Optimal Block Designs with Limited Resources

Bo Jin

Dissertation submitted to the Faculty of Virginia Polytechnic Institute and State University in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

in

Statistics

John P. Morgan, chair

Eric P. Smith

Boxin Tang

George R. Terrell

Keying Ye

Nov. 12, 2004

Blacksburg, Virginia

Keywords: block designs, optimal designs

Optimal Block Designs with Limited Resources

Bo Jin

Abstract

In this dissertation we present new results regarding optimality of block designs with limited resources. The dissertation is organized as follows. The *first* chapter outlines the theory of optimal block design. The *second* chapter shows new work in optimal minimally connected block designs with spatial correlation structure. The *third* chapter details the discovery of the optimal incomplete designs with two blocks. The *fourth* chapter does the same for the optimal binary incomplete designs with three blocks. The *fifth* chapter summarizes the techniques used and new results found and lists possible future research topics.

Acknowledgements

I would like to thank Dr. J. P. Morgan, who has been there for me every step of the way, teaching, encouraging and helping. I greatly appreciate the time and efforts he has given to me and to my work. I have enjoyed working with him. What he has taught in the past few years will benefit me all my life.

I would also like to recognize the contribution of my committee members, Dr. Eric P. Smith, Dr. Boxin Tang, Dr. George Terrell and Dr. Keying Ye. I am so thankful to them for serving on my committee and for their helpful and constructive suggestions.

Contents

List of Figures

List of Tables

Chapter 1

Theory of Optimal Block Design

1.1 Summary

In this chapter we present an overview of the theory of optimal block design. Section 1.2 contains the linear model set-up for block designs. In section 1.3 we discuss several optimality criteria that are commonly used. In section 1.4 we present a general procedure for finding optimal block designs.

1.2 The Linear Model

In this section we consider the linear model set-up for block designs.

Definition 1.1. Suppose there are v treatments to be compared using n experimental units. The units are partitioned into b groups (blocks) of k units each ($n = bk$). A block design is an assignment of the v treatments to the bk units. Denote the class of all possible such assignments as $D(v, b, k)$.

Usually we will assume the observation-vector $\underline{Y}_{n\times 1}$ for a design $d \in D(v, b, k)$ follows a standard linear model,

$$y_{ju} = \mu + \tau_{d[j,u]} + \beta_j + e_{ju} \tag{1.1}$$

where y_{ju} is the yield of unit u in block j, μ is the overall mean, $\tau_{d[j,u]}$ is the effect of the treatment assigned to unit u in block j by design d, β_j is block effect, and e_{ju} is the error term assumed to have mean zero and positive definite variance matrix.

Written in matrix form, with the observation vector ordered $\underline{Y} = (y_{11}, y_{12}, \ldots, y_{1k}, y_{21}, y_{22}, \ldots, y_{2k}, \ldots, y_{bk})'$, the model in 1.1 becomes

$$\begin{aligned} \underline{Y} &= \mu\underline{1} + A_d\underline{\tau} + L\underline{\beta} + \underline{e} && (1.2) \\ Cov(\underline{e}) &= \Sigma && (1.3) \end{aligned}$$

where Σ is a positive definite $n \times n$ matrix (usually $\sigma^2 I_n$) and $L = I_b \otimes \underline{1}_k$. In any row of A_d $(n \times v)$ there is exactly one 1 and the rest are 0's. If the row corresponds to plot u in block j, then the 1 lies in the column $i \in \{1, 2, \ldots, v\}$ if and only if $\tau_{d[j,u]} = i$.

Suppose $Cov(\underline{\varepsilon}) = \sigma^2 I_n$. Then the reduced normal equations for $\underline{\tau}$ are

$$C_d\underline{\tau} = Q \tag{1.4}$$

where

$$\begin{aligned} C_d &= A_d'A_d - \frac{1}{k}A_d'LL'A_d && (1.5) \\ Q &= A_d'(I - \frac{1}{k}LL')\underline{Y}. && (1.6) \end{aligned}$$

Denote

$$N_d = A_d'L. \tag{1.7}$$

N_d $(v \times b)$ is called the incidence matrix of the design $d \in D(v, b, k)$ and its $(i, j)th$ element, denoted as n_{dij}, is the number of times that treatment i is used in block j. In addition, we have the (i, i') element, where $i, i' \in \{1, 2, \cdots v\}$, of N_dN_d' is

$$(N_dN_d')_{ii'} = \sum_{j=1}^{b} n_{dij}n_{di'j}. \tag{1.8}$$

$(N_dN_d^{'})_{ii'}$ is the *concurrence* of treatments i and $i^{'}$ under the design d, denoted by $\lambda_{dii'}$.

Write

$$r_{di} = \sum_{j=1}^{b} n_{dij}. \tag{1.9}$$

Then r_{di} is the replicate number of treatment i. It can be seen that

$$A_d^{'}A_d = D(r_{di}) \tag{1.10}$$

where $D(r_{di})$ is a diagonal matrix with r_{di} on the diagonal.

By (1.5), (1.7) and (1.10), the matrix C_d is

$$C_d = D(r_{di}) - \frac{1}{k}N_dN_d^{'}. \tag{1.11}$$

C_d is called the *information matrix* of design d. One reason C_d is important is that a linear combination of treatment effects with coefficient vector $\underline{p}$ is estimable if and only if $\underline{p}$ belongs to its row space. Since $C_d\underline{1}_v = \underline{0}_v$, only the linear functions $\underline{p}^{'}\underline{\tau}$ with coefficient vector $\underline{p}$ satisfying $\underline{p}^{'}\underline{1}_v = \underline{0}_v$ can be estimated. Such linear functions are referred to as treatment contrasts. It is known that $rank(C_d) = v - 1$ if and only if all treatment contrasts are estimable, and in that case, the underlying design is said to be *connected*. In this dissertation, we will be exclusively dealing with connected designs.

1.3 Choice of Optimality Criteria

1.3.1 Basic Consideration

We address the problem of suggesting a suitable class of optimality criteria for comparison of experiments involving linear models in (1.2). Specifically, denote by Ω the class of available C_d matrices in a given experimental set up $D(v, b, k)$. Denote by Φ the class of optimality functions ϕ defined on the members in Ω. The optimality functionals may be aimed at providing symmetric measures of the lack of information contained in the C_d matrices. Shah and Sinha (1989) brought up four requirements to be satisfied by the optimality function ϕ, which are laid down as follows:

Definition 1.2. (**Shah and Sinha (1989)**)

A function ϕ is an *optimality function* if it satisfies the following four conditions:

1. $\phi(C_d) = \phi(C_{dg})$, where $C_{dg} = G_g^{'} C_d G_g$, g is any member of the symmetric group of permutations, and G_g denote the corresponding permutation matrix, i.e., the matrix obtained by applying g to the columns of the identity matrix. The condition says that the information contained in C_d is invariant to the symmetric group of permutations on the treatment symbols.

2. If $C_{d1} \succeq C_{d2}$, then $\phi(C_{d1}) \leq \phi(C_{d2})$. By $C_{d1} \succeq C_{d2}$, we mean that $C_{d1} - C_{d2}$ is a non-negative definite matrix.

3. If $\phi(C_{d1}) \geq \phi(C_{d2})$, then $\phi(tC_{d1}) \geq \phi(tC_{d2})$ and vice versa for any integer $t \geq 1$. The condition says that C_{d2} is ϕ better than C_{d1} if and only if so are t copies of the former design compared to the t copies of the latter.

4. $\phi(\sum t_g C_{dg}) \leq \phi((\sum t_g) C_d)$ for any integer numbers $t_g \geq 1$. This condition means a combination of various forms of d under permutations g would be no worse than an exclusive use of d itself.

In particular, (4) implies,

$4^{'}$ $\phi(\sum C_{dg}) \leq \phi(v! C_d)$ by taking all possible permutation of v treatment symbols and $t_g = 1$.

We may say that a design is *optimal* in a very general sense if the underlying C_d matrix minimizes each optimality functional ϕ satisfying conditions $1 - 4$.

As pointed out by Shah and Sinha (1989), the requirement $4^{'}$ is the *symmetry* requirement on the optimality functionals ϕ; the requirement 4 is in fact the property of *weak convexity*;

the requirements of 1 and 3 together with convexity condition implies 4; and 4 is satisfied by all functions of the form $\phi(C_d) = \pi(f(C_d))$ where π is monotone increasing, and f is convex satisfying 1 and 3.

