begin{aligned} s_4 &= -27(pq + p + q), & s_3 &= -2qs_4, \\ s_2 &= -3(3p^3q^3 + 4p^2q^3 + 12pq^3 + 9q^3 + 3p^3q^2 + 2p^2q^2 + 12pq^2 - 3p^3q - 2p^2q - 3p^3), \\ s_1 &= -p(q + 1)(-8p^2q^3 - 13pq^3 - 9q^3 + 2p^3q^2 + 5pq^2 + 8p^2q - 2p^3), \\ s_0 &= -p^2q(q + 1)^2(pq - p + q)^2. \end{aligned}$$

Coefficients  $s_4$ ,  $s_2$ , and  $s_0$  are negative. Also  $s_0 + s_1u$  and  $s_2 + s_3u$  are negative at the maximum value of  $u$ , which is  $\frac{q}{2}$ . Thus, (3.50) is negative at  $x = 0$  for any  $r_1 < \frac{p(q+1)}{3}$ .

Setting  $x = q - 2u$ , we obtain another quartic polynomial in  $u$  with coefficients:

$$\begin{aligned} s_4 &= 81(pq + p + q), & s_3 &= -\frac{4}{3}qs_4, & s_2 &= \frac{1}{9}(3p^2q^2 + pq^2 + 3q^2 + pq - 3p^2)s_4, \\ s_1 &= -3p^2(q + 1)(6pq^3 + 7q^3 - 2p^2q^2 + q^2 - 6pq + 2p^2), \\ s_0 &= -p^2q(q + 1)^2(p^2q^2 - 2pq^2 - 4q^2 + 2p^2q + 2pq - 3p^2). \end{aligned}$$

Note that  $s_4$  is positive, and also  $s_2 + 3s_3u > 0$  since  $0 \leq u \leq \frac{2q-p}{3}$ . Thus, the second derivative of the above polynomial is positive. Also, the polynomial is negative both at  $u = 0$  and at  $u = \frac{q}{2}$ . Thus, (3.50) is negative at  $x = q - 2u$  for any  $r_1 < \frac{p(q+1)}{3}$ , and by the earlier discussion, (3.50) is in fact negative for any  $x$  and  $u$ . Henceforth, only uniform designs with  $r_i \in [\frac{q(p-1)}{3}, \frac{q(p+2)}{3}]$  need to be considered.

**Step 4.** In this step we will show that among the remaining competitors,  $d^*$  is  $A$ -optimal. The problem will be divided into two subparts. First, for a given  $r_1$  it will be shown that the  $A$ -best design is the one with the minimum  $r_3$ . Then it will be shown that among such designs, the  $A$ -best design is  $d^*$ .

Similar to the previous step, write  $r_1 = \frac{q(p+2)}{3} - u$  with  $0 \leq u \leq \frac{2q-1}{3}$ ,  $r_3 = \frac{q(p-1)}{3} + x$ ,  $r_2 = pq - r_1 - r_3 = \frac{q(p-1)}{3} - x + u$  with  $0 \leq x \leq \frac{u}{2}$ . Also, for any given  $u$  we must also have  $x \geq 2u - q$ . Restrictions for  $u$  and  $x$  follow directly from  $r_1 \geq r_2 \geq r_3$  and  $r_i \in [\frac{q(p-1)}{3}, \frac{q(p+2)}{3}]$ . We will show that  $A$  is a decreasing function of  $x$ . By (3.5) and just like in (3.50):

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} \frac{27p^3q^3}{8} \{ (c'_2 + c'_3) [(\sum c_i)^2 + 2 \sum c_i^2] - 4(c_2c'_2 + c_3c'_3)(\sum c_i) \}, \quad (3.51)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ . Similar to the previous step, (3.51) has two different forms depending on  $\text{int}[\frac{r_1}{p}]$ . If  $r_1 \geq \frac{p(q+1)}{3}$ , which is equivalent to  $u \leq \frac{2q-p}{3}$ , (3.51) becomes a linear function of  $x$  with coefficients:

$$\begin{aligned} s_1 &= -2p(-4p^3 + 18p^2q - 13pq^2 - 8p^2q^2 - 3p^3q^2 - 18q^3 + 22pq^3 + 2p^2q^3 + 2p^3q^3 + 8pq^4 - 8p^2q^4) \\ &\quad -6(-9p^3 + 20p^2q + 4p^3q + 12pq^2 - 22p^2q^2 - 2p^3q^2 - 9q^3 + 9pq^3 - 3p^2q^3 + 3p^3q^3)u \\ &\quad -18(-6p^2 + pq + 5p^2q + 6q^2 - 6pq^2)u^2 - 54(pq - p - q)u^3, \\ s_0 &= -\frac{u}{2}s_1. \end{aligned}$$

When  $x$  is at its maximum of  $\frac{u}{2}$ , (3.51) becomes 0, and when  $x = 0$ , (3.51) is  $-\frac{u}{2}s_1$ . The coefficient  $s_1$  is decreasing in  $u$  for  $u \in [0, \frac{2q-p}{3}]$  and is positive at  $u = \frac{2q-p}{3}$ . Thus (3.51) is increasing in  $x$ , and is negative for any  $x$ . Thus, when  $r_1 \geq \frac{p(q+1)}{3}$  the  $A$ -best designs have  $r_3 = \frac{q(p-1)}{3}$ . Next, suppose  $r_1 < \frac{p(q+1)}{3}$ . In this case (3.51) is another linear function of  $x$  with coefficients:

$$\begin{aligned} s_1 &= -4p^2(q+1)(-p^2 + 4pq - 5q^2 + p^2q^2 + 4q^3 - 4pq^3) - 18(pq + p - q)(p^2q^2 - p^2 + 3q^2)u \\ &\quad + 108q(pq + p - q)u^2 - 54(pq + p - q)u^3, \\ s_0 &= -\frac{u}{2}s_1. \end{aligned}$$

Again, (3.51) is 0 at  $x = \frac{u}{2}$ . The coefficient  $s_1$  is decreasing in  $u$  and is positive at the maximum value of  $u$ , which is  $\frac{2q-1}{3}$ , making  $s_1$  positive everywhere. Hence (3.51) is negative for any  $r_1 < \frac{p(q+1)}{3}$  as well. Thus, for given  $r_1$ ,  $A$ -best designs are the ones with minimum  $r_3$ ; that is  $r_3 = \frac{q(p-1)}{3}$  if  $r_1 \geq \frac{pq - q(p-1)/3}{2} = \frac{q(2p+1)}{6}$ , and  $r_3 = pq - 2r_1$  if  $r_1 < \frac{q(2p+1)}{6}$ .

To find the  $A$ -optimal design among the remaining competitors, write  $r_1 = \frac{q(p+2)}{3} - x$ . It will be shown that  $A$  is an increasing function of  $x$  for  $x \leq \frac{q}{2}$ , and a decreasing function of  $x$  for  $x \geq \frac{q}{2}$ .

First, for  $x \leq \frac{q}{2}$ ,  $r_2 = \frac{q(p-1)}{3} + x$  and  $r_3 = \frac{q(p-1)}{3}$ , similar to previous cases we have:

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} \frac{27p^3q^3}{8} \{(c'_1 + c'_2)[(\sum c_i)^2 + 2 \sum c_i^2] - 4(c_1c'_1 + c_2c'_2)(\sum c_i)\}, \quad (3.52)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ . Again, this equation takes two forms depending on  $\text{int}[\frac{r_1}{p}]$ . If  $x \leq \frac{2q-p}{3}$ , then (3.52) becomes a quadratic function of  $x$  with coefficients:

$$\begin{aligned} s_2 &= -3p^2q(p-1)(q-2), \\ s_1 &= 2p^2[4p^2 + (7-4p-6p^2)q^2 + (-4+p+4p^2)q^3 + (1-p)q^4], \\ s_0 &= p^2[4p^3 - 4p^2q + (3p-6p^3)q^2 + (-7+2p+7p^2+2p^3)q^3 + (4-6p^2+p^3)q^4 + (p-1)q^5]. \end{aligned}$$

The coefficient of  $x^2$  is negative, and this quadratic is positive both at  $x=0$  and  $x=\frac{q}{2}$ . So (3.52) is positive for any  $x \in [0, \frac{2q-p}{3}]$ . If  $x > \frac{2q-p}{3}$ , then (3.52) becomes a linear function of  $x$  with coefficients:

$$s_1 = -2p^2(q+1)^2(pq^2 - q^2 + 2p^2q - pq - 2p^2), \quad s_0 = -\frac{q}{2}s_1.$$

This is decreasing in  $x$  and it equals 0 at  $x = \frac{q}{2}$ . Hence (3.52) is positive for any  $x \leq \frac{q}{2}$ .

Now suppose  $x > \frac{q}{2}$ , and so  $r_2 = r_1 = \frac{q(p+2)}{3} - x$ ,  $r_3 = pq - 2r_1 = \frac{q(p-4)}{3} + 2x$ , and also  $c_1 = c_2$ . We will show that  $A$  is a decreasing function of  $x$ . Similar to previous cases:

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} \frac{27p^3q^3}{16} [c'_3(8c_1^2 - 4c_1c_3 - c_3^2) + 6c_3^2c'_1], \quad (3.53)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ . Using (3.14) this becomes a quartic function of  $x$  with coefficients:

$$\begin{aligned} s_4 &= -81(pq + p - q), \quad s_3 = -\frac{8}{3}qs_4, \quad s_2 = \frac{1}{3}(p^2q^2 + 7q^2 - p^2)s_4, \\ s_1 &= -6[-p^4 + (7p^3 - p^4)q + (-8p^2 + 7p^3 + p^4)q^2 + (-9p - p^2 - 7p^3 + p^4)q^3 \\ &\quad + (9 - 9p + 7p^2 - 7p^3)q^4], \\ s_0 &= -4p^2q(q+1)(4pq^3 - 4q^3 - p^2q^2 + 5q^2 - 4pq + p^2). \end{aligned}$$

Note that  $s_4$  is negative, and  $s_2 + 3s_3x < 0$  for any  $x \in [\frac{q}{2}, \frac{2q-1}{3}]$  and  $q \geq p+1 \geq 5$ . Hence, the above polynomial must be concave; also its first derivative is positive at  $x = \frac{2q-1}{3}$ , and so the polynomial is increasing in  $x$ . The polynomial is negative at  $x = \frac{2q-1}{3}$ , and so negative for any  $x$  in the above interval. Hence,  $A$  is a decreasing function of  $x$ .

We have shown that for a given  $r_1$ , the  $A$ -best design has  $r_3$  minimum (with the restriction  $r_3 \geq \frac{q(p-1)}{3}$ ). Among these designs,  $A$  increases as  $r_1$  goes from  $\frac{pq+1}{3}$  to  $\frac{q(2p+1)}{6}$  and it

decreases as  $r_1$  goes from  $\frac{q(2p+1)}{6}$  to  $\frac{q(p+2)}{3}$ . It is then clear that when  $q$  is even,  $d^*$  is  $A$ -optimal (remember that  $r_1^* = r_2^* = \frac{q(2p+1)}{6}$ ,  $r_3^* = \frac{q(p-1)}{6}$  when  $q < 2p$  and  $q$  even). Note however that if  $q$  is odd, one cannot in fact have  $r_1 = \frac{q(2p+1)}{6}$  because  $r_1$  must be an integer. So, when  $q$  is odd there are two competitor designs:

$$\begin{aligned} d' & \text{ with } r_1 = r_2 = \frac{q(2p+1)-3}{6}, \quad r_3 = \frac{q(p-1)}{3} + 1, \text{ and} \\ d^* & \text{ with } r_1 = \frac{q(2p+1)+3}{6}, \quad r_2 = \frac{q(2p+1)-3}{6}, \quad r_3 = \frac{q(p-1)}{3}. \end{aligned}$$

To show that  $d^*$  is in fact  $A$ -superior to  $d'$ , use (3.5) and (3.14) to compute  $A_{d^*} - A_{d'}$ .

$$\begin{aligned} A_{d^*} - A_{d'} &= \frac{2}{3pq(4p^2-3)(q-1)[4p^2(q+1)-3(q+3)]} [p(2p+3)^2(4p-3) - (2p+3)(14p^2 \\ &\quad - 3p-9)q - (16p^4 + 36p^3 - 80p^2 - 27p + 54)q^2 + (p-1)(28p^2 - 27)q^3] \end{aligned}$$

The numerator and the denominator of the above fraction are both positive for any  $5 \leq p+1 \leq q \leq 2p-3$ . Thus  $d^*$  is  $A$ -superior to  $d'$ . With this we conclude the proof of Theorem 3.4.

### 3.4.5 Case 5: $p \equiv 2 \pmod{3}$ and $q \equiv 1 \pmod{3}$

In this case, a strategy similar to previous cases is employed for finding the  $A$ -optimal design. Depending on how large  $q$  is relative to  $p$ , the replications for the  $A$ -optimal design change.

**Theorem 3.5.** *The uniform design  $d^*$  with replications*

$$\begin{aligned} r_1^* = r_2^* &= \frac{p(2q+1)}{6}, \quad r_3^* = \frac{p(q-1)}{3}, & \text{if } p \text{ is even, and } q \leq \frac{3p}{2}, \\ r_1^* &= \frac{p(2q+1)+3}{6}, \quad r_2^* = \frac{p(2q+1)-3}{6}, \quad r_3^* = \frac{p(q-1)}{3}, & \text{if } p \text{ is odd, and } q \leq \frac{3(p-1)}{2}, \\ r_1^* = r_2^* &= \frac{pq+1}{3}, \quad r_3^* = \frac{pq-2}{3}, & \text{otherwise.} \end{aligned}$$

*is  $A$ -optimal.*

The proof of this theorem will be presented in two parts, with each part divided further into several steps. For the first part of the proof assume  $p \leq q \leq 2p$ , while for the second part assume  $q > 2p$ . Each part will be divided as follows:

- (1) Eliminate all designs with  $r_3 < \frac{q(p-2)}{3}$  or  $r_1 > \frac{p(q+2)}{3}$ ,
- (2) Eliminate all nonuniform designs with replications inside the interval determined in step (1),
- (3) Eliminate all designs with  $r_3 < \frac{p(q-1)}{3}$ ,
- (4) Reduce the competitors to three possible replication sets among remaining uniform designs,
- (5) Find the relations between  $p$  and  $q$  which dictate which replication set yields the  $A$ -optimal design,

**Part I.** In this first part of the proof assume  $p \leq q \leq 2p$ . For  $p = 2$ , under the restriction  $q \leq 2p$ , the only viable parameters are  $p = 2$  and  $q = 4$ . It has been shown numerically that  $d^*$  is  $A$ -optimal by going through all possible  $2 \times 4$  row-column designs. So also assume  $p \geq 5$ .

Note that  $c_i$  is an increasing function of  $r_i$  by Lemma 2.1 for any uniform treatment  $i$  with  $r_i \leq \frac{p(q-1)}{3}$ . Also, for uniform treatments, if  $r_i \leq \frac{p(q+2)}{3}$ , we have from (2.5) and (2.7):

$$3pq(c_i[r_i + 1] - c_i[r_i]) = \begin{cases} 3 - p + q - pq + 6r_i & \text{if } \frac{p(q-1)}{3} \leq r_i < \frac{q(p+1)}{3} \\ 3 - p - 5q - pq + 6r_i & \text{if } \frac{q(p+1)}{3} \leq r_i \leq \frac{p(q+2)}{3} \end{cases} . \quad (3.54)$$

Both are positive for  $p \geq 5$ , so  $c_i$  is an increasing function of  $r_i$  for all  $r_i \leq \frac{p(q+2)}{3}$ .

**Step 1.** We start by eliminating all designs with  $r_1 > \frac{p(q+2)}{3}$  using Lemma 3.4. First, construct the uniform design  $d^0$  with replications:

$$r_1^0 = \frac{p(q+2)}{3}, \quad r_2^0 = r_3^0 = \frac{p(q-1)}{3}.$$

We will show that any design  $d(c_1, c_2, c_3)$  with replication  $r_1 > \frac{p(q+2)}{3}$  is  $A$ -inferior to  $d^0$ . To do this create the symmetrized design  $\bar{d}(c_1, \bar{c}_2, \bar{c}_2)$ , where  $\bar{c}_2 = \frac{c_2 + c_3}{2}$ . Now

$$2(\sqrt{3} - 1)c_2^0 - c_1^0 = \frac{1}{9p}[-2p(\sqrt{3}p + \sqrt{3} - 6) + 2q(2\sqrt{3}p^2 - 3p^2 - 2\sqrt{3})].$$

This is positive, and thus condition (a) of Lemma 3.4 is met. The trace of  $d$  is no more than the trace of its column component design, which for fixed replications is maximized when  $d$  is uniform in columns. Let  $n_{ij}$  denote the number of times treatment  $i$  occurs in column  $j$ . Then:

$$\begin{aligned} \text{trace}(C_{\bar{d}}) &\leq pq - \frac{1}{p} \sum_{j=1}^q \sum_{i=1}^3 n_{ij}^2 \\ &\leq pq - \frac{1}{p} h(pq, 3q) - \frac{2}{p} \left[ r_1 - \frac{q(p+1)}{3} \right] \\ &< pq - \frac{1}{p} h(pq, 3q) - \frac{2}{p} \left[ r_1^0 - \frac{q(p+1)}{3} \right] = \text{trace}(C_{d^0}), \end{aligned}$$

since  $r_1 > r_1^0$ , and  $\sum_{j=1}^q \sum_{i=1}^3 n_{ij}^2$  increases by at least 2 above  $h(pq, 3q)$  for each unit  $r_1$  is above  $\frac{q(p+1)}{3}$ . So condition (b) of Lemma 3.4 is met as well.

To show condition (c), we need  $c_2 + c_3 < 2c_2^0$ . Note that

$$\begin{aligned} c_2 + c_3 &\leq pq - r_1 - \frac{1}{p} \sum_{j=1}^q \sum_{i=2}^3 n_{ij}^2 \\ &\leq pq - r_1 - \frac{1}{p} h(pq - r_1, 2q) < pq - r_1^0 - \frac{1}{p} h(pq - r_1^0, 2q) = 2c_2^0, \end{aligned}$$

where the last inequality follows directly from an application of Lemma 2.1 for a treatment replicated  $pq - r_1$  times in a block design with  $2q$  blocks of size  $p$ , since  $pq - r_1 \leq \frac{2q(p-1)}{2}$ . Hence, all conditions of Lemma 3.4 are met, and so any design  $d$  with  $r_1 > \frac{p(q+2)}{3}$  is  $A$ -inferior to  $d^0$ .

Next, consider a design  $d$  with  $r_3 < \frac{q(p-2)}{3}$  and  $r_1 \leq \frac{p(q+2)}{3}$ . We will show that such a design is  $A$  inferior to  $d_0$ , the uniform design with replications

$$r_{01} = r_{02} = \frac{q(p+1)}{3}, \quad r_{03} = \frac{q(p-2)}{3}.$$

Again, we symmetrize  $d(c_1, c_2, c_3)$  to obtain  $\bar{d}(\bar{c}_1, \bar{c}_1, c_3)$ , with  $\bar{c}_1 = \frac{c_1+c_2}{2}$ . An upper bound for the trace of  $C_{\bar{d}}$  is found when columns of  $d$  are permutations of one another. Letting  $n_{ij}$

denote the number of times treatment  $i$  occurs in row  $j$  of  $d$ , we have:

$$\begin{aligned} \text{trace}(C_{\bar{d}}) = \text{trace}(C_d) &\leq pq - \frac{1}{q} \sum_{j=1}^p \sum_{i=1}^3 n_{ij}^2 \\ &\leq pq - \frac{1}{q} h(pq, 3p) - \frac{2}{q} \left[ \frac{p(q-1)}{3} - r_3 \right] \\ &< pq - \frac{1}{q} h(pq, 3p) - \frac{2}{q} \left[ \frac{p(q-1)}{3} - r_{03} \right] = \text{trace}(C_{d_0}), \end{aligned}$$

since  $r_3 < r_{03}$  and  $\sum_{j=1}^p \sum_{i=1}^3 n_{ij}^2$  increases by at least 2 above  $h(pq, 3p)$  for each unit  $r_3$  is under  $\frac{p(q-1)}{3}$ . Condition (a) of Lemma 3.5 is met, and by Lemma 2.1 we also have condition (b), that is,  $c_3 < c_{03}$ . Thus  $d_0$  is  $A$ -superior to  $\bar{d}$ , which in turn is better than  $d$ , and so all designs with  $r_3 < \frac{q(p-2)}{3}$  are also eliminated.

**Step 2.** In this step we eliminate all nonuniform designs with replications not shown inadmissible in the previous step. To apply Lemma 3.3, we will verify that the inequality  $(\sqrt{3}-1)(c_2 + c_3) - c_1 > 0$  holds for any uniform design  $d(c_1, c_2, c_3)$  with these replications. As discussed in the previous step  $c_i$  is an increasing function of  $r_i$  for  $r_i \leq \frac{p(q+2)}{3}$ . If  $r_2 \geq r_3 \geq \frac{p(q-1)}{3}$ , then  $c_2 \geq c_3 \geq c_2^0$  and  $c_1 \leq c_1^0$ . Since  $2(\sqrt{3}-1)c_2^0 - c_1^0 > 0$ , it follows that  $(\sqrt{3}-1)(c_2 + c_3) - c_1 > 0$  for any  $r_3 \geq \frac{p(q-1)}{3}$ .

Next, let  $r_3 = \frac{p(q-1)}{3} - x$ , with  $0 < x \leq \frac{2q-p}{3} \leq p$ . The difference  $(\sqrt{3}-1)(c_2 + c_3) - c_1$  is a decreasing function of  $r_1$ , and will be minimized when  $r_1 = \frac{p(q+2)}{3}$  and  $r_2 = \frac{p(q-1)}{3} + x$ . With these replications we have:

$$\begin{aligned} \text{int}\left[\frac{r_1}{p}\right] &= \frac{q+2}{3}, & \text{int}\left[\frac{r_2}{p}\right] &= \frac{q-1}{3}, & \text{int}\left[\frac{r_3}{p}\right] &= \frac{q-4}{3}, \\ \text{int}\left[\frac{r_1}{q}\right] &= \frac{p+1}{3}, & \text{int}\left[\frac{r_2}{q}\right] &= \text{int}\left[\frac{r_3}{q}\right] &= \frac{p-2}{3}, \end{aligned} \quad (3.55)$$

since  $q \leq 2p$ . At the boundary point  $(q, x) = (2p, p)$  we have  $r_2 = r_1$ , but the value of  $c_2$  can be computed with the above values of  $\text{int}\left[\frac{r_2}{p}\right]$  and  $\text{int}\left[\frac{r_2}{q}\right]$  since  $h(r, b)$  is a continuous function of  $r$ . Thus, for fixed  $x$ , the minimum of  $(\sqrt{3}-1)(c_2 + c_3) - c_1$  is

$$\frac{1}{9pq} [18(\sqrt{3}-1)x^2 - 18p(\sqrt{3}-1)x + 2q(2\sqrt{3}p^2q - 3p^2q - 2\sqrt{3}q - \sqrt{3}p^2 - \sqrt{3}p + 6p)]$$

which itself is minimized at  $x = \frac{p}{2}$ . Setting  $x = \frac{p}{2}$ , we have an increasing function of  $p$ , positive for any  $p \geq 5$ . With this, all nonuniform designs are eliminated.

**Step 3.** In this step we further restrict the replication range by eliminating all designs with  $r_3 < \frac{p(q-1)}{3}$ . For a fixed  $r_1 = \frac{p(q+2)}{3} - u$  with  $0 \leq u \leq \frac{p}{2}$ , let  $r_3 = \frac{p(q-1)}{3} - x$  and  $r_2 = \frac{p(q-1)}{3} + x + u$ . Since  $r_1 \geq r_2 \geq r_3$ , we have  $0 \leq x \leq p - 2u$ . Also, since  $r_3 \geq \frac{q(p-2)}{3}$  it must be that  $x \leq \frac{2q-p}{3}$  as in the previous step. We will show that  $A$  defined in (3.5) is a decreasing function of  $x$ . Similar to (3.50):

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} \frac{27p^3q^3}{8} \{(c'_2 + c'_3)[(\sum c_i)^2 + 2 \sum c_i^2] - 4(c_2c'_2 + c_3c'_3)(\sum c_i)\}, \quad (3.56)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ . The value of  $\text{int}[\frac{r_1}{q}]$  is  $\frac{p+1}{3}$  when  $u \leq \frac{2p-q}{3}$ , and  $\frac{p-2}{3}$  when  $u > \frac{2p-q}{3}$ . The value of  $\text{int}[\frac{r_1}{p}]$  is  $\frac{q-1}{3}$  for  $u > 0$ , and when  $u = 0$  this value can still be used since  $h(r_1, q)$  is a continuous function of  $u$ . All the other integer parts values are given in (3.55). If  $u \leq \frac{2p-q}{3}$ , then (3.56) becomes a quadratic function in  $x$  with coefficients:

$$\begin{aligned} S_2 &= 3p(1+p)q(q+pq+3u), \\ S_1 &= 2\{p^4q^2(2q+1) + q(q+3u)^2(4q+3u) + p^3q[-2q(q^2+4q+5) - 9u(q^2+q+1)] \\ &\quad - 3p(q+3u)[6q^2+4qu(q+2) + 3u^2(q+1)] + p^2[q^2(3q^2+8q+25) \\ &\quad + 3qu(2q^2+16q+15) + 9u^2(4q+3)]\}, \\ S_0 &= -pq^2(p^2q+2q+p^2-5p)^2 - qu(45p^3-9p^4-112p^2q+46p^3q-13p^4q+48pq^2-8p^4q^2-4q^3 \\ &\quad - 14p^2q^2+20p^3q^2-3p^2q^3+2p^3q^3) - 3u^2(9p^3-45p^2q+12p^3q+48pq^2-26p^2q^2+4p^3q^2 \\ &\quad - 9q^3+4pq^3-2p^2q^3+3p^3q^3) - 9u^3(-6p^2+13pq-6p^2q-6q^2+5pq^2) - 27u^4(pq+p-q). \end{aligned}$$

The coefficient of  $x^2$  is positive. To show that the expression is negative, consider its values at the maximum and minimum of  $x$ . At  $x = 0$ , it reduces to  $S_0 = s_4u^4 + s_3u^3 + s_2u^2 + s_1u + s_0$ , where  $s_i$  are as shown above. Note that  $s_4$ ,  $s_2$ , and  $s_0$  are negative for any  $7 \leq p+2 \leq q \leq 2p$ . Also,  $s_0 + s_1u$  and  $s_2 + s_3u$  are negative at  $u = \frac{p}{2}$ , and so for any  $0 \leq u \leq \frac{p}{2}$ ; thus (3.56) is negative at  $x = 0$ . At  $x = \frac{2q-p}{3}$ , (3.56) reduces to another quartic function in  $u$  with

coefficients:

$$\begin{aligned}
s_4 &= -27(pq + p - q), \quad s_3 = -9(-8p^2 + 19pq - 8p^2q - 10q^2 + 9pq^2), \\
s_2 &= -3(15p^3 - 75p^2q + 20p^3q + 96pq^2 - 52p^2q^2 + 4p^3q^2 - 33q^3 + 24pq^3 - 2p^2q^3 + 3p^3q^3), \\
s_1 &= q[-74p^3 + 16p^4 + q(220p^2 - 94p^3 + 19p^4) + q^2(-166p + 90p^2 - 36p^3 + 14p^4) \\
&\quad + q^3(40 - 16p + 11p^2 - 14p^3)], \\
s_0 &= -\frac{q^2}{3}[124p^3 - 52p^4 + 4p^5 + q(-192p^2 + 76p^3 - 46p^4 + 10p^5) + q^2(88p - 40p^2 + 46p^3 \\
&\quad - 12p^4 + 3p^5) + q^3(-16 - 12p^2 + 8p^3)].
\end{aligned}$$

Here all coefficients are negative, so again (3.56) is negative. Hence, when  $u \leq \frac{2p-q}{3}$ , the function  $A$  is decreasing in  $x$ .

Next, suppose  $u > \frac{2p-q}{3}$ . In this case (3.56) becomes a similar quadratic function of  $x$  with coefficients:

$$\begin{aligned}
S_2 &= 3pq(p+1)(pq+q+3u), \\
S_1 &= 2\{q^2(p+1)^2[p^2+2q(p-q)(p-1)] - 9uq(p+1)[p^2+pq(p-1)+q^2(p^2-1)] \\
&\quad + 9u^2p[3p+4q(p+1)] - 27u^3(pq+p+q)\}, \\
S_0 &= -pq^2(p+1)^2(pq+p-q)^2 + uq(p+1)(9p^3 - 5p^2q + 13p^3q - 8pq^2 + 8p^3q^2 + 2q^3 \\
&\quad - 2p^2q^3) - 3u^2(9p^3 + 12p^2q + 12p^3q - 2pq^2 + 2p^2q^2 + 4p^3q^2 - 3q^3 - 3pq^3 \\
&\quad + 3p^2q^3 + 3p^3q^3) + 54u^3p(pq+p+q) - 27u^4(pq+p+q).
\end{aligned}$$

The coefficient of  $x^2$  is positive. Consider this quadratic at  $x = 0$  and  $x = p - 2u$ . When  $x = 0$ , it reduces to  $S_0 = s_4u^4 + s_3u^3 + s_2u^2 + s_1u + s_0$ . Note that  $s_4, s_2$  and  $s_0$  are negative, as are  $s_0 + s_1u$  and  $s_2 + s_3u$  at  $u = \frac{p}{2}$ , so the quadratic is negative at  $x = 0$ . At  $x = p - 2u$ , (3.56) becomes a quartic polynomial in  $u$  with coefficients:

$$\begin{aligned}
s_4 &= 81(pq + p + q), \quad s_3 = -\frac{4}{3}ps_4, \quad s_2 = \frac{1}{9}(3p^2 + pq + p^2q - 3q^2 + 3p^2q^2)s_4, \\
s_1 &= -3q^2(p+1)(p^2 + 7p^3 - 6pq + 6p^3q + 2q^2 - 2p^2q^2), \\
s_0 &= -pq^2(p+1)^2(-4p^2 + 2pq - 2p^2q - 3q^2 + 2pq^2 + p^2q^2).
\end{aligned}$$

The second derivative of this polynomial with respect to  $u$  is positive because  $3s_3u + s_2 > 0$  for any  $0 \leq u \leq \frac{p}{2}$ . Also, the polynomial is negative both at  $u = 0$  and at  $u = \frac{p}{2}$ , and thus negative everywhere in this interval. Therefore (3.56) is negative and  $A$  is decreasing in  $x$  for any  $u$ , implying  $A$ -best designs have  $r_3 \geq \frac{p(q-1)}{3}$ .

**Step 4.** All remaining competitors are uniform and have  $r_i \in [\frac{p(q-1)}{3}, \frac{p(q+2)}{3}]$ . Construct the uniform designs  $d^{**}$ ,  $d^*$ , and  $d'$  with replications:

$$\begin{aligned} r_1^{**} = r_2^{**} &= \frac{p(2q+1)}{6}, & r_3^{**} &= \frac{p(q-1)}{3}, & \text{if } p \text{ is even,} \\ r_1^{**} &= \frac{p(2q+1)+3}{6}, & r_2^{**} &= \frac{p(2q+1)-3}{6}, & r_3^{**} &= \frac{p(q-1)}{3}, & \text{if } p \text{ is odd,} \\ r_1^* &= r_2^* &= \frac{pq+1}{3}, & r_3^* &= \frac{pq-2}{3}, \\ r_1' &= r_2' &= \frac{p(2q+1)-3}{6}, & r_3' &= \frac{p(q-1)}{3} + 1, & \text{if } p \text{ is odd.} \end{aligned}$$

Note that  $d'$  is defined only for  $p$  odd. In this step we show that one of the three designs ( $d^{**}$ ,  $d^*$  or  $d'$ ) is  $A$ -optimal. The problem will be divided into two subparts. First, it will be shown that for any given  $r_3$ , the function  $A$  is decreasing in  $x$ , where  $x = r_1 - r_2$ . Then, among designs with minimum  $x$ , it will be shown that one of the three designs is  $A$ -optimal.