1.3.2 Universal Optimality

Kiefer's version. Kiefer (1975) introduced the notion of *Universal Optimality* in the following manner. Consider optimality functionals ϕ satisfying the following conditions:

$$
\begin{aligned}
&i)\ \phi(C_d) = \phi(C_{dg}) \text{ (same as requirement 1 in last section.)}\\
&ii)\ \phi(tC_d) \text{ is non-increasing in } t \text{ where } t \geq 0.\\
&iii)\ \phi(\theta C_{d1} + (1-\theta)C_{d2}) \leq \theta\phi(C_{d1}) + (1-\theta)\phi(C_{d2}) \text{ for } 0 < \theta < 1.
\end{aligned}
\tag{1.12}
$$

If a design is optimal with respect to all such optimal functionals ϕ, it is said to be *universally optimal.*

As pointed out by Shah and Sinha (1989), the condition of convexity (1.12)(iii) imposed on the optimality functionals implies weak convexity 4 and hence the symmetry condition $4'$. However, the usual convexity does not appear to have any statistical interpretation while $4'$ (or even 4 of which $4'$ is a special case) is appealing in a reasonable statistical sense. Furthermore, 4 (or $4'$) relates only to a set of feasible C_d matrices while the usual convexity may not relate to feasible ones when considering arbitrary convex combinations. Therefore, Shah and Sinha (1989) set forth a definition of extended universal optimality.

Extended Universal Optimality A design is said to be universally optimal in an extended sense in a given design class if the underlying C_d matrix minimizes every optimality function ϕ satisfying the requirements of 1,2,3 and $4'$ among all possible C_d matrices in that class.

The theorem below (Shah and Sinha (1989)) is a modified version of the universal optimality theorem by Kiefer (1975) in terms of extended universal optimality. For the detailed proof one may refer to Shah and Sinha (1989).

Theorem 1.1. If there is a feasible C_d matrix which is completely symmetric and has maximum trace, then the underlying design is universally optimal in the extended sense of minimizing ϕ simultaneously for all functionals ϕ satisfying 1,2,3,and $4'$.

Now we will present some known universal optimal designs.

Definition 1.3. A design $d \in D(v, b, k)$ is said to be *binary* if $n_{dij} \in \{0, 1\}$ $\forall$ i, j; is said to be generally binary if $n_{dij} \in \{\lfloor \frac{k}{v} \rfloor, \lfloor \frac{k}{v} \rfloor + 1\}$ $\forall$ i, j.

Definition 1.4. A design $d \in D(v, b, k)$ is said to be *combinatorially balanced* if it is equally replicated ($r_{di} = \frac{bk}{v}$) and $\lambda_{dii'}$ are constant ($\lambda_{dii'} = \frac{r(k-1)}{v-1}$) for any $i \neq i'$.

Definition 1.5. BIBD. A design $d \in D(v, b, k)$ with $k < v$ is called a *balanced incomplete block design* (BIBD) if it satisfies:

1) d is binary, i.e., $n_{dij} \in \{0, 1\}$, and

2) d is combinatorially balanced.

Definition 1.6. BBD. A design $d \in D(v, b, k)$ is said to be a *bottom-stratum balanced design* (BBD) if

1) d is generally binary, and

2) d is combinatorially balanced.

Below is a modified version of a theorem given by Kiefer (1975).

Theorem 1.2. If there exists a design $d^* \in D(v, b, k)$ which is a BIBD or BBD, then d^* is a universally optimal design in $D(v, b, k)$.

1.3.3 Specific Optimality Criteria

The values of (v, b, k) for which usually the universally optimal designs exist are fairly rare. In this section we discuss different *specific* optimality criteria currently in use. We first present the Type I-criteria introduced by Cheng (1978). Then we will specialize to the specific criteria, namely the A-, D- and E-optimality functions.

Type I-optimality. Following Cheng (1978), let us consider a class of optimality functions (to be minimized) of the form

$$\phi_f(C_d) = \sum_{i=1}^{v-1} f(z_{di}) \tag{1.13}$$

where f is a non-increasing and convex real valued function and z_{di}'s are $v-1$ positive eigenvalues of C_d. Without loss of generality let $0 < z_{d1} \leq z_{d2} \leq \cdots \leq z_{d,v-1}$. A design is said to be ϕ_f-optimal in $D(v,b,k)$ provided $\phi_f(C_d)$ is minimal over all designs in $D(v,b,k)$.

Definition 1.7. The function ϕ_f of (1.13) is called a Type I-optimality criterion if f satisfies the following conditions:

(1) f is continuously differentiable on $(0, max_{d\in D(v,b,k)} tr(C_d))$, and $f' < 0$,$f'' > 0$, $f''' < 0$ on $(0, max_{d\in D(v,b,k)} tr(C_d))$.

(2) f is continuous at 0 and $lim_{x\to 0} f(x) = f(0) = \infty$.

Two of the most widely used criteria, called A- and D-, are Type I-criteria, corresponding to $f(z_{di}) = \frac{1}{z_{di}}$ and $f(z_{di}) = -log(z_{di})$ respectively. Specifically, they are defined as follows:

Definition 1.8. A-optimality. A design $d^* \in D(v,b,k)$ is A-optimal if it minimizes $\sum_{i=1}^{v-1} \frac{1}{z_{di}}$ over all possible designs in $D(v,b,k)$.

Definition 1.9. D-optimality. A design $d^* \in D(v,b,k)$ is D-optimal if it minimizes $\sum_{i=1}^{v-1}(-log(z_{di}))$ (or equivalently minimizes $\prod_{i=1}^{v-1} \frac{1}{z_{di}}$) over all possible designs in $D(v,b,k)$.

There is another commonly used criterion which is not of Type I-.

Definition 1.10. E-optimality. A design $d^* \in D(v,b,k)$ is E-optimal design if it minimizes $\frac{1}{z_{d1}}$ (maximizes z_{d1}) over all possible designs in $D(v,b,k)$.

A-, D- and E-optimality criteria were widely used well before the Type I-class was introduced. These arise quite naturally in various statistical inference problems. We explain the statistical meanings of the three criteria for block designs next.

The idea of E-optimality arises in the following situations: Suppose we want to estimate all (normalized) linear contrasts of the treatment effects $\underline{\tau}$. Then the maximum variance of such a contrast is the inverse of the smallest positive eigenvalue of C_d, i.e, z_{d1}. The E-optimal design is the one that minimizes this maximum variance among all possible designs.

Next suppose we are interested in the $100(1-\alpha)$ percent confidence ellipsoid for a complete orthonormal set of treatment contrasts, assuming normality of the linear model (1.2). It is known that the volume of this ellipsoid is proportional to the square root of the inverse of the product of positive eigenvalues of C_d. This inverse is called the *generalized variance*. The D-optimal design is the one that minimizes the generalized variance.

For A-optimality, the idea is to minimize the average variance for any orthonormal set of treatment contrasts. It turns out that this average is just the sum of the inverses of the positive eigenvalues of C_d. Furthermore, this sum is also proportional to the average variance of all $\binom{v}{2}$ pairwise elementary treatment contrasts, so A-optimal designs also minimize the average variance.

It is important to study relationships among various criteria, because if optimality criteria are included in a larger class, a design which is optimal with respect to each criterion in the larger class is optimal with respect to each criterion in the smaller class. For instance, if we are able to use a general technique to prove optimality with respect to all Type I-criteria, we get specific optimality of interest, such as A- and D-.

From the previous discussion, the extended universal optimality criteria form the largest class. Progressively smaller, are the universal optimality criteria class and Type I-criteria class, and finally the A- and D-criteria. The E- criterion is not covered by the Type I-criteria class, but is by universal optimality and extended universal optimality. In fact, the E- criterion is the point-wise limit of a sequence of Type I- criteria (see Shah and Sinha

(1989, page 9)).

1.4 General Procedure for Finding Optimal Block Designs

The following are several facts based on the current state of research for optimal block designs.

1) Extended universal (or universal) optimal block designs are usually non-achievable. The conditions on (v, b, k) under which BBD or BIBD designs exist are very strict. In other settings, there may be different optimal designs with respect to different criteria.

2) A design may be known to be optimal in many senses in $D(v, b, k)$, but current theory does not allow universal optimality to be established.

3) There are many settings (v, b, k) for which optimal designs are still not known.

In light of these facts, we employ this general procedure for finding optimal block designs:

1) Propose a design as potentially optimal with respect to some criterion. Usually the proposed design is binary, as combinatorially balanced as possible.

2) Compare the proposed design with other designs using known inequalities and theorems. In the following chapters, we will discuss these inequalities and theorems in detail. Sometimes we also need to use combinatorial arguments.

3) If some other design is discovered to be better than the proposed design, then set this design as the proposed optimal design and repeat 1) and 2). Continue this procedure until we cannot find a better design than the proposed design. Hopefully, the proposed design will be found to be optimal in $D(v, b, k)$ with respect to some criterion.

There are some known results with respect to different criteria including those for BIBDs and BBDs detailed above. These typically require binarity, equal replication, and close approximation to combinatorial balance. One may refer to Shah and Sinha (1989) for a more extensive summary. However, as is already mentioned, in many situations optimal designs remain unknown. Even for a specific criterion, there is no denying the fact that a satisfactory study of optimality aspects of designs is quite difficult using currently known inequalities and theorems and available results are not extensive. Additional difficulty is found in the fact that for a specific optimality problem, combinatorial structure study is sometimes very tough.

In the chapters that follow we will work on problems where experimental resources are limited. When experimental resources are limited, we are usually unable to attain any reasonable degree of "closeness" to combinatorial balance in our choice of design. In such situations the intuition engendered by work on BIBDs or other nearly balanced designs can fail. Indeed, in some cases, optimality will require nonbinarity, and in others, replication numbers that are not as equal as possible.

Three specific problems are attacked in chapters 2 through chapter 4. Chapter 2 presents new work on optimal minimally connected block designs with spatial correlation structure. Chapter 3 details the discovery of the optimal incomplete designs with two blocks. Chapter 4 does the same for the optimal binary incomplete designs with three blocks.

Chapter 2

Optimal Minimally Connected Designs For Correlated Observations

2.1 Summary

A- and MV-optimal block designs are identified in the class of minimally connected designs when the observations within blocks are spatially correlated. A sufficient condition for E-optimal designs is presented.

2.2 The Problem

Consider the situation where an experimenter is planning a block design experiment d for comparing the relative effectiveness of v treatments. It is well known that all treatment contrasts are estimable under d if and only if d is connected. If n denotes the total number of experimental units in d, then a necessary condition for d to be connected is that $n \geq b + v - 1 = n_0$.

Several papers have appeared in the literature which discuss optimality of connected block designs when the number of experimental units is minimal, or equivalently, $n = n_0$. Let $D(v, b, k)$ denote the class of all connected block designs having v treatments, b blocks and constant block size $k \geq 2$ satisfying

$$bk = b + v - 1 \tag{2.1}$$

It is known that there is an uniquely A-, MV-, and E-optimal design $d \in D$ when observations within blocks are uncorrelated (Bapat and Dey (1991), Mandal, Shah and Sinha (1991)).

In this chapter, the A- , MV- and E-optimality of block designs are studied in the class $D(v, b, k)$ when observations within blocks are spatially correlated. Let the experimental units be sequentially ordered $u = 1, 2, \ldots, k$ in j^{th} block and as usual let y_{ju} denote the observation for the u^{th} experimental unit in the j^{th} block. Consider the spatial correlation structure

$$Cov(y_{ju}, y_{j'u'}) = \begin{cases} \sigma^2 & \text{if } j = j', u = u' \\ 0 & \text{if } j \neq j' \\ \rho_{|u-u'|}\sigma^2 & \text{if } j = j', u \neq u' \end{cases} \tag{2.2}$$

where

$$1 > \rho_1 \geq \rho_2 \geq \rho_3 \geq \ldots \geq \rho_{k-1} \geq 0. \tag{2.3}$$

In addition we assume that the corresponding variance-covariance matrix Σ for observations $\underline{y}$ is positive definite, i.e.

$$\underline{a}^{'}\Sigma\underline{a} > 0 \text{ for any } \underline{a} \neq 0 \tag{2.4}$$

The chapter proceeds as follows. Section 2.3 discusses the basic properties of minimally connected designs. In section 2.4 we identify A-optimal designs in the class $D(v, b, k)$ under the conditions (2.1), (2.2), (2.3) and (2.4). It turns out that the A-optimal designs are also the MV-optimal designs, as shown in section 2.5. In section 2.6 we study E-optimal designs in $D(v, b, k)$.

2.3 Properties of Minimally Connected Designs

In this section we first present three results on the structure of designs in the class *D(v,b,k)* under condition (3.1). Proofs for the first two lemmas were given by Bapat and Dey (1991). All three lemmas also hold for the spatial correlation structure, since estimability depends only on first-order moments.

Lemma 2.1. Under (2.1) any connected design $d \in D$ is necessarily binary.

Let the blocks of $d \in D$ be numbered as $B_1, B_2, B_3, \ldots, B_b$ in such a manner that $B_1 \cap B_2 \neq \emptyset, B_3 \cap (B_1 \cup B_2) \neq \emptyset, \ldots, (B_b \cap (B_1 \cup B_2 \cup \ldots \cup B_{b-1}) \neq \emptyset$, where $\emptyset$ is the empty set. This is clearly possible because design d is assumed to be connected. Define $S_j = B_1 \cup B_2 \cup \ldots \cup B_{j-1}, j = 2, \ldots, b$, and let S_j^c be the complement of S_j with respect to the set of treatment symbols, $\Omega = \{1, 2, \ldots, v\}$. Let

$$x_j = |\{\tau_l : \tau_l \in (B_j \cap S_j^c)\}| \tag{2.5}$$

where $j = 2, 3, \ldots, b$; $l = 1, 2, \ldots, v$; and $|.|$ denotes the number of elements in a set. It can be seen that x_j is the number of treatments in block j not occurring in the previous $j-1$ blocks.

Lemma 2.2. Under (2.1) for any design $d \in D$, $x_j = k - 1$.

Corollary 2.1. Under (2.1) for any connected design $d \in D$, no pair of blocks have more than one treatment in common, that is, no pair of treatments occurs in more than one block.

Lemma 2.3. Under (2.1) for any connected design $d \in D$, there is only one unbiased estimate for any treatment contrast $\underline{l}'\underline{\tau}$, thus the ordinary least squares estimate (OLSE) and the general least squares estimate (GLSE) for $\underline{l}'\underline{\tau}$ are the same.

Proof. Suppose there are two unbiased estimates $\underline{l}_1'\underline{y}$ and $\underline{l}_2'\underline{y}$ ($\underline{l}_1' \neq \underline{l}_2'$) for $\underline{l}'\underline{\tau}$. Then $E(\underline{l}_2' - \underline{l}_1')\underline{y} = 0$ and $Var(\underline{l}_2' - \underline{l}_1')\underline{y} = (\underline{l}_2' - \underline{l}_1')\Sigma(\underline{l}_2 - \underline{l}_1) > 0$ since Σ is positive definite. Therefore, $(\underline{l}_2' - \underline{l}_1')\underline{y}$ provides a degree of freedom for estimating σ^2. However, for a minimally connected design there is no degree of freedom for estimating σ^2, a contradiction. □

Definition 2.1. A *chain* in a block design is a sequence of experimental units such that two consecutive units either share the same treatment or the same block, but not both.

Corollary 2.2. Under (2.1) any two blocks are connected by exactly one chain.

We define the *elementary treatment contrast* for the l^{th} and m^{th} treatments as $\tau_l - \tau_m$, where $l \neq m$. For later use we need to clarify two kinds of elementary treatment contrasts in minimally connected designs. If two treatments appear in the same block then their elementary contrast estimate is the difference between the corresponding observations for the two treatments. We call this a *within-block elementary contrast* and its corresponding estimate a *within-block elementary contrast estimate.* If two treatments never appear in the same block then their elementary contrast is estimated by the unique chain of observations connecting them. We call this a *between-blocks elementary contrast* and its corresponding estimate a *between-blocks elementary contrast estimate.*

Example 2.3.1. Consider a design $d \in D(7, 3, 3)$:

$$\begin{array}{llll} B_1: & 1 & 2 & 3 \\ B_2: & 4 & 1 & 5 \\ B_3: & 5 & 6 & 7 \end{array}$$

$\widehat{\tau}_2 - \widehat{\tau}_3 = y_{12} - y_{13}$ is a *within-block elementary treatment contrast estimate.* $\widehat{\tau}_4 - \widehat{\tau}_7 = (y_{21} - y_{23}) - (y_{33} - y_{31})$ is a *between-blocks elementary treatment contrast estimate.*

2.4 A-optimal Designs

Now consider a design $d^* \in D$

$$\begin{array}{lccccccccc} B_1: & 1 & 2 & \dots & l-1 & l & l+1 & \dots & k-1 & k \\ B_2: & k+1 & k+2 & \dots & k+l-1 & l & k+l & \dots & 2k-2 & 2k-1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ B_b: & v-k+2 & v-k+3 & \dots & v-k+l & l & v-k+l+1 & \dots & v-1 & v \end{array}$$

where treatment $l = \lfloor \frac{k+1}{2} \rfloor$ is placed on experiment unit $u = \lfloor \frac{k+1}{2} \rfloor$ in every block. If the block size k is odd then treatment l is at the the middle unit in each block; and if the block size k is even then treatment l could be at either of the middle two units in each block, though for clarity we choose unit $u = \frac{k}{2}$.

Theorem 2.1. Under condition (2.1)-(2.4) design d^* is A-optimal in $D(v, b, k)$.

Proof. Recall that A-optimal designs minimize the average variance of all elementary treatment contrasts, i.e., the A-value is proportional to $\sum_i \sum_{j<i} \frac{Var(\hat{\tau}_i - \hat{\tau}_j)}{\sigma^2}$, which can be split into two parts. One part is due to within-block elementary treatment contrast, which will be the same for any design $d \in D(v, b, k)$, denoted as A_1. The other part is due to between-blocks elementary treatment contrast, denoted as A_2. We will compute A_2 for d^*, as well as competing designs, then show that d^* minimizes A_2. In the following we first show that d^* minimizes A_2 when there are only two blocks. Then we prove that d^* minimizes A_2 for any $b > 2$.