For a fixed  $r_3 = \frac{p(q-1)}{3} + u$  with  $0 \leq u \leq \frac{p-2}{3}$ , let  $r_1 = \frac{p(2q+1)-3u+3x}{6}$  and  $r_2 = \frac{p(2q+1)-3u-3x}{6}$ , for some  $x \in [0, p-3u]$ . For these replications

$$\begin{aligned} \text{int}\left[\frac{r_1}{p}\right] &= \frac{q-1}{3}, & \text{int}\left[\frac{r_2}{p}\right] &= \frac{q-1}{3}, & \text{int}\left[\frac{r_3}{p}\right] &= \frac{q-1}{3}, \\ \text{int}\left[\frac{r_1}{q}\right] &= \begin{cases} \frac{p+1}{3} & \text{if } r_1 \geq \frac{q(p+1)}{3} \\ \frac{p-2}{3} & \text{if } r_1 < \frac{q(p+1)}{3} \end{cases}, & \text{int}\left[\frac{r_2}{q}\right] &= \text{int}\left[\frac{r_3}{q}\right] &= \frac{p-2}{3}. \end{aligned} \quad (3.57)$$

We will now show that  $A$  is decreasing in  $x$ . Similar to (3.52), we have:

$$\frac{\partial A}{\partial x} \stackrel{\text{sign}}{=} 27p^3q^3\{(c'_1 + c'_2)[(\sum c_i)^2 + 2\sum c_i^2] - 4(c_1c'_1 + c_2c'_2)(\sum c_i)\}, \quad (3.58)$$

where  $c'_i = \frac{\partial c_i}{\partial x}$ . Again, (3.58) takes two forms depending on  $\text{int}[\frac{r_1}{q}]$  given in (3.57). If

$r_1 \geq \frac{q(p+1)}{3}$ , then (3.58) becomes a quadratic function of  $x$  with coefficients:

$$\begin{aligned} S_2 &= 3pq(q-1)(pq-2q-3u), \\ S_1 &= -2q^2[-8p^2+5p^3-2p^4+q(2p^2+p^3+2p^4)+q^2(-8+12p^2-8p^3)]+6pq[9p+q(10-8p \\ &\quad -6p^2)+q^2(2-7p+6p^2)]u-18(-6p^2-pq+6p^2q+6q^2-5pq^2)u^2+108(pq-p-q)u^3, \\ S_0 &= -q^2[-6p^3+3p^4+q(12p^2-2p^3+p^4)+q^2(4p^3-8p^4)+q^3(16-24p^2+8p^3+4p^4)] \\ &\quad -3pq(-3p^2+12pq+5p^2q+24q^2-12pq^2-10p^2q^2-12pq^3+8p^2q^3)u \\ &\quad -9q(10p^2+6pq-11p^2q-12q^2+6pq^2+p^2q^2)u^2-27q(3pq-3p-4q)u^3. \end{aligned}$$

The coefficient  $S_2$  of  $x^2$  is positive. Also,  $S_0$  is negative since it is a cubic polynomial in  $u$  with all coefficients negative, so (3.58) is negative at  $x=0$ . At the maximum value of  $x$ , which is  $p-3u$ , (3.58) becomes a quartic polynomial in  $u$  with coefficients:

$$\begin{aligned} s_4 &= -324(pq-p-q), \quad s_3 = \frac{4}{3}(q-p)s_4, \quad s_2 = \frac{1}{9}(3p^2-11pq+3q^2-pq^2+3p^2q^2)s_4, \\ s_1 &= 12q(6p^3-5p^2q-2p^3q-4p^4q-6pq^2+8p^2q^2-2p^3q^2+4p^4q^2-4q^3+9p^2q^3-6p^3q^3), \\ s_0 &= -4q^2(-7p^3+4p^4-p^5+3p^2q+2p^3q+p^5q-4pq^2+7p^3q^2-6p^4q^2+4q^3 \\ &\quad -6p^2q^3+2p^3q^3+p^4q^3). \end{aligned}$$

All coefficients are negative, except  $s_1$  for some values of  $p$  and  $q$ . However,  $s_0+s_1u$  is negative even at the maximum value of  $u$ , which is  $\frac{p-2}{3}$ , implying (3.58) is negative at maximum  $x$  and so at all  $x$ . Therefore,  $A$  is a decreasing function of  $x$  when  $r_1 \geq \frac{q(p+1)}{3}$ . Next, suppose  $r_1 < \frac{q(p+1)}{3}$ . In this case, (3.58) becomes a linear function of  $x$  with intercept 0 and slope  $S_1 = s_3u^3 + s_2u^2 + s_1u + s_0$ , where:

$$\begin{aligned} s_3 &= 108(pq-p+q), \quad s_2 = -ps_3, \quad s_1 = \frac{1}{3}q^2(p^2-1)s_4, \\ s_0 &= -4q^2(p+1)^2(-p^2-pq+p^2q-2q^2+2pq^2). \end{aligned}$$

Coefficients  $s_2$  and  $s_0$  are negative. Also, for any  $u \leq \frac{p-2}{3}$ , we have  $s_0+s_1u < 0$  and  $s_2+s_3u < 0$ . Therefore,  $S_1$  is negative and  $A$  is a decreasing function of  $x$  when  $r_1 < \frac{q(p+1)}{3}$  as well as when  $r_1 \geq \frac{q(p+1)}{3}$ . So for a given  $r_3$ , we now know that the  $A$ -best design will have  $x = r_1 - r_2$  minimized.

Now we move on to showing that the  $A$ -optimal design is one of the three competitors  $d^{**}$ ,  $d^*$  and  $d'$ . First, we need the following result about continuous differentiable functions.

**Lemma 3.6.** *Let  $g(t) : [a, b] \rightarrow \mathcal{R}$  be a continuous, three times differentiable function. If  $g'''(t) < 0$  for all  $t \in (a, b)$ , and  $g'(b) > 0$ , then the maximum value of  $g$  is  $g(a)$  or  $g(b)$ .*

*Proof.* Suppose there exists a local maximum of  $g$  at some  $\xi \in (a, b)$ . Then  $g'(\xi) = 0$  and  $g''(\xi) \leq 0$ . Since  $g'''(t) < 0$ , it follows that  $g''(t) < 0$  for any  $t > \xi$ . However, this implies that  $g'(t) < g'(\xi) = 0$  for any  $t > \xi$ , which contradicts  $g'(b) > 0$ .  $\square$

Now consider uniform designs  $d(c_1, c_1, c_3)$  with  $r_3 = \frac{p(q-1)}{3} + u$  where  $0 \leq u \leq \frac{p-2}{3}$ , and  $r_1 = r_2 = \frac{p(2q+1)-3u}{6}$ . We do not require  $r_1$  and  $r_2$  to be integers at this point (the word ‘‘design’’ is used loosely here). For such replications,  $A$  is a continuous differentiable function of  $u$ . Similar to (3.53):

$$\frac{\partial A}{\partial u} \stackrel{\text{sign}}{=} 27p^3q^3[c'_3(8c_1^2 - 4c_1c_3 - c_3^2) + 6c_3^2c'_1], \quad (3.59)$$

where  $c'_i = \frac{\partial c_i}{\partial u}$ . Using (3.14) and (3.57) with  $r_1 < \frac{q(p+1)}{3}$ , this becomes a quartic function of  $u$  with coefficients:

$$\begin{aligned} s_4 &= -\frac{81}{2}(pq - p + q), & s_3 &= -\frac{4}{3}ps_4, & s_2 &= \frac{2}{3}(-p^2 - 2q^2 + 2p^2q^2)s_4, \\ s_1 &= 6(9p^4 - 9p^3q - 9p^4q + 14p^2q^2 + 4p^3q^2 - 10p^4q^2 - 10pq^3 - 10p^2q^3 + 10p^3q^3 + 10p^4q^3 \\ &\quad + 4q^4 + 4pq^4 - 4p^2q^4 - 4p^3q^4), \\ s_0 &= -\frac{1}{2}p(27p^4 - 27p^3q - 27p^4q + 44p^2q^2 + 16p^3q^2 - 28p^4q^2 - 28pq^3 - 28p^2q^3 + 28p^3q^3 \\ &\quad + 28p^4q^3 + 16q^4 + 16pq^4 - 16p^2q^4 - 16p^3q^4). \end{aligned}$$

First, note that  $A'''(u) = 12s_4u^2 + 6s_3u + 2s_2 < 0$  since  $12s_4u^2$  and  $2s_2 + 6s_3u$  are both negative for any  $0 \leq u \leq \frac{p-2}{3}$ . Also,

$$A'\left(\frac{p-2}{3}\right) = 8(p+1)^2(q-1)^2(p-2p^2-q+3pq-2p^2q-2q^2+2pq^2) > 0,$$

since  $7 \leq p+2 \leq q$ . Hence, by Lemma 3.6,  $A$  is maximum at  $u = 0$  or at  $u = \frac{p-2}{3}$ .

Design  $d^*$  has the replications corresponding to  $u = \frac{p-2}{3}$ . If  $p$  is even, design  $d^{**}$  has replications corresponding to  $u = 0$ . However, if  $p$  is odd and  $u = 0$ , there is no design with  $r_3 = \frac{p(q-1)}{3}$  and  $r_1 = r_2 = \frac{p(2q+1)}{6}$  since  $\frac{p(2q+1)}{6}$  is not an integer. But by Lemma 3.6 we still know that any design with  $r_3 > \frac{p(q-1)}{3} + 1$  (i.e. with  $u > 1$ ) is  $A$ -inferior to  $d'$  which has  $u = 1$ . We also know that when  $p$  is odd, for fixed  $r_3 = \frac{p(q-1)}{3}$ , the  $A$ -best design is  $d^{**}$  since  $A$  is a decreasing function of  $x = r_1 - r_2$  and  $r_1^{**} - r_2^{**} = 1$ .

In conclusion, we have shown that when  $p$  is even,  $d^*$  or  $d^{**}$  is  $A$ -optimal, and if  $p$  is odd, the three competitors are  $d^*$ ,  $d^{**}$ , and  $d'$ . In the next step of the proof we eliminate  $d'$ , and establish the conditions under which  $d^*$  is  $A$ -superior to  $d^{**}$ .

**Step 5.** First, assume that  $p$  is even. To determine which design between  $d^*$  and  $d^{**}$  is  $A$ -optimal, simply compute  $A_{d^*} - A_{d^{**}}$ . Using (3.5) and (3.14), we have:

$$A_{d^*} - A_{d^{**}} = \frac{2(p^2 - p - 2)[2q^3(p-1)(p+2) - pq^2(p-1)(3p+4) - 3p^2q + 3p^3]}{9pq(p-1)(q+1)(4p^2q^2 - 3p^2 - 4q^2)}.$$

Note that the denominator is positive, and

$$A_{d^*} - A_{d^{**}} \stackrel{\text{sign}}{=} 2q^3(p-1)(p+2) - pq^2(p-1)(3p+4) - 3p^2q + 3p^3. \quad (3.60)$$

Equation (3.60) tells us when  $d^*$  is  $A$ -optimal for even  $p$ . First, (3.60) is increasing in  $q$  since  $7 \leq p+2 \leq q$ . Setting  $q = \frac{3p+2}{2}$ , (3.60) becomes a quartic polynomial in  $p$ , positive for any  $p \geq 2$ . Setting  $q = \frac{3p-4}{2}$ , (3.60) becomes a similar quartic polynomial in  $p$ , negative for any  $p \geq 2$ . Note that we cannot have  $\frac{3p-4}{2} < q < \frac{3p+2}{2}$  since  $q \equiv 1 \pmod{3}$ . Therefore, for even  $p$  we can say that if  $q \geq \frac{3p+2}{2}$ , then  $d^*$  is  $A$ -optimal, and otherwise  $d^{**}$  is  $A$ -optimal.

Now suppose  $p$  is odd. We will eliminate design  $d'$  by showing that  $A_{d^*} - A_{d'} > 0$  for any  $q \geq \frac{3}{2}p - 1$ , and  $A_{d^{**}} - A_{d'} > 0$  for any  $q < \frac{3}{2}p - 1$ . First, note that if  $p = 5$ , then  $d^*$  and  $d'$  are in fact the same design, so assume  $p \geq 11$ . Using (3.5) and (3.14), we have:

$$A_{d^*} - A_{d'} = \frac{2(p-5)[3p(p^2 - 2p + 3) - 3q(p^2 - 2p + 3) - q^2(p+1)(3p^2 - 8p + 9) + 2q^3(p^2 - 1)]}{9pq(p-1)(q+1)(4q^2p - 3p + 4q^2 - 9)}.$$

The denominator is positive, and so

$$A_{d^*} - A_{d'} \stackrel{\text{sign}}{=} 3p(p^2 - 2p + 3) - 3q(p^2 - 2p + 3) - q^2(p+1)(3p^2 - 8p + 9) + 2q^3(p^2 - 1). \quad (3.61)$$

Now, (3.61) is increasing in  $q$ , and it can be checked that it is positive for any  $q \geq \frac{3p}{2} - 1$  and  $p \geq 11$ . Next, comparing  $d'$  to  $d^{**}$ :

$$A_{d^{**}} - A_{d'} = \frac{2}{3pq(p-1)(4q^2-3)(4q^2p-3p+4q^2-9)} \\ \times [27p(p-1)^2 - 27q(p-1)^2(p+1) - 4q^2p(7p^2-20p+9) + 4q^3(p^2-1)(7p-9) - 16q^4(p^2-1)].$$

The denominator is positive, and the numerator is a concave function in  $q$ , its second derivative being strictly negative in  $q > p$ . The numerator is positive for any  $q \in [p+2, \frac{3p}{2}-1]$  because it is positive both at  $q = p+2$ , and at  $q = \frac{3p}{2}-1$ , for any  $p \geq 11$ . Therefore  $d'$  is  $A$ -inferior to either  $d^*$  or  $d^{**}$ .

Finally, we compare designs  $d^*$  and  $d^{**}$  for  $p$  odd and  $p \geq 5$ . Using (3.5) and (3.14), we have:

$$A_{d^*} - A_{d^{**}} = \frac{2(p+1)(-6p+3p^2+6q-3pq+6q^2+5pq^2-3p^2q^2-2q^3+2pq^3)}{9pq(p-1)(q+1)(4q^2-3)},$$

and so  $A_{d^*} - A_{d^{**}} \stackrel{\text{sign}}{\equiv} -6p+3p^2+6q-3pq+6q^2+5pq^2-3p^2q^2-2q^3+2pq^3$ . (3.62)

Analogous to the  $p$  even case, (3.62) is increasing in  $q$ . Setting  $q = \frac{3p-1}{2}$ , (3.62) becomes a cubic polynomial in  $p$ , positive for any  $p \geq 5$ . Setting  $q = \frac{3p-7}{2}$ , (3.62) becomes another cubic polynomial in  $p$ , negative for any  $p \geq 5$ . Also, since  $q \equiv 1 \pmod{3}$ , we cannot have  $\frac{3p-7}{2} < q < \frac{3p-1}{2}$ . Therefore, when  $p$  is odd, design  $d^*$  is  $A$ -optimal if and only if  $q \geq \frac{3p-1}{2}$ .

**Part II.** We now move on to the second part of the proof, where the assumption is  $q > 2p$ . First, we show that  $d^*$  is  $A$ -optimal when  $p = 2$ . Create the uniform design  $d^0(c_1^0, c_2^0, c_2^0)$  with replications:

$$r_1^0 = \frac{2q+4}{3}, \quad r_2 = r_3 = \frac{2q-2}{3}. \quad (3.63)$$

Note that  $d^0$  is of maximal trace because the two rows are permutations of each other, and the design is generalized binary in columns. Similar to step 1 below, all designs with  $r_1 \geq \frac{2q+4}{3}$  are not  $A$ -superior to  $d^0$ , provided that  $2(\sqrt{3}-1)c_2^0 - c_1^0 > 0$ . This inequality holds for any  $q \geq 10$ . Indeed, we have

$$2(\sqrt{3}-1)c_2^0 - c_1^0 = \frac{1}{\sqrt{3}}(2q - q\sqrt{3} - 2).$$

By the same inequality, nonuniform designs can be eliminated using Lemma 3.3 when  $r_1 \leq \frac{2q+4}{3}$  and  $q \geq 10$ . The only designs with  $q \geq 10$  left to consider are uniform designs with replications as in  $d^0$  or  $d^*$ . Using (3.5) and (3.14), we get:

$$A_{d^*} - A_{d^0} = \frac{2(q+2)}{3q(q+1)} > 0,$$

and so  $d^*$  is  $A$ -optimal. For  $2 \times 7$  row-column designs, it can be shown that  $d^*$  is  $A$ -optimal by enumeration.

So for steps 1 through 5 take  $p \geq 5$ . Most calculations needed in this part of the proof were performed in part I.

**Step 1.** In this step we eliminate all designs with  $r_1 > \frac{p(q+2)}{3}$ . Since  $q > 2p$  this will also eliminate designs with  $r_3 < \frac{q(p-2)}{3}$ . We will again use lemma 3.4 to show that design  $d^0$  defined in part I is  $A$ -superior to any competitor  $d$  with  $r_1 > \frac{p(q+2)}{3}$ . First,

$$2(\sqrt{3}-1)c_2^0 - c_1^0 = \frac{1}{9p}[-2\sqrt{3}p(p+1) + 2q(2\sqrt{3}-3)(p-1)(p+1)].$$

This is positive, and thus condition (a) of Lemma 3.4 is met. Conditions (b) and (c) of Lemma 3.4 are also satisfied (see part I), so all designs with  $r_1 > \frac{p(q+2)}{3}$  are eliminated.

**Step 2.** In this step we eliminate all nonuniform designs with replications not shown inadmissible in the previous step. Nonuniform designs with  $r_3 \geq \frac{p(q-1)}{3}$  are eliminated same way as in part I.

For designs with  $\frac{q(p-2)}{3} \leq r_3 < \frac{p(q-1)}{3}$  we apply lemma 3.3. By (3.54),  $c_i$  is an increasing function of  $r_i$  for  $r_i \leq \frac{p(q+2)}{3}$ . So for fixed  $r_3 = \frac{p(q-1)}{3} - x$ , the difference  $(\sqrt{3}-1)(c_2+c_3) - c_1$  is minimized when we set  $r_1 = \frac{p(q+2)}{3}$  and  $r_2 = \frac{p(q-1)}{3} + x$  (see part I). For these replications, the difference  $(\sqrt{3}-1)(c_2+c_3) - c_1$  changes from that computed in part I, because for  $q > 2p$  we have  $\text{int}[\frac{r_1}{q}] = \frac{p-2}{3}$ . We are interested in the minimum of

$$(\sqrt{3}-1)(c_2+c_3) - c_1 = \frac{1}{9pq}[18(\sqrt{3}-1)x^2 - 18p(\sqrt{3}-1)x + 2q(p+1)(2\sqrt{3}pq - 3pq - 2\sqrt{3}q + 3q - \sqrt{3}p)].$$

Just as before, the difference is minimum at  $x = \frac{p}{2}$ , where it becomes an increasing function of  $p$ , positive for any  $p \geq 5$ . By lemma 3.3, all nonuniform designs are eliminated.

**Steps 3 through 5.** These steps are covered in part I of the proof. All arguments deal with maximizing the quantity  $A$  given in (3.5), as a function of the replication numbers  $r_i$ . The subcases that appeared in part I were due to  $\text{int}[\frac{r_i}{q}]$  taking two different values depending on  $r_1$ . When  $q > 2p$ , we have  $\text{int}[\frac{r_i}{q}] = \frac{p-1}{3}$  for all designs with  $r_1 \leq \frac{p(q+2)}{3}$ . Therefore, all the forms that  $A$  can take for uniform designs with replications in the ranges considered were included in part I.  $\square$

### 3.4.6 Discussion

One common characteristic of  $A$ -optimal designs with three treatments is that they are all uniform. In fact, there are no known non-uniform  $A$ -optimal block or row-column designs. This seems to be due to the relationship between the diagonal elements and the inverses of eigenvalues of the information matrix. Distributing a treatment replicated  $r_i$  times uniformly throughout the design maximizes the diagonal element of the information matrix corresponding to that treatment. That is, for fixed replications, uniformity maximizes trace. As it can be seen from the form of  $A$  given in (3.5), in the case of three treatments, an ideal design would maximize  $\sum c_i$ , while minimizing  $\sum c_i^2$ . Naturally, this cannot be achieved simultaneously, and so the  $A$ -optimal design is in many cases a compromise between the two.

We now summarize the main results in this section. Under the general assumptions  $p \leq q$ , and  $r_1 \geq r_2 \geq r_3$ , replications for all  $A$ -optimal designs are given in Table 3.1. The proofs of the main results in this section eliminate all other designs from consideration. As discussed earlier, all  $A$ -optimal designs are uniform.

In some cases, treatments are as nearly equireplicated as possible, but in other cases not. For example, when  $p \equiv q \equiv 1 \pmod{3}$ , treatment 1 is replicated  $p$  more times than the other two treatments. This is against the “conventional wisdom” that optimal designs should have replications as close as possible.

Knowing the replications for a design with three treatments, and the fact that it is uniform,

Table 3.1: Replications for  $A$ -optimal row-column designs (under the assumption  $p \leq q$ )

$p \pmod 3$	$q \pmod 3$	Additional Information	$r_1$	$r_2$	$r_3$	Source
0	0,1,2	-	$\frac{pq}{3}$	$\frac{pq}{3}$	$\frac{pq}{3}$	(GYD)
0,1,2	0	-	$\frac{pq}{3}$	$\frac{pq}{3}$	$\frac{pq}{3}$	(GYD)
1	1	-	$\frac{p(q+2)}{3}$	$\frac{p(q-1)}{3}$	$\frac{p(q-1)}{3}$	Theorem 3.2
1	2	$q \geq 2p$	$\frac{p(q+1)}{3}$	$\frac{p(q+1)}{3}$	$\frac{p(q-2)}{3}$	Theorem 3.4
		$q < 2p, q$ even	$\frac{q(2p+1)}{6}$	$\frac{q(2p+1)}{6}$	$\frac{q(p-1)}{3}$	
		$q < 2p, q$ odd	$\frac{q(2p+1)+3}{6}$	$\frac{q(2p+1)-3}{6}$	$\frac{q(p-1)}{3}$	
2	1	$q \geq \frac{3p+2}{2}, p$ even, or $q \geq \frac{3p-1}{2}, p$ odd	$\frac{pq+1}{3}$	$\frac{pq+1}{3}$	$\frac{pq-2}{3}$	Theorem 3.5
		$q < \frac{3p+2}{2}, p$ even	$\frac{p(2q+1)}{6}$	$\frac{p(2q+1)}{6}$	$\frac{p(q-1)}{3}$	
		$q < \frac{3p-1}{2}, p$ odd	$\frac{p(2q+1)+3}{6}$	$\frac{p(2q+1)-3}{6}$	$\frac{p(q-1)}{3}$	
2	2	-	$\frac{pq+2}{3}$	$\frac{pq-1}{3}$	$\frac{pq-1}{3}$	Theorem 3.3

is sufficient for obtaining the design's information matrix. This is not true in general for designs with more than three treatments, where uniform designs with the same replications might have different information matrices, based on treatment concurrences (i.e. the number of times two treatments occur together in the blocks of a blocking factor). An algorithm for constructing uniform designs with three treatments and given replications is developed in Section 4.4.

# Chapter 4

## *E*-optimal Designs with Three Treatments

### 4.1 The *E*-value of a $3 \times 3$ Information Matrix

As discussed in section 3.1, the *C*-matrix of a design with three treatments can be written in terms of its diagonal elements  $(c_1, c_2, c_3)$ . The *C*-matrix has two non-zero eigenvalues which can be written as  $Z_{1,2} = \frac{1}{2}(\sum c_i \pm \sqrt{2 \sum_{i < j} (c_i - c_j)^2})$ . From now on *Z* will only refer to the smaller non-zero eigenvalue:

$$Z = \frac{1}{2} \left( \sum c_i - \sqrt{2 \sum_{i < j} (c_i - c_j)^2} \right). \quad (4.1)$$

*E*-optimal designs maximize *Z*. The expression for *Z* simplifies when some of the  $c_i$ 's are equal:

$$c_1 = c_2 \geq c_3 \text{ implies } Z = \frac{3}{2}c_3 \quad (4.2)$$

$$c_1 \geq c_2 = c_3 \text{ implies } Z = c_2 + c_3 - \frac{1}{2}c_1 \quad (4.3)$$

In some cases there are multiple designs which are *E*-optimal. One way to discriminate among them is to find the design which is *M*-optimal in the entire class of *E*-optimal designs.

**Definition 4.1.** A design  $d^*$  is said to be *E* – *M*-optimal in  $\mathcal{D}$ , if  $d^*$  is *M*-optimal in the class of *E*-optimal designs in  $\mathcal{D}$ .

Note that when  $v = 3$ , it is sufficient to show that the trace of  $C_{d^*}$  for an  $E$ -optimal design  $d^*$  is maximal among all  $E$ -optimal designs, in order to say that  $d^*$  is  $E - M$ -optimal.

The next result by Morgan and Reck [24] is very useful in finding upper bounds for the smallest eigenvalue of the  $C$ -matrix.

**Theorem 4.1.** *Consider a design  $d$  with information matrix  $C_d$  partitioned as*

$$C_d = \begin{pmatrix} C_{d11} & C_{d12} \\ C_{d21} & C_{d22} \end{pmatrix},$$

where  $C_{d11}$  and  $C_{d22}$  are square matrices of orders  $p$  and  $v - p$ . Let  $w$  be any normalized vector of length  $p$ , and  $x = w'1$ . Then  $Z$ , the smallest non-zero eigenvalue of  $C_d$ , satisfies

$$Z \leq \frac{v}{v - x^2} w' C_{d11} w.$$

Two relevant lemmas, which follow immediately from the above result are given below. First let  $p = 1$  and  $w = 1$  in theorem 4.1.

**Lemma 4.1.** *For a design  $d$  with information matrix  $C_d$ , the minimum non-zero eigenvalue  $Z$  of  $C_d$  satisfies:*

$$Z \leq \frac{v}{v - 1} \min(c_{dii}).$$

Next, let  $p = 2$  and  $w' = (\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})$  in theorem 4.1.

**Lemma 4.2.** *For a design  $d$  with information matrix  $C_d$ , the minimum non-zero eigenvalue  $Z$  of  $C_d$  satisfies:*

$$Z \leq \frac{c_{dii} + c_{di'i'} - 2c_{dii'}}{2},$$

for any  $i$  and  $i'$ .

The bounds given in the above two lemmas can also be obtained by the averaging technique of Constantine [9], symmetrizing on  $p = 1$  and  $p = 2$  treatments, respectively. Similar bounds were developed by Jacroux [15], using other methods. In the following sections,  $E$ -optimal designs will be found for different blocking schemes. Throughout this chapter, it will be assumed, without loss of generality, that  $r_1 \geq r_2 \geq r_3$ .

## 4.2 $E$ -optimal designs with One Blocking Factor

The block design setting  $\{v, b, k\}$  denotes:

- $v$  treatments to be compared, using
- $b$  blocks of experimental material, each composed of
- $k$  experimental units

Associated with the setting, define two auxiliary parameters as follows:

- $r = \text{int}(\frac{bk}{v}) =$  maximized minimum replication
- $p = bk - vr =$  excess plots over those needed for equal replication

In a block design  $d(v, b, k)$ , suppose treatment  $i$  has replication  $r_i$ , with block-wise replications  $n_{il}$ ,  $l = 1, 2, \dots, b$ . Then the diagonal elements of the design,  $C_d$ , are given by  $c_{ii} = r_i - \frac{1}{k} \sum_{l=1}^b (n_{il})^2$ . If treatment  $i$  is uniform, then  $c_{ii}^0 = r_i - \frac{1}{k} h(r_i, b)$ . The nonuniformity of treatment  $i$  is defined as  $NU_i = c_{ii}^0 - c_{ii} \geq 0$  (see section 2.1).

The  $E$ -optimal designs will be found based on the different values of  $b$  and  $k \pmod 3$ .

### 4.2.1 Case 1: $bk \equiv 0 \pmod 3$

In this case we can see that  $r = \frac{bk}{3}$ , and  $p = 0$ . For this setting we can create a generalized binary balanced design (BBD), which is universally optimal. The diagonal elements of  $C_d$  for such a design will be  $c_i = \frac{b(k-1)}{3}$ . The  $E$ -value can be computed to be  $Z = \frac{b(k-1)}{2}$ .

To build a BBD, follow these steps:

- (a) If  $3 \nmid k$ , then build a GRBD (generalized randomized block design) which has each treatment occurring  $\frac{k}{3}$  times in each block.

(b) If  $3 \nmid k$ , then we must have  $3 \mid b$ . Create an equireplicated, generalized binary design.

Because there are only 3 treatments, and the design is generalized binary,  $C_d$  is completely symmetrical and of maximum trace. Therefore it is universally optimal by theorem 2.1.

#### 4.2.2 Case 2: $bk \equiv 2 \pmod{3}$

**Theorem 4.2.** *A design in  $\mathcal{D}(3, b, k)$  with  $bk \equiv 2 \pmod{3}$ , is E-optimal if and only if it satisfies one of the following conditions:*

- (a)  $r_1 = r_2 = \frac{bk+1}{3}$ ,  $r_3 = \frac{bk-2}{3}$ , treatment 3 uniform and treatments 1 and 2 nonuniform in any way such that  $c_1 = c_2 \geq c_3$ .
- (b)  $\text{int}(\frac{b}{3}) \geq \text{int}(\frac{k}{3})$ ,  $r_1 = \frac{bk+4}{3}$ ,  $r_2 = r_3 = \frac{bk-2}{3}$ , treatments 2 and 3 uniform, and treatment 1 nonuniform in  $x = \text{int}(\frac{k+1}{3})$  blocks.

The E – M-optimal design is uniform and has replications  $r_1 = r_2 = \frac{bk+1}{3}$ ,  $r_3 = \frac{bk-2}{3}$ . Such a design is generalized binary, and thus of higher trace than the other E-optimal designs.

*Proof.* In this case we have  $r = \frac{bk-2}{3}$ , and  $p = 2$ . First create a generalized binary design  $d^0$  with  $r_1 = r_2 = r + 1$ , and  $r_3 = r$ . For this design  $c_1^0 = c_2^0 > c_3^0$ , and the E-value of this design is  $Z_{d^0} = \frac{3}{2}c_3^0$  by (4.2). Any design  $d$  with  $r_3 < r$  will have  $c_3 < c_3^0$ , and therefore  $Z_d < Z_{d^0}$ , by lemma 4.1. Also note that any other design with  $r_i = r$  must be binary in treatment  $i$ , otherwise it would be E-inferior to  $d^0$ . In general, any design will have  $r_3 \leq r$ , and so  $Z_d \leq Z_{d^0}$ , because  $Z_d \leq \frac{3}{2}c_3 \leq \frac{3}{2}c_3^0$ . So  $d^0$  is E-optimal.

Now consider designs with same replications as  $d^0$ , but not necessarily uniform in treatments 1 and 2. Obviously, in order for such a design to have the same E-value as  $d^0$ , it needs to have  $c_1 \geq c_3$ , and also  $c_2 \geq c_3$ . Furthermore, if  $c_1 \neq c_2$ , then  $Z_d < Z_{\bar{d}}$ , where  $C_{\bar{d}}$  has diagonal elements  $(\frac{c_1+c_2}{2}, \frac{c_1+c_2}{2}, c_3)$ . This is true by majorization: the sum of the two eigenvalues is equal for  $d$  and  $\bar{d}$ , but they have different sum of squares.

Let's now consider a design  $d$  with  $r_1 = r + 2$ , and  $r_2 = r_3 = r$ . In order for this design to have  $Z_d = Z_{d^0}$ , treatments 2 and 3 will have to be uniform, while treatment 1 will have to be nonuniform in such a way that  $c_1 = c_2 = c_3$ . Otherwise  $Z_d = 2c_2 - \frac{c_1}{2} < \frac{3}{2}c_2 = Z_{d^0}$ . Since treatments 2 and 3 are uniform, the nonuniformity of treatment 1 will be  $NU_1 = \frac{2}{k}x$ , where  $x$  will be the number of blocks in which treatment 1 is nonuniform. In general, maximum nonuniformity for treatment 1 with treatments 2 and 3 forced to be uniform, will be obtained by the following block assignments:

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

In the above display,  $xmax$  denotes the maximum number of blocks in which treatment 1 can be nonuniform, while keeping treatments 2 and 3 uniform. Using the formula for  $c_{ii}$  for a uniform design with replications  $(r + 2, r, r)$ , we get  $c_1^0 - c_2^0 = \begin{cases} \frac{2(k+1)}{3k}, & \text{when } b \equiv 1 \text{ and } k \equiv 2; \\ \frac{2(k-1)}{3k}, & \text{when } b \equiv 2 \text{ and } k \equiv 1. \end{cases}$  In order to make  $c_1 = c_2$ , we need to make treatment 1 nonuniform in

$$x = \begin{cases} \frac{k+1}{3}, & \text{when } b \equiv 1 \text{ and } k \equiv 2; \\ \frac{k-1}{3}, & \text{when } b \equiv 2 \text{ and } k \equiv 1 \end{cases} \quad (4.4)$$

blocks. By the above discussion about maximum nonuniformity of treatment 1, we can see that this will be possible if and only if  $int(\frac{b}{3}) \geq int(\frac{k}{3})$ . □

### 4.2.3 Case 3: $bk \equiv 1 \pmod{3}$

In this case  $r = \frac{bk-1}{3}$ , and  $p = 1$ . Create the generalized binary design  $d^0$ , with replications  $(r + 1, r, r)$ . Computing the values of the diagonal elements of  $C_{d^0}$ , we get:

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

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

The  $E$ -value of this design will be:

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

Suppose a design  $d$  has  $r_3 \leq r - 1$ . Then by (3.10):

$$Z_d \leq \frac{3}{2}c_3 \leq \begin{cases} \frac{1}{3k}(bk^2 - b - 2k + 2), & \text{when } b \equiv 1 \text{ and } k \equiv 1; \\ \frac{1}{3k}(bk^2 - b - 2k - 2), & \text{when } b \equiv 2 \text{ and } k \equiv 2; \end{cases} < Z_{d^0}.$$

Therefore all the  $E$ -optimal designs must have same replications as  $d^0$ , (i.e. they must have replications as close as possible, called replication balanced designs). From now on we'll only consider this type of designs.

However,  $d^0$  will not be in general  $E$ -optimal, because we can create designs with treatment 1 nonuniform, while keeping treatments 2 and 3 uniform with replication  $r$ , in such a way that  $Z_{d^0} < 2c_2 - \frac{c_1}{2}$ . Let  $\mathcal{D}_R$  denote the subclass of  $\mathcal{D}(v, b, k)$  replication balanced designs, which are also generalized binary in treatments 2 and 3. Note that in this subclass the diagonal elements  $c_2$  and  $c_3$  are  $c_2 = c_3 = c_2^0$ . Below are the block assignments which obtain maximum nonuniformity of treatment 1, within  $\mathcal{D}_R$ :

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

Again, just like in case 2,  $xmax$  denotes the maximum number of blocks in which treatment 1 is nonuniform, given that the design is in  $\mathcal{D}_R$ . In order to see how nonuniform we should make treatment 1 and get  $c_1$  as close as possible to  $c_2$ , compute:

$$diff = c_1^0 - c_2^0 = \begin{cases} \frac{k-1}{3k}, & \text{when } b \equiv k \equiv 1; \\ \frac{k+1}{3k}, & \text{when } b \equiv k \equiv 2. \end{cases} \quad (4.5)$$

Create design  $d^*$  by making treatment 1 nonuniform in  $x^* = \min(xmax, \text{int}(\frac{diff}{2/k}))$  blocks.

**Theorem 4.3.** *In the class  $\mathcal{D}(3, b, k)$  with  $bk \equiv 1 \pmod{3}$ , consider a design  $d^*$  that satisfies:*

$$(a) \quad r_1 = \frac{bk+2}{3}, \quad r_2 = r_3 = \frac{bk-1}{3},$$

(b) treatments 2 and 3 are uniform

(c) treatment 1 is nonuniform in  $x^*$  blocks, where  $x^* = \min[\frac{b-1}{3}, \text{int}(\frac{k-1}{6})]$  if  $b \equiv k \equiv 1 \pmod{3}$ , and  $x^* = \min[\frac{b+1}{3}, \text{int}(\frac{k+1}{6})]$  if  $b \equiv k \equiv 2 \pmod{3}$ ;

then  $d^*$  is E-optimal. A necessary, but not sufficient condition for other E-optimal designs to exist is  $x_{max} + 2 < \text{int}(\frac{diff}{2/k})$ . When other E-optimal designs exist,  $d^*$  is E - M-optimal.

*Proof.* Designs which are not replication balanced have already been ruled out, so all competitors have  $r_1 = r + 1$ ,  $r_2 = r_3 = r$ .

First let's look at settings where

$$x_{max} \geq \text{int}\left(\frac{diff}{2/k}\right) = \begin{cases} \text{int}(\frac{k-1}{6}), & \text{when } b \equiv k \equiv 1; \\ \text{int}(\frac{k+1}{6}), & \text{when } b \equiv k \equiv 2 \end{cases},$$

and so  $x^* = \text{int}(\frac{diff}{2/k})$ . Under this setting, any design  $d$  in  $\mathcal{D}_R$  with treatment 1 nonuniform in less than  $x^*$  blocks will have  $c_1 > c_1^*$ . So  $Z_d = 2c_2^0 - \frac{c_1}{2} < 2c_2^0 - \frac{c_1^*}{2} = Z_{d^*}$ . Note that  $c_1^* = c_2^0 + diff - \frac{2}{k}\text{int}(\frac{diff}{2/k})$ , and any other design in  $\mathcal{D}_R$  will have  $c_1 = c_2^0 + diff - \frac{2}{k}x$ , where  $x$  is the number of blocks in which treatment 1 is nonuniform,  $x^* < x \leq x_{max}$ .

In order to compare  $d^*$  to other designs which are nonuniform in treatments 2 or 3, or nonuniform in treatment 1 in more than  $x^*$  blocks, let's compute  $Z_{d^*}$  using (4.2) and (4.3):

$$(a) \quad b \equiv k \equiv 1, \text{ and } k \text{ even. In this case } x = \frac{k-4}{6}, \text{ and } Z_{d^*} = \frac{3}{2}c_2^0 - \frac{1}{2k}.$$

$$(b) \quad b \equiv k \equiv 1, \text{ and } k \text{ odd. In this case } x = \frac{k-1}{6}, \text{ and } Z_{d^*} = \frac{3}{2}c_2^0.$$

$$(c) \quad b \equiv k \equiv 2, \text{ and } k \text{ even. In this case } x = \frac{k-2}{6}, \text{ and } Z_{d^*} = \frac{3}{2}c_2^0 - \frac{1}{2k}.$$

$$(d) \quad b \equiv k \equiv 2, \text{ and } k \text{ odd. In this case } x = \frac{k+1}{6}, \text{ and } Z_{d^*} = \frac{3}{2}c_2^0.$$

Looking at the definition of  $diff$  in (4.5), we can see that  $diff - \frac{2}{k}\text{int}(\frac{diff}{2/k}) = \begin{cases} \frac{1}{k}, & \text{when } k \text{ is even} \\ 0, & \text{when } k \text{ is odd} \end{cases}$ .

If  $x > x^*$  for a design  $d$  in  $\mathcal{D}_R$ , then  $c_1 \leq c_1^* - \frac{2}{k} = c_2^0 + \text{diff} - \frac{2}{k}(\text{int}(\frac{\text{diff}}{2/k}) + 1) \leq c_2^0 - \frac{1}{k}$ . By lemma 4.1  $Z_d \leq \frac{3}{2}c_2^0 - \frac{3}{2k} < Z_{d^*}$ .

Any design which is nonuniform in treatment 3 (similarly for 2), will have  $c_3 \leq c_2^0 - \frac{2}{k}$ , and hence  $Z_d \leq \frac{3}{2}c_3 \leq \frac{3}{2}c_2^0 - \frac{3}{k} < Z_{d^*}$  (for any of the values  $Z_{d^*}$  takes from the above list).

Next, suppose  $\text{int}(\frac{\text{diff}}{2/k}) - 2 \leq x_{\max} < \text{int}(\frac{\text{diff}}{2/k})$ . We have  $x^* = x_{\max}$  and  $c_1^* \leq c_2^0 + \text{diff} - \frac{2}{k}\text{int}(\frac{\text{diff}}{2/k}) + \frac{4}{k} \leq c_2^0 + \frac{5}{k}$ ; then by (4.3),  $Z_{d^*} = 2c_2^0 - \frac{1}{2}c_1^* > \frac{3}{2}c_2^0 - \frac{3}{k} \geq Z_d$  for any design  $d$  nonuniform in treatment 2 or 3. Therefore, when  $x_{\max} \geq \text{int}(\frac{\text{diff}}{2/k}) - 2$ ,  $d^*$  is  $E$ -optimal, and there are no other  $E$ -optimal designs (i.e. with treatments 2 or 3 nonuniform, or with treatment 1 nonuniform in  $x \neq x^*$  blocks). The condition  $x_{\max} \geq \text{int}(\frac{\text{diff}}{2/k}) - 2$ , under which all  $E$ -optimal designs have  $x = x^*$  as identified in the theorem statement, is equivalent to:

- (a)  $b \geq \frac{k-14}{2}$  when  $b \equiv k \equiv 1$  and  $k$  even;
- (b)  $b \geq \frac{k-11}{2}$  when  $b \equiv k \equiv 1$  and  $k$  odd;
- (c)  $b \geq \frac{k-16}{2}$  when  $b \equiv k \equiv 2$  and  $k$  even;
- (d)  $b \geq \frac{k-13}{2}$  when  $b \equiv k \equiv 2$  and  $k$  odd.

Finally let's look at settings where  $x_{\max} < \text{int}(\frac{\text{diff}}{2/k}) - 2$ , so  $x^* = x_{\max}$ , and  $Z_{d^*} = 2c_2^0 - \frac{1}{2}(c_1^0 - x_{\max}\frac{2}{k}) = Z_{d^0} + \frac{x_{\max}}{k} = \frac{bk-1}{3}$  (this is easy to check by the formulas given at the beginning of the section). We'll show that  $d^*$  is  $E$ -optimal, and also state some characteristics of the other  $E$ -optimal designs in this class.

By (3.1) and lemma 4.2, it is known that  $Z_d \leq c_2 + c_3 - \frac{c_1}{2} = ub_d$ , where  $ub_d$  denotes the upper bound for design  $d$ . As usual, let  $n_{ij}$  denote the number of times treatment  $i$  appears in block  $j$ . Now, let  $n_{1j} = n_1 + e_j$ , where  $n_1 = \text{int}(\frac{r_1}{b}) = \text{int}(\frac{bk+2}{3b})$ , and  $\sum_{j=1}^b e_j = r_1 - bn_1 = r+1 - bn_1$ . The  $e_j$ 's are the deviations from equal block-wise replications for treatment 1. For a given set of  $e_j$ 's,  $ub$  will be maximized when we maximize  $c_2 + c_3 = 2r - \frac{1}{k} \sum_{j=1}^b (n_{2j}^2 + n_{3j}^2)$ . The following assignment pattern for  $n_{2j}$ 's and  $n_{3j}$ 's maximizes  $c_2 + c_3$  for a given  $c_1$ :

$$n_{2j} = n_{3j} = \frac{k-n_{1j}}{2} = \frac{1}{2}(k - n_1 - e_j)$$

$j$	$n_{1j}$	$n_{2j}$	$n_{3j}$
1	$n_1 + e_1$	$\frac{1}{2}(k - n_1 - e_1)$	$\frac{1}{2}(k - n_1 - e_1)$
2	$n_1 + e_2$	$\frac{1}{2}(k - n_1 - e_2)$	$\frac{1}{2}(k - n_1 - e_2)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$b$	$n_1 + e_b$	$\frac{1}{2}(k - n_1 - e_b)$	$\frac{1}{2}(k - n_1 - e_b)$

Note that when  $x^* = xmax$ ,  $d^*$  is a special case of this assignment pattern (see the block-wise replications of  $d^*$  at the beginning of this section). In general, call this assignment pattern  $\bar{d}$ ; a design with these block-wise replications does not exist if  $k - n_1 - e_j$  is odd for some  $j$ . However, the bound  $\overline{ub}$  will be useful in showing the optimality of  $d^*$ .  $C_{\bar{d}}$  has the following diagonal elements:

$$c_1 = r + 1 - \frac{1}{k} \sum_{j=1}^b (n_1 + e_j)^2$$

$$c_2 = c_3 = r - \frac{1}{4k} \sum_{j=1}^b (k - n_1 - e_j)^2$$

Next we'll show that  $\overline{ub}$  does not actually depend on the values of the  $e_j$ 's:

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

First, note that  $Z_{d^*} = \overline{ub}$ , which means that  $d^*$  is  $E$ -optimal. The only question left to answer is which are the other  $E$ -optimal designs. Note that for any design  $Z_d \leq c_2 + c_3 - \frac{c_1}{2} = \overline{ub}_d$ . However,  $\overline{ub}_d$  does not reach its upper bound  $\overline{ub}$  for most designs. For a given block assignment of treatment 1, if  $n_{2j} \neq n_{3j}$  for some  $j$ , then it follows that  $\overline{ub}_d < \overline{ub}$ . Also, if  $n_{2j} = n_{3j}$  for all  $j$ 's, then  $c_2 = c_3$ . If  $c_1 < c_2 = c_3$ , then  $Z_d = \frac{3c_1}{2} < \overline{ub}_d$ . Therefore, when  $xmax < int(\frac{diff}{2/k}) - 2$  a design will be  $E$ -optimal if and only if  $n_{2j} = n_{3j}$  for all  $j$ , and  $c_1 \geq c_2$  (i.e. treatment 1 cannot be made nonuniform in such a way that its diagonal element falls under the diagonal elements of treatments 2 and 3).

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

As a simple example of a design, other than  $d^*$ , which is  $E$ -optimal, consider the setting

$b = 2, k = 50$ . The block assignments are given below for designs  $d^*$  and  $d'$ , both of them being  $E$ -optimal with  $Z_{d^*} = Z_{d'} = r = 33$ :

$d^*$				$d'$			
$j$	$n_{1j}$	$n_{2j}$	$n_{3j}$	$j$	$n_{1j}$	$n_{2j}$	$n_{3j}$
1	16	17	17	1	14	18	18
2	18	16	16	2	20	15	15

### 4.3 $E$ -optimal Designs with Three Treatments in Settings with Multiple Blocking Factors

As discussed in section 2.2, in settings with multiple blocking factors, the experimental units are arranged in an  $n$ -dimensional hyperrectangle ( $n \geq 2$ ) of size  $b_1 \times b_2 \times \dots \times b_n$ , where  $b_i$  is the number of levels of the  $i$ th factor, and  $b_1 \leq b_2 \leq \dots \leq b_n$ . The total number of experimental units to be assigned to treatments is  $m = b_1 b_2 \dots b_n$ . The size of each block in direction  $j$  is  $mb_j^{-1}$ . Let  $N_j$  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 [7], we have:

$$C_d = \text{diag}(r_1, \dots, r_v) - \frac{1}{m} \sum_{j=1}^n b_j N_j N_j' + \frac{n-1}{m} \mathbf{r} \mathbf{r}', \quad (4.6)$$

where  $\mathbf{r}$  is the  $3 \times 1$  replication vector. From the above equation it follows that the  $i$ th diagonal element of  $C_d$  can be computed as:

$$c_i = r_i - \frac{1}{m} \sum_{j=1}^n (b_j \sum_{l=1}^{b_j} n_{ijl}^2) + \frac{n-1}{m} r_i^2, \quad (4.7)$$

where  $n_{ijl}$  is the number of times treatment  $i$  occurs in block  $l$  of factor  $j$ . Formulas for  $c_i$  when treatment  $i$  is uniform, as well as the nonuniformity of a treatment, are given in section 2.2.

The problem is divided in two main parts - first the replication numbers are found for  $E$ -optimal designs, then the uniformity characteristics are studied. Both parts are further divided into cases, depending on the value of  $m \bmod 3$ .

### 4.3.1 $E$ -optimal Designs when $m \equiv 0 \pmod{3}$

Under this setting,  $r = \frac{m}{3}$ , and we can create design  $d^0$  which has  $r_1 = r_2 = r_3 = r$ , and is generalized binary in all  $n$  directions (factors). Note that  $C^0$  is completely symmetrical, and thus  $Z_{d^0} = \frac{3c_i^0}{2}$ . Since any other design will have either  $r_3 < r$ , or will be nonbinary in some treatment, at least one diagonal element will be less than  $c_i^0$ . Therefore any other design would have  $Z < \frac{3c_i^0}{2} = Z_{d^0}$ , and thus be  $E$ -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 [7]).

### 4.3.2 Replication Numbers for $E$ -optimal Designs when $m \equiv 1 \pmod{3}$

Under this setting,  $r = \frac{m-1}{3}$ , and we can create design  $d^0$  which has  $r_1 = r + 1$ , and  $r_2 = r_3 = r$ , and is binary in all directions. We'll use the inequality  $Z_d \leq \frac{3}{2}c_i$  to show that  $d^0$  with  $E$ -value

$$Z_{d^0} = 2c_2^0 - \frac{c_1^0}{2} \quad (4.8)$$

is  $E$ -superior to any design which has  $r_3 \leq r - 1$ . So  $E$ -optimal designs will be shown to have same replication numbers as  $d^0$ .

We'll show that  $Z_{d^0} - \frac{3}{2}c_3 \geq 0$ , where  $c_3$  is the diagonal element of a generalized binary treatment with replication  $r_3 = r - 1$ . This implies that  $Z_{d^0} - \frac{3}{2}c_3 \geq 0$  for any  $r_3 \leq r - 1$ , and thus by Lemma 4.1,  $d^0$  is  $E$ -superior to any design which has  $r_3 \leq r - 1$ .

To do this, we'll need the following identities:

$$r \pmod{b_j} = r_{(b_j)} = \begin{cases} \frac{b_j-1}{3} & \text{when } b_j \equiv 1 \pmod{3}; \\ \frac{2b_j-1}{3} & \text{when } b_j \equiv 2 \pmod{3}. \end{cases} \quad (4.9)$$

$$r - 1 \pmod{b_j} = (r - 1)_{(b_j)} = \begin{cases} \frac{b_j-4}{3} & \text{when } b_j \equiv 1 \pmod{3}; \\ \frac{2b_j-4}{3} & \text{when } b_j \equiv 2 \pmod{3}. \end{cases} \quad (4.10)$$

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

$$\begin{aligned}
b_j[2h(r, b_j) - \frac{1}{2}h(r+1, b_j) - \frac{3}{2}h(r-1, b_j)] &= -b_j[\frac{1}{2}\Delta h(r, b_j) - \frac{3}{2}\Delta h(r-1, b_j)] \\
&= -b_j[\frac{1}{2} + \frac{1}{b_j}(r - r_{(b_j)}) - \frac{3}{2} - \frac{1}{b_j}(r-1 - (r-1)_{(b_j)})] \\
&= b_j + 2(r - r_{(b_j)})
\end{aligned} \tag{4.11}$$

Now, we are ready to compute  $Z_{d^0} - \frac{3}{2}c_3$ , using equations (4.8) and (2.5):

$$\begin{aligned}
Z_{d^0} - \frac{3}{2}c_3 &= 2r - \frac{r+1}{2} - \frac{3(r-1)}{2} + \frac{n-1}{m}[2r^2 - \frac{1}{2}(r+1)^2 - \frac{3}{2}(r-1)^2] \\
&\quad - \frac{1}{m} \sum_{j=1}^n b_j[2h(r, b_j) - \frac{1}{2}h(r+1, b_j) - \frac{3}{2}h(r-1, b_j)] \\
&\stackrel{(4.11)}{=} 1 + \frac{2}{m}(n-1)(r-1) - \frac{1}{m} \sum_{j=1}^n (b_j + 2r - 2 - 2(r-1)_{(b_j)}) \\
&= \frac{1}{m}(m + 2(n-1)(r-1) - \sum b_j - 2nr + 2n + 2 \sum (r-1)_{(b_j)}) \\
&= \frac{1}{m}(m - 2r + 2 - \sum b_j + 2 \sum (r-1)_{(b_j)}) \\
&= \frac{1}{3m}(m + 8 - 3 \sum b_j + 6 \sum (r-1)_{(b_j)}),
\end{aligned} \tag{4.12}$$

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

- (a)  $b_1 \equiv b_2 \equiv 1 \pmod{3}$ . In this case  $y \stackrel{(4.10)}{=} (b_1 - 1)(b_2 - 1) - 9 \geq 0$  with equality if and only if  $b_1 = b_2 = 4$ .
- (b)  $b_1 \equiv b_2 \equiv 2 \pmod{3}$ . In this case  $y \stackrel{(4.10)}{=} (b_1 + 1)(b_2 + 1) - 9 \geq 0$  with equality if and only if  $b_1 = b_2 = 2$ .

From (4.10) we can say that  $(r-1)_{(b_j)} \geq \frac{b_j-4}{3}$ , 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 we have  $y \geq 0$  for any  $n \geq 2$ , and  $y = 0$  if and only if  $n = 2$  and  $b_1 = b_2 = 4$  or  $b_1 = b_2 = 2$ .

As a conclusion, when  $m \equiv 1 \pmod{3}$  and  $n > 2$ , any design with  $r_3 \leq r - 1$  will be  $E$ -inferior to  $d^0$ . When  $n = 2$  and  $b_1 = b_2 = 4$ , or  $b_1 = b_2 = 2$ , other designs with different replications than  $d^0$  which are  $E$ -equal to  $d^0$  might exist. When  $b_1 = b_2 = 2$ , there is no connected design, and when  $b_1 = b_2 = 4$ , we have an  $E$ -optimal design with  $r_1 = r_2 = 6$ , and  $r_3 = 4$ , different than  $d^0$ , with  $r_1 = 6$ ,  $r_2 = r_3 = 5$ , which is also  $E$ -optimal.

### 4.3.3 Replication Numbers for $E$ -optimal Designs when $m \equiv 2 \pmod{3}$

Under this setting,  $r = \frac{m-2}{3}$ , and we can create a design  $d^0$  which has  $r_1 = r_2 = r + 1$ , and  $r_3 = r$ , and is generalized binary in all directions. For this design  $Z_{d^0} = \frac{3}{2}c_3^0$ . Note that any other design will have some  $r_i \leq r$ , which implies  $c_i \leq c_3^0$ , and hence will have  $Z_d \leq \frac{3}{2}c_i \leq Z_{d^0}$ . Therefore  $d^0$  is  $E$ -optimal.

Designs that have  $r_3 < r$ , will have  $c_3 < c_3^0$ , and hence by Lemma 4.1,  $Z_d < Z_{d^0}$ . Since  $r_3 \geq r$ , the only replication assignment different than  $d^0$  is  $r_1 = r + 2$ , and  $r_2 = r_3 = r$ . Section 4.3.5 gives the conditions under which a design with those replications can also be  $E$ -optimal.

### 4.3.4 Uniformity of Treatments for $E$ -optimal Designs when $m \equiv 1 \pmod{3}$

As shown in section 4.3.2, the replications of  $E$ -optimal designs for this case are  $r_1 = r + 1$ , and  $r_2 = r_3 = r$ . The only special case when a design with different replications may be  $E$ -optimal is  $n = 2$ , and  $b_1 = b_2 = 4$ .

Let's look at the design with  $n = 2$ ,  $b_1 = b_2 = 4$ . The two candidate designs are  $d_1$  and  $d_2$ , which are both generalized binary, and have replications  $r_1 = 6, r_2 = r_3 = 5$  for  $d_1$ , and

$r_1 = r_2 = 6, r_3 = 4$  for  $d_2$ . Both designs have the same  $E$ -value,  $Z_{d_1} = 2c_2 - \frac{c_1}{2} = 4.5$ , and  $Z_{d_2} = \frac{3c_3}{2} = 4.5$ , where the  $c_i$ 's are the diagonal elements for their respective designs. The two designs are given below (up to column or row permutations):

$d_1$		$d_2$					
1	2	3	1	3	2	1	1
2	3	1	2	1	3	2	1
3	1	2	3	2	1	3	2
1	2	3	1	2	1	2	3

For uniform designs with replications  $r_1 = r_2 = 6, r_3 = 4$ , we have  $c_1 = c_2 = 6 - \frac{2}{4}h(6, 4) + \frac{36}{16} = \frac{13}{4}$ , and  $c_3 = 4 - \frac{2}{4}h(4, 4) + \frac{16}{16} = 3$ . In general, if any binary treatment is made nonbinary in factor  $j$ , then the diagonal element corresponding to that treatment decreases by at least  $\frac{2b_j}{m} = \frac{1}{2}$  when  $b_1 = b_2 = 4$  (this is because  $\sum_{k=1}^{b_j} n_{ijk}^2$  increases by at least 2). Note that  $c_1 - c_3 = \frac{1}{4}$ . Hence if treatment 1 (or 2) is non-binary, then  $c_1 < c_3$ , which implies  $Z_d \leq \frac{3}{2}c_1 < Z_{d_2}$ , by lemma 4.1. Obviously, if treatment 3 is nonbinary, then the  $E$ -value would be less than that for  $d_2$ , also by lemma 4.1. For the same reasons no treatments can be made nonbinary in designs with same replications as  $d_1$ .

Now consider designs with replications (7,5,4) or (8,4,4). By the same argument as above, treatments 2 and 3 must be kept generalized binary, which will also force treatment 1 to be generalized binary. A generalized binary design with replications (7,5,4) or (8,4,4) is  $E$ -inferior to  $d_1$  and  $d_2$  because  $c_1 \neq c_2$ , and so  $Z_d < \frac{3}{2}c_3$ . Design  $d_2$  is the only  $E$ -optimal design which is not nearly balanced (for the case  $m \equiv 1 \pmod{3}$ ).

With the exception of the special case described above, all  $E$ -optimal designs have replications  $r_1 = r + 1$ , and  $r_2 = r_3 = r$ . It turns out that  $E$ -optimal designs have treatments 2 and 3 generalized binary, while treatment 1 is nonbinary in such a way that the  $C$ -matrix is made as close as possible to a completely symmetrical matrix (i.e.  $c_1$  will be brought down close to  $c_2 = c_3$ ).

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. Since treatments 2 and 3 must be 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 (4.9)  $\text{int}(\frac{r}{b_j}) = \frac{mb_j^{-1}-1}{3}$ . 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  $n_{1jl} = \frac{mb_j^{-1}-4}{3}$ . Define the nonuniformity ( $NU$ ) of treatment 1 due to factor  $j$  as  $\frac{2}{mb_j^{-1}}x_j$ , where  $x_j$  is the number of blocks of factor  $j$  in which  $n_{1jl} = \frac{mb_j^{-1}-4}{3}$ . Note that for any design which is uniform in treatments 2 and 3,  $c_1 = c_1^0 - NU$ . We need to find what the maximum nonuniformity of treatment 1 in factor  $j$  is, when treatments 2 and 3 are constrained to be uniform. The maximum nonuniformity for treatment 1 is obtained with the following block assignments:

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

$\textit{max}_j$  denotes the maximum number of blocks in which treatment 1 can be nonuniform in factor  $j$ . Similar, when  $b_j \equiv 2 \pmod{3}$  we define the nonuniformity of treatment 1 due to factor  $j$  as  $\frac{2}{mb_j^{-1}}x_j$ , where  $x_j$  is the number of blocks of factor  $j$  in which  $n_{1jl} = \frac{mb_j^{-1}-4}{3}$ . We can see that  $\textit{max}_j = \frac{b_j+1}{3}$  when  $b_j \equiv 2 \pmod{3}$ . This is obtained with the following block assignments:

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

Design  $d^0$  was defined in section 4.3.2 as the generalized binary design with replications  $r_1 = r + 1$ , and  $r_2 = r_3 = r$ . Let  $D$  denote the difference between  $c_1^0$  and  $c_2^0$ .

$$\begin{aligned}
D = c_1^0 - c_2^0 &= 1 - \frac{1}{m} \sum_{j=1}^n b_j \Delta h(r, b_j) + \frac{n-1}{m} (2r+1) = \\
&= \frac{2mn + m + n - 1}{3m} - \frac{1}{m} \sum_{j=1}^n [b_j + 2(r - r_{(b_j)})] \tag{4.13}
\end{aligned}$$

The next step is to create designs  $d^*$  and  $d_*$  generalized binary in treatments 2 and 3, and nonuniform in treatment 1 in such a way that  $c_1$  gets as close as possible to  $c_2^0$ ; for  $d^*$  we have  $c_1^* \geq c_2^0$ , and for  $d_*$  we have  $c_{1*} \leq c_2^0$ . To find the number of blocks  $x_j^*$  and  $x_{j*}$  of factor  $i$  in which treatment 1 should be made nonuniform, solve the following integer minimization/maximization problems:

$$\text{maximize } \frac{2}{m} \sum_{j=1}^n (b_j x_j^*), \quad \text{subject to } 0 \leq x_j^* \leq \text{max}_j \text{ and } \frac{2}{m} \sum_{j=1}^n (b_j x_j^*) \leq D \tag{4.14}$$

$$\text{minimize } \frac{2}{m} \sum_{j=1}^n (b_j x_{j*}), \quad \text{subject to } 0 \leq x_{j*} \leq \text{max}_j \text{ and } \frac{2}{m} \sum_{j=1}^n (b_j x_{j*}) \geq D \tag{4.15}$$

Note that (4.15) may not have a solution. This occurs exactly when  $\frac{2}{m} \sum_{j=1}^n (b_j \text{max}_j) < D$ .

**Theorem 4.4.** *For any setting with multiple blocking factors and  $m \equiv 1 \pmod{3}$ , the  $E-M$ -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  $\frac{2}{m} \sum_{j=1}^n (b_j \text{max}_j) < D$ .*

When  $n = 2, b_1 = b_2 = 4$ , an  $E-M$ -optimal design different from  $d^*$  and  $d_*$  exists, as discussed at the beginning of this section.

*Proof.* The  $E$ -values for the two designs are

$$Z^* = 2c_2^0 - \frac{c_1^*}{2} \text{ and } Z_* = \frac{3}{2}c_{1*}, \quad (4.16)$$

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  $c_1^* > c_{1*}$ . When  $c_2$  and  $c_3$  are fixed to be equal to  $c_2^0$ , the  $E$ -value of any design is  $Z_d = \begin{cases} 2c_2^0 - \frac{c_1}{2} & \text{if } c_1 \geq c_2^0 \\ \frac{3}{2}c_1 & \text{if } c_1 < c_2^0 \end{cases}$ . By the conditions on  $d^*$  and  $d_*$ , we have  $Z^* > 2c_2^0 - \frac{c_1}{2}$  if  $c_1 \geq c_2^0$  and  $Z_* > \frac{3}{2}c_1$  if  $c_1 < c_2^0$ . We need to show that any design nonuniform in treatments 2 or 3 will not have a higher  $E$ -value than both  $d^*$  and  $d_*$ , so that for  $E - M$ -optimal designs  $c_2 = c_3 = c_2^0$ .

First, note that by the conditions on  $d^*$ ,  $c_1^* - c_2^0 \geq \frac{2b_j}{m}$  implies that  $x_j^* = x \max_j$ , otherwise treatment 1 could have been made nonuniform in 1 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:

- (a)  $x_{j*} = 0$ , for otherwise making treatment 1 nonuniform in  $x_{j*} - 1$  blocks in direction  $j$ , would have brought  $c_1$  closer to  $c_2^0$  than at least one of  $c_1^*$  or  $c_{1*}$ ;
- (b)  $x_j^* = x \max_j$  for all  $j$  and equation (4.15) 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

$$\begin{aligned} c_1^* - c_2^0 &\geq \frac{2b_j}{m} \text{ for all } j < s \\ c_1^* - c_2^0 &< \frac{2b_j}{m} \text{ for all } j \geq s \end{aligned} \quad (4.17)$$

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

$$x_j^* = x \max_j \text{ and } x_{j*} = 0 \text{ for all } j < s. \quad (4.18)$$

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 4.1, (4.16)

and (4.17),  $Z_d \leq \frac{3}{2}c_2 \leq \frac{3}{2}c_2^0 - \frac{3b_j}{m} < Z^*$ ; 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  $NU_{\geq s}$  denote the nonuniformity of treatment 1 in directions  $j \geq s$ .

$$NU_{\geq s} = \frac{1}{m} \sum_{j=s}^n (b_j \sum_{l=1}^{b_j} n_{1jl}^2) - \frac{1}{m} \sum_{j=s}^n b_j h(r+1, b_j) \quad (4.19)$$

Similarly, define  $NU_{< s}$  as the nonuniformity of treatment 1 in directions  $j < s$ . Also let  $NU_{\geq s}^*$  and  $NU_{\geq s^*}$  represent treatment 1 nonuniformity in directions  $j \geq s$  in designs  $d^*$  and  $d_*$ . By (4.14) and (4.15) 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  $NU_{\geq s}^* < NU'_{\geq s} < NU_{\geq s^*}$ . We claim that this is not possible because it would contradict the latter statement:

- (a) If  $NU'_{\geq s} \geq D$ , 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 (4.18).
- (b) If  $D - \frac{2b_{s-1}}{m} < NU'_{\geq s} < D$ , 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 (4.17),  $c_1^* - c_2^0 \geq \frac{2b_j}{m}$  for all  $j < s$ .
- (c) If  $NU'_{\geq s} \leq D - \frac{2b_{s-1}}{m}$  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  $NU_{\geq s}^* < NU'_{\geq s}$ , 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  $NU_{\geq s}^* < NU'_{\geq s}$ , the ending value must satisfy  $c'_1 < c_1^*$ .

Under all possibilities, we obtained  $c_{1*} < c'_1 < c_1^*$  with a uniform arrangement of treatments 2 and 3 in  $d'$ , which contradicts (4.14) and (4.15). Hence, there is no competitor design, uniform in treatments 2 and 3 in directions  $j \geq s$ , which has  $NU_{\geq s}^* < NU_{\geq s} < NU_{\geq s*}$ . Also, any design which has  $NU_{\geq s} > NU_{\geq s*}$ , will have  $c_1 < c_{1*}$  by (4.18), 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  $NU_{\geq s} \leq NU_{\geq s}^*$ .

By lemma 4.2, it is known that for any design we have the inequality  $Z_d \leq c_2 + c_3 - \frac{c_1}{2}$ . Call this upper bound  $ub_d$ . Using (2.3) and (2.5), for the competitor designs remaining, the above upper bound can be computed as:

$$\begin{aligned}
ub_d &= 2r - \frac{r+1}{2} + \frac{n-1}{m} \left( 2r^2 - \frac{(r+1)^2}{2} \right) - \frac{1}{m} \sum_{j=1}^n \left[ b_j \sum_{l=1}^{b_j} (n_{2jl}^2 + n_{3jl}^2 - \frac{n_{1jl}^2}{2}) \right] \\
&= const_1 - \frac{1}{m} \sum_{j=1}^{s-1} \left[ b_j \sum_{l=1}^{b_j} (n_{2jl}^2 + n_{3jl}^2 - \frac{n_{1jl}^2}{2}) \right] \\
&\quad - \frac{1}{m} \sum_{j=s}^n \left[ 2b_j h(r, b_j) - b_j \frac{h(r+1, b_j)}{2} \right] + \frac{1}{2} NU_{\geq s} \\
&= const_2 - \frac{1}{m} \sum_{j=1}^{s-1} \left[ b_j \sum_{l=1}^{b_j} (n_{2jl}^2 + n_{3jl}^2 - \frac{n_{1jl}^2}{2}) \right] + \frac{1}{2} NU_{\geq s}, \tag{4.20}
\end{aligned}$$

where  $const_1$  and  $const_2$  are constants, depending only on  $s$  and the dimensions of the hyperrectangle. Expression (4.20) 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 we show that the  $ub_d$  for any other design uniform in treatments 2 and 3 in directions  $j \geq s$  and with  $NU_{\geq s} \leq NU_{\geq s}^*$  cannot be higher than  $ub^*$ . Since  $NU_{\geq s} \leq NU_{\geq s}^*$ , it is sufficient to show that  $d^*$  minimizes  $\sum_{l=1}^{b_j} (n_{2jl}^2 + n_{3jl}^2 - \frac{n_{1jl}^2}{2})$  for each  $j \leq s-1$ . Given a set of block assignments for treatment 1,  $(n_{1j1}, n_{1j2}, \dots, n_{1jb_j})$ , the above sum is minimized if we force  $n_{2jl} = n_{3jl} = \frac{1}{2}(mb_j^{-1} - n_{1jl})$  for all  $l$ . Then the above sum becomes:

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

Note that the above minimum 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 (4.18) and block assignments in direction  $j$  when  $x_j^* = \text{xmax}_j$  at the beginning of this section). Thus  $ub$  is maximized by  $d^*$ .

This also proves that  $d^*$  is  $E$ -optimal when (4.15) has no solution (i.e. when  $x_j^* = \text{xmax}_j$  for all  $j$ ). In this case  $d^*$  reaches the absolute maximum of (4.20) because  $n_{2jl}^* = n_{3jl}^*$  for any  $j$  and  $l$ .  $\square$

In some cases, other  $E$ -optimal designs might exist, by making treatments 2 and 3 nonuniform. However,  $C_{d^*}$  or  $C_{d_*}$  will have higher trace, and thus one of them will be  $E-M$ -optimal. Equations (4.14) and (4.15) must be solved numerically, for any given hyperrectangle of size  $b_1 \times b_2 \times \dots \times b_n$ . The computer is always a valuable tool when dealing with such problems. *ESolver* [26] is a program written in *Mathematica* that computes  $x_j^*$  and  $x_{j*}$  for all  $j$ , and it also decides whether  $d^*$  or  $d_*$  is the  $E-M$ -optimal design.