Step 1. **Prove the result for** $b = 2$. By Lemma 2.1 and 2.2 any minimally connected design $d \in D$ with $b = 2$ is binary, and there is only one common treatment, say l, in the two blocks. Lemma 2.2 implies that all other treatments have only one replicate each. Denote the replicate of treatment l in block 1 as $l_{[s]}$, which is at the s^{th} unit of block 1, and the replicate of treatment l in block 2 as $l_{[t]}$, which is at t^{th} unit in block 2. WLOG let $s \le t \le \lfloor \frac{k+1}{2} \rfloor$. Then any minimally connected design d with $b = 2$ is of the following pattern:

$$\begin{array}{lcccccccccc} B_1: & 1 & 2 & \dots & s-1 & l_{[s]} & s+1 & \dots & \dots & k-1 & k \\ B_2: & k+1 & k+2 & \dots & \dots & k+t-1 & l_{[t]} & k+t & \dots & 2k-2 & 2k-1 \end{array} \quad (2.6)$$

By Lemma 2.3 there is only one unbiased estimate for any between-blocks treatment contrast, which must be of the form

$$(y_{1u_1} - y_{1s}) - (y_{2u_2} - y_{2t}) \quad (2.7)$$

where

$$u_1 \in \{1, 2, \dots, k\}/\{s\} \text{ and } u_2 \in \{k+1, k+2, \dots, 2k\}/\{t\}$$

Define $\sum_{h=1}^{0} \rho_h = 0$. Then we have

$$A_2 = 4(k-1)^2 - 2(k-1)A_p \tag{2.8}$$

where

$$A_p = \sum_{h=1}^{s-1} \rho_h + \sum_{h=1}^{k-s} \rho_h + \sum_{h=1}^{t-1} \rho_h + \sum_{h=1}^{k-t} \rho_h \tag{2.9}$$

So A_2 is minimized by maximizing the value of A_p. It can be seen that A_p consists of $2(k-1)$ terms and no ρ_h can appear more than four times in A_p. Now consider two cases.

Case I: k is an odd number, i.e., $k = 2m+1$ for some integer $m > 1$. A_p is maximized when it is the sum of the $\frac{2(k-1)}{4} = m$ largest ρ_h's occurring four times each in A_p, which is achieved by d^*. Denoting A_p and A_2 for d^* as A_p^* and A_2^* respectively, we have

$$\begin{aligned} max(A_p) &= A_p^* &&= 4\sum_{h=1}^{m} \rho_h \\ min(A_2) &= A_2^* &&= 4(k-1)^2 - 8(k-1)\sum_{h=1}^{m} \rho_h \end{aligned} \tag{2.10}$$

Case II: k is an even number, i.e., $k = 2m$ where $m > 0$ is an integer. If $m = 1$, there are no competing designs for d^* since d^* is the only connected design in $D(v, b, k)$. So we only need consider $m > 1$. Now $\frac{2(k-1)}{4}$ is not an integer. A_p is maximized when it is the sum of the $m-1$ largest ρ_h's occurring four times each in A_p and ρ_m occurring twice, which is achieved by d^*.

$$\begin{aligned} max(A_p) &= A_p^* &&= 4\sum_{h=1}^{m-1} \rho_h + 2\rho_m \\ min(A_2) &= A_2^* &&= 4(k-1)^2 - 8(k-1)\sum_{h=1}^{m-1} \rho_h - 4(k-1)\rho_m \end{aligned} \tag{2.11}$$

Step 2. Prove the result for $b > 2$. When $b > 2$, A_2 value can be decomposed into $\binom{b}{2}$ pieces, i.e.,

$$A_2 = \sum_{i=1}^{\frac{b(b-1)}{2}} A_{2i} \tag{2.12}$$

where A_{2i} is the A_2 value for two from b blocks. Since A_1 contains exactly $\frac{bk(k-1)}{2}$ elementary contrasts for every design in $D(v, b, k)$, A_2 must contain exactly $\frac{v(v-1)}{2} - \frac{bk(k-1)}{2}$ elementary contrasts. In fact, A_{2i} contains exactly $\frac{(\frac{v(v-1)}{2}-\frac{bk(k-1)}{2})}{b(b-1)/2}=(k-1)^2$ elementary contrasts, and as will be seen later, these elementary contrasts are between the treatments in one block and the treatments in the other excluding two *linking treatments*.

For the design d^*, we have

$$A_2^* = \sum_{i=1}^{\frac{b(b-1)}{2}} A_{2i}^* \tag{2.13}$$

where A_{2i}^* can be expressed exactly as the same as in (2.10) and (2.11) for $k = 2m+1$ and $k = 2m$ separately. We now show that

$$A_{2i} \geq A_{2i}^* \tag{2.14}$$

for any other design $d \in D(v, b, k)$.

Let's choose two blocks, say B_1 and B_2 out of the b blocks. If these two blocks share one treatment in common (by lemma 2.2 they will have at most one treatment in common), then step 1 has already shown that $A_{2i} \geq A_{2i}^*$. The equality sign holds when the common treatment is at the middle unit in each of the two blocks.

If B_1 and B_2 have no common treatment, then there must be a unique chain linking the two blocks so that the between-blocks treatment contrasts can be estimated by Corollary 2.2. This chain is of the following pattern:

$$\begin{array}{llllll} B_1: & \ldots & l_1 & \ldots & \ldots & \ldots \\ B_{j_1}: & \ldots & l_1 & \ldots & l_2 & \ldots \\ B_{j_2}: & \ldots & l_2 & \ldots & l_3 & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ B_{j_w}: & \ldots & l_w & \ldots & l_{w+1} & \ldots \\ B_2: & \ldots & l_{w+1} & \ldots & \ldots & \ldots \end{array} \tag{2.15}$$

We call B_{j_1}, B_{j_2}, ..., B_{j_w} the *linking blocks* and treatments l_1, l_2, ..., l_{w+1} the *linking treatments*. The subscripts for the linking treatments are not their positions and different subscripts are just used to indicate different treatments.

Note that the elementary treatment contrasts involving the linking treatments are not between-blocks treatment contrasts for B_1 and B_2 because they are either within-block treatment contrasts, or between-blocks treatment contrasts for other pairs of blocks. For example, the elementary contrast between l_1 and l_2 is a within-block treatment contrast for B_{j_1} and the elementary contrast between l_1 and l_3 is a between-blocks treatment contrast for B_{j_1} and B_{j_2}. Therefore, when we calculate the A_{2i} value for B_1 and B_2, we should not consider the elementary treatment contrasts involving the linking treatments.

Denote p_{lj} as the position of the lth linking treatment in jth linking block. We have

$$A_{2i} = A'_{2i} + (k-1)^2\Delta \tag{2.16}$$

where

$$\Delta = 2w - 2\sum_{m=1}^{w} \rho_{|p_{l_m j_m} - p_{l_{m+1} j_m}|} = 2\sum_{m=1}^{w}(1 - \rho_{|p_{l_m j_m} - p_{l_{m+1} j_m}|}) \tag{2.17}$$

and A'_{2i} is the A_2 value for the two blocks assuming they have one common treatment, which can be expressed in the same form as (2.8). (2.16) says that A_{2i} can be divided into two parts: one is if the two blocks had one common treatment, and the other is due to the unique chain when we don't have a common treatment in the two blocks.

By step 1, $A'_{2i} \geq A^*_{2i}$, and it is easy to see that $\Delta > 0$. Therefore, $A_{2i} > A^*_{2i}$ if B_1 and B_2 have no common treatment. In fact, $\Delta > 0$ implies that for fixed linking positions, the variance of any elementary contrast is increasing in number of linking blocks.

As illustration consider example 2.3.1, For B_1 and B_3, $w = 1$, $\Delta = 2 - 2\rho_1$ and $A'_{2i} = 4(k-1)^2 - 4(k-1)(\sum_{h=1}^{k-1}\rho_h) = 16 - 8(\rho_1 + \rho_2)$. Then $A_{2i} = 24 - 16\rho_1 - 8\rho_2$.

In summary, any design $d \in D(v, b, k)$ will have $A_{2i} \geq A^*_{2i}$ for each pair of blocks so that $A_2 \geq A^*_2$ for $b > 2$. □

Depending on the ρ_h's, d^* may or may not be uniquely A-optimal. Uniqueness is guaranteed by $\rho_1 > \rho_2 > \ldots > \rho_{k-1} > 0$.

Corollary 2.3. Treatment l in d^* can shift to any position in each block if $\rho_1 = \rho_2 = \rho_3 = \ldots = \rho_{k-1}$ and the resulting designs are still A-optimal.

2.5 MV-optimal Designs

Definition 2.2. The MV-value for a design is defined as

$$MV_d = \frac{1}{\sigma^2} max_{i \neq i'} Var(\widehat{\tau_i} - \widehat{\tau_{i'}}) \tag{2.18}$$

A design d is said to be MV-optimal over $D(v, b, k)$ if and only if its MV-value is minimum over $D(v, b, k)$.

Theorem 2.2. Under condition (2.1), (2.2), (2.3) and (2.4) design d^* is MV-optimal in $D(v, b, k)$.

Proof. For d^*, the largest variance for within-block elementary contrast estimates is $1 - \rho_{k-1}$ while the largest variance for between-blocks elementary contrast estimates is $2 - 2\rho_{\lfloor \frac{k}{2} \rfloor}$. Then

$$MV_{d^*} = max\{1 - \rho_{k-1}, 2 - 2\rho_{\lfloor \frac{k}{2} \rfloor}\} \tag{2.19}$$

For any other design $d \in D(v, b, k)$, the largest variance for within-block elementary contrast estimates is still $1 - \rho_{k-1}$. If two blocks have one treatment in common, suppose this treatment is at the s^{th} unit in block one and at the t^{th} unit in block two, then the largest variance for between-blocks elementary contrast estimates in these two blocks is $2 - \rho_{p_1} - \rho_{p_2}$ where $p_1 = max\{s-1, k-s\}$ and $p_2 = max\{t-1, k-t\}$. If two blocks have no treatment in common, then consider the unique chain as in (2.15) linking the two blocks. If the linking treatment is at the s^{th} unit in block one and at the t^{th} unit in block two, then the the largest variance for between-blocks elementary contrast estimates in the two blocks is $2 - \rho_{p_1} - \rho_{p_2} + \Delta$, where Δ can be expressed by (2.17). So we have

$$MV_d = max\{1 - \rho_{k-1}, 2 - \rho_{p_1} - \rho_{p_2}\} \text{ or } max\{1 - \rho_{k-1}, 2 - \rho_{p_1} - \rho_{p_2} + \Delta\} \tag{2.20}$$

It is easy to check that $2-\rho_{p_1}-\rho_{p_2}\geq 2-2\rho_{\lfloor\frac{k}{2}\rfloor}$ and $2-\rho_{p_1}-\rho_{p_2}+\Delta > 2-2\rho_{\lfloor\frac{k}{2}\rfloor}$.

So we conclude $MV_{d^*}\leq MV_d$. □

Corollary 2.4. Treatment l in d^* can shift to any position in each block if $\rho_1=\rho_2=\rho_3=\ldots=\rho_{k-1}$ and the resulting designs are still MV-optimal.

2.6 E-optimal Designs

In this section we study the E-optimal designs in $D(v,b,k)$. Since E-optimality problems are concerned with the smallest eigenvalue of the information matrix C_d or equivalently the largest eigenvalue of the Moore-Penrose inverse matrix $C_d^\dagger$, one or both of the matrices are needed under the covariance structure of (2.2), (2.3) and (2.4) .

Lemma 2.4. For any connected block design $d(v,b,k)$,

$$C_d^\dagger=(I_v-\frac{1}{v}J_v)Cov(\underline{\hat{\tau}})(I_v-\frac{1}{v}J_v) \tag{2.21}$$

where I_v is a $v\times v$ identity matrix, J_v is a $v\times v$ matrix whose elements are all one, and $Cov(\underline{\hat{\tau}})$ is the variance-covariance matrix for a solution $\underline{\hat{\tau}}$ to the reduced normal equation for estimating linear functions of treatment effects.

Proof. Led C_d be the information matrix for a design $d(v,b,k)$. By spectral decomposition we have

$$C_d=\sum_{i=1}^{v-1} z_{di}\underline{s_i}\underline{s_i}'$$

where as usual the eigenvalues of C_d are $z_{d0}=0<z_{d1}\leq z_{d2}\leq\ldots\leq z_{d,v-1}$. Let a set of orthonomal eigenvectors of C_d be $\{\underline{s}_0=\frac{1}{\sqrt{v}}\underline{1}_v,\underline{s}_1,\underline{s}_2,\ldots,\underline{s}_{v-1}\}$. Then the Moore-Penrose inverse Matrix of C_d is $C_d^\dagger=\sum_{i=1}^{v-1}\frac{1}{z_{di}}\underline{s}_i\underline{s}_i'$.

Denote any generalized inverse of C_d by C_d^-. We know that for any estimable contrasts, say, $\underline{s}'\underline{\tau}$ and $\underline{m}'\underline{\tau}$ where $\underline{s}'\underline{1} = \underline{m}'\underline{1} = 0$,

$$Cov(\underline{s}'\hat{\underline{\tau}}, \underline{m}'\hat{\underline{\tau}}) = \underline{s}'Cov(\hat{\underline{\tau}})\underline{m} = \sigma^2 \underline{s}' C_d^- \underline{m} \tag{2.22}$$

is invariant to the choice of C_d^-.

Write

$$C_d^p = (I_v - \frac{1}{v}J_v)Cov(\hat{\underline{\tau}})(I_v - \frac{1}{v}J_v).$$

Notice that

$$\underline{s}_i'(I_v - \frac{1}{v}J_v) = \begin{cases} 0 & \text{if } i = 0 \\ \underline{s}_i' & \text{if } i > 0. \end{cases}$$

Then for any i,

$$\underline{s}_0' C_d^p \underline{s}_i = 0$$

for any $i > 0$,

$$\underline{s}_i' C_d^p \underline{s}_i = \frac{1}{z_{di}}$$

and for any $i \neq j \neq 0$,

$$\underline{s}_i' C_d^p \underline{s}_j = 0.$$

Write

$$L = (\underline{s}_0, \underline{s}_1, \ldots, \underline{s}_{v-1})$$

and let $D^+(z_{di})$ be a $v \times v$ diagonal matrix whose diagonal elements are 0 and $\frac{1}{z_{di}}$. Noting that L is orthogonal, we have

$$L'C_d^p L = D^+(z_{di})$$

and

$$C_d^p = LL^{'}C_d^pLL^{'} = LD^+(z_{di})L' = \sum_{i=1}^{v-1} \frac{1}{z_{di}} \underline{s}_i\underline{s}_i^{'} = C_d^{\dagger}.$$

□

Corollary 2.5. $C_{d^*}^{\dagger}$ for the design d^* is of the form:

$$C_{d^*}^{\dagger} = \begin{pmatrix} \frac{b}{v^2}\underline{1}_{k-1}'V\underline{1}_{k-1} & -\frac{1}{v}\underline{1}_b' \otimes [\underline{1}_{k-1}'V(I_{k-1} - \frac{b}{v}J_{k-1})] \\ -\frac{1}{v}\underline{1}_b \otimes [(I_{k-1} - \frac{b}{v}J_{k-1})V\underline{1}_{k-1}] & I_b \otimes V - \frac{1}{v}J_b \otimes (VJ_{k-1} + J_{k-1}V) + \frac{b}{v^2}J_b \otimes (J_{k-1}VJ_{k-1}) \end{pmatrix} \tag{2.23}$$

where V is *(k-1)×(k-1)* matrix,

$$V = Cov(y_{11} - y_{1,\lfloor\frac{k+1}{2}\rfloor}, y_{12} - y_{1,\lfloor\frac{k+1}{2}\rfloor}, \cdots, y_{1,\lfloor\frac{k+1}{2}\rfloor-1} - y_{1,\lfloor\frac{k+1}{2}\rfloor}, y_{1,\lfloor\frac{k+1}{2}\rfloor+1} - y_{1,\lfloor\frac{k+1}{2}\rfloor}, \cdots, y_{1k} - y_{1,\lfloor\frac{k+1}{2}\rfloor}). \tag{2.24}$$

Proof. For d^*, we can get one solution $\underline{\hat{\tau}}$ to the reduced normal equation by letting the estimator for treatment l at the position $j = \lfloor\frac{k+1}{2}\rfloor$ be zero, i.e.,

$$\underline{\hat{\tau}} = (0, \underline{\hat{\tau}}_0^{'})' \tag{2.25}$$

where

$$\begin{aligned} \underline{\hat{\tau}}_0 = (&y_{11} - y_{1,\lfloor\frac{k+1}{2}\rfloor}, y_{12} - y_{1,\lfloor\frac{k+1}{2}\rfloor}, \cdots, y_{1,\lfloor\frac{k+1}{2}\rfloor-1} - y_{1,\lfloor\frac{k+1}{2}\rfloor}, y_{1,\lfloor\frac{k+1}{2}\rfloor+1} - y_{1,\lfloor\frac{k+1}{2}\rfloor}, \cdots, y_{1k} - y_{1,\lfloor\frac{k+1}{2}\rfloor}, \\ &y_{21} - y_{2,\lfloor\frac{k+1}{2}\rfloor}, y_{22} - y_{2,\lfloor\frac{k+1}{2}\rfloor}, \cdots, y_{2,\lfloor\frac{k+1}{2}\rfloor-1} - y_{2,\lfloor\frac{k+1}{2}\rfloor}, y_{2,\lfloor\frac{k+1}{2}\rfloor+1} - y_{2,\lfloor\frac{k+1}{2}\rfloor}, \cdots, y_{2k} - y_{2,\lfloor\frac{k+1}{2}\rfloor}, \\ &\cdots, y_{b1} - y_{b,\lfloor\frac{k+1}{2}\rfloor}, y_{b2} - y_{b,\lfloor\frac{k+1}{2}\rfloor}, \cdots, y_{b,\lfloor\frac{k+1}{2}\rfloor-1} - y_{b,\lfloor\frac{k+1}{2}\rfloor}, y_{b,\lfloor\frac{k+1}{2}\rfloor+1} - y_{b,\lfloor\frac{k+1}{2}\rfloor}, \cdots, y_{bk} - y_{b,\lfloor\frac{k+1}{2}\rfloor})'. \end{aligned} \tag{2.26}$$

Note that for convenience of later discussions, in (2.25) we have put the estimator for treatment l, which is zero, at the first position, while estimators for all other treatments are otherwise listed in order.