### 4.3.5 Uniformity of Treatments for $E$ -optimal Designs when $m \equiv 2 \pmod{3}$

As discussed in section 4.3.3, there are two possible replications for  $E$ -optimal designs:  $d_1$  with  $(r+1, r+1, r)$  and  $d_2$  with  $(r+2, r, r)$ . The design  $d^0$  has same replications as  $d_1$ , and is generalized binary in all directions. The  $E$ -value of design  $d^0$ , is  $Z_{d^0} = \frac{3}{2}c_3^0$ . Since  $Z_d \leq \frac{3}{2}c_3$ ,  $E$ -optimal designs must be generalized binary in treatment 3. Also, by Lemma 4.1, for  $d_1$  we must have  $c_1 = c_2 \geq c_3$ , and for  $d_2$  treatment 1 should be nonuniform in such a way that  $c_1 = c_2 = c_3$ , in order for the  $E$ -value to reach this bound. In some cases, due to

the discrete nature of the problem, design 2 cannot be constructed such that  $c_1 = c_2 = c_3$ . Also, the  $E - M$ -optimal design in this case is  $d^0$  (i.e.  $C_d$  has highest trace when  $c_1$  and  $c_2$  are maximized, which is achieved by making treatments 1 and 2 uniform). We give this result in the form of a theorem.

**Theorem 4.5.** *For any setting with multiple blocking factors and  $m \equiv 2 \pmod{3}$ , the  $E - M$ -optimal design is generalized binary with replications  $r_1 = r_2 = \frac{m+1}{3}$ ,  $r_3 = \frac{m-2}{3}$ .*

## 4.4 Construction of $A$ - and $E$ -optimal Designs

In this section we will give methods for constructing designs with three treatments. In the construction of designs with more than one blocking factor, the theory of *Systems of Distinct Representatives* (SDR) proved to be useful in many situations. If  $S_1, S_2, \dots, S_n$  are  $n$  subsets of a finite set  $S$  then we say that  $(a_1, a_2, \dots, a_n)$  is an SDR for the sets  $S_1, S_2, \dots, S_n$  if  $a_i$  is an element of  $S_i$  and all  $a_i$ 's are distinct. The necessary and sufficient condition in order that  $S_1, S_2, \dots, S_n$  possess an SDR is that the union of any  $k$  of the sets contain at least  $k$  distinct elements, for every  $k \leq n$ . A natural generalization of this was given by Agrawal in [1].

**Definition 4.2.** If  $S_1, S_2, \dots, S_n$  are  $n$  subsets of a finite set  $S$ , then  $(O_1, O_2, \dots, O_n)$  will be called an  $(m_1, m_2, \dots, m_n)$  SDR if:

- (a)  $O_i \subseteq S_i$ ,
- (b)  $|O_i| = m_i$ ,
- (c)  $O_i \cap O_j = \emptyset$ , for any  $i \neq j$ ,

where  $|O_i|$  is the number of elements in set  $O_i$ .

**Theorem 4.6** (Agrawal, 1966). *A necessary and sufficient condition for sets  $S_1, S_2, \dots, S_n$  to possess an  $(m_1, m_2, \dots, m_n)$  SDR is that*

$$|S_{i_1} \cup S_{i_2} \cup \dots \cup S_{i_k}| \geq \sum_{j=1}^k m_{i_j},$$

for any  $k \leq n$  and  $1 \leq i_1 < i_2 < \dots < i_k \leq n$ .

#### 4.4.1 Construction of Designs with One Blocking Factor

As discussed in earlier sections, when  $bk \equiv 0 \pmod{3}$  the universally optimal design is a BBD. For *A*- and *E*-optimal block designs with  $bk \equiv 1 \pmod{3}$  and  $bk \equiv 2 \pmod{3}$ , the replications and uniformity of treatments are given in theorems 3.1, 4.3, and 4.2. Knowing the replications and uniformity characteristics of treatments gives us the values of  $n_{dij}$ 's, the elements of the block-treatment incidence matrix of a design  $d$ .

**Example 4.1.** Construct the *A*-optimal and *E*-optimal designs with  $v = 3$  treatments in  $b = 5$  blocks of size  $k = 8$ .

By Theorem 3.1, the *A*-optimal design is uniform and has replications  $r_1 = 14, r_2 = r_3 = 13$ . Thus  $n_{ij} \in \{2, 3\}$ , and we also know the number of blocks in which each treatment occurs 2 or 3 times (e.g. treatment 2 must occur 2 times in 2 blocks and 3 times in 3 blocks). The 3 candidate blocks are:

$b_1$	$b_2$	$b_3$
1	1	1
1	1	1
1	1	2
2	2	2
2	2	2
2	3	3
3	3	3
3	3	3

In order to obtain the desired replications, one must use two copies of  $b_1$ , two copies of  $b_2$ , and one copy of  $b_3$ .

By Theorem 4.3, the  $E - M$ -optimal design must have  $r_1 = 14, r_2 = r_3 = 13$ , treatments 2 and 3 uniform, and treatment 1 nonuniform in one block. Hence,  $n_{1j} = 4$  in one block (say block 1),  $n_{1j} \in \{2, 3\}$  for  $j > 1$ , and  $n_{2j}, n_{3j} \in \{2, 3\}$  for any  $j$ . To obtain the desired replications, one must therefore use one copy of  $b_1$ , one copy of  $b_2$ , two copies of  $b_3$ , and the additional block with  $n_{1j} = 4$  and  $n_{2j} = n_{3j} = 2$ . The  $A$ -optimal design  $d_A$  and the  $E$ -optimal design  $d_E$  can also be represented as:

	$n_{1j}$	$n_{2j}$	$n_{3j}$	no. of blocks		$n_{1j}$	$n_{2j}$	$n_{3j}$	no. of blocks	
$d_A$ :	3	3	2	2	,	$d_E$ :	4	2	2	1
	3	2	3	2			3	3	2	1
	2	3	3	1			3	2	3	1
							2	3	3	2

The above display basically gives the block-treatment incidence matrix  $N$ , up to permutations of blocks. For  $d_A$ , two columns of  $N$  will be  $\begin{pmatrix} 3 \\ 3 \\ 2 \end{pmatrix}$ , another two columns will be  $\begin{pmatrix} 3 \\ 2 \\ 3 \end{pmatrix}$ , and one column  $\begin{pmatrix} 2 \\ 3 \\ 3 \end{pmatrix}$ . □

$A$ -optimal designs with three treatments are uniform, and so  $n_{1j} \in \{\bar{n}_1, \bar{n}_1 + 1\}$ ,  $n_{2j} \in \{\bar{n}_2, \bar{n}_2 + 1\}$ , and  $n_{3j} \in \{\bar{n}_3, \bar{n}_3 + 1\}$ , where  $\bar{n}_i = \text{int}[\frac{r_i}{b}]$ . Since  $\sum_i \frac{r_i}{b} = k$ , it must be that  $\sum_i \bar{n}_i = k - \sum_i \text{frac}(\frac{r_i}{b}) \geq k - 2$ , where  $\text{frac}(\frac{r_i}{b})$  stands for the fractional part of  $\frac{r_i}{b}$ . Thus,  $k - 2 \leq \sum_i \bar{n}_i \leq k$ , and there will always be at most three candidate blocks. We state this in the form of a lemma.

**Lemma 4.3.** *Let design  $d$  be a uniform block design with  $v = 3$  treatments in  $b$  blocks of size  $k$  with replications  $r_1, r_2$ , and  $r_3$ . Also, let  $N$  denote the  $v \times b$  block-treatment incidence matrix and  $\bar{n}_i = \text{int}[\frac{r_i}{b}]$ . Then*

- (a) if  $\sum \bar{n}_i = k$ , the only candidate column of  $N$  is  $\begin{pmatrix} \bar{n}_1 \\ \bar{n}_2 \\ \bar{n}_3 \end{pmatrix}$ ;
- (b) if  $\sum \bar{n}_i = k - 1$ , the three candidate columns of  $N$  are  $\begin{pmatrix} \bar{n}_1 + 1 \\ \bar{n}_2 \\ \bar{n}_3 \end{pmatrix}$ ,  $\begin{pmatrix} \bar{n}_1 \\ \bar{n}_2 + 1 \\ \bar{n}_3 \end{pmatrix}$ , and

$$\begin{pmatrix} \bar{n}_1 \\ \bar{n}_2 \\ \bar{n}_3 + 1 \end{pmatrix};$$

(c) if  $\sum \bar{n}_i = k - 2$ , the three candidate columns of  $N$  are  $\begin{pmatrix} \bar{n}_1 \\ \bar{n}_2 + 1 \\ \bar{n}_3 + 1 \end{pmatrix}$ ,  $\begin{pmatrix} \bar{n}_1 + 1 \\ \bar{n}_2 \\ \bar{n}_3 + 1 \end{pmatrix}$ , and

$$\begin{pmatrix} \bar{n}_1 + 1 \\ \bar{n}_2 + 1 \\ \bar{n}_3 \end{pmatrix};$$

Obviously, when there is only one candidate column for  $N$ , the design is clear. When there are three candidate columns, let  $s_1$ ,  $s_2$ , and  $s_3$  denote the multiplicities of the three candidate columns  $u_1$ ,  $u_2$ , and  $u_3$  respectively. These multiplicities can always be found by solving the simple system of equations:

$$s_1 u_1 + s_2 u_2 + s_3 u_3 = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix}. \quad (4.21)$$

In the above example, with  $b = 5$  and  $k = 8$ , the following system of equations was solved to find  $d_A$ :

$$s_1 \begin{pmatrix} 3 \\ 3 \\ 2 \end{pmatrix} + s_2 \begin{pmatrix} 3 \\ 2 \\ 3 \end{pmatrix} + s_3 \begin{pmatrix} 2 \\ 3 \\ 3 \end{pmatrix} = \begin{pmatrix} 14 \\ 13 \\ 13 \end{pmatrix}.$$

As discussed throughout this chapter, treatments 2 and 3 of  $E - M$ -optimal designs are also uniform, but sometimes treatment 1 must be made nonuniform in  $x$  number of blocks to obtain the  $E$ -optimal design. This happens in the case  $bk \equiv 1 \pmod{3}$ . Here, the problem changes only slightly.  $E$ -optimal designs have  $r_1 = \frac{bk+2}{3}$ ,  $r_2 = r_3 = \frac{bk-1}{3}$ , and so  $\sum \bar{n}_i = k - 1$  if  $k \equiv 1 \pmod{3}$ , or  $\sum \bar{n}_i = k - 2$  if  $k \equiv 2 \pmod{3}$ . Beside the three candidate columns of  $N$  described earlier, it will be required that  $N$  contain  $s_4 = x$  copies of either column  $\begin{pmatrix} \bar{n}_1 - 1 \\ \bar{n}_2 + 1 \\ \bar{n}_3 + 1 \end{pmatrix}$

if  $\sum \bar{n}_i = k - 1$ , or column  $\begin{pmatrix} \bar{n}_1 + 2 \\ \bar{n}_2 \\ \bar{n}_3 \end{pmatrix}$ , if  $\sum \bar{n}_i = k - 2$ . Letting  $u_4$  denote this column which appears  $x$  times in  $N$ , the multiplicities of the other columns will be again found by solving

the similar system of equations:

$$s_1 u_1 + s_2 u_2 + s_3 u_3 = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix} - x u_4. \quad (4.22)$$

In the above example,  $d_E$  had to have  $x = 1$  block in which treatment 1 was nonuniform, and that block corresponded to column  $u_4 = \begin{pmatrix} 4 \\ 2 \\ 2 \end{pmatrix}$ . The multiplicities of the other columns were found by solving:

$$s_1 \begin{pmatrix} 3 \\ 3 \\ 2 \end{pmatrix} + s_2 \begin{pmatrix} 3 \\ 2 \\ 3 \end{pmatrix} + s_3 \begin{pmatrix} 2 \\ 3 \\ 3 \end{pmatrix} = \begin{pmatrix} 10 \\ 11 \\ 11 \end{pmatrix} = \begin{pmatrix} 14 \\ 13 \\ 13 \end{pmatrix} - \begin{pmatrix} 4 \\ 2 \\ 2 \end{pmatrix}.$$

To summarize, the *A*-optimal designs and *E*-optimal designs for all cases except  $bk \equiv 1 \pmod{3}$  can be constructed following these steps:

- (a) Determine replication numbers  $r_1$ ,  $r_2$ , and  $r_3$ ,
- (b) Determine the candidate columns for  $N$ , knowing that the designs must be uniform,
- (c) Solve (4.21) to determine the multiplicity of each candidate column.

For *E*-optimal designs with  $bk \equiv 1 \pmod{3}$ , one must also determine  $x$ , the number of blocks in which treatment 1 is to be made nonuniform, and  $u_4$ , the column of  $N$  corresponding to the block with treatment 1 nonuniform. Then equation (4.22) must be solved to determine the multiplicities of the other columns in  $N$ . Once the columns of  $N$  are known, the design is unique up to block permutations.

#### 4.4.2 Construction of Row-Column Designs

We start by building row-column designs which are uniform in columns. Suppose we want to build  $d$ , a  $p \times q$  row-column design uniform in columns, with replications  $r_1, r_2, r_3$ . Start by constructing  $d_C$ , the column-component design with the  $v \times q$  column-treatment incidence matrix  $N = (n_{ij})$ . Then select one treatment from each column to form row 1; after deleting

the selected treatments, the remaining column-component design  $d_C^{(1)}$  will have  $q$  columns of size  $p-1$ . For row 2, select one treatment from each column of  $d_C^{(1)}$ , and repeat the procedure until all  $p$  rows are formed. Below we describe a method which guarantees this can be done in a way that yields the desired row-treatment incidence  $M = (m_{ij})$ .

**Lemma 4.4.** *Let  $d_C$  be the column-component design of a  $p \times q$  row-column design uniform in columns. One treatment from each column of  $d_C$  can be selected such that we select  $m_{11}$  1s,  $m_{21}$  2s, and  $m_{31}$  3s, with  $\sum_i m_{i1} = q$ , and  $d_C^{(1)}$  is uniform.*

*Proof.* Let  $N^{(1)}$  denote the incidence matrix of the resulting column-component design after deleting one treatment from each column. We need to verify that  $|n_{ij}^{(1)} - n_{ij'}^{(1)}| \leq 1$ , for any  $i$  and any  $(j, j')$ . As described in Lemma 4.3, there are three possibilities for the type of columns in  $N$ . We will verify the claim for each possibility.

- (a) All columns of  $N$  are of the form  $\begin{pmatrix} \bar{n}_1 \\ \bar{n}_2 \\ \bar{n}_3 \end{pmatrix}$ . In this case it doesn't matter from which columns we select the treatments; obviously,  $n_{ij}^{(1)} \in \{\bar{n}_i - 1, \bar{n}_i\}$  for all  $i$  and  $j$ .
- (b) The columns of  $N$  are  $\begin{pmatrix} \bar{n}_1 + 1 \\ \bar{n}_2 \\ \bar{n}_3 \end{pmatrix}$  w.m.  $s_1$ ,  $\begin{pmatrix} \bar{n}_1 \\ \bar{n}_2 + 1 \\ \bar{n}_3 \end{pmatrix}$  w.m.  $s_2$ , and  $\begin{pmatrix} \bar{n}_1 \\ \bar{n}_2 \\ \bar{n}_3 + 1 \end{pmatrix}$  w.m.  $s_3$  with  $\sum s_i = q$ . Let  $g_i = \min[s_i, m_{i1}]$ . If  $g_i = s_i$  for all  $i$  or  $g_i = m_{i1}$  for all  $i$ , it follows that  $s_i = m_{i1}$ . In this case select symbol  $i$  from all columns of type  $i$ , and  $N^{(1)}$  will have columns as in case (a) of Lemma 4.3.

If  $g_1 = s_1$ ,  $g_2 = s_2$ , and  $g_3 = m_{31}$ , then select the required  $m_{31}$  3's from columns of type 3, select 1's from all columns of type 1, select 2's from all columns of type 2, and select the remaining  $m_{11} - s_1$  1's and  $m_{21} - s_2$  2's randomly from the columns of type 3 from which symbol 3 was not already chosen. In this case  $N^{(1)}$  will have columns of the same form as those in (c) of Lemma 4.3, but with incidence numbers  $\bar{n}_1^{(1)} = \bar{n}_1 - 1$ ,  $\bar{n}_2^{(1)} = \bar{n}_2 - 1$ , and  $\bar{n}_3^{(1)} = \bar{n}_3$ .

If  $g_1 = s_1$ ,  $g_2 = m_{21}$ , and  $g_3 = m_{31}$  select 1s from all columns of type 1, select 2s from  $m_{21}$  columns of type 2, select 3s from  $m_{31}$  columns of type 3, and select 1s from the

remaining  $s_2 + s_3 - m_{21} - m_{31} = m_{11} - s_1$  columns of types 2 and 3. In this case,  $N^{(1)}$  will have columns of the same form as those in (b) of Lemma 4.3, with  $\bar{n}_1^{(1)} = \bar{n}_1 - 1$ ,  $\bar{n}_2^{(1)} = \bar{n}_2$ , and  $\bar{n}_3^{(1)} = \bar{n}_3$ .

(c) The columns of  $N$  are  $\begin{pmatrix} \bar{n}_1 \\ \bar{n}_2 + 1 \\ \bar{n}_3 + 1 \end{pmatrix}$  w.m.  $s_1$ ,  $\begin{pmatrix} \bar{n}_1 + 1 \\ \bar{n}_2 \\ \bar{n}_3 + 1 \end{pmatrix}$  w.m.  $s_2$ , and  $\begin{pmatrix} \bar{n}_1 + 1 \\ \bar{n}_2 + 1 \\ \bar{n}_3 \end{pmatrix}$  w.m.  $s_3$ .

Now let  $g_i = \min[q - s_i, m_{i1}]$ . Suppose we could have  $q - s_1 < m_{11}$  and  $q - s_2 < m_{21}$ .

This would imply  $2q - s_1 - s_2 < m_{11} + m_{21}$ , which is equivalent to  $q + s_3 < q - m_{31}$ .

This is not possible, and so for any  $i$ ,  $q - s_i < m_{i1}$  implies  $q - s_{i'} \geq m_{i'1}$  for all  $i' \neq i$ .

If  $g_1 = q - s_1$ ,  $g_2 = m_{21}$ , and  $g_3 = m_{31}$ , then select 1s from all columns of types 2 and 3 and  $m_{11} - s_2 - s_3$  columns of type 1, select 2s from  $m_{21}$  columns of type 1, and select 3s from the remaining  $m_{31}$  columns of type 1. In this case  $N^{(1)}$  will have columns of the same form as those in (c) of Lemma 4.3, with  $\bar{n}_1^{(1)} = \bar{n}_1 - 1$ ,  $\bar{n}_2^{(1)} = \bar{n}_2$ , and  $\bar{n}_3^{(1)} = \bar{n}_3$ .

If  $g_i = m_{i1}$  for all  $i$ , then let  $S_1 = \{j: \text{column } j \text{ of } N \text{ is of type 2 or 3}\}$ ,  $S_2 = \{j: \text{column } j \text{ of } N \text{ is of type 1 or 3}\}$ ,  $S_3 = \{j: \text{column } j \text{ of } N \text{ is of type 1 or 2}\}$ . Note that  $|S_i \cup S_j| = q$  for any  $i$  and  $j$ . Then by Theorem 4.6,  $S_1, S_2, S_3$  possess some  $(O_1, O_2, O_3)$  as an  $(m_{11}, m_{21}, m_{31})$  SDR. Select symbol  $i$  from column  $j$  if  $j \in O_i$ . Hence treatment  $i$  will be selected only from columns with  $n_{ij} = \bar{n}_i + 1$ , and so  $d_C^{(1)}$  will remain uniform.

□

The next theorem is an important result that follows directly from the above lemma.

**Theorem 4.7.** *Let  $d_C$  be the column component design of a  $p \times q$  row-column design uniform in columns. The treatments can be arranged in columns to obtain a row-column design with any row-treatment incidence matrix  $M = (m_{ij})$  consistent with the given replications.*

*Proof.* Start by selecting the first row with  $m_{11}$  1s,  $m_{21}$  2s, and  $m_{31}$  3s as described in Lemma 4.4. Since  $d_C^{(1)}$  is uniform, we can select another row, with  $m_{12}$  1s,  $m_{22}$  2s, and  $m_{32}$  3s, the left-over symbols forming another uniform column-component design  $d_C^{(2)}$ . Using the

procedure described above repeatedly, we can construct all  $p$  rows with any row-treatment incidence matrix  $M = (m_{ij})$ .  $\square$

All  $A$ -optimal row-column designs given in Table 3.1 are uniform both in rows and in columns, as are the  $E - M$ -optimal row-column designs with  $pq \equiv 0 \pmod{3}$  or  $pq \equiv 2 \pmod{3}$ . To construct such designs, first find the incidence matrices  $N$  and  $M$ . Then construct  $d_C$  and build one row at a time, with row counts given in  $M$ .

**Example 4.2.** We give an example of how to build a uniform row-column design, in particular the  $A$ -optimal  $4 \times 5$  row-column design, using the method given in Lemma 4.4.

As given in Table 3.1, the  $A$ -optimal design will be uniform with replications  $r_1 = 8$ ,  $r_2 = 7$ , and  $r_3 = 5$ . The columns of the column-component ( $N$ ), and row-component ( $M$ ), incidence matrices are:

$$N : \begin{array}{ccc} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \\ \hline w.m. & 3 & 2 & 0 \end{array} \quad M : \begin{array}{ccc} 2 & 2 & 1 \\ 2 & 1 & 2 \\ 1 & 2 & 2 \\ \hline w.m. & 3 & 1 & 0 \end{array}$$

We first write the column component design  $d_C$ :

$$\begin{array}{ccccc} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 2 & 2 \\ 2 & 2 & 2 & 2 & 2 \\ 3 & 3 & 3 & 3 & 3 \end{array}$$

Now select the rows one at a time such that  $d_C^{(1)}$ ,  $d_C^{(2)}$ , and  $d_C^{(3)}$  are uniform. One possible choice of rows gives us the desired uniform row column design  $d_A$ :

$$\begin{array}{ccccc} 1 & 1 & 3 & 2 & 2 \\ 1 & 2 & 1 & 2 & 3 \\ 2 & 1 & 1 & 3 & 2 \\ 3 & 3 & 2 & 1 & 1 \end{array}$$

The columns of the incidence matrices  $N$  and  $M$  are as given two paragraphs earlier, ordered from left to right. Also, note that if we delete the first  $l$  rows of  $d_A$  for any  $l \leq 3$ , the remaining  $(4 - l) \times 5$  row-column design is uniform in columns.  $\square$

Next, we give a method for building the *E*-optimal row-column designs for the cases  $pq \equiv 1 \pmod 3$ , as given in Theorem 4.4. These designs have replications  $r_1 = \frac{pq+2}{3}$ ,  $r_2 = r_3 = \frac{pq-1}{3}$  and are uniform for treatments 2 and 3. However, treatment 1 is non-uniform in  $x_1$  columns and  $x_2$  rows, where  $x_{1(2)} \leq \frac{q(p)-1}{3}$  if  $p \equiv q \equiv 1 \pmod 3$  and  $x_{1(2)} \leq \frac{q(p)+1}{3}$  if  $p \equiv q \equiv 2 \pmod 3$ . The columns of  $N$  and  $M$  are found by solving equation (4.22). The columns of  $N$  are:

$$\begin{array}{cccc}
 \frac{p-4}{3} & \frac{p+2}{3} & \frac{p-1}{3} & \frac{p-1}{3} \\
 \frac{p+2}{3} & \frac{p-1}{3} & \frac{p+2}{3} & \frac{p-1}{3} \\
 \frac{p+2}{3} & \frac{p-1}{3} & \frac{p-1}{3} & \frac{p+2}{3} \\
 \hline
 w.m. & x_1 & \frac{q+2}{3} + x_1 & \frac{q-1}{3} - x_1 \\
 \hline
 Type & I & II & III
 \end{array}$$

if  $p \equiv q \equiv 1 \pmod 3$ ,

and

$$\begin{array}{cccc}
 \frac{p+4}{3} & \frac{p-2}{3} & \frac{p+1}{3} & \frac{p+1}{3} \\
 \frac{p-2}{3} & \frac{p+1}{3} & \frac{p-2}{3} & \frac{p+1}{3} \\
 \frac{p-2}{3} & \frac{p+1}{3} & \frac{p+1}{3} & \frac{p-2}{3} \\
 \hline
 w.m. & x_1 & \frac{q-2}{3} + x_1 & \frac{q+1}{3} - x_1 \\
 \hline
 Type & I & II & III
 \end{array}$$

if  $p \equiv q \equiv 2 \pmod 3$ .

Interchanging  $p$  and  $q$ , and replacing  $x_1$  with  $x_2$  gives the columns of the row incidence matrix  $M$ . We use a similar method of constructing such designs as for uniform designs. In fact, when  $x_{1(2)} = 0$ , we can construct the uniform column(row)-component design, and then select one row(column) at a time as described in Lemma 4.4. From now on assume  $x_1 \geq 1$  and  $x_2 \geq 1$ .

First consider the case  $p \equiv q \equiv 1 \pmod 3$ , and start by constructing the column component design. We can construct two rows corresponding to two columns of type  $\begin{pmatrix} \frac{q+2}{3} \\ \frac{q-1}{3} \\ \frac{q-1}{3} \end{pmatrix}$  of  $M$  in such a way that  $d_C^{(2)}$  is uniform. We do this by carefully selecting 1s, 2s, and 3s from the target columns of  $N$  shown above. For row 1 select 2s from the  $x_1$  columns of type I and from the  $\frac{q-1}{3} - x_1$  columns of type III, select 3s from  $x_1$  columns of type II and from the

$\frac{q-1}{3} - x_1$  columns of type IV, and select 1s from the remaining  $\frac{q+2}{3}$  columns of type II. For row 2 select 2s from  $x_1$  columns of type II from which we selected 1s for row 1, and from the  $\frac{q-1}{3} - x_1$  columns of type III, select 3s from the  $x_1$  columns of type I and from the  $\frac{q-1}{3} - x_1$  columns of type IV, and select 1s from the remaining  $\frac{q+2}{3}$  columns of type II. After removing these treatments, the columns of  $N^{(2)}$  are:

$$\begin{array}{ccc} \frac{p-4}{3} & \frac{p-1}{3} & \frac{p-1}{3} \\ \frac{p-1}{3} & \frac{p-4}{3} & \frac{p-1}{3} \\ \frac{3}{3} & \frac{3}{3} & \frac{3}{3} \\ \frac{p-1}{3} & \frac{p-1}{3} & \frac{p-4}{3} \\ \hline w.m. & \frac{q+2}{3} & \frac{q-1}{3} \end{array}$$

Thus  $d_C^{(2)}$  is uniform, and the remaining rows can be formed by the procedure described in Lemma 4.7.

When  $p \equiv q \equiv 2 \pmod{3}$ , start again by building the column-component design  $d_C$ . Let  $S_1 = \{\text{all columns of } d_C \text{ of types III or IV}\}$ ,  $S_2 = \{\text{all columns of } d_C \text{ of types II or IV}\}$ , and  $S_3 = \{\text{all columns of } d_C \text{ of types II or III}\}$ .

If  $x_2 < \frac{p+1}{3}$ , we can select one row corresponding to one column of type  $\begin{pmatrix} \frac{q+1}{3} \\ \frac{q-2}{3} \\ \frac{q+1}{3} \end{pmatrix}$  of  $M$  in such a way that  $d_C^{(1)}$  is uniform. To achieve this, first select 1s from the  $x_1$  columns of type I. Next obtain an  $(\frac{q+1}{3} - x_1, \frac{q-2}{3}, \frac{q+1}{3})$ -SDR from  $S_1, S_2, S_3$ , call it  $O_1, O_2, O_3$ , which is possible by Theorem 4.6. Now remove  $i$  from all columns in  $O_i$  for  $i = 1, 2, 3$ . The remaining treatments form  $d_C^{(1)}$  which is uniform with the columns of  $N^{(1)}$ :

$$\begin{array}{ccc} \frac{p+1}{3} & \frac{p-2}{3} & \frac{p-2}{3} \\ \frac{p-2}{3} & \frac{p+1}{3} & \frac{p-2}{3} \\ \frac{3}{3} & \frac{3}{3} & \frac{3}{3} \\ \frac{p-2}{3} & \frac{p-2}{3} & \frac{p+1}{3} \\ \hline w.m. & \frac{q+1}{3} & \frac{q-2}{3} \end{array}$$

If  $x_2 = \frac{p+1}{3}$  and  $x_1 < \frac{q+1}{3}$ , select a row corresponding to one column of type  $\begin{pmatrix} \frac{q-2}{3} \\ \frac{q+1}{3} \\ \frac{q+1}{3} \end{pmatrix}$  of  $M$  in such a way that  $d_C^{(1)}$  is uniform. To achieve this, select 1s from all  $x_1$  columns of type I and then select an  $(\frac{q-2}{3} - x_1, \frac{q+1}{3}, \frac{q+1}{3})$ -SDR from  $S_1, S_2, S_3$ . In order for such an SDR to exist

one must have  $|S_2 \cup S_3| \geq 2\frac{q+1}{3}$ , which is equivalent to  $x_1 \leq \frac{q-2}{3}$ . The remaining treatments form  $d_C^{(1)}$ , which is uniform, with  $n_{ij} \in \{\frac{p-2}{3}, \frac{p+1}{3}\}$ .

The only designs left to build have  $x_1 = \frac{q+1}{3}$  and  $x_2 = \frac{p+1}{3}$ , in which case column types III and IV have multiplicity 0. The columns of  $N$  and  $M$  for such designs are

$$N : \begin{array}{c} \frac{p+4}{3} \quad \frac{p-2}{3} \\ \frac{p-2}{3} \quad \frac{p+1}{3} \\ \frac{p-2}{3} \quad \frac{p+1}{3} \\ \hline w.m. \quad \frac{q+1}{3} \quad \frac{2q-1}{3} \\ \hline Type \quad I \quad II \end{array} \qquad M : \begin{array}{c} \frac{q+4}{3} \quad \frac{q-2}{3} \\ \frac{q-2}{3} \quad \frac{q+1}{3} \\ \frac{q-2}{3} \quad \frac{q+1}{3} \\ \hline w.m. \quad \frac{p+1}{3} \quad \frac{2p-1}{3} \\ \hline Type \quad I \quad II \end{array}$$

It turns out that such a design can be built only if  $q \geq p \geq 5$ . If  $p = 2$  then only  $\frac{q+1}{3}$  columns contain 1s, and thus a row of type I cannot be created. In conclusion, when  $p = 2$  only designs with  $x_1 \leq \frac{q-2}{3}$  or  $x_2 = 0$  can be constructed.

If  $p > 2$  we can select two rows of type I such that  $d_C^{(2)}$  is uniform in columns. For both rows select 1s from the  $\frac{q+1}{3}$  columns of type I. For row 1 select an additional 1 from column 1 of type II, and for row 2 select an additional 1 from column 2 of type II. Treatments 2 and 3 can then be selected from columns of type II such that a symbol is not selected twice from the same column. For instance, with columns of Type I numbered  $\frac{2q+2}{3}, \dots, q$ , select:

	Row 1	Row 2
Treatment	columns	columns
1	1, $\frac{2q+2}{3}$ through $q$	2, $\frac{2q+2}{3}$ through $q$
2	2 through $\frac{q+1}{3}$	$\frac{q+4}{3}$ through $\frac{2q-1}{3}$
3	$\frac{q+4}{3}$ through $\frac{2q-1}{3}$	1, 3 through $\frac{q+1}{3}$

After these two rows are selected, the columns of  $N_C^{(2)}$  will be:

$$\begin{array}{c} \frac{p-2}{3} \quad \frac{p-5}{3} \quad \frac{p-5}{3} \\ \frac{p-2}{3} \quad \frac{p+1}{3} \quad \frac{p-2}{3} \\ \frac{p-2}{3} \quad \frac{p-2}{3} \quad \frac{p+1}{3} \end{array}$$

Note that  $d_C^{(2)}$  is uniform in columns, and thus the remaining rows can be selected by Lemma 4.7.

**Example 4.3.** We demonstrate the construction method by building a  $5 \times 5$  row-column design with replications  $r_1 = 9$ ,  $r_2 = r_3 = 8$ , nonuniform in 2 columns and 2 rows. Such a design is not *E*-optimal, but we present it here to aid in the discussion.

The column component design  $d_C$  is given below.

$$\begin{array}{ccccc} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 2 & 2 & 2 \\ 1 & 1 & 2 & 2 & 2 \\ 2 & 2 & 3 & 3 & 3 \\ 3 & 3 & 3 & 3 & 3 \end{array}$$

Treatment 1 is not uniform in the first two columns. Next, select the first two rows such that 1 appears three times in each row, while 2 and 3 appear once in each of them. Finally, select the remaining three rows in which 1 appears once in each of them, while 2 and 3 each appear twice in a row. The resulting row-column design is:

$$\begin{array}{ccccc} 1 & 1 & 1 & 2 & 3 \\ 1 & 1 & 3 & 1 & 2 \\ 1 & 3 & 2 & 3 & 2 \\ 2 & 1 & 2 & 3 & 3 \\ 3 & 2 & 3 & 2 & 1 \end{array}$$

The above design has the required replications with treatment 1 nonuniform in the first two columns and the first two rows.  $\square$

Remember that the number of rows and columns in which treatment 1 should be made nonuniform is determined by the difference  $D = c_1^0 - c_2^0$ , where  $c_1^0$  and  $c_2^0$  are the diagonal elements of a uniform treatment replicated  $\frac{pq+2}{3}$  and  $\frac{pq-1}{3}$  times, respectively. When  $p \equiv q \equiv 2 \pmod{3}$ , this difference reduces to  $D = \frac{(p+1)(q+1)}{3pq}$ , which becomes  $D = \frac{q+1}{2q}$  when  $p = 2$ .

When  $p = 2$ , each row in which treatment 1 is made nonuniform reduces  $c_1$  by  $\frac{2}{q}$ , while each column in which treatment 1 is made nonuniform reduces  $c_1$  by  $\frac{2}{p} = 1$ . Making treatment 1 nonuniform in one column already brings  $c_1$  under  $c_2^0$ . Thus, to obtain  $d^*$ , make treatment 1 nonuniform in one row and zero columns, and to obtain  $d_*$ , make treatment 1 nonuniform in zero rows and one column. Therefore, all *E*-optimal row-column designs can be constructed.

### 4.4.3 Construction of $E$ -optimal Hyperrectangles

Consider a hyperrectangle of size  $b_1 \times b_2 \times \cdots \times b_n$  with  $m = \prod b_j$  total experimental units. The construction is divided into cases according to the value of  $m \bmod 3$ . Unlike in sections 2.2 and 4.3, we no longer require  $b_1 \leq b_2 \leq \cdots \leq b_n$ .