Obviously the first row and column elements in $Cov(\underline{\hat{\tau}})$ are all zero and the bottom right *(v-1)×(v-1)* sub-matrix is a diagonal block matrix with b diagonal blocks V which can be expressed by (2.24).

By substituting $Cov(\underline{\hat{\tau}})$ into (2.21) and after some simplification one obtains (2.23). □

The following lemma is used for the proof of the next theorem.

Lemma 2.5. Let λ_A and λ_B be the largest eigenvalue of non-negative definite matrices A and B respectively. Also suppose AB is non-negative definite with largest eigenvalue λ. Then

$$\lambda \leq \lambda_A \lambda_B. \tag{2.27}$$

Proof. We use the concept of matrix 2-norm and its properties to do the proof. For this concept and its properties, refer to Mayer (2000), page 280-282.

Denote the 2-norm of matrix A as $\parallel A \parallel_2$. It is known that if A is non-negative definite,

$$\parallel A \parallel_2 = \lambda_A. \tag{2.28}$$

Also by the property of matrix 2-norm,

$$\parallel AB \parallel_2 \leq \parallel A \parallel_2 \parallel B \parallel_2 \tag{2.29}$$

or equivalently

$$\lambda \leq \lambda_A \lambda_B. \tag{2.30}$$

□

Theorem 2.3. The largest eigenvalue of $C^{\dagger}_{d^*}$ is the same as that of V for the design d^*.

Proof. Factoring $|C^{\dagger}_{d^*} - \lambda I_v|$ gives $|C^{\dagger}_{d^*} - \lambda I_v| = -\frac{\lambda}{v}|V - \lambda I_{k-1}|^{b-1}|V(I_{k-1} - \frac{b}{v}J_{k-1}) - \lambda I_{k-1}|$. Thus the non-zero eigenvalues of $C^{\dagger}_{d^*}$ are the eigenvalues of V with frequency $b-1$ each and the eigenvalues of $V(I_{k-1} - \frac{b}{v}J_{k-1})$. Both matrices must be positive definite because $C^{\dagger}_{d^*}$ is a non-negative definite matrix with only one zero eigenvalue.

By Lemma 2.5, since the largest eigenvalue of $I_{k-1} - \frac{b}{v}J_{k-1}$ is 1,

$$\lambda_{max}(V(I_{k-1} - \frac{b}{v}J_{k-1})) \leq \lambda_{max}(V)\lambda_{max}(I_{k-1} - \frac{b}{v}J_{k-1}) \leq \lambda_{max}(V), \tag{2.31}$$

and so the largest eigenvalue of $C^{\dagger}_{d^*}$ is the largest eigenvalue of V. □

Theorem 2.3 gives us a tool for comparing any other design, say d, to d^* in terms of the E-criterion. If we can find a normalized treatment contrast for d with variance no less than the largest eigenvalue of V, design d cannot be E-superior to d^*. The question is how to pick such a contrast for an arbitrary d.

In fact for any minimally connected design, we can always find two blocks with one common treatment, say l, in the two blocks. The pattern of these two blocks is shown in (2.6).

By setting the estimator for treatment l to zero, one *partial* solution to the reduced normal equations is

$$\begin{aligned} \underline{\hat{\tau}} = (0, y_{11} - y_{1s}, y_{12} - y_{1s}, \cdots, y_{1,s-1} - y_{1s}, y_{1,s+1} - y_{1s}, \cdots, y_{1k} - y_{1s}, \\ y_{21} - y_{2t}, y_{22} - y_{2t}, \cdots, y_{2,t-1} - y_{2t}, y_{2,t+1} - y_{2t}, \cdots, y_{2k} - y_{2t}, \cdots, \cdots)'. \end{aligned} \tag{2.32}$$

Note that we put the estimator for treatment l at the first position in above solution for convenience of later discussions. Also the solution is only a partial solution in the sense that we only explicitly write down the estimators for the treatments in the blocks B_1 and B_2. By Lemma 2.3 these estimators are a basis for the only unbiased estimators for the contrasts of these treatments. The reason we consider this partial solution is simply because we may be able to write down partial expressions for the matrix $Cov(\underline{\hat{\tau}})$ (some sub-matrix in $Cov(\underline{\hat{\tau}})$) and thus get the variances for certain treatment contrasts. We illustrate this idea in detail below.

Suppose V_1 and V_2 are the *(k-1)*$\times$*(k-1)* matrices

$$\begin{aligned} V_1 &= Cov(y_{11} - y_{1s}, y_{12} - y_{1s}, \cdots, y_{1,s-1} - y_{1s}, y_{1,s+1} - y_{1s}, \cdots, y_{1k} - y_{1s}) \\ V_2 &= Cov(y_{21} - y_{2t}, y_{22} - y_{2t}, \cdots, y_{2,t-1} - y_{2t}, y_{2,t+1} - y_{2t}, \cdots, y_{2k} - y_{2t}) \end{aligned}$$

Then the partial expression of $Cov(\underline{\hat{\tau}})$ corresponding to (2.32) is:

$$Cov(\underline{\hat{\tau}}) = \begin{pmatrix} 0 & \underline{0}'_{k-1} & \underline{0}'_{k-1} & \underline{0}'_{(b-2)(k-1)} \\ \underline{0}_{k-1} & V_1 & 0_{k-1,k-1} & \cdots \\ \underline{0}_{k-1} & 0_{k-1,k-1} & V_2 & \cdots \\ \underline{0}_{(b-2)(k-1)} & \cdots & \cdots & \cdots \end{pmatrix} \tag{2.33}$$

Lemma 2.6. If $\lambda_{max}(\frac{V_1+V_2}{2}) \geq \lambda_{max}(V)$, no design d can be E-superior to design d^*.

Proof. Suppose the nomalized eigenvector corresponding to the largest eigenvalue of $\frac{V_1+V_2}{2}$ is $\underline{x}_{(k-1)\times 1}$, Consider a vector of the form

$$\underline{l}_d = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ \underline{x}_{(k-1)\times 1} \\ -\underline{x}_{(k-1)\times 1} \\ \underline{0}_{((b-2)(k-1))\times 1} \end{pmatrix} \tag{2.34}$$

We may see that

$$Var_d(\underline{l}_d\underline{\hat{\tau}}) = \underline{l}_d^{'}Cov_d(\underline{\hat{\tau}})\underline{l}_d = \lambda_{max}(\frac{V_1+V_2}{2}) \tag{2.35}$$

If $\lambda_{max}(\frac{V_1+V_2}{2}) \geq \lambda_{max}(V)$, (2.35) implies that there is an orthonormal treatment contrast with variance no less that the largest eigenvalue of V. Therefore, design d cannot be E-superior to d^*. □

We introduce a new notation so that we can write V, V_1 and V_2 in a universal form. The variance-covariance structure $\Sigma_{n\times n}$ can be expressed as $\Sigma_{n\times n} = I_b \otimes \Sigma^0_{k\times k}$ by (3.2). Define H_u as a $k \times k$ matrix with its u^{th} column elements are 1's and all other elements are 0's, where $u = 1, 2, \cdots, k$. Compute $(I - H_u)\Sigma^0(I - H_u^{'})$ then remove the u^{th} row and the u^{th} column and name the resulting matrix Γ_u. It can be seen that Γ_u is a positive definite *(k-1)×(k-1)* matrix.

Using Γ_u's, where $u = 1, 2, \cdots, k$, we can write,

$$\begin{aligned} V &= \Gamma_{\lfloor \frac{k+1}{2} \rfloor} \\ V_1 &= \Gamma_s \\ V_2 &= \Gamma_t \end{aligned} \tag{2.36}$$

Theorem 2.4. Design d^* is E-optimal if $min(\lambda_{max}(\frac{\Gamma_{u_1}+\Gamma_{u_2}}{2})) = \lambda_{max}(\Gamma_{\lfloor \frac{k+1}{2} \rfloor})$, where the minimum is over $1 \leq u_1 \leq u_2 \leq \lfloor \frac{k+1}{2} \rfloor$.

Proof. Suppose WLOG in design d treatment l is at the u_1^{th} unit in B_1 and at the u_2^{th} unit in B_2 where $u_1 \leq u_2 \leq \lfloor \frac{k+1}{2} \rfloor$. Note that we have enumerated all distinct possibilities for positions u_1 and u_2 by setting $u_1 \leq u_2 \leq \lfloor \frac{k+1}{2} \rfloor$. Lemma 2.6 says that if $\lambda_{max}(\frac{\Gamma_{u_1}+\Gamma_{u_2}}{2}) \geq \lambda_{max}(\Gamma_{\lfloor \frac{k+1}{2} \rfloor})$ then design d cannot be E-superior to d^*. □

Note that the sufficient condition as stated in Theorem 2.4 is one of a family of sufficient conditions for d^* to be E-optimal. In the set of indices $\{1, 2, \ldots, \lfloor \frac{k+1}{2} \rfloor\}$, any member, say u, can be replaced by $k+1-u$. Consequently, there are $2^{\lfloor \frac{k+1}{2} \rfloor}$ sets of sufficient conditions, although some of these are identical. One of these will be employed in the proof for Corollary 2.8.

Any design d with two blocks sharing a common treatment at the middle position in each block cannot be E-superior to d^*. To see this, consider the vector in the form of (2.34). Now $V_1 = V_2 = \Gamma_{\lfloor \frac{k+1}{2} \rfloor}$ and

$$\underline{l}_d' C_d^{\dagger} \underline{l}_d = \lambda_{max}(\Gamma_{\lfloor \frac{k+1}{2} \rfloor}) \tag{2.37}$$

(2.37) implies that there is an orthonormal treatment contrast with variance equal to the largest eigenvalue of V. Therefore, design d cannot be E-superior to design d^*.

Theorem 2.4 provides a method for trying to show d^* is E-optimal, but it requires comparing largest eigenvalues for $\lfloor \frac{k+1}{2} \rfloor - 1 + \binom{\lfloor \frac{k+1}{2} \rfloor}{2}$ matrices with that of C_{d^*}, i.e., enumerating all possibilities for u_1 and u_2 except $u_1 = u_2 = \lfloor \frac{k+1}{2} \rfloor$. It is impossible to enumerate all of these possibilities when k is large. In this sense the sufficient condition in Theorem 2.4 is very strong.

This not withstanding, Theorem 2.4 can be used to find E-optimal designs in some cases. Below are three examples.

Corollary 2.6. Treatment l in d^* can shift to any other positions in each block if $\rho_1 = \rho_2 = \rho_3 = \ldots = \rho_{k-1}$ and the resulting designs are E-optimal.

Corollary 2.6 also follows from the fact that OLSE's are the same as GLSE's when the observations within blocks are equally correlated, so that optimal designs for uncorrelated data are also optimal for equally correlated data. This same observation holds for Corollaries 2.3 and 2.4.

Corollaries 2.3, 2.4 and 2.6 apply to the model with random block effects:

$$y_{ij} = \mu + \tau_i + B_j + e_{ij} \tag{2.38}$$

where

$$\begin{aligned} B_j &\sim i.i.d.\ N(0, \sigma_B^2) \\ e_{ij} &\sim i.i.d.\ N(0, \sigma^2) \end{aligned}$$

For this model, $\rho_1 = \rho_2 = \rho_3 = \ldots = \rho_{k-1} = \frac{\sigma_B^2}{\sigma_B^2 + \sigma^2}$.

Corollary 2.7. Design d^* is E-optimal when $k = 3$.

Corollary 2.8. Design d^* is E-optimal when $k = 4$ and the covariance structure is defined as $\rho_s = \rho^s$ where $0 < \rho < 1$.

The detailed proofs for Corollaries 2.7 and 2.8 are given in Appendix A.

2.7 D-optimal Designs

Bapat and Dey (1991) have shown that all minimally connected designs are D-equal when the observations are uncorrelated. Any block design d can be expressed by a unique multigraph H_d. By graph theory, when observations are uncorrelated, the D-value of a connected design is determined by the number of spanning trees of H_d, and for any minimally connected design H_d has exactly one spanning tree.

When the observations are correlated within each block, we cannot use graph theory to solve the D-optimality problem. Perhaps we have to find an expression for D-value in terms of the eigenvalues and/or elements of C_d, which appears to be a very tough task. We will not tackle the D-optimality problem for correlated data in this dissertation.

Chapter 3

Optimal Incomplete Designs with Two Blocks

3.1 Summary

In this chapter we study optimal incomplete block designs when there are two blocks and their sizes are equal. It turns out that a binary design of a certain pattern is A- and D-optimal in the class of designs $D(v, 2, k)$ with $v/2 < k < v$. The same design is also E-optimal design in $D(v, 2, k)$ when $v/2 < k < 5v/6$. If $5v/6 < k < v$ a non-binary design with a certain pattern is E-optimal. If $k = 5v/6$ both the binary design and the non-binary design are E-optimal.

3.2 Majorization Theorem and Average Matrix

In this section we will be discussing two useful techniques used in optimal block design problems. The majorization theorem is used for convex function optimality problems, therefore applies to every Type I-criteria, including A- and D-optimality problems. The average matrix technique is an extended version of the majorization theorem, which can also be used for E-optimality problems.

To begin with, we give the definition of majorization for two vectors.

Definition 3.1. let $\underline{x} = (x_1, x_2, \cdots x_n)'$ and $\underline{y} = (y_1, y_2, \cdots y_n)'$ be two vectors with their elements in non-decreasing order $x_1 \le x_2 \le \cdots \le x_n$ and $y_1 \le y_2 \le \cdots \le y_n$. Then $\underline{x}$ is majorized by $\underline{y}$,denoted as $\underline{x} \preceq \underline{y}$ if

$$\begin{array}{l} i)\ \sum_{i=1}^{l} x_{n+1-i} \le \sum_{i=1}^{l} y_{n+1-i}\ for\ l = 1, 2, \cdots, n \\ ii)\ \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i \end{array} \tag{3.1}$$

The following majorization theorem is well known. One may refer to Marshall and Olkin (1979) for a proof.

Theorem 3.1. For every convex function f, $\sum_{i=1}^{n} f(x_i) \le \sum_{i=1}^{n} f(y_i)$ where x_i and y_i are elements of vectors defined as above if and only if $\underline{x} \preceq \underline{y}$.

For optimal simple block design problems, we consider two vectors of $v-1$ eigenvalues of two designs d_1 and d_2 in $D(v, b, k)$. Suppose their information matrices have the same trace, i.e., the sum of the eigenvalues are the same. If we have $\sum_{i=1}^{l} z_{d_1, v-i} \le \sum_{i=1}^{l} z_{d_2, v-i}$ for $l = 1, 2, \cdots, v-1$ then d_1 is better than d_2 with respect to every convex functionals. We will be giving a version of majorization theorem in terms of design information matrix C_d. The proof of the theorem needs the following result given by Haemers (1980).

Lemma 3.1. Let $A_{n\times n}$ be a symmetric matrix with eigenvalues $x_1, x_2, \cdots, x_n$,where $x_1 \le x_2 \le \cdots \le x_n$ and their corresponding eigenvectors are $\underline{u}_1, \underline{u}_2, \cdots, \underline{u}_n$.Denote the linear span of a set of vectors $\underline{u}_1, \underline{u}_2, \cdots, \underline{u}_i$ as $\langle \underline{u}_1, \underline{u}_2, \cdots, \underline{u}_i \rangle$ where $i = 1, 2, \cdots, n$. Then,

$i)\ x_i \le \frac{\underline{u}' A \underline{u}}{\underline{u}' \underline{u}}\ for\ \underline{u} \in \langle \underline{u}_i, \underline{u}_{i+1}, \cdots, \underline{u}_n \rangle,\ \underline{u} \ne \underline{0},\ i = 1, 2, \cdots, n$

equality holds if and only if $\underline{u}_i$ is an eigenvector of A for x_i;

$ii)\ x_i \ge \frac{\underline{u}' A \underline{u}}{\underline{u}' \underline{u}} for\ \underline{u} \in \langle \underline{u}_1, \underline{u}_2, \cdots, \underline{u}_i \rangle,\ \underline{u} \ne \underline{0}, i = 1, 2, \cdots, n.$

equality holds if and only if $\underline{u}_i$ is an eigenvector of A for x_i.

Lemma 3.2 follows immediately from Lemma 3.1.

Lemma 3.2. Let $A_{n\times n}$ be a symmetric matrix with eigenvalues $x_1, x_2, \cdots, x_n$, where $x_1 \leq x_2 \leq \cdots \leq x_n$ and corresponding eigenvectors $\underline{u}_1, \underline{u}_2, \cdots, \underline{u}_n$. Then for $l = 1, 2, \cdots, n$,

$$max(\sum_{i=1}^{l} \frac{\underline{l}_i' A \underline{l}_i}{\underline{l}_i' \underline{l}_i}) = \sum_{i=1}^{l} x_{n+1-i}, \tag{3.2}$$

where $\underline{l}_i' \underline{l}_{i'} = 0, \forall\, i \neq i'$ and $\underline{l}_i' \underline{l}_i = 1$.