#### Case 1: $m \equiv 0 \pmod{3}$

When  $v = 3$  and  $3|m$ , a Youden hyperrectangle is universally optimal and can always be constructed as given in Corollary 2.1.1 of Cheng [8]. We present a simple method for constructing a YHR with 3 treatments.

Without loss of generality assume  $3|b_1$ . Start by constructing a hyperrectangle of size  $b_2 \times b_3 \times \cdots \times b_n$  with  $b_1$  experimental units per cell, each treatment occurring  $\frac{b_1}{3}$  times in each cell. This design reduces to GRBDs in each direction  $j \geq 2$ . Order the cells 1 to  $b_2 \times b_3 \times \cdots \times b_n$ . Next, select treatment  $i$  from cell  $j$  if  $i \equiv j \pmod{3}$  (e.g. select treatment 3 from cells 3, 6, ...). These will represent the first block in direction 1. For block 2 of factor 1, select treatment  $i$  from cell  $j$  if  $i + 1 \equiv j \pmod{3}$ . Continue the procedure to build the remaining  $b_1 - 2$  blocks of direction 1. For block  $w$  of factor 1, select treatment  $i$  from cell  $j$  if  $i + w - 1 \equiv j \pmod{3}$ . After selecting  $3s$  blocks, each cell will contain  $\frac{b_1}{3} - s$  copies of each treatment. In this fashion each block in direction 1 will be generalized binary, and since  $v = 3$  and the design is equireplicated, it reduces to a BBD in direction 1.

#### Case 2: $m \equiv 2 \pmod{3}$

In this case, the  $E$ -optimal hyperrectangle is uniform with replications  $r_1 = r_2 = \frac{m+1}{3}$  and  $r_3 = \frac{m-2}{3}$ . Such a design can be constructed cyclically. Number the cells of the hyperrectangle as follows:

$$\text{coordinate } (a_1 \times a_2 \times \cdots \times a_n) \rightarrow \text{cell number } \sum_{j=1}^{n-1} \left[ (a_j - 1) \prod_{k=j+1}^n b_k \right] + a_n \quad (4.23)$$

For example, if  $n = 3$  this numbering system will order the cells as:

$$(1, 1, 1) \rightarrow (1, 1, 2) \rightarrow \cdots \rightarrow (1, 1, b_3) \rightarrow (1, 2, 1) \rightarrow \cdots \rightarrow (b_1, b_2, b_3 - 1) \rightarrow (b_1, b_2, b_3)$$

$$\begin{matrix} 1 & 2 & & b_3 & & b_3+1 & & b_1 b_2 b_3 - 1 & & b_1 b_2 b_3 \end{matrix}$$

Assigning treatment  $(j - 1 \pmod 3) + 1$  to cell  $j$  yields a uniform design with the desired replications. In other words, assign treatment 1 to cells  $(1, 4, 7, \dots)$ , treatment 2 to cells  $(2, 5, 8, \dots)$ , and treatment 3 to cells  $(3, 6, 9, \dots)$ . It is easy to see that such an assignment yields  $r_1 \geq r_2 \geq r_3$  and  $|r_i - r_{i'}| \leq 1$  regardless of  $m$ . When  $m \equiv 2 \pmod 3$  the resulting replications are  $r_1 = r_2 = \frac{m+1}{3}$ ,  $r_3 = \frac{m-2}{3}$ . To see that the design is uniform, consider a block  $l$  in direction  $j$ . Since  $3 \nmid \prod_{k \geq j+1}^n b_k$ , block  $l$  in direction  $j$  will constitute a piece of either sequence

$$\begin{aligned} &\dots 3, 1, 2, 3, 1, 2, 3, 1, \dots \text{ if } \prod_{k \geq j+1}^n b_k \equiv 1 \pmod 3 \text{ or,} \\ &\dots 2, 1, 3, 2, 1, 3, 2, 1, \dots \text{ if } \prod_{k \geq j+1}^n b_k \equiv 2 \pmod 3. \end{aligned}$$

Thus the design is generalized binary. This method can be used to construct generalized binary hyperrectangles with  $v > 3$  treatments. However, when  $v > 3$  treatment concurrences are not determined only by the number of times each treatment appears in each block, as is the case with  $v = 2$  or  $v = 3$ , so there is no guarantee of a good design.

**Example 4.4.** We construct the *E*-optimal hyperrectangle of size  $4 \times 5 \times 4$  by the above method. This design has replications  $r_1 = r_2 = 27$ ,  $r_3 = 26$ , and is uniform in all directions (see Theorem 4.5). To better visualize the design, consider the slices as factor 1, the rows as factor 2, and the columns as factor 3. Note that the 4 slices below are crossed, not nested. Column 1 of the hyperrectangle is the union of the first columns in each of the slices, and the same applies to the rest of the columns and the rows.

Slice 1				Slice 2				Slice 3				Slice 4			
1	2	3	1	3	1	2	3	2	3	1	2	1	2	3	1
2	3	1	2	1	2	3	1	3	1	2	3	2	3	1	2
3	1	2	3	2	3	1	2	1	2	3	1	3	1	2	3
1	2	3	1	3	1	2	3	2	3	1	2	1	2	3	1
2	3	1	2	1	2	3	1	3	1	2	3	2	3	1	2

□

**Case 3:**  $m \equiv 1 \pmod 3$

In this case,  $E$ -optimal designs have replications  $r_1 = \frac{m+2}{3}$  and  $r_2 = r_3 = \frac{m-1}{3}$ . As given in Theorem 4.4,  $E$ -optimal designs must be uniform in treatments 2 and 3, but nonuniform in treatment 1 in  $x_j$  blocks of direction  $j$ , where  $x_j \leq \begin{cases} \frac{b_j-1}{3} & \text{if } b_j \equiv 1 \pmod{3}, \\ \frac{b_j+1}{3} & \text{if } b_j \equiv 2 \pmod{3} \end{cases}$ . Treatment 1 will be made nonuniform in block  $l$  of direction  $j$ , by permuting treatments in the design such that  $n_{1jl} = \begin{cases} \frac{mb_j^{-1}-4}{3} & \text{if } b_j \equiv 1 \pmod{3}, \\ \frac{mb_j^{-1}+4}{3} & \text{if } b_j \equiv 2 \pmod{3} \end{cases}$ . We will construct such a hyperrectangle in several steps.

Let the first  $s_1$  dimensions of the hyperrectangle be  $b_1 \equiv b_2 \equiv \dots \equiv b_{s_1} \equiv 2 \pmod{3}$ , and the last  $n - s_1$  dimensions be  $b_{s_1+1} \equiv \dots \equiv b_n \equiv 1 \pmod{3}$ . Since  $m \equiv 1 \pmod{3}$ ,  $s_1$  must be even. Start by constructing the uniform  $b_1 \times b_2 \times \dots \times b_{s_1}$  hyperrectangle  $d_2$  by the cyclical method described earlier. In this hyperrectangle,  $r_1 = \frac{(\prod_{j \leq s_1} b_j)+2}{3}$  and  $r_2 = r_3 = \frac{(\prod_{j \leq s_1} b_j)-1}{3}$ . Now take the  $b_1 \times b_2$  row-column design formed by fixing  $b_3 = b_4 = \dots = b_{s_1} = 1$ . Following directly from the construction, the  $b_1 \times b_2$  row-column design is:

$$\begin{array}{cccccc} 1 & 2 & 3 & 1 & \dots & 1 & 2 \\ 3 & 1 & 2 & 3 & \dots & 3 & 1 \\ 2 & 3 & 1 & 2 & \dots & 2 & 3 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 3 & 1 & 2 & 3 & \dots & 3 & 1 \end{array}$$

Furthermore, if these treatments are deleted from  $d_2$ , each treatment will appear the same number of times in each block of direction 1 and in each block of direction 2. The above  $b_1 \times b_2$  row-column design is uniform with replications  $r_1 = \frac{b_1 b_2 + 2}{3}$  and  $r_2 = r_3 = \frac{b_1 b_2 - 1}{3}$ .

We fix position (1,1) in the  $b_1 \times b_2$  row-column design, and by permuting treatments within rows and within columns we can make treatment 1 nonuniform in  $x_1 \leq \frac{b_1+1}{3}$  columns and  $x_2 \leq \frac{b_2+1}{3}$ . We know about the existence of these types of row-column designs from section 4.4.2. After these permutations, design  $d_2$  is still uniform in treatments 2 and 3, but nonuniform in treatment 1 in  $x_1$  blocks of direction 1 and  $x_2$  blocks of direction 2.

Next, select the  $b_3 \times b_4$  row-column design by fixing  $b_1 = b_2 = b_5 = \dots = b_{s_1} = 1$ . Make the  $b_3 \times b_4$  design nonuniform in  $x_3$  columns and  $x_4$  rows, again fixing the element in the

(1,1) position. Note that the only position from  $d_2$  selected here, as well as in the  $b_1 \times b_2$  row-column design is the  $(1, 1, \dots, 1)$  position occupied by treatment 1. This guarantees that the nonuniformity achieved for the first two directions is not disturbed. The procedure can be repeated until the final two dimensions  $b_{s_1-1}$  and  $b_{s_1}$ .

We now have a  $b_1 \times b_2 \times \dots \times b_{s_1}$  hyperrectangle nonuniform in  $x_j$  blocks of direction  $j$ . Let this hyperrectangle represent the last block of factor  $s_1 + 1$ . To this last block, prepend a  $b_1 \times b_2 \times \dots \times b_{s_1} \times (b_{s_1+1} - 1)$  Youden hyperrectangle to form a new  $b_1 \times b_2 \times \dots \times b_{s_1} \times b_{s_1+1}$  hyperrectangle, uniform in direction  $s_1 + 1$ . The YHR is to be constructed cyclically such that blocks  $1, 4, \dots, b_{s_1+1} - 3$  of direction  $s_1 + 1$  contain one more '1' than the other blocks. In this YHR,  $3|(b_{s_1+1} - 1)$  and thus each treatment appears an equal number of times in each block of direction  $j$  for all  $j \leq s_1$ . Thus, treatments 2 and 3 are still uniform in directions  $j \leq s_1$ , while treatment 1 is nonuniform in  $x_j$  blocks of direction  $j$  for all  $j \leq s_1$ .

The block-treatment incidence matrix in direction  $s_1 + 1$  of the  $b_1 \times b_2 \times \dots \times b_{s_1} \times b_{s_1+1}$  hyperrectangle is  $N_{s_1+1} = (n_{il})_{s_1+1}$ , where:

$$(n_{1l}, n_{2l}, n_{3l}) = \begin{cases} \frac{1}{3}(\prod_{j \leq s_1} b_j + 2, \prod_{j \leq s_1} b_j - 1, \prod_{j \leq s_1} b_j - 1) & \text{if } l \equiv 1 \pmod{3}, \\ \frac{1}{3}(\prod_{j \leq s_1} b_j - 1, \prod_{j \leq s_1} b_j + 2, \prod_{j \leq s_1} b_j - 1) & \text{if } l \equiv 2 \pmod{3}, \\ \frac{1}{3}(\prod_{j \leq s_1} b_j - 1, \prod_{j \leq s_1} b_j - 1, \prod_{j \leq s_1} b_j + 2) & \text{if } l \equiv 0 \pmod{3}. \end{cases}$$

The next step is to make treatment 1 nonuniform in  $x_{s_1+1}$  blocks of direction  $s_1 + 1$ . This will be achieved by performing several permutations of treatments among blocks in this direction. Take for instance blocks 2 and 3 of factor  $s_1 + 1$ . Positions  $(1, 1, \dots, 1, 2)$ ,  $(1, 1, \dots, 2, 2)$ ,  $(1, 1, \dots, 1, 3)$ , and  $(1, 1, \dots, 2, 3)$  in the hyperrectangle are occupied by treatments 2,3,3, and 1, respectively. Interchanging  $(1, 1, \dots, 1, 2)$  with  $(1, 1, \dots, 1, 3)$  and  $(1, 1, \dots, 2, 2)$  with  $(1, 1, \dots, 2, 3)$  will not affect the block-wise replication numbers in directions  $j \leq s_1$ . However, after these permutations, we will have

$$\begin{aligned} n_{1(s_1+1)2} &= \frac{\prod_{j \leq s_1} b_j + 2}{3}, & n_{2(s_1+1)2} &= n_{3(s_1+1)2} = \frac{\prod_{j \leq s_1} b_j - 1}{3}, \\ n_{1(s_1+1)3} &= \frac{\prod_{j \leq s_1} b_j - 4}{3}, & n_{2(s_1+1)3} &= n_{3(s_1+1)3} = \frac{\prod_{j \leq s_1} b_j + 2}{3}. \end{aligned}$$

Treatments 2 and 3 remain uniform, while treatment 1 is made nonuniform in block 3 of

direction  $s_1 + 1$ . In a similar way, treatment 1 can be made nonuniform in any block  $l \equiv 0 \pmod 3$ , and so it can be made nonuniform in any number  $x_{s_1+1} \leq \frac{b_{s_1+1}-1}{3}$  of blocks in direction  $s_1 + 1$ . Now pad the  $b_1 \times b_2 \times \cdots \times b_{s_1+1}$  hyperrectangle with a  $b_1 \times b_2 \times \cdots \times b_{s_1+1} \times (b_{s_1+2} - 1)$  YHR. The resulting  $b_1 \times b_2 \times \cdots \times b_{s_1+1} \times b_{s_1+2}$  hyperrectangle can then be made nonuniform in  $x_{s_1+2} \leq \frac{b_{s_1+2}-1}{3}$  blocks of direction  $s_1 + 2$ . This padding procedure can be used repeatedly to create hyperrectangles of higher dimensions, ending with the desired  $b_1 \times b_2 \times \cdots \times b_n$   $E$ -optimal hyperrectangle.

If  $b_j \equiv 1 \pmod 3$  for all  $j \leq n$ , the construction starts with a  $b_1 \times b_2$  row-column design nonuniform for treatment 1 in  $x_1$  columns and  $x_2$  rows. The padding procedure can then be used to build the  $b_1 \times b_2 \times \cdots \times b_n$   $E$ -optimal hyperrectangle, one dimension at a time.

**Example 4.5.** We construct the  $E$ -optimal  $5 \times 5 \times 4$  hyperrectangle. By Theorem 4.4 the  $E - M$ -optimal design has replications  $r_1 = 34$ ,  $r_2 = r_3 = 33$ , and treatment 1 nonuniform in  $x_j$  blocks of direction  $j$ , where  $j = 1, 2, 3$ . Solving (4.14) and (4.15) gives  $x_1 = 1$ ,  $x_2 = 2$  and  $x_3 = 0$ .

We start with a  $5 \times 5$  row-column design with replications  $r_1 = 9$ ,  $r_2 = r_3 = 8$ , and with treatment 1 nonuniform in column 1 and in rows 1 and 2. This will represent the last block in direction 3 of the  $5 \times 5 \times 4$  hyperrectangle.

Slice 4				
1	1	1	2	3
1	2	3	1	1
1	3	2	3	2
2	1	3	2	3
3	2	1	3	2

Pad this row-column design with the following  $5 \times 5 \times 3$  YHR. Since  $x_3 = 0$ , no permutations are needed to make treatment 1 nonuniform in direction 3.

Slice 1				
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

Slice 2				
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

Slice 3				
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

Note that if we would have had  $x_3 = 1$ , treatment 1 could be made nonuniform in slice 3 by interchanging position (1, 1, 2) with (1, 1, 3) and position (1, 2, 2) with (1, 2, 3). This would not affect the uniformity in the incidence matrices in directions 1 and 2, and it will also keep treatments 2 and 3 uniform in direction 3. □

**Example 4.6.** We next construct an  $E - M$ -optimal  $5^4$  hypercube with  $v = 3$  by the above method. By Theorem 4.4 the  $E - M$ -optimal design has replications  $r_1 = 209$ , and  $r_2 = r_3 = 208$ , and treatment 1 is nonuniform in 2 blocks of each direction. Start by building the uniform design with  $r_1 = 209$ , and  $r_2 = r_3 = 208$  as shown in Table 4.1. Large rows, large columns, small rows, and small columns represent blocking factor 1,2,3, and 4 respectively. Remember that the factors are crossed; for instance, the first block in direction 4 is comprised of the union of all first columns of the 25 smaller row-column designs.

Note that when we fix  $b_1 = b_2 = 1$ , the design reduces to a  $5 \times 5$  uniform row-column design, same as when we fix  $b_3 = b_4 = 1$ . The row-column design

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

can be rearranged as in Example 4.3 to be make treatment 1 nonuniform in 2 rows and 2 columns:

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

Perform this operation both for the row-column design determined by  $a_1 = a_2 = 1$  and by the row-column design determined by  $a_3 = a_4 = 1$ . After these rearrangements, the  $5^4$  hypercube will have treatment 1 nonuniform in 2 blocks of each direction, while treatments 2 and 3 will still be uniform. Note that the block-treatment incidence matrices are

$$N_j = \begin{pmatrix} 43 & 43 & 41 & 41 & 41 \\ 41 & 41 & 42 & 42 & 42 \\ 41 & 41 & 42 & 42 & 42 \end{pmatrix},$$

for  $j = 1, \dots, 4$ . The  $E - M$ -optimal design summarized by the above incidence matrices is displayed in Table 4.2.

Table 4.1: A  $5^4$  uniform hypercube

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## 4.5 Deciding between the *E*-optimal and *A*-optimal Designs

A comparison of *A*-optimal and *E*-optimal designs with three treatments will be performed in this section. The purpose of this comparison is to facilitate the choice for a good design. Such a choice will be made easier by having the *E*-efficiency of the *A*-optimal design for a given setting, as well as the *A*-efficiency of the *E* – *M*-optimal design for that setting. These efficiencies will answer the questions: “How much will the average variance of all contrasts increase if I guard against a very large variance for some contrast versus minimizing the average variance?” and “How much does the largest variance increase if I minimize the average variance of all contrasts versus guarding against a very large variance for some contrast?”. The comparison will be performed for simple block designs and row-column designs. Throughout this section let  $E_{eff}(d_A)$  denote the *E*-efficiency of the *A*-optimal design, and  $A_{eff}(d_E)$  denote the *A*-efficiency of the *E*-optimal design. In some of the cases there exists a design  $d^*$  that is both *A*-optimal and *E* – *M*-optimal, and so  $E_{eff}(d_A) = A_{eff}(d_E) = 1$ .

We start by comparing block designs. If  $bk \equiv 0 \pmod 3$  or  $bk \equiv 2 \pmod 3$  both the *A*-optimal and *E* – *M*-optimal designs are generalized binary and have the same replications. This also happens if  $b \equiv k \equiv 1 \pmod 3$  and  $\min[\frac{b-1}{3}, \text{int}(\frac{k-1}{6})] = 0$ , or  $b \equiv k \equiv 2 \pmod 3$  and  $\min[\frac{b+1}{3}, \text{int}(\frac{k+1}{6})] = 0$ . A comparison of *A*-optimal and *E* – *M*-optimal block designs with  $4 \leq b \leq 20$  blocks of size  $5 \leq k \leq 20$  and  $3 \nmid bk$  is given in Table 4.3.

Table 4.3: Comparison of *A*-optimal and *E* – *M*-optimal block designs with  $3 \nmid bk$

<i>k</i>		<i>b</i>											
		4	5	7	8	10	11	13	14	16	17	19	20
5	$E_{eff}(d_A)$	1	0.9744	1	0.9841	1	0.9885	1	0.9910	1	0.9926	1	0.9937
	$A_{eff}(d_E)$	1	0.9774	1	0.9853	1	0.9891	1	0.9914	1	0.9929	1	0.9939
7	$E_{eff}(d_A)$	0.9841	1	0.9910	1	0.9937	1	0.9952	1	0.9961	1	0.9967	1
	$A_{eff}(d_E)$	0.9853	1	0.9914	1	0.9939	1	0.9953	1	0.9962	1	0.9968	1
8	$E_{eff}(d_A)$	1	0.9903	1	0.9940	1	0.9956	1	0.9966	1	0.9972	1	0.9976
	$A_{eff}(d_E)$	1	0.9912	1	0.9943	1	0.9958	1	0.9967	1	0.9973	1	0.9977

Table 4.3: (continued)

$k$		$b$											
		4	5	7	8	10	11	13	14	16	17	19	20
10	$E_{eff}(d_A)$	0.9923	1	0.9956	1	0.9970	1	0.9977	1	0.9981	1	0.9984	1
	$A_{eff}(d_E)$	0.9929	1	0.9958	1	0.9970	1	0.9977	1	0.9981	1	0.9984	1
11	$E_{eff}(d_A)$	1	0.9899	1	0.9937	1	0.9954	1	0.9964	1	0.9971	1	0.9975
	$A_{eff}(d_E)$	1	0.9904	1	0.9939	1	0.9955	1	0.9965	1	0.9971	1	0.9975
13	$E_{eff}(d_A)$	0.9955	1	0.9949	1	0.9964	1	0.9972	1	0.9978	1	0.9981	1
	$A_{eff}(d_E)$	0.9958	1	0.9950	1	0.9965	1	0.9973	1	0.9978	1	0.9981	1
14	$E_{eff}(d_A)$	1	0.9938	1	0.9961	1	0.9972	1	0.9978	1	0.9982	1	0.9985
	$A_{eff}(d_E)$	1	0.9941	1	0.9962	1	0.9973	1	0.9978	1	0.9982	1	0.9985
16	$E_{eff}(d_A)$	0.9970	1	0.9966	1	0.9976	1	0.9982	1	0.9985	1	0.9988	1
	$A_{eff}(d_E)$	0.9972	1	0.9967	1	0.9977	1	0.9982	1	0.9985	1	0.9988	1
17	$E_{eff}(d_A)$	1	0.9958	1	0.9961	1	0.9972	1	0.9978	1	0.9982	1	0.9984
	$A_{eff}(d_E)$	1	0.9960	1	0.9962	1	0.9972	1	0.9978	1	0.9982	1	0.9984
19	$E_{eff}(d_A)$	0.9979	1	0.9976	1	0.9975	1	0.9981	1	0.9984	1	0.9987	1
	$A_{eff}(d_E)$	0.9980	1	0.9977	1	0.9975	1	0.9981	1	0.9984	1	0.9987	1
20	$E_{eff}(d_A)$	1	0.9970	1	0.9972	1	0.9979	1	0.9984	1	0.9987	1	0.9989
	$A_{eff}(d_E)$	1	0.9971	1	0.9972	1	0.9980	1	0.9984	1	0.9987	1	0.9989

One can see that both the  $A$ -optimal and  $E - M$ -optimal block designs have a high efficiency with respect to the other criterion. The  $A$ -efficiency of  $E - M$ -optimal designs is in general slightly higher than the  $E$ -efficiency of  $A$ -optimal designs. Also, as the size of the designs increases, these efficiencies get closer to each other, and closer to 1.

We now move on to  $p \times q$  row-column designs, with the general assumption  $p \leq q$ . As discussed in earlier sections, If  $pq \equiv 0 \pmod{3}$ , an universally optimal GYD exists. If  $p \equiv q \equiv 2 \pmod{3}$  or  $p \equiv 2 \pmod{3}$ ,  $q \equiv 1 \pmod{3}$  and  $q \gg p$ , a generalized binary design with  $r_i \in \{\text{int}[\frac{pq}{3}], \text{int}[\frac{pq}{3}] + 1\}$  is  $A$ -optimal as well as  $E - M$ -optimal. In these cases  $E_{eff}(d_A) = A_{eff}(d_E) = 1$ . Similar to the comparison for block design, we present the  $E$ -efficiency of  $A$ -optimal row-column designs and the  $A$ -efficiency of  $E$ -optimal row-column designs in Table 4.4 for  $p \times q$  row-column designs with  $4 \leq p \leq q \leq 20$  and  $3 \nmid pq$ .

Table 4.4: Comparison of  $A$ -optimal and  $E - M$ -optimal row-column designs with  $3 \nmid pq$ 

$p$		$q$											
		4	5	7	8	10	11	13	14	16	17	19	20
2	$E_{eff}(d_A)$	1	0.9	1	0.9642	1	0.9818	1	0.989	1	0.9926	1	0.9947
	$A_{eff}(d_E)$	1	0.9697	1	0.9818	1	0.9887	1	0.9924	1	0.9946	1	0.9959
4	$E_{eff}(d_A)$	0.8889	0.9332	0.9274	0.9412	0.9388	0.9541	0.9531	0.9625	0.962	0.9684	0.9681	0.9726
	$A_{eff}(d_E)$	0.975	0.9975	0.9919	0.9935	0.9883	0.9966	0.9931	0.9979	0.9954	0.9986	0.9968	0.999
5	$E_{eff}(d_A)$	-	0.973	1	0.9838	1	0.9884	1	0.9909	1	0.9926	1	0.9937
	$A_{eff}(d_E)$	-	0.9777	1	0.9854	1	0.9892	1	0.9914	1	0.9929	1	0.9939
7	$E_{eff}(d_A)$	-	-	0.9038	0.9545	0.9282	0.9513	0.9435	0.9515	0.9528	0.9593	0.9601	0.965
	$A_{eff}(d_E)$	-	-	0.9861	0.9993	0.9932	0.9989	0.9938	0.9987	0.9957	0.9991	0.9961	0.9994
8	$E_{eff}(d_A)$	-	-	-	0.9939	0.9649	0.9936	1	0.9946	1	0.9958	1	0.9966
	$A_{eff}(d_E)$	-	-	-	0.9943	0.9999	0.9939	1	0.9947	1	0.9959	1	0.9967
10	$E_{eff}(d_A)$	-	-	-	-	0.9231	0.9625	0.9395	0.9624	0.9497	0.9616	0.9575	0.9615
	$A_{eff}(d_E)$	-	-	-	-	0.9952	0.9998	0.9966	0.9996	0.9969	0.9996	0.9971	0.9995
11	$E_{eff}(d_A)$	-	-	-	-	-	0.9954	0.9697	0.9964	1	0.997	1	0.9974
	$A_{eff}(d_E)$	-	-	-	-	-	0.9955	$\simeq 1$	0.9965	1	0.9971	1	0.9974
13	$E_{eff}(d_A)$	-	-	-	-	-	-	0.9371	0.9696	0.9477	0.9689	0.9557	0.9689
	$A_{eff}(d_E)$	-	-	-	-	-	-	0.9964	0.9999	0.9974	0.9999	0.998	0.9998
14	$E_{eff}(d_A)$	-	-	-	-	-	-	-	0.9978	0.9745	0.9976	0.9781	0.9981
	$A_{eff}(d_E)$	-	-	-	-	-	-	-	0.9978	$\simeq 1$	0.9976	$\simeq 1$	0.9982
16	$E_{eff}(d_A)$	-	-	-	-	-	-	-	-	0.9467	0.974	0.9547	0.9739
	$A_{eff}(d_E)$	-	-	-	-	-	-	-	-	0.9981	0.9999	0.9984	0.9999
17	$E_{eff}(d_A)$	-	-	-	-	-	-	-	-	-	0.9982	0.9776	0.9984
	$A_{eff}(d_E)$	-	-	-	-	-	-	-	-	-	0.9982	$\simeq 1$	0.9984
19	$E_{eff}(d_A)$	-	-	-	-	-	-	-	-	-	-	0.954	0.9776
	$A_{eff}(d_E)$	-	-	-	-	-	-	-	-	-	-	0.9984	$\simeq 1$
20	$E_{eff}(d_A)$	-	-	-	-	-	-	-	-	-	-	-	0.9989
	$A_{eff}(d_E)$	-	-	-	-	-	-	-	-	-	-	-	0.9989

## 4.6 Conclusions

In some situations there are circumstances where the estimation of certain treatment contrasts is more important than the estimation of others. For instance, if treatment 1 is a control, then we might be interested in the difference between treatments 1 and 2, treatments 1 and 3, and maybe not as interested in the difference between treatments 2 and 3. However, when the estimation of all possible contrasts between treatments is equally

important to the researcher, one should use some optimality criteria  $\Phi$  which are invariant to permutations of the treatment set (i.e.  $\Phi(C_d) = \Phi(P'C_dP)$  for any permutation matrix  $P$ ). Also, if all contrasts are equally important and the optimality criteria are functions of the eigenvalues of  $C_d$ , then the functions should preserve the majorization ordering, as described in Definition 1.2. The  $A$  and  $E$  criteria have been used so much in literature for good reason:  $A$  guarantees minimization of the average variance of all contrast estimates, while  $E$  minimizes the largest variance among all variances of contrast estimates.

In the previous section we presented a method of comparing the  $E$ -optimal and  $A$ -optimal designs, in settings with one and two blocking factors. In the one blocking factor case, the  $A$  and  $E$  optimal designs are either the same, or very close to each other. For that reason, their efficiencies with respect to the other criterion are very close to 1. The situation is different in the two blocking factor case. In general,  $E$ -optimal row-column designs have  $A$ -efficiency that is larger than the  $E$ -efficiency of  $A$ -optimal designs. By this metric, if one is undecided about the optimality criterion to use, the  $E$ -optimal design should be chosen.

# Chapter 5

## Robustness of BIBDs to the Removal of Observations

### 5.1 Introduction

Balanced incomplete block designs are commonly used in experiments, which is not surprising, for being universally optimal they are the incomplete block design of choice whenever available. BIBDs have been extensively studied by both mathematicians and statisticians, so that much is known about their construction and existence (a good starting point to explore mathematical properties of BIBDs is Mathon and Rosa [22]). Frequently there is more than one isomorphically distinct BIBD for given  $v$ ,  $b$ , and  $k$ ; in such cases, is there some advantage to selecting one over another? To distinguish between BIBDs with the same parameters, a statistically sensible approach is to look at their robustness against missing data. In this chapter, a BIBD with  $v$  treatments having concurrence  $\lambda$ , in blocks of size  $k$ , will be denoted by  $(v, k, \lambda)$ .

A fundamental requirement for a design to be robust is that it remain connected after the removal of either a small number of plots or a small number of blocks. It was shown by Ghosh [13] that a BIBD remains connected after the removal of any  $r - 1$  observations, where  $r$  is the replication number for the original BIBD. Baksalary and Tabis [2] also showed that a BIBD remains connected after the removal of any  $r - 1$  blocks. These facts are true for all

BIBDs, and thus offer no help in choosing among nonisomorphic  $(v, k, \lambda)$  competitors.

In any case, when a small number of observations or blocks are lost, BIBDs remain connected. Another approach for judging robustness is to measure the efficiency of the residual design with respect to the original design. One such criterion of robustness, called *Criterion 2* in the literature, is the  $A$ -efficiency of the residual design given by:

$$Eff = \frac{\text{Sum of reciprocals of non-zero eigenvalues of } C_0}{\text{Sum of reciprocals of non-zero eigenvalues of } C_t}, \quad (5.1)$$

where  $C_0$  and  $C_t$  are the information matrices of the original design and the residual design respectively.

The paper by Lal et. al. [19] gives a comprehensive study on the  $A$ -efficiency of residual designs from several classes of block designs. The efficiencies are computed for the loss of all observations in one or two blocks, and also for the loss of two observations. In the following sections, their work is extended to calculating robustness values of symmetric balanced incomplete block designs (SBIBDs) to the loss of all observations in three blocks. The greater scope of this work, which has not yet appeared in the literature, is to compare nonisomorphic BIBDs and SBIBDs via robustness criteria.

For example, there are 4 nonisomorphic  $(7, 3, 2)$  designs as shown in Table A.1. It makes sense to ask whether one of them is superior to another based on some robustness measure. If we consider the loss of two blocks, there are  $\binom{b}{2}$  possible residual designs for each original design. Comparisons among nonisomorphic designs will be made based on the efficiencies of all their possible residuals. The minimum and average  $A$ -efficiency of all residuals of a design, and the minimum and average  $E$ -efficiency of all residuals of a design, will be the criteria used to distinguish among the nonisomorphic competitors. In order to compute these efficiencies, the eigenvalues of the information matrices of residual designs are needed.

The  $C$ -matrix of a residual design can be computed as follows:

$$C_t = C_0 - C_b, \quad (5.2)$$

where  $C_t, C_0$ , and  $C_b$  are the information matrices of the residual design, of the original

design, and of the blocks removed, respectively.

## 5.2 The information matrix of $t = 3$ blocks from a SBIBD

The information matrix of a SBIBD is given by:

$$C_0 = (k - 1 + \frac{1}{k}\lambda)I_v - \lambda J_v. \quad (5.3)$$

Now, suppose 3 blocks are removed from a SBIBD. Without loss of generality assume that:

- (a) treatments 1 through  $n_3$  occur 3 times in the removed blocks
- (b) treatments  $n_3 + 1$  through  $n_3 + n_2$  occur 2 times in the removed blocks
- (c) treatments  $n_3 + n_2 + 1$  through  $n_3 + n_2 + n_1$  occur 1 time in the removed blocks
- (d) treatments  $n_3 + n_2 + n_1 + 1$  through  $n_3 + n_2 + n_1 + n_0$  occur 0 times in the removed blocks

The following conditions hold for the  $n_i$ 's:

- (a)  $n_i \geq 0$
- (b)  $n_3 + n_2 + n_1 + n_0 = v$
- (c)  $3n_3 + 2n_2 + n_1 = 3k$
- (d)  $3n_3 + n_2 = 3\lambda$

The last condition follows from the fact that any two blocks in a SBIBD have  $\lambda$  treatments in common. If we set  $n_3 = q$ , from the above conditions, we have:

$$\begin{aligned}
 n_3 &= q \\
 n_2 &= 3\lambda - 3q \\
 n_1 &= 3k - 6\lambda + 3q \\
 n_0 &= v - 3k + 3\lambda - q
 \end{aligned}
 \tag{5.4}$$

Because  $n_i \geq 0$ , a necessary condition for  $q$  is:

$$\max(0, 2\lambda - k) \leq q \leq \min(\lambda, 3k - 3\lambda + v)
 \tag{5.5}$$

Depending on which  $n_i$ 's are strictly positive, there are eight possible values that the matrix  $C_b$  can take. Note that out of the 16 possibilities of choosing  $n_i = 0$  or  $n_i > 0$ , only eight can actually occur (for instance we cannot have  $n_3 = n_2 = 0$ , since that would mean that  $q = \lambda = 0$ ). Following is a list of the 8 cases that cannot take place:

Case	$n_3$	$n_2$	$n_1$	$n_0$
1	0	0	0	0
2	0	0	0	+
3	0	0	+	0
4	0	0	+	+
5	0	+	0	0
6	0	+	+	0
7	+	0	0	0
8	+	0	0	+

Note that  $n_3 = n_0 = 0$  implies  $v = 3k - 3\lambda$ , which can be rewritten as  $3k(v - k) = v(v - 1)$ . However  $3k(v - k) \leq 3\frac{v^2}{4} < v(v - 1)$  for any  $v \geq 5$  (designs with  $v = b < 5$  will not be considered since three missing blocks will cause such a design not to be connected). Also, we could not have  $n_2 = n_1 = 0$  because that would imply  $k = \lambda$ , which is not possible in a SBIBD.

For the remaining 8 cases the information matrix of the residual design, along with its eigenvalues will be computed. To compute the information matrix, the following well known

expression will be used:

$$C_b = D(\underline{r}) - \frac{1}{k} N_3 N_3', \quad (5.6)$$

where  $N_3$  is the 3-block incidence matrix, and  $D(\underline{r})$  is the diagonal matrix formed from the replication vector:

$$\underline{r} = \begin{pmatrix} 3 \cdot \mathbf{1}_{n_3} \\ 2 \cdot \mathbf{1}_{n_2} \\ \mathbf{1}_{n_1} \\ \mathbf{0}_{n_0} \end{pmatrix}$$

**Case i.**  $n_i > 0$  for all  $i$ 's. The incidence matrix  $N_3$  of the three blocks is:

$$N_3 = \begin{pmatrix} \mathbf{1}_{n_3} & \mathbf{1}_{n_3} & \mathbf{1}_{n_3} \\ \mathbf{1}_{n_2/3} & \mathbf{1}_{n_2/3} & \mathbf{0}_{n_2/3} \\ \mathbf{1}_{n_2/3} & \mathbf{0}_{n_2/3} & \mathbf{1}_{n_2/3} \\ \mathbf{0}_{n_2/3} & \mathbf{1}_{n_2/3} & \mathbf{1}_{n_2/3} \\ \mathbf{1}_{n_1/3} & \mathbf{0}_{n_1/3} & \mathbf{0}_{n_1/3} \\ \mathbf{0}_{n_1/3} & \mathbf{1}_{n_1/3} & \mathbf{0}_{n_1/3} \\ \mathbf{0}_{n_1/3} & \mathbf{0}_{n_1/3} & \mathbf{1}_{n_1/3} \\ \mathbf{0}_{n_0} & \mathbf{0}_{n_0} & \mathbf{0}_{n_0} \end{pmatrix}$$

The  $v \times v$  matrix  $N_3 N_3'$  can be partitioned in the following constant matrices (note that  $J_{m \times n}$  stands for an  $m \times n$  matrix of ones):

$$\begin{pmatrix} 3 \cdot J_{n_3 \times n_3} & 2 \cdot J_{n_3 \times \frac{n_2}{3}} & 2 \cdot J_{n_3 \times \frac{n_2}{3}} & 2 \cdot J_{n_3 \times \frac{n_2}{3}} & J_{n_3 \times \frac{n_1}{3}} & J_{n_3 \times \frac{n_1}{3}} & J_{n_3 \times \frac{n_1}{3}} & \mathbf{0}_{n_3 \times n_0} \\ 2 \cdot J_{\frac{n_2}{3} \times n_3} & 2 \cdot J_{\frac{n_2}{3} \times \frac{n_2}{3}} & J_{\frac{n_2}{3} \times \frac{n_2}{3}} & J_{\frac{n_2}{3} \times \frac{n_2}{3}} & J_{\frac{n_2}{3} \times \frac{n_1}{3}} & J_{\frac{n_2}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_2}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_2}{3} \times n_0} \\ 2 \cdot J_{\frac{n_2}{3} \times n_3} & J_{\frac{n_2}{3} \times \frac{n_2}{3}} & 2 \cdot J_{\frac{n_2}{3} \times \frac{n_2}{3}} & J_{\frac{n_2}{3} \times \frac{n_2}{3}} & J_{\frac{n_2}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_2}{3} \times \frac{n_1}{3}} & J_{\frac{n_2}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_2}{3} \times n_0} \\ 2 \cdot J_{\frac{n_2}{3} \times n_3} & J_{\frac{n_2}{3} \times \frac{n_2}{3}} & J_{\frac{n_2}{3} \times \frac{n_2}{3}} & 2 \cdot J_{\frac{n_2}{3} \times \frac{n_2}{3}} & \mathbf{0}_{\frac{n_2}{3} \times \frac{n_1}{3}} & J_{\frac{n_2}{3} \times \frac{n_1}{3}} & J_{\frac{n_2}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_2}{3} \times n_0} \\ J_{\frac{n_1}{3} \times n_3} & J_{\frac{n_1}{3} \times \frac{n_2}{3}} & J_{\frac{n_1}{3} \times \frac{n_2}{3}} & \mathbf{0}_{\frac{n_1}{3} \times \frac{n_2}{3}} & J_{\frac{n_1}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_1}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_1}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_1}{3} \times n_0} \\ J_{\frac{n_1}{3} \times n_3} & J_{\frac{n_1}{3} \times \frac{n_2}{3}} & \mathbf{0}_{\frac{n_1}{3} \times \frac{n_2}{3}} & J_{\frac{n_1}{3} \times \frac{n_2}{3}} & \mathbf{0}_{\frac{n_1}{3} \times \frac{n_1}{3}} & J_{\frac{n_1}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_1}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_1}{3} \times n_0} \\ J_{\frac{n_1}{3} \times n_3} & \mathbf{0}_{\frac{n_1}{3} \times \frac{n_2}{3}} & J_{\frac{n_1}{3} \times \frac{n_2}{3}} & J_{\frac{n_1}{3} \times \frac{n_2}{3}} & \mathbf{0}_{\frac{n_1}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_1}{3} \times \frac{n_1}{3}} & J_{\frac{n_1}{3} \times \frac{n_1}{3}} & \mathbf{0}_{\frac{n_1}{3} \times n_0} \\ \mathbf{0}_{n_0 \times n_3} & \mathbf{0}_{n_0 \times \frac{n_2}{3}} & \mathbf{0}_{n_0 \times \frac{n_2}{3}} & \mathbf{0}_{n_0 \times \frac{n_2}{3}} & \mathbf{0}_{n_0 \times \frac{n_1}{3}} & \mathbf{0}_{n_0 \times \frac{n_1}{3}} & \mathbf{0}_{n_0 \times \frac{n_1}{3}} & \mathbf{0}_{n_0 \times n_0} \end{pmatrix} \quad (5.7)$$

For the other seven cases,  $N_3 N_3'$  will be same as above, with some rows and columns deleted. For instance, if  $n_2 = 0$ , rows and column partitions 2, 3, and 4 are deleted from the partitioned matrix  $N_3 N_3'$  of (5.7). Using equation (5.6), the information matrix of  $S_3$  can be found.

**Case ii.**  $n_3 = 0$ ,  $n_i > 0$  for  $i < 3$ . Delete first row and column of  $N_3N_3'$  from (5.7).

**Case iii.**  $n_3 = n_1 = 0$ ,  $n_2 > 0$  and  $n_0 > 0$ . This can occur in SBIBDS with  $k = 2\lambda$ . Delete rows and columns 1, 5, 6, and 7 of  $N_3N_3'$  from (5.7).

**Case iv.**  $n_2 = 0$ ,  $n_i > 0$  for  $i \neq 2$ . Delete rows and columns 2, 3, and 4 of  $N_3N_3'$  from (5.7).

**Case v.**  $n_2 = n_0 = 0$ ,  $n_3 > 0$  and  $n_1 > 0$ . This can occur in SBIBDS with  $v = 3k - 2\lambda$ . Delete rows and columns 2, 3, 4, and 8 of  $N_3N_3'$  from (5.7).

**Case vi.**  $n_1 = 0$ ,  $n_i > 0$  for  $i \neq 1$ . Delete rows and columns 5, 6, and 7 of  $N_3N_3'$  from (5.7).

**Case vii.**  $n_1 = n_0 = 0$ ,  $n_i > 0$  for  $i > 1$ . This can occur in SBIBDS with  $v = 2k - \lambda$ . Delete rows and columns 5, 6, 7, and 8 of  $N_3N_3'$  from (5.7).

**Case viii.**  $n_0 = 0$ ,  $n_i > 0$  for  $i \neq 0$ . Delete last row and column of  $N_3N_3'$  from (5.7).

### 5.3 Eigenvalues of the information matrices of residual designs

In this section, the eigenvalues of a residual design formed by removing 3 blocks from a SBIBD are computed. Also, the eigenvalues of a residual design formed by removing 2 blocks from a BIBD are given. These were computed by Bhaumik and Whittinghill III in [3]. These eigenvalues are needed for computing the efficiency of a residual design. It will be shown that they are functions of the original design parameters  $(v, k, \lambda)$ , and  $q$ , which is the number of treatments in the intersection of the 3 removed blocks from a SBIBD, or the 2 removed blocks from a BIBD.

**Definition 5.1.** A symmetric matrix  $X$  will be called a generalized block-diagonal matrix

if it can be partitioned as follows:

$$\begin{pmatrix} A_{n_1 \times n_1} & c_{12} J_{n_1 \times n_2} & \cdots & c_{1p} J_{n_1 \times n_p} \\ c_{21} J_{n_2 \times n_1} & A_{n_2 \times n_2} & \cdots & c_{2p} J_{n_2 \times n_p} \\ \dots & \dots & \dots & \dots \\ c_{p1} J_{n_p \times n_1} & c_{p2} J_{n_p \times n_2} & \cdots & A_{n_p \times n_p} \end{pmatrix},$$

where all matrices  $A_{n_i \times n_i}$  are completely symmetric matrices (i.e. constant on the diagonal, and constant off the diagonal).

The following two lemmas are needed to compute the eigenvalues of a generalized block-diagonal matrix.

**Lemma 5.1.** *Let  $A$  be a completely symmetric matrix which can be written as:*

$$A = xI_n + yJ_n$$

*Then the eigenvalues of  $A$  are  $x$  with multiplicity  $n - 1$  and  $x + ny$  with multiplicity 1.*

The proof of this lemma requires checking the following identities:

- (a)  $A \cdot \mathbf{c}_{ni} = x\mathbf{c}_{ni}$
- (b)  $A \cdot \mathbf{1}_n = (x + ny)\mathbf{1}_n$

where the  $\mathbf{c}_{ni}$ 's are a complete set of orthonormal contrasts. This also gives the spectral decomposition of a completely symmetric matrix  $A$ :

$$A = x \sum \mathbf{c}_{ni} \mathbf{c}'_{ni} + \left(\frac{x}{n} + y\right) J_n$$

**Lemma 5.2.** *Let  $X$  be a generalized block-diagonal matrix as given in Definition 5.1. Also let matrices  $A_{n_i \times n_i}$  have eigenvalues  $\theta_i$  with multiplicity  $n_i - 1$  and  $a_i$  with multiplicity 1. Then the eigenvalues of  $X$  are  $\theta_i$  with multiplicity  $n_i - 1$ , and the right eigenvalues of the (not necessarily symmetric) matrix:*

$$X_r = \begin{pmatrix} a_1 & c_{12} \cdot n_2 & \cdots & c_{1p} \cdot n_p \\ c_{21} \cdot n_1 & a_2 & \cdots & c_{2p} \cdot n_p \\ \dots & \dots & \dots & \dots \\ c_{p1} \cdot n_1 & c_{p2} \cdot n_2 & \cdots & a_p \end{pmatrix}$$

The eigenvectors corresponding to eigenvalues  $\theta_i$  are of the form  $(\mathbf{0}_f, \mathbf{c}'_{n_i}, \mathbf{0}_g)'$ , where the  $\mathbf{c}_{n_i}$ 's are a set of  $n_i - 1$  orthonormal contrasts,  $f = \sum_{j < i} n_j$  and  $g = \sum_{j > i} n_j$ . Now, let  $z = (z_1, z_2, \dots, z_p)'$  be an eigenvector of  $X_r$  corresponding to an eigenvalue  $\gamma$ . Then  $\gamma$  is also an eigenvalue of  $X$ , with the eigenvector  $z = (z_1 \cdot \mathbf{1}_{n_1}, z_2 \cdot \mathbf{1}_{n_2}, \dots, z_p \cdot \mathbf{1}_{n_p})'$ .

From (5.3) and (5.6), the information matrix of the residual design of a SBIBD when three blocks are removed is:

$$C_t = (k - 1 + \frac{\lambda}{k})I_v - D(\underline{r}) - \frac{\lambda}{k}J_v + \frac{1}{k}N_3N_3' \quad (5.8)$$

Note that  $C_t$  is of rank  $v - 1$ , since the residual design is connected. Also,  $C_t$  is a generalized block-diagonal matrix with number of partitions  $p \leq 8$ , depending on the structure of  $N_3N_3'$ . Thus, Lemma 5.2 can be used to find the eigenvalues of  $C_t$ . Using the notation of Definition 5.1, the matrix  $C_t$  has the following sub-matrices on the diagonal when  $n_i > 0$  for all  $i \geq 0$ :

$$\begin{aligned} A_1 &= (k - 4 + \frac{\lambda}{k})I_{n_3} + \frac{3 - \lambda}{k}J_{n_3} \\ a_1 &= k - 4 + 3\frac{n_3}{k} - (n_3 - 1)\frac{\lambda}{k} \\ A_2 &= A_3 = A_4 = (k - 3 + \frac{\lambda}{k})I_{n_2/3} + \frac{2 - \lambda}{k}J_{n_2/3} \\ a_2 &= a_3 = a_4 = k - 3 + 2\frac{n_2}{3k} - (n_2/3 - 1)\frac{\lambda}{k} \\ A_5 &= A_6 = A_7 = (k - 2 + \frac{\lambda}{k})I_{n_1/3} + \frac{1 - \lambda}{k}J_{n_1/3} \\ a_5 &= a_6 = a_7 = k - 2 + \frac{n_1}{3k} - (n_1/3 - 1)\frac{\lambda}{k} \\ A_8 &= (k - 1 + \frac{\lambda}{k})I_{n_0} + \frac{-\lambda}{k}J_{n_0} \\ a_8 &= k - 1 - (n_0 - 1)\frac{\lambda}{k} \end{aligned} \quad (5.9)$$

The eigenvalues of  $C_t$  originating from the matrices given above are:  $\frac{v\lambda}{k} - 3$ ,  $\frac{v\lambda}{k} - 2$ ,  $\frac{v\lambda}{k} - 1$ , and  $\frac{v\lambda}{k}$  with multiplicities  $n_3 - 1$ ,  $n_2 - 3$ ,  $n_1 - 3$ , and  $n_0 - 1$  respectively. Note that some of these eigenvalues do not appear in cases ii. through viii. The other eigenvalues of  $C_t$  are

computed from the matrix  $X_r$  (see Lemma 5.2) given below:

$$\frac{1}{k} \begin{pmatrix} k \cdot a_1 & (2 - \lambda) \frac{n_2}{3} & (2 - \lambda) \frac{n_2}{3} & (2 - \lambda) \frac{n_2}{3} & (1 - \lambda) \frac{n_1}{3} & (1 - \lambda) \frac{n_1}{3} & (1 - \lambda) \frac{n_1}{3} & -\lambda n_0 \\ (2 - \lambda) n_3 & k \cdot a_2 & (1 - \lambda) \frac{n_2}{3} & (1 - \lambda) \frac{n_2}{3} & (1 - \lambda) \frac{n_1}{3} & (1 - \lambda) \frac{n_1}{3} & -\lambda \frac{n_1}{3} & -\lambda n_0 \\ (2 - \lambda) n_3 & (1 - \lambda) \frac{n_2}{3} & k \cdot a_3 & (1 - \lambda) \frac{n_2}{3} & (1 - \lambda) \frac{n_1}{3} & -\lambda \frac{n_1}{3} & (1 - \lambda) \frac{n_1}{3} & -\lambda n_0 \\ (2 - \lambda) n_3 & (1 - \lambda) \frac{n_2}{3} & (1 - \lambda) \frac{n_2}{3} & k \cdot a_4 & -\lambda \frac{n_1}{3} & (1 - \lambda) \frac{n_1}{3} & (1 - \lambda) \frac{n_1}{3} & -\lambda n_0 \\ (1 - \lambda) n_3 & (1 - \lambda) \frac{n_2}{3} & (1 - \lambda) \frac{n_2}{3} & -\lambda \frac{n_2}{3} & k \cdot a_5 & -\lambda \frac{n_1}{3} & -\lambda \frac{n_1}{3} & -\lambda n_0 \\ (1 - \lambda) n_3 & (1 - \lambda) \frac{n_2}{3} & -\lambda \frac{n_2}{3} & (1 - \lambda) \frac{n_2}{3} & -\lambda \frac{n_1}{3} & k \cdot a_6 & -\lambda \frac{n_1}{3} & -\lambda n_0 \\ (1 - \lambda) n_3 & -\lambda \frac{n_2}{3} & (1 - \lambda) \frac{n_2}{3} & (1 - \lambda) \frac{n_2}{3} & -\lambda \frac{n_1}{3} & -\lambda \frac{n_1}{3} & k \cdot a_7 & -\lambda n_0 \\ -\lambda n_3 & -\lambda \frac{n_2}{3} & -\lambda \frac{n_2}{3} & -\lambda \frac{n_2}{3} & -\lambda \frac{n_1}{3} & -\lambda \frac{n_1}{3} & -\lambda \frac{n_1}{3} & k \cdot a_8 \end{pmatrix}$$

Next, we give the  $v - 1$  non-zero eigenvalues of  $C_t$  in terms of  $q$ ,  $v$ ,  $\lambda$ , and  $k$  for the eight cases described in the previous section. Note that some rows and columns of  $X_r$  are deleted for cases ii. through viii. before computing its eigenvalues. Remember that  $q$  denotes the number of treatments that occur in all 3 blocks removed.

**Case i.**  $q \notin \{0, \lambda, 2\lambda - k, v - 3k + 3\lambda\}$

Eigenvalues	With Multiplicity
$\frac{v\lambda}{k} - 3$	$q - 1$
$\frac{v\lambda}{k} - 2$	$3\lambda - 3q - 3$
$\frac{v\lambda}{k} - 1$	$3k - 6\lambda + 3q - 3$
$\frac{v\lambda}{k}$	$v - 3k + 3\lambda - q$
$\frac{v\lambda}{k} - 2 - \frac{k-2\lambda+\sqrt{(k+2\lambda)^2-8kq}}{2k}$	1
$\frac{v\lambda}{k} - 2 - \frac{k-2\lambda-\sqrt{(k+2\lambda)^2-8kq}}{2k}$	1
$\frac{v\lambda}{k} - 1 - \frac{\lambda+\sqrt{(2k-\lambda)^2-4k(\lambda-q)}}{2k}$	2
$\frac{v\lambda}{k} - 1 - \frac{\lambda-\sqrt{(2k-\lambda)^2-4k(\lambda-q)}}{2k}$	2

**Case ii.**  $q = 0, k \neq 2\lambda$

Eigenvalues	With Multiplicity
$\frac{v\lambda}{k} - 2$	$3\lambda - 3$
$\frac{v\lambda}{k} - 1$	$3k - 6\lambda - 3$
$\frac{v\lambda}{k}$	$v - 3k + 3\lambda$
$\frac{v\lambda}{k} - 2 + \frac{2\lambda}{k}$	1
$\frac{v\lambda}{k} - 1 - \frac{\lambda+\sqrt{(2k-\lambda)^2-4k\lambda}}{2k}$	2
$\frac{v\lambda}{k} - 1 - \frac{\lambda-\sqrt{(2k-\lambda)^2-4k\lambda}}{2k}$	2

**Case iii.**  $q = 0, k = 2\lambda$

Eigenvalues	With Multiplicity
$\frac{v-4}{2}$	$3\lambda - 3$
$\frac{v-3}{2}$	2
$\frac{v}{2}$	$v - 3\lambda$

**Case iv.**  $q = \lambda, v \neq 3k - 2\lambda$

Eigenvalues	With Multiplicity
$\frac{v\lambda}{k} - 3$	$\lambda - 1$
$\frac{v\lambda}{k} - 3 + \frac{2\lambda}{k}$	1
$\frac{v\lambda}{k} - 1$	$3k - 3\lambda - 3$
$\frac{v\lambda}{k} - \frac{\lambda}{k}$	2
$\frac{v\lambda}{k}$	$v - 3k + 2\lambda$

**Case v.**  $q = \lambda$ ,  $v = 3k - 2\lambda$

Eigenvalues	With Multiplicity
$\frac{v\lambda}{k} - 3$	$\lambda - 1$
$\frac{v\lambda}{k} - 3 + \frac{2\lambda}{k}$	1
$\frac{v\lambda}{k} - 1$	$v - \lambda - 3$
$\frac{v\lambda}{k} - \frac{\lambda}{k}$	2

**Case vi.**  $q = 2\lambda - k > 0$ ,  $v \neq 2k - \lambda$

Eigenvalues	With Multiplicity
$\frac{v\lambda}{k} - 3$	$2\lambda - k - 1$
$\frac{v\lambda}{k} - 4 + \frac{2\lambda}{k}$	1
$\frac{v\lambda}{k} - 2$	$3k - 3\lambda - 3$
$\frac{v\lambda}{k} - 1 - \frac{\lambda}{k}$	2
$\frac{v\lambda}{k}$	$v - 2k + \lambda$

**Case vii.**  $q = 2\lambda - k > 0$ ,  $v = 2k - \lambda$

Eigenvalues	With Multiplicity
$\frac{v\lambda}{k} - 3$	$2\lambda - k - 1$
$\frac{v\lambda}{k} - 4 + \frac{2\lambda}{k}$	1
$\frac{v\lambda}{k} - 2$	$3k - 3\lambda - 3$
$\frac{v\lambda}{k} - 1 - \frac{\lambda}{k}$	2

**Case viii.**  $0 < q = v - 3k + 3\lambda < \lambda$ ,  $v \neq 2k - \lambda$

Eigenvalues	With Multiplicity
$\frac{v\lambda}{k} - 3$	$v - 3k + 3\lambda - 1$
$\frac{v\lambda}{k} - 2$	$9k - 3v - 6\lambda - 3$
$\frac{v\lambda}{k} - 1$	$3v - 6k + 3\lambda - 3$
$\frac{v\lambda}{k} - 2 - \frac{k-2\lambda+\sqrt{(5k-2\lambda)^2-8kv}}{2k}$	1
$\frac{v\lambda}{k} - 2 - \frac{k-2\lambda-\sqrt{(5k-2\lambda)^2-8kv}}{2k}$	1
$\frac{v\lambda}{k} - 1 - \frac{\lambda+\sqrt{-8k^2+4kv+4k\lambda+\lambda^2}}{2k}$	2
$\frac{v\lambda}{k} - 1 - \frac{\lambda-\sqrt{-8k^2+4kv+4k\lambda+\lambda^2}}{2k}$	2

Note that the trace of  $C_t$  is  $v\lambda(v-1)/k - 3(k-1)$ , and it does not depend on  $q$ . Next, we present the eigenvalues of a residual design formed by removing 2 blocks from a BIBD. Here,  $q$  denotes the number of treatments in common in the 2 blocks. Obviously,  $0 \leq q \leq k$ .

**Case i.**  $q = 0$

Eigenvalues	With Multiplicity
$\frac{v\lambda}{k}$	$v - 2k + 1$
$\frac{v\lambda}{k} - 1$	$2(k - 1)$

**Case ii.**  $0 < q < k$

Eigenvalues	With Multiplicity
$\frac{v\lambda}{k}$	$v - 2k + q$
$\frac{v\lambda}{k} - \frac{q}{k}$	1
$\frac{v\lambda}{k} - 1$	$2(k - q - 1)$
$\frac{v\lambda}{k} - 2 + \frac{q}{k}$	1
$\frac{v\lambda}{k} - 2$	$q - 1$

**Case iii.**  $q = k$

Eigenvalues	With Multiplicity
$\frac{v\lambda}{k}$	$v - k$
$\frac{v\lambda}{k} - 2$	$k - 1$

Again, note that the trace of  $C_t$  is  $v\lambda(v - 1)/k - 2(k - 1)$ , and it does not depend on  $q$ .

## 5.4 Comparison of nonisomorphic designs

Now, we have the tools needed for computing the efficiencies of different residual designs. However, finding all nonisomorphic designs for a given set of parameters  $(v, k, \lambda)$  is quite a difficult task in many cases. Using a new package in GAP (see [29]), developed by Leonard H. Suicher [30], one can perform an exhaustive computer search for these designs. Unfortunately, the job may take days even for a relatively small design. An additional obstacle is the fact that for some parameter sets, the number of nonisomorphic designs is extremely large. For instance, it is known that there are more than  $1.25 \times 10^8$  nonisomorphic  $(9, 4, 6)$  designs. A good reference containing parameter sets of BIBDs, as well as the number of nonisomorphic designs for each parameter set is Table 1.28 in [10].

The eigenvalues of a BIBD are  $v\lambda/k$  with multiplicity  $v - 1$ , and 0 with multiplicity 1. The  $v - 1$  non-zero eigenvalues of residual designs for connected BIBDs with 2 blocks removed, and connected SBIBDs with 3 blocks removed are  $z_1, z_2, \dots, z_{v-1}$ , as given in the previous section. Using these eigenvalues, the following efficiencies of a residual design can be computed:

$$A - efficiency = \frac{\frac{k(v-1)}{v\lambda}}{\sum_{i=1}^{v-1} \frac{1}{z_i}} \quad (5.10)$$

$$E - efficiency = \frac{k \min(z_i)}{v\lambda} \quad (5.11)$$

For each nonisomorphic design, the average and minimum  $A$ - and  $E$ - efficiencies of all its residual designs are reported. When  $t$  blocks are removed from a design there are  $\binom{b}{t}$  possible residuals.

The third criterion which will be computed is the average and minimum  $MV$ - efficiency. This criterion minimizes the maximum variance of pair-wise treatment differences.

**Definition 5.2.** A design  $d^* \in D$  is  $MV$ -optimal in the class  $D$  if  $\max_{d^*} [Var(\hat{\tau}_i - \hat{\tau}_j)] \leq \max_d [Var(\hat{\tau}_i - \hat{\tau}_j)]$  for any design  $d \in D$ .

The maximum variance of pair-wise treatment differences for a BIBD is  $\frac{2k}{v\lambda}\sigma^2$ . For each possible residual design  $d$  of a BIBD, the  $MV$ -efficiency can be computed as:

$$MV - efficiency = \frac{2k/v\lambda}{\max[c_{ii}^+ + c_{jj}^+ - 2c_{ij}^+]}, \quad (5.12)$$

where the  $c_{ij}^+$ 's are elements of  $C_t^+$ , and  $C_t^+$  is any generalized inverse of  $C_t$ .

### 5.4.1 A generalized inverse of $C_2$

$C_2$  is the information matrix of a BIBD with two blocks removed, and the two blocks' intersection number is  $q$ . When  $0 < q < k$ ,  $C_2$  has the following form:

$$C_2 = \begin{pmatrix} A_1 & \frac{1}{k}J_{q \times (k-q)} & \frac{1}{k}J_{q \times (k-q)} & 0_{q \times (v-2k+q)} \\ \frac{1}{k}J_{(k-q) \times q} & A_2 & 0_{(k-q) \times k-q} & 0_{(k-q) \times (v-2k+q)} \\ \frac{1}{k}J_{(k-q) \times q} & 0_{(k-q) \times (k-q)} & A_3 & 0_{(k-q) \times (v-2k+q)} \\ 0_{(v-2k+q) \times q} & 0_{(v-2k+q) \times (k-q)} & 0_{(v-2k+q) \times (k-q)} & A_4 \end{pmatrix} - \frac{\lambda}{k}J_{v \times v}, \quad (5.13)$$

where  $A_i$  are the nonsingular completely symmetric matrices given below.

$$A_1 = \left(\frac{v\lambda}{k} - 2\right)I_q + \frac{2}{k}J_q \quad (5.14)$$

$$A_2 = A_3 = \left(\frac{v\lambda}{k} - 1\right)I_{(k-q)} + \frac{1}{k}J_{(k-q)} \quad (5.15)$$

$$A_4 = \frac{v\lambda}{k}I_{(v-2k+q)} \quad (5.16)$$

In order to better compare two residuals obtained by removing two blocks from a BIBD, a generalized inverse of  $C_2$  will be found. The following results are needed for this.

**Lemma 5.3.** *Let  $A_{v \times v}$  be a matrix with  $\mathbf{1}_v$  as an eigenvector and corresponding eigenvalue  $\alpha$ .*

(a) *If  $A$  is nonsingular then  $(A - xJ_v)^{-1} = A^{-1} + \frac{x}{\alpha(\alpha-xv)}J_v$ , for any  $x \neq \frac{\alpha}{v}$*

(b) *If  $\alpha = 0$  and  $A$  is of rank  $v - 1$ , then  $(A - xJ_v)^{-1}$  is a generalized of  $A$ , for any  $x \neq 0$ .*

The proof is straightforward, using the spectral decomposition of  $A$ .

**Lemma 5.4.** *Let  $A_{v \times v} = xI_v + yJ_v$  be a nonsingular completely symmetric matrix. Then  $A^{-1} = \frac{1}{x}I_v - \frac{y}{x(x+yv)}J_v$ .*

Simple algebra gives the above result. Now let

$$T_4 = C_2 + \frac{\lambda}{k}J_{v \times v}. \quad (5.17)$$

The matrix  $T_4$  is nonsingular, and  $T_4^{-1}$  is a generalized inverse of  $C_2$ . Let

$$B_3 = \begin{pmatrix} A_1 & \frac{1}{k}J_{q \times (k-q)} & \frac{1}{k}J_{q \times (k-q)} \\ \frac{1}{k}J_{(k-q) \times q} & A_2 & 0_{(k-q) \times (k-q)} \\ \frac{1}{k}J_{(k-q) \times q} & 0_{(k-q) \times (k-q)} & A_3 \end{pmatrix}, \quad (5.18)$$

$$T_3 = B_3 - \frac{1}{k}J_{(2k-q) \times (2k-q)}. \quad (5.19)$$

$T_3$  has  $\mathbf{1}_{(2k-q)}$  as an eigenvector with corresponding eigenvalue  $\alpha_3 = \frac{v\lambda-2k+q}{k}$ . Now let

$$B_2 = \begin{pmatrix} A_2 - \frac{1}{k}J_{(k-q) \times (k-q)} & -\frac{1}{k}J_{(k-q) \times (k-q)} \\ -\frac{1}{k}J_{(k-q) \times (k-q)} & A_3 - \frac{1}{k}J_{(k-q) \times (k-q)} \end{pmatrix}, \quad (5.20)$$

$$T_2 = B_2 + \frac{1}{k} J_{(2k-2q) \times (2k-2q)}. \quad (5.21)$$

$T_2$  has  $\mathbf{1}_{(2k-2q)}$  as an eigenvector with corresponding eigenvalue  $\alpha_2 = \frac{v\lambda-q}{k}$ . Thus, by Lemma 5.3:

$$T_2^{-1} = \begin{pmatrix} A_2^{-1} & 0 \\ 0 & A_3^{-1} \end{pmatrix}, \quad (5.22)$$

$$B_2^{-1} = T_2^{-1} + \frac{k}{(v\lambda - 2k + q)(v\lambda - q)} J_{(2k-2q)}. \quad (5.23)$$

Repeating the process:

$$T_3^{-1} = \begin{pmatrix} (A_1 - \frac{1}{k} J_q)^{-1} & 0 \\ 0 & B_2^{-1} \end{pmatrix}, \quad (5.24)$$

$$B_3^{-1} = T_3^{-1} - \frac{k}{(v\lambda - 2k + q)v\lambda} J_{(2k-q)}. \quad (5.25)$$

Finally,

$$T_4^{-1} = \begin{pmatrix} B_3^{-1} & 0 \\ 0 & A_4^{-1} \end{pmatrix}. \quad (5.26)$$

Plugging in the inverses of the completely symmetric matrices  $A_1 - \frac{1}{k} J_q$ ,  $A_2$ , and  $A_3$ , we get:

$$B_3^{-1} = \begin{pmatrix} \frac{k}{v\lambda-2k} I_q - \frac{2k(v\lambda-k)}{v\lambda(v\lambda-2k)(v\lambda-2k+q)} J_q & \frac{-k}{v\lambda(v\lambda-2k+q)} J_{q \times (k-q)} & \frac{-k}{v\lambda(v\lambda-2k+q)} J_{q \times (k-q)} \\ \frac{-k}{v\lambda(v\lambda-2k+q)} J_{(k-q) \times q} & M_{(k-q) \times (k-q)} & \frac{kq}{v\lambda(v\lambda-q)(v\lambda-2k+q)} J_{(k-q)} \\ \frac{-k}{v\lambda(v\lambda-2k+q)} J_{(k-q) \times q} & \frac{kq}{v\lambda(v\lambda-q)(v\lambda-2k+q)} J_{(k-q)} & M_{(k-q) \times (k-q)} \end{pmatrix}, \quad (5.27)$$

where  $M_{(k-q) \times (k-q)} = \frac{k}{v\lambda-k} I_{(k-q)} - \frac{k[v^2\lambda^2 - k(2v\lambda-q)]}{v\lambda(v\lambda-k)(v\lambda-q)(v\lambda-2k+q)} J_{(k-q)}$ . Adding the fact that  $A_4^{-1} = \frac{k}{v\lambda} I_{(v-2k+q)}$ , we have a generalized inverse of  $C_2$  given in (5.26). The variance of a pairwise treatment comparison is

$$Var[\hat{\tau}_i - \hat{\tau}_j] / \sigma^2 = T_{4_{ii}} + T_{4_{jj}} - 2T_{4_{ij}}, \quad (5.28)$$

and is displayed in Table 5.1. The variances in Table 5.1 also apply for  $q = 0$  and  $q = k$ , but some of the cases cannot occur in these situations.

## 5.4.2 Robustness of BIBDs to the removal of two blocks

First, note that when one block is removed from a BIBD, all the information matrices of residual designs are the same up to row and column permutation. Thus, if we want to

Table 5.1: Variance of pairwise treatment contrasts when two blocks are removed from a BIBD

Case	$Var[\hat{\tau}_i - \hat{\tau}_j]/\sigma^2$
$i$ and $j$ occur in both blocks	$V_1 = \frac{2k}{v\lambda - 2k}$
$i$ occurs in both blocks, $j$ occurs in one block	$V_2$
$i$ and $j$ both occur once, in the same block	$V_3 = \frac{2k}{v\lambda - k}$
$i$ occurs in both blocks, $j$ does not occur in either block	$V_4$
$i$ and $j$ both occur once, in different blocks	$V_5 = \frac{2k(v\lambda - q - 1)}{(v\lambda - k)(v\lambda - q)}$
$i$ occurs in one block, $j$ does not occur in either block	$V_6$
$i$ and $j$ do not occur in the removed blocks	$V_7 = \frac{2k}{v\lambda}$

$$\begin{aligned}
 V_2 &= \frac{k(q-1)}{q(v\lambda - 2k)} + \frac{k(k-q-1)}{(k-q)(v\lambda - k)} + \frac{k}{2(k-q)(v\lambda - q)} + \frac{k(2k-q)}{2q(k-q)(v\lambda - 2k+q)} \\
 V_4 &= \frac{k(2k-q+1)}{v\lambda(2k-q)} + \frac{k(q-1)}{q(v\lambda - 2k)} + \frac{2k(k-q)}{q(2k-q)(v\lambda - 2k+q)} \\
 V_6 &= \frac{k(2k-q+1)}{v\lambda(2k-q)} + \frac{k(k-q-1)}{(k-q)(v\lambda - k)} + \frac{k}{2(k-q)(v\lambda - q)} + \frac{kq}{2(k-q)(2k-q)(v\lambda - 2k+q)}
 \end{aligned}$$

distinguish between two nonisomorphic designs, the robustness against the loss of two blocks must be studied. Further, as discussed in a previous section, the information matrix  $C_2$  of a residual design depends only on  $q$ , the intersection number of the two removed blocks. Since for a SBIBD  $q$  is the constant  $\lambda$  not depending on the pair of blocks removed, robustness of designs against loss of two blocks will not discriminate amongst SBIBDs.

This section presents comparisons of nonisomorphic designs for several parameter sets of non-symmetric BIBDs. Besides the average and minimum efficiencies of the residual designs, the block intersection numbers for each design, labelled  $q$  in the previous section, are also presented. For each  $q$ , the number of pairs of blocks that intersect in  $q$  treatments are given. Note that  $0 \leq q \leq k$ . An ordering of BIBDs will be developed based on this vector of intersection numbers.

Let  $\mathcal{D}(v, k, \lambda)$  be a class of BIBDs with the specified parameters. For every  $d \in \mathcal{D}$ , we have  $\mathcal{R}(d, 2)$ , the set of  $\binom{b}{2}$  designs derived from  $d$  by removing two blocks (see [3]). We are interested in comparing the minimum  $\Phi$ -efficiency of residuals designs of  $d_i$

$$\min_{d \in \mathcal{R}(d_i, 2)} \left[ \frac{\Phi(d_i)}{\Phi(d)} \right],$$

and the average  $\Phi$ -efficiency of residuals designs of  $d_i$

$$\sum_{d \in \mathcal{R}(d_i, 2)} \left[ \frac{\Phi(d_i)}{\Phi(d)} \right],$$

where  $d_i \in \mathcal{D}(v, k, \lambda)$ , and  $\Phi$  is some optimality criterion.

Table 5.2: Comparison of  $(7, 3, 2)$  designs robustness against loss of 2 blocks

Design no.	Int. numbers				A-efficiency		E-efficiency		MV-efficiency	
	0	1	2	3	average	min	average	min	average	min
1	0	84	0	7	0.833134	0.8	0.637363	0.571429	0.69172	0.571429
2	4	72	12	3	0.833073	0.8	0.637363	0.571429	0.683955	0.571429
3	6	66	18	1	0.833042	0.8	0.637363	0.571429	0.680072	0.571429
4	7	63	21	0	0.833027	0.820046	0.637363	0.571429	0.678131	0.571429

Table 5.3: Worst case scenarios of  $(7, 3, 2)$  designs robustness against loss of 2 blocks

Maximum q	Impact of MIA design			
	Designs	A-impact	E-impact	MV-impact
2	4 (MIA)	-	-	-
3	1-3	0.933333	0.8	0.816667

**Example 5.1.** Consider the BIBD with parameters  $v = 7$ ,  $k = 3$ ,  $\lambda = 2$ , and thus  $b = 14$ . The four nonisomorphic BIBDs with these parameters are given in Table A.1.

Efficiencies of the four nonisomorphic designs are displayed in Table 5.2. First note that design 2 is uniformly better than design 3, the only differences between them occurring in the average  $A$ -efficiency and average  $MV$ -efficiency of their residuals. Design 1 is better than the rest if we are interested in minimizing the average variance of pair-wise treatment differences (see average  $A$ -efficiency), while design 4 is best if we want to guard against worst case scenarios (see minimum  $A$ -efficiency). The design that maximizes average  $A$  and  $MV$  efficiency (design 1 here), does not do very well in worst case scenarios. This will be a feature

in future examples as well; also, designs that perform best in worst case scenarios (such as design 4 here), do not have high average efficiencies. The following result by Bhaumik and Whittinghill [3] will give some clarification on this phenomenon.

Let  $C_2(q)$  denote the information matrix of a design obtained by removing 2 blocks with intersection number  $q$  from a BIBD. Also, let  $\mu\{C_2(q)\}$  denote the vector of eigenvalues of the matrix  $C_2(q)$ .

**Theorem 5.1** (Bhaumik and Whittinghill 1991). *The vectors of eigenvalues of residual designs obtained by removing 2 blocks from a BIBD satisfy:*

$$\mu\{C_2(0)\} \prec \mu\{C_2(1)\} \prec \cdots \prec \mu\{C_2(k)\}, \quad (5.29)$$

and thus

$$\Phi\{C_2(0)\} \leq \Phi\{C_2(1)\} \leq \cdots \leq \Phi\{C_2(k)\}, \quad (5.30)$$

for any majorization criterion  $\Phi$ .

For the  $A$ - and  $D$ - optimality criteria  $\Phi_A$  and  $\Phi_D$  respectively, we have  $\Phi_A\{C_2(0)\} < \Phi_A\{C_2(1)\} < \cdots < \Phi_A\{C_2(k)\}$ , and  $\Phi_D\{C_2(0)\} < \Phi_D\{C_2(1)\} < \cdots < \Phi_D\{C_2(k)\}$ .

The above result orders the residual designs of a BIBD based on the intersection numbers of the removed blocks. This explains why design 4 in Example 5.1 maximizes the minimum  $A$ -efficiency. Note that design 4 does not contain any identical blocks, and thus its minimum  $A$ -efficiency is  $\frac{\Phi_A\{C_0\}}{\Phi_A\{C_2(3)\}}$ , while for the other designs the minimum  $A$ -efficiency is  $\frac{\Phi_A\{C_0\}}{\Phi_A\{C_2(4)\}}$ .

Building on the previous theorem, we present a way to differentiate between designs, without having to compute efficiencies of majorization criteria. Let  $\eta = [\eta_0(d), \eta_1(d), \dots, \eta_k(d)]'$  denote the  $k + 1 \times 1$  vector of intersection numbers of a BIBD  $d$ , where  $\eta_j$  gives the number of pairs of blocks whose intersection number is  $j$ . For instance, in  $d_1$  of example 5.1, 84 of the 91 pairs of blocks intersect in one treatment, while the other seven pairs each intersect in 3 treatments, so  $\eta(d_1) = [0, 84, 0, 7]'$ . We define the following aberration criterion, based on  $\eta(d)$ .

**Definition 5.3.** Let  $d_1$  and  $d_2$  be two balanced incomplete block designs, and  $t$  be the largest integer such that  $\eta_t(d_1) \neq \eta_t(d_2)$ . Then design  $d_1$  is said to have *less intersection aberration* than  $d_2$  if  $\eta_t(d_1) < \eta_t(d_2)$ . A design  $d \in \mathcal{D}(v, k, \lambda)$  has *minimum intersection aberration* (MIA), if no other design in  $\mathcal{D}(v, k, \lambda)$  has less intersection aberration than  $d$ .

The next result follows immediately from Theorem 5.1.

**Theorem 5.2.** *Let  $d_1$  and  $d_2$  be two nonisomorphic BIBDs with the same parameters. If  $d_1$  has less intersection aberration than  $d_2$  then*

$$\min_{d \in \mathcal{R}(d_1, 2)} \left[ \frac{\Phi(d_1)}{\Phi(d)} \right] \geq \min_{d \in \mathcal{R}(d_2, 2)} \left[ \frac{\Phi(d_2)}{\Phi(d)} \right],$$

for any majorization criterion  $\Phi$ .

Table 5.4: Comparison of (8, 4, 3) designs for robustness against loss of 2 blocks

Design no.	Int. numbers					A-efficiency		E-efficiency		MV-efficiency	
	0	1	2	3	4	average	min	average	min	average	min
1	3	12	72	4	0	0.841905	0.832737	0.677656	0.666667	0.684874	0.666667
2	1	18	66	6	0	0.841908	0.832737	0.67674	0.666667	0.687568	0.666667
3	0	21	63	7	0	0.84191	0.832737	0.676282	0.666667	0.688915	0.666667
4	7	0	84	0	0	0.841897	0.840917	0.679487	0.666667	0.679487	0.666667

Table 5.5: Worst case scenarios of (8, 4, 3) designs for robustness against loss of 2 blocks

Maximum q	Impact of MIA design			
	Designs	A-impact	E-impact	MV-impact
2	4 (MIA)	1.0	1.0	1.0
3	1-3	0.983332	0.888889	0.874242

**Example 5.2.** Consider the BIBD with parameters  $v = 8$ ,  $k = 4$ ,  $\lambda = 3$ , and thus  $b = 14$ . The four nonisomorphic BIBDs with these parameters are given in Table A.2, and a comparison of their robustness against the loss of two blocks is presented in Table 5.4. Note

that design 4 has no blocks intersecting in more than two treatments, while designs 1, 2, and 3 contain blocks intersecting in 3 treatments. Therefore, design 4 has MIA, and thus maximizes the minimum efficiency of its residuals with respect to all majorization criteria.

Next, note that the minimum  $E$ -efficiency, as well as the minimum  $MV$ -efficiency is common to all 4 designs. The smallest nonzero eigenvalue of a residual design is  $\frac{v\lambda}{k} - 2$ , unless  $q \leq 1$ . We will next concentrate our attention on further analysis of the worst case scenarios for each design. Since most of the eigenvalues of  $C_2(q)$  are the same as the eigenvalues of  $C_2(q + 1)$ , it is reasonable to compare the different eigenvalues of two such residuals, and not the entire sets of eigenvalues. This is formally defined below.

**Definition 5.4.** Consider  $d_1$  and  $d_2$  whose information matrices have eigenvalues  $\mu(d_1)$  and  $\mu(d_2)$ . Let  $\mu^-(d_1)$  denote the eigenvalues in  $\mu(d_1)$  after removing the common eigenvalues in  $\mu(d_1)$  and  $\mu(d_2)$ . Also, let  $\mu^-(d_2)$  represent the same for  $d_2$ . Define the  $\Phi$ -impact of using design  $d_2$  over  $d_1$ , as the  $\Phi$ -efficiency of design  $d_2$  to design  $d_1$ , where  $\Phi$  is a majorization criterion defined on  $\mu^-(d_1)$  and  $\mu^-(d_2)$ .

The  $MV$ -impact will be computed in a similar manner, as the ratio of the two minimum and **non-equal** variances of pairwise treatment contrasts. For a BIBD with two blocks removed, these variances are given in Table 5.1. The above technique allows to better differentiate between designs. Eliminating the common eigenvalues from the comparison is statistically equivalent to comparing only variances of contrasts which are indeed different, while throwing away the contrasts that have equal variances in the two designs. For instance, instead of comparing the minimum eigenvalues of two designs (as the  $E$ -criterion does), the  $E$ -impact will give a comparison of the two minimum and **non-equal** eigenvalues.

Returning to example 5.1, an analysis of worst case scenarios for  $(7, 3, 2)$  BIBDs is presented in Table 5.3. The worst case residuals for designs 1, 2 and 3 have  $q = 3$ , while the worst case residual for design 4, the MIA design, has  $q = 2$ . Thus, the table presents a comparison of the non-common eigenvalues of residuals  $C_2(3)$  and  $C_2(2)$  for  $(7, 3, 2)$  designs. The numbers

in this table show that there is indeed a lot to be gained in using design 4. For instance, in the worst case scenario, even though the largest variance of pairwise treatment comparison is 0.571429 for all designs, the ratio of the first non-equal variances of design 4 worst residual and other designs' worst residuals is 0.816667. The same can be said about design 4 of  $(8, 4, 3)$  BIBDs, as shown in Table 5.5.

 Table 5.6: Comparison of  $(9, 4, 3)$  designs robustness against loss of 2 blocks

Design no.	Int. numbers					A-efficiency		E-efficiency		MV-efficiency	
	0	1	2	3	4	average	min	average	min	average	min
1	1	60	84	8	0	0.87746	0.870097	0.719196	0.703704	0.738631	0.703704
2	5	48	96	4	0	0.877458	0.870097	0.720165	0.703704	0.735713	0.703704
3	2	57	87	7	0	0.877459	0.870097	0.719438	0.703704	0.737902	0.703704
4	3	54	90	6	0	0.877459	0.870097	0.71968	0.703704	0.737172	0.703704
5	3	54	90	6	0	0.877459	0.870097	0.71968	0.703704	0.737172	0.703704
6	5	48	96	4	0	0.877458	0.870097	0.720165	0.703704	0.735713	0.703704
7	1	60	84	8	0	0.87746	0.870097	0.719196	0.703704	0.738631	0.703704
8	1	60	84	8	0	0.87746	0.870097	0.719196	0.703704	0.738631	0.703704
9	0	63	81	9	0	0.877461	0.870097	0.718954	0.703704	0.739361	0.703704
10	1	60	84	8	0	0.87746	0.870097	0.719196	0.703704	0.738631	0.703704
11	9	36	108	0	0	0.877456	0.875792	0.721133	0.703704	0.732794	0.703704

 Table 5.7: Worst case scenarios of  $(9, 4, 3)$  designs robustness against loss of 2 blocks

Maximum q	Designs	Impact of MIA design		
		A-impact	E-impact	MV-impact
2	11 (MIA)	-	-	-
3	1-10	0.987475	0.904762	0.890807

**Example 5.3.** Consider the BIBD with parameters  $v = 9$ ,  $k = 4$ ,  $\lambda = 3$ , and thus  $b = 18$ . The 11 nonisomorphic BIBDs with these parameters are given in Table A.3, and a comparison of their robustness against the loss of two blocks is presented in Tables 5.6 and 5.7. Design 11 has minimum intersection aberration, since any two blocks of this design intersect in

no more than 2 treatments. Again, the MIA design performs about the same as others on average, but in worst case scenarios it outperforms its competitors.

Table 5.8: Comparison of  $(10, 5, 4)$  designs robustness against loss of 2 blocks

Design no.	Int. numbers						A-efficiency		E-efficiency		MV-efficiency	
	0	1	2	3	4	5	average	min	average	min	average	min
1	0	4	96	48	5	0	0.880536	0.874841	0.750654	0.75	0.751848	0.75
2	0	6	90	54	3	0	0.880536	0.874841	0.75098	0.75	0.752772	0.75
3	0	8	84	60	1	0	0.880535	0.874841	0.751307	0.75	0.753696	0.75
4	0	8	84	60	1	0	0.880535	0.874841	0.751307	0.75	0.753696	0.75
5	0	4	96	48	5	0	0.880536	0.874841	0.750654	0.75	0.751848	0.75
6	0	4	96	48	5	0	0.880536	0.874841	0.750654	0.75	0.751848	0.75
7	0	6	90	54	3	0	0.880536	0.874841	0.75098	0.75	0.752772	0.75
8	0	0	108	36	9	0	0.880536	0.874841	0.75	0.75	0.75	0.75
9	0	7	87	57	2	0	0.880536	0.874841	0.751144	0.75	0.753234	0.75
10	0	4	96	48	5	0	0.880536	0.874841	0.750654	0.75	0.751848	0.75
11	0	7	87	57	2	0	0.880536	0.874841	0.751144	0.75	0.753234	0.75
12	0	9	81	63	0	0	0.880535	0.878427	0.751471	0.75	0.751848	0.75
13	0	8	84	60	1	0	0.880535	0.874841	0.751307	0.75	0.753696	0.75
14	0	8	84	60	1	0	0.880535	0.874841	0.751307	0.75	0.753696	0.75
15	0	4	96	48	5	0	0.880536	0.874841	0.750654	0.75	0.751848	0.75
16	0	6	90	54	3	0	0.880536	0.874841	0.75098	0.75	0.752772	0.75
17	0	9	81	63	0	0	0.880535	0.878427	0.751471	0.75	0.754158	0.75
18	0	8	84	60	1	0	0.880535	0.874841	0.751307	0.75	0.753696	0.75
19	0	6	90	54	3	0	0.880536	0.874841	0.75098	0.75	0.752772	0.75
20	0	8	84	60	1	0	0.880535	0.874841	0.751307	0.75	0.753696	0.75
21	0	8	84	60	1	0	0.880535	0.874841	0.751307	0.75	0.753696	0.75

**Example 5.4.** Consider the BIBD with parameters  $v = 10$ ,  $k = 5$ ,  $\lambda = 4$ , and thus  $b = 18$ . The 21 nonisomorphic BIBDs with these parameters are given in Table A.4, and a comparison of their robustness against the loss of two blocks is presented in Tables 5.8 and 5.9. Designs 12 and 17 have minimum intersection aberration, since any two blocks of these designs intersect in no more than 3 treatments. Either of these designs is preferable to the others.

Table 5.9: Worst case scenarios of  $(10, 5, 4)$  designs robustness against loss of 2 blocks

Maximum q	Designs	Impact of MIA design		
		A-impact	E-impact	MV-impact
3	12, 17 (MIA)	-	-	-
4	1-11, 13-16, 18-21	0.990911	0.909091	0.914122

In order to differentiate between designs 12 and 17, their robustness against the loss of more than two blocks must be studied. However, there is no clear way to determine a worst case scenario when three or more blocks are lost. Average and minimum efficiencies of residual designs for three and four blocks removed were computed numerically, and the results are given in Appendix B and Appendix C, respectively. The tables, similar to the ones in this section, show no major differences between designs 12 and 17. Appendices B and C contain comparisons of the other designs in this section, in terms of their robustness to the removal of more than two blocks. Since these tables do not show major differences between the nonisomorphic BIBDs, it seems that looking at design robustness to the removal of two blocks is sufficient.

### 5.4.3 MIA balanced incomplete block designs

The minimum intersection aberration criterion gives us a clear method of differentiating between designs. Obviously, finding the block intersection numbers for a design is not computationally intensive. One easy way to do it is to compute the block intersection matrix as  $N'N$ , where  $N$  is the block-treatment incidence matrix. However, finding all nonisomorphic BIBDs for a parameter set is no easy task, even with the aid of computers. Better software, and more importantly, much faster computers are needed to make the search for BIBDs with larger parameters possible.

There are a couple of conditions on the values of block intersection numbers for a BIBD that we will invoke here. Let  $q_j$  denote the number of treatments in common for a pair  $j$  of

blocks, with  $j = 1, \dots, \binom{b}{2}$ . Then

$$\sum_{j=1}^{\binom{b}{2}} q_j = \frac{1}{2} [\mathbf{1}'_b (N'N - kI_b) \mathbf{1}_b] = \frac{bk(r-1)}{2}. \quad (5.31)$$

Note that any BIBDs with  $\lambda = 1$  must have identical distributions of block intersection numbers, since  $q_j \in \{0, 1\}$  and  $\sum q_j$  is constant. Therefore only nonisomorphic BIBDs with  $\lambda \geq 2$  should be compared in terms of their robustness to the loss of two blocks.

Another property refers to the block intersection numbers for the complement of a BIBD. If we let  $B_1, B_2, \dots, B_b$  denote the  $b$  sets forming a BIBD, and  $B'_i = \{1, 2, \dots, v\} - B_i$ , then the  $b$  sets  $B'_i$  form another BIBD called the complement of the original design. The new BIBD has parameters

$$v_1 = v, \quad b_1 = b, \quad r_1 = b - r, \quad k_1 = v - k, \quad \lambda_1 = b - 2r + \lambda.$$

All nonisomorphic BIBDs with parameters  $v_1, b_1, r_1, k_1$ , and  $\lambda_1$  can be found as the complements of the nonisomorphic BIBDs with parameters  $v, b, r, k$ , and  $\lambda$ . Also, if  $|B_i \cap B_j| = q$ , then  $|B'_i \cap B'_j| = v - 2k + q$ . Therefore, if a BIBD has minimum intersection aberration, then its complement also has minimum intersection aberration.

Hence, only nonisomorphic BIBDs with  $\lambda \geq 2$  and  $k \leq \frac{v}{2}$  need to be enumerated in order to find MIA designs. Admissible parameter sets of such BIBDs with the bounding restrictions  $v \leq 10$  and  $r \leq 15$  are given in Table 5.10. The column “ $N_d$ ” contains the number of nonisomorphic BIBDs with parameters  $v, b, r, k, \lambda$ , while “ $N_{MIA}$ ” contains the number of MIA nonisomorphic BIBDs. Only parameter sets with  $N_d > 1$  are included in the table. One MIA design for each parameter set is given in Appendix D.

#### 5.4.4 Robustness of SBIBDs to the removal of three blocks

Any two blocks in a SBIBD intersect in  $\lambda$  treatments. Therefore, all nonisomorphic SBIBDs are equally robust against the loss of two blocks, and so their robustness against the loss of three or more blocks must be studied.

Table 5.10: Parameters of BIBDs with  $v \leq 10$ ,  $r \leq 15$ ,  $\lambda \geq 2$ ,  $k \leq \frac{v}{2}$ 

$v$	$b$	$r$	$k$	$\lambda$	$N_d$	$N_{MIA}$
6	20	10	3	4	4	1
6	30	15	3	6	6	1
7	14	6	3	2	4	1
7	21	9	3	3	10	1
7	28	12	3	4	35	1
7	35	15	3	5	109	1
8	14	7	4	3	4	1
8	28	14	4	6	2310	1
9	24	8	3	2	36	13
9	36	12	3	3	22521	332
9	18	8	4	3	11	1
10	30	9	3	2	960	394
10	15	6	4	2	3	3
10	30	12	4	4	$> 1.7 \times 10^6$	1
10	18	9	5	4	21	2

Let  $q$  denote the number of treatments in common in the three blocks removed. As shown in sections 5.2 and 5.3, the information matrix of a residual design obtained by removing three blocks from a SBIBD and its eigenvalues depend only on  $q$ . If we write this matrix as  $C_3(q)$ , intuitively it would seem that  $\mu\{C_3(q)\} \prec \mu\{C_3(q+1)\}$ , similar to the result given in Theorem 5.1. Unfortunately, majorization does not hold in this case. For a numerical counterexample see Example 5.5 below. Thus, one cannot say that one residual is worse than another with respect to all majorization criteria, and so an undisputed worst-case scenario does not exist here. However,  $C_3(q+1)$  is inferior to  $C_3(q)$  under a criterion that will be discussed in this section.

**Example 5.5.** Consider the SBIBD with parameters  $v = b = 15$ ,  $k = 7$ ,  $\lambda = 3$ . The 5 nonisomorphic SBIBDs with these parameters are given in Table A.5, and a comparison of their robustness against the loss of three blocks is presented in Table 5.11. For each design there are  $\binom{b}{3}$  possible residuals; the column containing the intersection numbers gives the number of block triplets that intersect in  $q$  treatments for  $q \in \{0, 1, 2, 3\}$ .

Table 5.11: Comparison of  $(15, 7, 3)$  designs robustness against loss of 3 blocks

Design no.	Int. numbers				A-efficiency		E-efficiency		MV-efficiency	
	0	1	2	3	average	min	average	min	average	min
1	0	420	0	35	0.779886	0.775591	0.55764	0.533333	0.607253	0.533333
2	16	372	48	19	0.779886	0.775591	0.560332	0.533333	0.604275	0.533333
3	28	336	84	7	0.779886	0.775591	0.562351	0.533333	0.602042	0.533333
4	24	348	72	11	0.779886	0.775591	0.561678	0.533333	0.602786	0.533333
5	28	336	84	7	0.779886	0.775591	0.562351	0.533333	0.602042	0.533333

The minimum eigenvalue of any residual obtained by removing three blocks from a SBIBD, with their intersection  $q > 1$ , is  $\frac{v\lambda}{k} - 3$  with multiplicity  $q - 1$ . Thus  $C_3(q + 1)$  has one additional minimum eigenvalue. In statistical terms, a residual obtained by removing three blocks intersecting in  $q + 1$  treatments has one additional contrast of maximum variance, compared to a residual obtained by removing three blocks intersecting in  $q$  treatments. This justifies using the minimum intersection aberration criterion to differentiate between designs. In this example, designs 3 and 5 have MIA, because only 7 block triplets have intersection number  $q = 3$ . This means that designs 3 and 5 are less likely than the others to produce a residual with  $q = 3$ .

Next, let's look at the eigenvalues of possible residual designs, displayed in Table 5.12. We have four possible vectors of eigenvalues. There is no majorization relation between any two of the four vectors. Thus, there is no worst residual with respect to all majorization criteria. However, a residual with  $q = 3$  is  $A$ -inferior to all other residuals, and it has two eigenvalues equal to the overall minimum eigenvalue 3.42857, while other residuals have either one or no eigenvalues less than or equal to 3.42857. In conclusion, designs 3 and 5 are preferable because they have a smaller chance of yielding a residual with  $q = 3$ .

Due to the lack of a definite majorization ordering among residuals, one should always look at the eigenvalues of possible residuals, not only at the number of different possible residuals yielded by each nonisomorphic SBIBD.

Table 5.12: Eigenvalues ( $\iota$ ) of possible residuals obtained by removing 3 blocks from a (15, 7, 3) SBIBD

Intersection number ( $q$ )							
0		1		2		3	
$\iota$	multiplicity	$\iota$	multiplicity	$\iota$	multiplicity	$\iota$	multiplicity
4.42857	6	3.59785	1	3.42857	1	3.42857	2
4.7798	2	4.42857	3	3.81787	1	4.28571	1
5.28571	1	4.63841	2	4.52545	2	5.42857	9
5.64877	2	5.11644	1	4.89642	1	6	2
6.42857	3	5.42857	3	5.42857	6		
		5.79016	2	5.90312	2		
		6.42857	2	6.42857	1		

Table 5.13: Comparison of (19, 9, 4) designs robustness against loss of 3 blocks

Design no.	Int. numbers					A-efficiency		E-efficiency		MV-efficiency	
	0	1	2	3	4	average	min	average	min	average	min
1	12	363	549	45	0	0.8308	0.829846	0.651796	0.644737	0.895585	0.818936
2	9	372	540	48	0	0.8308	0.829846	0.651568	0.644737	0.89538	0.818936
3	33	300	612	24	0	0.8308	0.829846	0.653391	0.644737	0.895971	0.818936
4	0	399	513	57	0	0.8308	0.829846	0.650884	0.644737	0.895235	0.818936
5	9	372	540	48	0	0.8308	0.829846	0.651568	0.644737	0.895488	0.818936
6	21	336	576	36	0	0.8308	0.829846	0.65248	0.644737	0.89573	0.818936

**Example 5.6.** Consider the SBIBD with parameters  $v = b = 19$ ,  $k = 9$ ,  $\lambda = 4$ . The 6 nonisomorphic SBIBDs with these parameters are given in Table A.6, and a comparison of their robustness against the loss of three blocks is presented in Table 5.13. Note that none of the designs have three blocks intersecting in  $q = \lambda = 4$  treatments.

The eigenvalues of residuals with  $q \in \{0, 1, 2, 3\}$  are presented in Table 5.14. Just like in the previous example, there is no majorization ordering between any two of the four possible vectors. However, a residual with  $q = 3$  can be considered worst because it has most eigenvalues (2) equal to the overall minimum eigenvalue, which is 5.44444. Furthermore, a residual with  $q = 3$  is also  $A$ -worst among the four possible residuals. By the MIA criterion, design 3 is the most robust out of the 6 nonisomorphic SBIBDs. Also, residuals derived from design 3 have the highest  $E$ - and  $MV$ - averaged efficiencies, compared to residuals derived from the other designs (see Table 5.13).

Table 5.14: Eigenvalues ( $\iota$ ) of possible residuals obtained by removing 3 blocks from a  $(19, 9, 4)$  SBIBD

Intersection number ( $q$ )							
0		1		2		3	
$\iota$	multiplicity	$\iota$	multiplicity	$\iota$	multiplicity	$\iota$	multiplicity
6.44444	9	5.5705	1	5.44444	1	5.44444	2
6.82161	2	6.44444	6	5.71991	1	5.91422	1
7.33333	1	6.70106	2	6.44444	3	6.51949	2
7.62284	2	7.20727	1	6.60358	2	6.86356	1
8.44444	4	7.44444	3	7.05787	1	7.44444	9
		7.74338	2	7.44444	6	7.92495	2
		8.44444	3	7.84086	2	8.44444	1
				8.44444	2		

An analysis of the robustness of the SBIBDs with the parameters of examples 5.5 and 5.6 is given in Appendix C. The efficiencies shown in Table C.5 and C.6 are quite close. When the number of blocks removed is increased, it becomes computationally intensive to compare the designs, and it must be done numerically, due to the many different possible information

matrices. Even though it might seem that it is not as easy to differentiate between SBIBDs under loss of 3 blocks as between BIBDs under loss of 2 blocks, sometimes one design proves to perform better overall than the other designs. This is the case with design 3 of the six nonisomorphic  $(19, 9, 4)$  designs. Therefore, one should take robustness into consideration when trying to decide on one of several nonisomorphic designs with the same parameters.

# Chapter 6

## Conclusions and Future Research

### 6.1 Optimality of designs with small number of treatments

*A*-optimal designs with three treatments in settings with one or two blocking factors were found in Chapter 3. The common characteristic of all these designs is uniformity. Until now, the only designs that have been found in the literature to be *A*-optimal, are designs which have number of experimental units a multiple of 3 - such designs are in fact universally optimal. The replication numbers of *A*-optimal row-column designs are given in Table 3.1.

*E*-optimal designs with three treatments in settings with any number of crossed blocking factors were found in Chapter 4. All *E*-optimal designs are equireplicated, or as close to being equireplicated as possible. As mentioned earlier, when the number of experimental units in the design setting is a multiple of 3, universally optimal designs exist. When the number of experimental units in the design is  $m \equiv 1 \pmod{3}$ , *E* - *M*-optimal designs are in general nonuniform in the treatment replicated  $r + 1$  times. When  $m \equiv 2 \pmod{3}$ , the *E* - *M*-optimal designs are uniform with replications  $r_1 = r_2 = r + 1$ , and  $r_3 = r$ .

Chapter 4 also contains a section dedicated to the construction of *A* and *E* optimal designs. Systems of distinct representatives theory was used for the construction of some of the designs with multiple blocking factors. Section 4.5 presents comparisons between *A*-optimal

and  $E$ -optimal block designs, as well as row-column designs. For block designs, the  $A$ -optimal and  $E$ -optimal designs are very similar, and thus their efficiencies with respect to the other criterion are close to 1. For row-column designs, some of the  $A$ -optimal designs perform poorly under the  $E$  criterion because of imbalance in their replication numbers. The  $E$ -optimal row-column designs have in general  $A$ -efficiency close to 1. Therefore, we think that when faced with a choice between  $A$ -optimal and  $E$ -optimal row-column designs, one should choose the  $E$ -optimal design, given no other outside considerations.

The search for optimal designs with 3 treatments could be extended to include some of the following settings:

- designs with correlated errors
- designs with nested blocking factors
- block designs with two or three block sizes

Extending this work to 4 treatments is possible, even though some settings where the problem was solved for 3 treatments might prove to be very complex. When moving from 3 treatments to 4 treatments, the number of variables that define the information matrix changes from 3 to 6. When finding optimal designs with 4 treatments, some concurrences must also be taken into account, which was not the case with 3 treatment designs.

When moving to larger number of treatments, the problem becomes increasingly complicated, but the search could be performed for useful and/or promising subsets of the parameter space. Some of these could be:

- restrict search to incomplete block settings
- restrict search to equireplicated designs
- restrict search to uniform designs

## 6.2 Robustness of designs to loss of data

In the last few years robustness has become a popular research topic in different areas of statistics. Robustness of models to changes in the assumed distribution of data and robustness of designs to changes in the underlying model are only two of the many examples. For block designs, many authors have studied robustness of different combinatorial designs to loss of data. Chapter 5 builds on a result in [3] and gives a method for selecting among nonisomorphic BIBDs and SBIBDs via robustness criteria. The minimum intersection aberration criterion (MIA) was introduced to help in choosing robust designs. To find MIA BIBDs, one must look at the intersection numbers of every pair of blocks in the design, while for MIA SBIBDs one must look at the intersection numbers of every block triplet.

All MIA BIBDs with  $v \leq 10$  and  $r \leq 15$  were found using the computer. The MIA BIBDs are displayed in Appendix D. This work can be extended to build tables of MIA BIBDs for larger parameters. Also, another natural extension would be to look at other widely used classes of designs such as partially balanced block designs, group divisible designs, generalized Youden designs, and others. It is expected that robustness to loss of data can be used for these other classes as well, to help select among nonisomorphic designs.

# Glossary

Acronym or Term	Description
$\lambda$	number of times each pair of treatments appears together in a balanced block design
$A$ -optimality	optimality criterion: minimizes $\sum \frac{1}{z_i}$
$b$	number of blocks in a block design
BBD	Balanced Block Design
BIBD	Balanced Incomplete Block Design
binary design	each treatment appears no more than once in a block
$C$ -matrix	Information matrix of a design
$c_i$	$i$ -th diagonal element of the information matrix (corresponds to treatment $i$ )
$D$ -optimality	optimality criterion: minimizes $\prod \frac{1}{z_i}$
$E$ -optimality	optimality criterion: minimizes $\frac{1}{z_i}$
generalized binary design	elements of the block-treatment incidence matrix satisfy $ n_{ij} - k/v  < 1$
GRBD	Generalized Randomized Block Design
GYD	Generalized Youden Design: row-column design whose rows and columns both form BBDs

$k$	size of blocks in a block design
LSD	Latin Square Design
$m$	total number of experimental units in designs with more than one blocking factor
$M$	row-treatment incidence matrix of a row-column design
MIA	minimum intersection aberration criterion
$n$	(1) number of blocking factors in designs with more than one blocking factor (2) total number of experimental units in designs with one blocking factor
$N$	block-treatment incidence matrix of a block design; also, the column-treatment incidence matrix of a row-column design
$n_{ij}$	element of $N$ : how many times treatment $i$ appears in block $j$
$N_j$	block-treatment incidence matrix of factor $j$ in a design with multiple blocking factors
$n_{ijl}$	element of $N_j$ : how many times treatment $i$ appears in block $l$ of factor $j$
$p$	number of rows in a row-column design
$q$	number of columns in a row-column design
$q_{ij}$	number of common treatments in blocks $i$ and $j$ of a BIBD
$r_i$	replication number of treatment $i$
RCBD	Randomized Complete Block Design
SBIBD	Symmetric Balanced Incomplete Block Design (BIBD with $v = b$ )
SDR	System of Distinct Representatives

uniform design	elements of the block-treatment incidence matrix satisfy $ n_{ij} - r_i/b  < 1$
$v$	number of treatments (varieties) in a design
YD	Youden Design: row-column design with rows forming an RCBD and columns forming a BIBD
YHR	Youden Hyper-Rectangle: design with multiple blocking factors which reduces to a BBD in any factor
$z_i$	$i$ -th non-zero eigenvalue of the $C$ -matrix

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# Appendix A

## Nonisomorphic Designs for Several Balanced Incomplete Block Settings

Table A.1: The 4 nonisomorphic  $(7, 3, 2)$  designs

1:	1	1	1	1	1	1	2	2	2	2	3	3	3	3
	2	2	4	4	6	6	4	4	5	5	4	4	5	5
	3	3	5	5	7	7	6	6	7	7	7	7	6	6
2:	1	1	1	1	1	1	2	2	2	2	3	3	3	3
	2	2	4	4	6	6	4	4	5	5	4	4	5	5
	3	3	5	5	7	7	6	7	6	7	6	7	6	7
3:	1	1	1	1	1	1	2	2	2	2	3	3	3	3
	2	2	4	4	5	6	4	4	5	6	4	4	5	5
	3	3	5	6	7	7	5	7	6	7	6	7	6	7
4:	1	1	1	1	1	1	2	2	2	2	3	3	3	4
	2	2	3	4	5	6	3	4	5	5	4	4	6	5
	3	4	5	6	7	7	6	7	6	7	5	7	7	6

Table A.2: The 4 nonisomorphic  $(8, 4, 3)$  designs

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

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

Table A.3: The 11 nonisomorphic (9, 4, 3) designs

1:	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	3	4	4	6	7	3	4	4	5	5	4	4	5	5
	3	3	6	6	5	5	8	8	8	6	6	7	7	7	7	6	6
	4	5	7	7	8	9	9	9	9	8	9	8	9	8	9	8	9
2:	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	3	4	4	6	7	3	4	4	5	5	4	4	5	5
	3	3	6	6	5	5	8	8	8	6	7	6	7	6	7	6	6
	4	5	7	7	8	9	9	9	9	8	9	9	8	9	8	8	9
3:	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	3	4	4	5	7	3	4	4	5	5	4	4	5	6
	3	3	6	6	5	6	8	8	7	6	8	6	7	5	7	6	7
	4	5	7	8	7	9	9	9	9	8	9	9	8	8	9	9	8
4:	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	3	4	4	5	7	3	4	4	5	5	4	4	5	6
	3	3	6	6	5	6	8	8	7	6	8	6	7	5	7	6	7
	4	5	7	8	7	9	9	9	9	8	9	9	8	9	8	8	9
5:	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	3	4	4	5	7	3	4	4	5	6	4	4	5	5
	3	3	6	6	5	6	8	8	8	5	7	6	7	6	7	6	7
	4	5	7	8	7	9	9	9	9	8	9	9	8	9	8	7	9
6:	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	3	4	4	5	7	3	4	4	5	5	4	4	5	6
	3	3	6	6	5	6	8	8	8	6	7	6	7	5	7	6	7
	4	5	7	8	7	9	9	9	9	8	9	9	8	9	8	7	9

7:	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	3	4	4	5	7	3	4	4	5	6	4	4	5	5	5
	3	3	6	6	5	6	7	8	7	5	7	6	8	6	8	6	7	6
	4	5	7	8	9	9	8	9	9	8	8	9	9	7	9	8	9	7
8:	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	3	4	4	5	7	3	4	4	5	6	4	4	5	5	5
	3	3	6	6	5	6	7	8	7	5	7	6	8	6	7	6	8	6
	4	5	7	8	9	9	8	9	9	8	8	9	9	8	9	7	9	7
9:	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	3	4	4	5	6	3	4	4	5	6	4	4	5	5	5
	3	3	6	6	5	7	7	8	8	5	7	8	7	6	7	6	7	6
	4	5	7	8	9	8	9	9	9	6	8	9	9	9	9	7	8	8
10:	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	3	4	4	5	5	3	4	4	5	6	4	4	5	6	5
	3	3	6	6	6	7	7	8	8	5	8	7	7	5	7	6	7	6
	4	5	7	8	9	9	8	9	9	6	9	9	8	7	8	9	9	8
11:	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4	5
	2	2	2	3	3	4	4	5	3	3	4	4	6	4	4	6	5	6
	3	5	7	5	6	6	7	8	5	7	5	6	8	5	8	7	7	7
	4	6	8	7	9	8	9	9	8	9	9	7	9	6	9	8	8	9

Table A.4: The 21 nonisomorphic  $(10, 5, 4)$  designs

1:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4	
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	5	5	
	3	3	5	5	6	6	7	7	6	7	8	6	6	6	5	5	6	6	
	4	4	7	9	7	9	8	9	8	8	9	7	8	7	7	8	7	8	
	5	6	8	10	8	10	9	10	10	10	10	10	10	9	9	10	9	10	
2:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4	
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	5	5	
	3	3	5	5	6	7	6	8	6	6	7	6	7	6	5	5	6	6	
	4	4	7	9	7	9	7	9	8	9	8	8	8	8	7	7	8	8	7
	5	6	8	10	8	10	9	10	10	10	10	10	10	9	9	10	9	10	
3:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4	
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	5	5	
	3	3	5	5	6	7	6	7	6	6	8	6	7	6	5	5	6	6	
	4	4	7	9	7	9	9	8	8	7	9	8	8	7	7	8	8	7	
	5	6	8	10	8	10	10	9	10	10	10	10	9	10	9	10	9	10	

4:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	5	5
	3	3	5	5	6	7	6	7	6	6	8	6	7	6	5	5	6	6
	4	4	7	9	7	8	8	9	8	7	9	8	8	7	7	9	8	7
	5	6	8	10	9	10	9	10	10	10	10	10	10	9	9	8	10	9
5:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	5	5
	3	3	5	6	5	6	7	7	6	7	8	5	6	6	5	6	6	6
	4	4	7	7	8	9	8	9	8	8	9	9	8	7	7	7	7	8
	5	6	8	9	10	10	10	10	9	9	10	10	10	10	9	8	10	9
6:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	5	5
	3	3	5	6	5	6	7	7	6	7	8	5	6	6	5	6	6	6
	4	4	7	9	7	8	8	9	8	8	9	8	7	7	9	7	7	8
	5	6	8	10	9	10	10	10	9	9	10	10	9	10	10	8	10	9
7:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	5	5
	3	3	5	7	5	6	6	8	6	6	7	5	6	6	5	7	6	6
	4	4	7	8	9	7	7	9	8	8	9	9	8	7	7	8	8	7
	5	6	8	9	10	9	10	10	10	10	10	10	10	9	10	8	10	9
8:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	5	5
	3	3	5	7	5	7	6	6	6	6	6	5	8	6	5	7	6	6
	4	4	7	8	9	9	7	8	8	7	8	9	9	7	7	8	8	7
	5	6	8	9	10	10	9	10	10	10	9	10	10	10	8	10	9	9
9:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	5	5
	3	3	5	7	5	6	6	8	6	6	7	5	6	6	5	7	6	6
	4	4	7	9	8	7	7	9	8	8	8	9	8	7	7	8	9	7
	5	6	8	10	9	9	10	10	10	10	10	10	10	9	9	10	9	10
10:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	5	5
	3	3	5	7	5	6	6	7	6	6	8	5	6	6	5	7	6	6
	4	4	7	9	8	7	8	8	9	8	9	9	7	7	7	8	7	8
	5	6	8	10	9	9	10	10	10	10	10	10	10	9	8	10	9	10
11:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	5	5
	3	3	5	7	5	6	6	7	6	6	7	5	6	6	5	8	6	6
	4	4	7	9	8	7	8	8	9	8	8	9	7	8	7	9	7	7
	5	6	8	10	9	10	9	10	10	10	9	10	10	9	10	10	9	8

12:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3
	2	2	2	2	3	4	4	5	6	3	4	4	5	5	4	4	4	5
	3	3	3	4	5	5	7	7	7	7	5	8	6	6	5	6	6	6
	4	6	8	6	8	6	8	9	8	9	7	9	7	8	7	7	9	8
	5	7	9	10	10	9	9	10	10	10	8	10	9	10	10	8	10	9
13:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	5	5	3	3	4	4	6	4	4	5	5
	3	3	4	5	4	8	6	6	7	5	6	5	7	7	5	7	6	6
	4	6	6	7	7	9	9	8	8	9	8	8	8	9	6	8	7	7
	5	7	8	9	10	10	10	9	10	10	10	10	9	10	9	9	8	10
14:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	5	5	3	3	4	4	5	4	4	6	5
	3	3	4	5	4	7	6	6	8	5	6	7	7	6	5	5	7	6
	4	6	6	7	8	8	9	7	9	8	9	8	9	8	6	7	8	7
	5	7	8	9	9	10	10	10	10	10	10	10	10	9	10	9	9	8
15:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	5	6	3	3	4	4	5	4	4	5	5
	3	3	4	5	4	5	7	6	7	6	7	5	7	6	5	6	7	6
	4	6	6	7	9	8	9	8	8	9	8	8	8	9	6	8	8	7
	5	7	8	9	10	10	10	10	9	10	10	9	10	10	7	9	9	10
16:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	5	6	3	3	4	4	5	4	4	5	5
	3	3	4	5	4	5	8	6	7	6	7	5	7	6	5	6	7	6
	4	6	6	9	7	8	9	7	8	9	8	7	8	8	6	9	8	7
	5	7	8	10	9	10	10	10	9	10	10	9	10	9	8	10	9	10
17:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	5	5	3	3	4	4	6	4	4	5	5
	3	3	4	5	4	6	7	6	7	5	7	5	6	7	5	8	6	6
	4	6	6	9	7	9	8	8	8	8	8	7	9	8	6	9	7	7
	5	7	8	10	9	10	10	10	9	9	10	10	10	9	8	10	10	9
18:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	5	5	3	3	4	4	6	4	4	5	5
	3	3	4	5	4	8	6	6	7	5	6	5	7	7	5	7	6	6
	4	6	6	9	7	9	9	7	8	8	8	7	8	9	6	8	7	8
	5	7	8	10	9	10	10	8	10	9	10	10	9	10	10	10	9	9
19:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	5	5	3	3	4	4	6	4	4	5	5
	3	3	4	5	4	6	7	6	7	5	7	5	6	8	5	7	6	6
	4	6	6	9	9	8	8	7	8	7	9	8	7	9	6	8	8	7
	5	7	8	10	10	9	10	9	10	8	10	9	10	10	10	9	10	9

20:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4
	2	2	2	2	3	3	4	5	5	3	3	4	4	7	4	4	5	5
	3	3	4	5	4	7	7	6	6	5	6	5	6	8	5	6	6	6
	4	6	6	9	9	8	8	7	8	7	8	8	7	9	7	9	8	7
	5	7	8	10	10	9	10	9	10	10	10	9	9	10	8	10	9	10
21:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	5
	2	2	2	2	3	3	4	4	5	3	3	4	4	5	4	4	4	6
	3	3	4	5	5	7	6	8	6	6	7	5	7	6	5	5	6	7
	4	6	6	9	8	8	7	9	7	9	8	7	8	8	6	7	9	8
	5	7	8	10	9	10	9	10	10	10	9	9	10	10	8	10	10	9

Table A.5: The 5 nonisomorphic  $(15, 7, 3)$  designs

1:	1	1	1	1	1	1	1	1	2	2	2	2	3	3	3	3
	2	2	2	4	4	6	6	4	4	5	5	4	4	5	5	
	3	3	3	5	5	7	7	6	6	7	7	7	7	6	6	
	4	8	12	8	10	8	10	8	9	8	9	8	9	8	9	
	5	9	13	9	11	9	11	10	11	10	11	11	10	11	10	
	6	10	14	12	14	14	12	12	13	13	12	12	13	13	12	
	7	11	15	13	15	15	13	14	15	15	14	15	14	14	15	
2:	1	1	1	1	1	1	1	2	2	2	2	3	3	3	3	
	2	2	2	4	4	6	6	4	4	5	5	4	4	5	5	
	3	3	3	5	5	7	7	6	6	7	7	7	7	6	6	
	4	8	12	8	10	8	10	8	9	8	9	8	9	8	9	
	5	9	13	9	11	9	11	10	11	10	11	11	10	11	10	
	6	10	14	12	14	14	12	12	13	13	12	13	12	12	13	
	7	11	15	13	15	15	13	14	15	15	14	14	15	15	14	
3:	1	1	1	1	1	1	1	2	2	2	2	3	3	3	3	
	2	2	2	4	4	5	6	4	4	5	6	4	4	5	5	
	3	3	3	5	6	7	7	5	6	7	7	7	7	6	6	
	4	8	12	8	8	10	9	9	10	8	8	8	9	8	9	
	5	9	13	9	10	11	11	11	11	10	9	11	10	11	10	
	6	10	14	12	14	12	13	14	12	13	12	13	12	12	13	
	7	11	15	13	15	14	15	15	13	15	14	14	15	15	14	

4:	1	1	1	1	1	1	1	2	2	2	2	3	3	3	4
	2	2	2	3	4	6	6	3	4	5	5	4	4	5	5
	3	3	4	5	5	7	7	6	6	7	7	7	7	6	6
	4	8	8	9	10	8	10	10	9	8	9	8	9	8	8
	5	9	12	12	11	9	11	12	11	11	10	10	11	11	9
	6	10	13	13	14	14	12	14	13	12	13	13	12	13	10
	7	11	14	15	15	15	13	15	15	15	14	15	14	14	12
5:	1	1	1	1	1	1	1	2	2	2	2	3	3	3	4
	2	2	2	3	4	6	6	3	4	5	5	4	4	5	5
	3	3	4	5	5	7	7	6	7	6	7	6	7	7	6
	4	8	8	9	10	8	10	10	9	8	9	9	8	8	8
	5	9	12	12	11	9	11	12	11	11	10	11	10	11	9
	6	10	13	13	14	14	12	14	12	13	13	13	13	12	10
	7	11	14	15	15	15	13	15	15	15	14	14	15	14	12

Table A.6: The 6 nonisomorphic  $(19, 9, 4)$  designs

1:	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4	
	2	2	2	2	3	4	4	6	7	3	4	4	5	5	4	4	5	6	5
	3	3	3	5	5	5	6	7	8	6	6	7	7	8	5	7	6	8	6
	4	4	7	6	8	9	8	9	9	9	8	9	8	9	9	8	7	9	7
	5	10	12	10	10	12	11	10	11	13	12	10	11	10	11	10	11	10	10
	6	11	15	11	13	14	14	13	12	14	13	11	13	12	13	14	12	11	12
	7	12	16	15	17	16	15	14	13	15	16	17	14	14	15	15	14	12	13
	8	13	18	16	18	17	18	16	15	17	17	18	16	15	16	16	17	16	15
	9	14	19	17	19	18	19	19	17	18	19	19	18	19	19	17	19	18	18
2:	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4	
	2	2	2	2	3	4	4	5	7	3	4	4	5	6	4	4	5	6	5
	3	3	3	5	5	6	8	6	8	8	5	6	7	7	5	6	6	7	7
	4	4	7	6	8	7	9	9	9	9	9	8	9	8	7	9	8	9	8
	5	10	12	10	10	11	11	12	10	11	10	12	11	10	13	10	11	10	10
	6	11	15	11	13	14	13	13	12	14	14	13	12	13	14	12	12	11	11
	7	12	16	15	17	17	15	14	14	15	16	16	13	14	15	15	14	13	12
	8	13	18	16	18	18	16	15	16	17	18	17	17	15	16	17	16	16	15
	9	14	19	17	19	19	18	19	17	19	19	19	18	18	17	18	18	19	19

3:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	2	3	4	4	5	6	3	4	4	5	6	4	4	5	6	5
	3	3	3	5	5	6	8	7	8	8	5	6	7	7	5	7	6	7	7
	4	4	7	6	8	7	9	9	9	9	9	8	8	9	6	9	9	8	8
	5	10	12	10	10	13	11	11	10	13	10	11	11	10	12	10	11	10	10
	6	11	15	11	13	14	12	13	12	14	14	13	12	12	14	11	12	11	12
	7	12	16	15	17	15	15	14	14	15	15	16	14	13	16	16	13	14	13
	8	13	18	16	18	17	17	16	16	16	18	18	17	17	17	17	15	15	15
	9	14	19	17	19	18	19	19	18	17	19	19	18	19	19	18	18	19	16
4:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3	4
	2	2	2	2	3	4	4	5	6	3	4	4	5	7	4	4	5	6	5
	3	3	3	5	5	6	7	8	7	8	5	6	6	8	5	6	6	7	7
	4	4	7	6	8	8	9	9	9	9	7	8	9	9	9	9	7	8	8
	5	10	12	10	10	11	10	12	11	11	13	12	10	10	11	10	11	10	10
	6	11	15	11	13	14	14	13	12	14	14	13	12	11	12	13	13	12	11
	7	12	16	15	17	15	16	14	13	16	15	16	14	13	15	15	14	14	12
	8	13	18	16	18	18	17	15	17	17	17	17	18	15	17	16	16	15	16
	9	14	19	17	19	19	18	16	19	19	19	18	19	18	18	19	18	17	19
5:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4	4
	2	2	2	2	3	3	4	5	7	3	3	4	4	6	4	5	6	5	5
	3	3	5	7	4	5	6	6	8	5	6	5	8	7	6	8	7	6	7
	4	4	6	8	9	7	8	9	9	8	9	7	9	9	7	9	8	8	9
	5	10	10	12	14	10	11	12	10	11	10	13	10	11	11	11	10	10	10
	6	11	11	13	15	12	13	13	11	14	13	14	12	12	12	12	13	12	11
	7	12	15	15	16	17	17	14	14	15	16	16	15	14	15	13	14	14	13
	8	13	16	16	17	18	18	15	16	18	18	17	17	17	16	16	15	16	15
	9	14	17	18	18	19	19	19	19	19	19	19	19	18	19	17	17	18	18
6:	1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	4	5
	2	2	2	2	3	3	4	4	5	3	3	4	4	6	4	4	6	5	6
	3	3	5	7	5	6	6	8	7	5	8	5	6	7	5	7	7	7	8
	4	4	6	8	7	8	9	9	9	9	9	8	7	9	6	9	8	8	9
	5	10	10	12	10	11	12	10	11	13	11	10	11	10	12	10	10	11	10
	6	11	11	13	12	14	14	13	13	14	12	14	13	12	13	11	13	12	11
	7	12	15	15	17	15	16	15	14	15	16	16	17	14	15	15	14	14	12
	8	13	16	16	18	18	17	17	16	17	17	18	18	15	16	16	16	15	13
	9	14	17	18	19	19	18	19	19	18	19	19	19	19	19	18	17	17	18

# Appendix B

## Robustness of Non-Symmetric BIBDs against Removal of 3 Blocks

Table B.1: Comparison of  $(7, 3, 2)$  designs robustness against loss of 3 blocks

Design no.	A-efficiency		E-efficiency		MV-efficiency	
	average	min	average	min	average	min
1	0.749314	0.718759	0.563039	0.449888	0.596607	0.486322
2	0.749122	0.718759	0.553776	0.443479	0.580014	0.484457
3	0.749025	0.718759	0.549144	0.443479	0.571718	0.484457
4	0.748977	0.7229	0.546828	0.443479	0.56757	0.484457

Table B.2: Comparison of  $(8, 4, 3)$  designs robustness against loss of 3 blocks

Design no.	A-efficiency		E-efficiency		MV-efficiency	
	average	min	average	min	average	min
1	0.762486	0.74708	0.582121	0.5	0.609594	0.5
2	0.762498	0.74708	0.58252	0.5	0.609619	0.5
3	0.762504	0.74708	0.58272	0.5	0.609632	0.5
4	0.762462	0.754163	0.581322	0.5	0.609544	0.5

Table B.3: Comparison of  $(9, 4, 3)$  designs robustness against loss of 3 blocks

Design no.	A-efficiency		E-efficiency		MV-efficiency	
	average	min	average	min	average	min
1	0.816031	0.802708	0.645385	0.555556	0.665621	0.555556
2	0.816024	0.802708	0.644657	0.555556	0.665102	0.555556
3	0.816029	0.802708	0.645203	0.555556	0.665491	0.555556
4	0.816027	0.802708	0.645021	0.555556	0.665361	0.555556
5	0.816027	0.802708	0.645021	0.555556	0.665361	0.555556
6	0.816024	0.802708	0.644657	0.555556	0.665102	0.555556
7	0.816031	0.802708	0.645385	0.555556	0.665621	0.555556
8	0.816031	0.802708	0.645385	0.555556	0.665621	0.555556
9	0.816033	0.802708	0.645567	0.555556	0.665751	0.555556
10	0.816031	0.802708	0.645385	0.555556	0.665621	0.555556
11	0.816017	0.807853	0.64393	0.555556	0.664583	0.555556

Table B.4: Comparison of  $(10, 5, 4)$  designs robustness against loss of 3 blocks

Design no.	A-efficiency		E-efficiency		MV-efficiency	
	average	min	average	min	average	min
1	0.820697	0.812197	0.666057	0.625	0.690907	0.625
2	0.820696	0.812197	0.666119	0.625	0.690698	0.625
3	0.820696	0.812197	0.66618	0.625	0.690489	0.625
4	0.820696	0.812197	0.666307	0.625	0.690283	0.625
5	0.820697	0.812197	0.666309	0.625	0.690495	0.625
6	0.820697	0.813478	0.666562	0.625	0.690082	0.625
7	0.820696	0.813478	0.666497	0.625	0.690079	0.625
8	0.820698	0.812197	0.666312	0.625	0.690706	0.625
9	0.820696	0.812197	0.666339	0.625	0.690284	0.625
10	0.820697	0.812197	0.666436	0.625	0.690288	0.625
11	0.820696	0.812197	0.666276	0.625	0.690387	0.625
12	0.820695	0.812197	0.666211	0.625	0.690385	0.625
13	0.820696	0.812197	0.666307	0.625	0.690283	0.625
14	0.820696	0.812197	0.66637	0.625	0.69018	0.625
15	0.820697	0.812197	0.666183	0.625	0.690701	0.625
16	0.820696	0.812197	0.666245	0.625	0.690492	0.625
17	0.820695	0.813791	0.666401	0.625	0.690075	0.625
18	0.820696	0.812197	0.666307	0.625	0.690283	0.625
19	0.820696	0.812197	0.666371	0.625	0.690286	0.625
20	0.820696	0.813478	0.666433	0.625	0.690077	0.625
21	0.820696	0.812197	0.666244	0.625	0.690386	0.625

# Appendix C

## Robustness of BIBDs against Removal of 4 Blocks

Table C.1: Comparison of  $(7, 3, 2)$  designs robustness against loss of 4 blocks

Design no.	A-efficiency		E-efficiency		MV-efficiency	
	average	min	average	min	average	min
1	0.665062	0.590164	0.460458	0.285714	0.501619	0.360902
2	0.664658	0.590164	0.451309	0.285714	0.486507	0.360902
3	0.664457	0.597015	0.446798	0.285714	0.478807	0.362812
4	0.664356	0.610869	0.444558	0.298764	0.474921	0.367498

Table C.2: Comparison of  $(8, 4, 3)$  designs robustness against loss of 4 blocks

Design no.	A-efficiency		E-efficiency		MV-efficiency	
	average	min	average	min	average	min
1	0.68269	0.658258	0.494199	0.391767	0.512322	0.426032
2	0.682717	0.658258	0.49431	0.391767	0.513411	0.426032
3	0.68273	0.658258	0.494391	0.391767	0.513959	0.426032
4	0.682636	0.668678	0.494177	0.401883	0.510176	0.426471

Table C.3: Comparison of  $(9, 4, 3)$  designs robustness against loss of 4 blocks

Design no.	A-efficiency		E-efficiency		MV-efficiency	
	average	min	average	min	average	min
1	0.754457	0.728374	0.566397	0.457154	0.586938	0.491362
2	0.754442	0.728374	0.565929	0.457154	0.586307	0.491362
3	0.754453	0.732467	0.566286	0.459349	0.586771	0.491694
4	0.754449	0.732467	0.566162	0.459349	0.586615	0.491694
5	0.754449	0.732467	0.566161	0.459349	0.586615	0.491694
6	0.754442	0.732467	0.565921	0.459349	0.586305	0.491694
7	0.754457	0.732467	0.566407	0.459349	0.586938	0.491694
8	0.754457	0.732467	0.566411	0.459349	0.586932	0.491694
9	0.75446	0.732467	0.566544	0.459349	0.587086	0.491694
10	0.754457	0.732467	0.566413	0.459349	0.586929	0.491694
11	0.754427	0.739735	0.565478	0.46834	0.585691	0.491918

Table C.4: Comparison of  $(10, 5, 4)$  designs robustness against loss of 4 blocks

Design no.	A-efficiency		E-efficiency		MV-efficiency	
	average	min	average	min	average	min
1	0.760761	0.745618	0.598158	0.5	0.613604	0.5
2	0.76076	0.745618	0.597849	0.5	0.613194	0.5
3	0.760758	0.745618	0.597546	0.5	0.612601	0.5
4	0.760758	0.745618	0.597443	0.5	0.612366	0.5
5	0.760761	0.745618	0.597881	0.5	0.613477	0.5
6	0.760761	0.746976	0.597597	0.5	0.613351	0.5
7	0.76076	0.746697	0.597423	0.5	0.613003	0.5
8	0.760764	0.745618	0.598325	0.5	0.614782	0.5
9	0.760759	0.745876	0.597489	0.5	0.612804	0.5
10	0.760761	0.745618	0.597712	0.5	0.613592	0.5
11	0.760759	0.745876	0.597556	0.5	0.612834	0.5
12	0.760758	0.745876	0.597405	0.5	0.612308	0.5
13	0.760758	0.745618	0.597394	0.5	0.612534	0.5
14	0.760758	0.745876	0.59734	0.5	0.612508	0.5
15	0.760761	0.745618	0.598006	0.5	0.613724	0.5
16	0.76076	0.745618	0.597704	0.5	0.61313	0.5
17	0.760758	0.747282	0.597195	0.5	0.612213	0.5
18	0.760758	0.745876	0.597441	0.5	0.612366	0.5
19	0.76076	0.745876	0.597561	0.5	0.613066	0.5
20	0.760758	0.746976	0.597262	0.5	0.612473	0.5
21	0.760758	0.745876	0.597478	0.5	0.61257	0.5

Table C.5: Comparison of  $(15, 7, 3)$  designs robustness against loss of 4 blocks

Design no.	A-efficiency		E-efficiency		MV-efficiency	
	average	min	average	min	average	min
1	0.705949	0.70179	0.498281	0.415302	0.520952	0.45598
2	0.705948	0.70179	0.495927	0.414923	0.515866	0.4559
3	0.705948	0.70179	0.494162	0.414923	0.512051	0.4559
4	0.705948	0.70179	0.49475	0.414923	0.513323	0.4559
5	0.705948	0.70179	0.494162	0.414923	0.512051	0.4559

Table C.6: Comparison of  $(19, 9, 4)$  designs robustness against loss of 4 blocks

Design no.	A-efficiency		E-efficiency		MV-efficiency	
	average	min	average	min	average	min
1	0.774243	0.77209	0.587875	0.526316	0.804336	0.686037
2	0.774243	0.77209	0.587874	0.526316	0.803831	0.686037
3	0.774243	0.77209	0.587877	0.526316	0.805341	0.686037
4	0.774243	0.77209	0.587873	0.526316	0.803481	0.686037
5	0.774243	0.77209	0.587874	0.526316	0.804031	0.686037
6	0.774243	0.77209	0.587876	0.526316	0.804686	0.686037

# Appendix D

## MIA Designs

Table D.1: A MIA (6, 3, 4) balanced incomplete block design

1	1	1	1	1	1	1	1	1	1	2	2	2	2	2	2	3	3	3	4
2	2	2	2	3	3	3	4	4	5	3	3	3	4	4	5	4	4	5	5
3	4	5	6	4	5	6	5	6	6	4	5	6	5	6	6	5	6	6	6

Table D.2: A MIA (6, 3, 6) balanced incomplete block design

1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	2	2	2	2	2	3	3	3	3	4	4	4	5	5	
3	3	4	4	5	6	4	5	5	6	5	6	6	6	6	
2	2	2	2	2	2	2	2	2	2	3	3	3	3	3	4
3	3	3	3	4	4	4	5	5	4	4	4	4	5	5	
4	5	6	6	5	5	6	6	6	6	5	5	6	6	6	

Table D.3: A MIA (7, 3, 2) balanced incomplete block design

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

Table D.4: A MIA (7, 3, 3) balanced incomplete block design

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

Table D.5: A MIA (7, 3, 4) balanced incomplete block design

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

Table D.6: A MIA (7, 3, 5) balanced incomplete block design

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

Table D.7: A MIA (8, 4, 3) balanced incomplete block design

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

Table D.8: A MIA (8, 4, 6) balanced incomplete block design

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

Table D.9: A MIA (9, 3, 2) balanced incomplete block design

1	1	1	1	1	1	1	1	2	2	2	2	2	2	3	3	3	3	3	4	4	4	4	4	4	4
2	2	3	5	5	6	7	8	3	5	5	6	7	8	5	5	6	6	7	5	5	6	6	7	7	7
3	4	4	6	7	8	9	9	4	6	7	8	9	9	8	9	7	9	8	8	9	7	9	8	8	8

Table D.10: A MIA (9, 3, 3) balanced incomplete block design

1	1	1	1	1	1	1	1	1	1	1	1	1	2	2	2	2	2	2	2	2	2	2	2	2	2
2	2	2	3	3	4	6	6	6	7	7	8	3	3	4	4	4	5	5	5	5	5	5	5	5	5
3	4	5	4	5	5	7	8	9	8	9	9	6	7	6	7	8	9	9	9	9	9	9	9	9	9
2	2	2	3	3	3	3	3	3	3	4	4	4	4	4	4	5	5	5	5	5	5	5	5	5	5
6	7	8	4	4	5	5	6	7	8	5	5	6	6	7	6	6	7	6	6	7	6	6	7	6	7
8	9	9	8	9	6	7	8	9	9	8	9	7	9	8	7	9	8	7	9	8	7	9	8	7	9

Table D.11: A MIA (9, 4, 3) balanced incomplete block design

1	1	1	1	1	1	1	1	2	2	2	2	2	2	3	3	3	4	5	5	5	5	5	5	5	5	5
2	2	2	3	3	4	4	5	3	3	4	4	6	4	4	4	6	5	6	5	6	5	6	5	6	5	6
3	5	7	5	6	6	7	8	5	7	5	6	8	5	8	7	7	7	7	7	7	7	7	7	7	7	7
4	6	8	7	9	8	9	9	8	9	9	7	9	6	9	8	8	9	8	9	8	9	8	9	8	9	8

Table D.12: A MIA (10, 3, 2) balanced incomplete block design

1	1	1	1	1	1	1	1	1	2	2	2	2	2	2
2	2	3	5	5	6	8	8	9	3	5	5	6	7	8
3	4	4	6	7	7	9	10	10	4	6	7	8	9	10
2	3	3	3	3	3	3	4	4	4	4	4	4	5	6
9	5	5	6	6	7	7	5	5	6	6	7	7	8	7
10	8	10	9	10	8	9	9	10	8	9	8	10	9	10

Table D.13: A MIA (10, 4, 2) balanced incomplete block design

1	1	1	1	1	1	2	2	2	2	3	3	3	4	4
2	2	3	4	6	7	3	4	5	6	4	5	6	5	5
3	5	5	8	8	9	8	7	8	7	6	9	7	6	7
4	6	7	9	10	10	9	10	10	9	10	10	8	9	8

Table D.14: A MIA (10, 4, 4) balanced incomplete block design

1	1	1	1	1	1	1	1	1	1	1	1	2	2	2
2	2	2	2	3	3	3	4	4	4	5	6	3	3	3
3	5	7	9	5	6	8	5	6	7	8	7	5	6	7
4	6	8	10	7	9	10	10	8	9	9	10	8	10	9
2	2	2	2	2	3	3	3	3	3	4	4	5	5	7
4	4	4	5	6	4	4	4	5	6	5	6	6	6	8
5	6	8	7	8	5	7	8	9	7	7	9	7	8	9
9	7	10	10	9	6	10	9	10	8	8	10	9	10	10

Table D.15: A MIA (10, 5, 4) balanced incomplete block design

1	1	1	1	1	1	1	1	1	2	2	2	2	2	3	3	3	3
2	2	2	2	3	4	4	5	6	3	4	4	5	5	4	4	4	5
3	3	3	4	5	5	7	7	7	7	5	8	6	6	5	6	6	6
4	6	8	6	8	6	8	9	8	9	7	9	7	8	7	7	9	8
5	7	9	10	10	9	9	10	10	10	8	10	9	10	10	8	10	9

# Vita

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