Now we are ready to give the following version of the majorization theorem in terms of information matrices.

Theorem 3.2. Let d_1 and d_2 be two designs in $D(v, b, k)$. Their information matrices C_{d1} and C_{d2} have the same trace. Define a new matrix as $\widetilde{C} = \theta C_{d1} + (1-\theta)C_{d2}$ for some $\theta \in [0, 1]$. Then

(1) $\widetilde{C}$ is also an information matrix, i.e., it is still a non-negative symmetric matrix with rank of $v - 1$, though it need not to correspond to any real design.

(2) if $\phi_f(C_d) = \sum_{i=1}^{v-1} f(z_{di})$, where f is a convex function, and $z_{d1} \leq z_{d2} \leq \cdots \leq z_{d,v-1}$ are positive eigenvalues of C_d then

$$\phi_f(\widetilde{C}) \leq \theta\phi_f(C_{d1}) + (1-\theta)\phi_f(C_{d2})$$

Proof. Part (1) can be easily verified. For (2), since $\widetilde{C} = \theta C_{d1} + (1-\theta)C_{d2}$, we have

$$L'\widetilde{C}L = \theta L' C_{d1} L + (1-\theta) L' C_{d2} L$$

and

$$tr(L'\widetilde{C}L) = \theta tr(L' C_{d1} L) + (1-\theta) tr(L' C_{d2} L).$$

Choose L so that its columns are k orthogonal eigenvectors of L corresponding to k largest eigenvalues of $\widetilde{C}$. By the property that the trace of a matrix is the sum of its eigenvalues and lemma 3.2, we have

$$\sum_{i=1}^{l} \overline{z}_{v-i} \leq \theta \sum_{i=1}^{l} z_{d1,v-i} + (1-\theta) \sum_{i=1}^{l} z_{d2,v-i}$$

for $l = 1, 2, \cdots, v-1$, which in fact says the vector of eigenvalues of $\widetilde{C}$ is majorized by the vector

$$(\theta z_{d1,1} + (1-\theta) z_{d2,1}, \theta z_{d1,2} + (1-\theta) z_{d2,2}, \cdots, \theta z_{d1,v-1} + (1-\theta) z_{d2,v-1})'.$$

By Theorem 3.1 and the property of convexity, we have

$$\begin{aligned}
\phi_f(\widetilde{C}) &= \sum_{i=1}^{v-1} f(\overline{z_i}) \\
&\leq \sum_{i=1}^{v-1} f(\theta z_{d1,i} + (1-\theta) z_{d2,i}) \\
&\leq \theta \sum_{i=1}^{v-1} f(z_{d1,i}) + (1-\theta) \sum_{i=1}^{v-1} f(z_{d2,i}) \\
&= \theta \phi_f(C_{d1}) + (1-\theta) \phi_f(C_{d2})
\end{aligned}$$

□

The above majorization theorem is for two information matrices with the same trace. In practice, researchers usually use an averaging technique, which is an extension of majorization theorem, to get the bounds for optimal designs. Below we first give the definition of an average matrix, followed by a theorem and a discussion.

Definition 3.2. Let σ_i be a colletion of t permutations on the symbols of $1, 2, \cdots, v$,where $1 \leq t \leq v!$. Define $\overline{C}_d = \frac{1}{t} \sum_{i=1}^{t} C_d^{\sigma_i}$,where $C_d^{\sigma_i} = P_i C_d P_i'$ with P_i representing the $v \times v$ matrix representation of σ_i. The matrix $\overline{C}_d$ is called an average matrix of C_d of order t.

Theorem 3.3. Suppose $\overline{C}_d$ is the average matrix of C_d of order t, then,

(1) $\overline{C}_d$ is nonnegative definite with zero row sums, $tr(\overline{C}_d) = tr(C_d)$.

(2) for any convex function f, $\phi_f(\overline{C}_d) \leq \phi_f(C_d)$ where $\phi_f(C_d) = \sum_{i=1}^{v-1} f(z_{di})$.

(3) $z_{d1} \leq \overline{z}_{d1}$ and more generally $\sum_{i=1}^{l} \overline{z}_{d,v-i} \leq \sum_{i=1}^{l} z_{d,v-i}$ for any $l \leq v-1$.

Proof. (1) is immediate. For (2), following the similar proof of Theorem 3.2, we have,

$$\phi_f(\overline{C}_d) \leq \frac{1}{t}\sum_{i=1}^{t}\phi_f(C_d^{\sigma_i}) = \phi_f(C_d).$$

The first part of (3) follows easily after observing that $z_{d1} = min_{\underline{l}}\frac{\underline{l}'C_d\underline{l}}{\underline{l}'\underline{l}}$ subject to the components of $\underline{l}$ summing to zero. The second part of (3) follows a proof similar to that for Theorem 3.2. □

In order to show that a design d^* is optimal with respect to some ϕ_f criterion (e.g. A- or D-criterion), by Theorem 3.3 it is enough to show that ϕ_f of some averaged version of C_d is no smaller than of C_{d^*}; and d^* is E-optimal if $\overline{z}_{d1}$ of some averaged version of C_d does not exceed the smallest non-zero eigenvalue z_{d^*1} of d^*. The question is how we should choose the average matrix. Let $i_1, i_2, \cdots, i_l$ be a subset of the treatments of $1, 2, \cdots, v$. Taking P_i ($i = 1, 2, \cdots, l!$), we will have the $v \times v$ matrix representation of the symmetric group on the symbols $i_1, i_2, \cdots, i_l$ extended to be the identity on the rest of the treatments. When averaging separately over g disjoint subsets of sizes p_i of treatments of $1, 2, \cdots, v$, where $1 \leq i \leq g$, we will have $p_1!p_2!\cdots p_g!$ permutation matrices to use in Definition 3.2. This averaging process transforms C_d into a matrix $\overline{C}_d$ which consists of completely symmetric blocks along the diagonal and blocks with equal entries elsewhere. In many cases it is a more tractable task to compute the eigenvalues of $\overline{C}_d$ than those of C_d. By Theorem 3.3 these eigenvalues help us relate a suspected optimal design d^* to an arbitrary design $d \in D(v, b, k)$.

Example 3.2.1. Constantine (1981) The matrix $\overline{C}_d$ obtained by averaging an information matrix C_d separately over varieties $1, 2, \cdots, i$ and $i+1, i+2, \cdots, v$ is of the form

$$\overline{C}_d = \frac{1}{k}\begin{pmatrix} (\overline{a}+\overline{\alpha})I_i - \overline{\alpha}J_i & -\overline{\beta}J_{i\times(v-i)} \\ -\overline{\beta}J_{(v-i)\times i} & (\overline{b}+\overline{\gamma})I_{v-i} - \overline{\gamma}J_{v-i} \end{pmatrix}$$

where $\overline{\alpha}$,$\overline{\beta}$,$\overline{\gamma}$, $\overline{a}$, $\overline{b}$ are constants depending on specific designs.

Apparently, $k\overline{C}_d$ has eigenvalues : $\overline{a}+\overline{\alpha}$ of multiplicity $i-1$, $\overline{b}+\overline{\gamma}$ of multiplicity $v-i-1$, $v\overline{\beta}$ of multiplicity 1, and 0 of multiplicity of 1, where $1 \leq i \leq v-1$.

3.3 A-optimal Designs

Write $bk = vr + p$ where p is a non-negative integer no larger than $v - 1$. Then p is the number of plots available for use in the particular design setting over and above the $n - p$ that would be used to replicate each treatment with equal frequency r. When $b = 2$ and $\frac{v}{2} < k < v$ we have $r = 1$ and $p = 2k - v$. There is only one binary design d_0 of the following pattern in this situation:

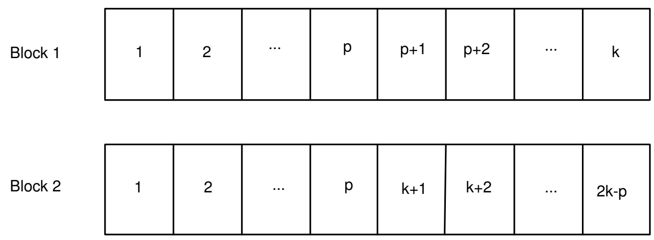

Figure 3.1: Binary design d_0

The information matrix C_{d_0} for this binary design is

$$C_{d_0} = \begin{pmatrix} 2I_p - \frac{2}{k}J_p & -\frac{1}{k}J_{p,k-p} & -\frac{1}{k}J_{p,k-p} \\ -\frac{1}{k}J_{k-p,p} & I_{k-p} - \frac{1}{k}J_{k-p} & 0_{k-p} \\ -\frac{1}{k}J_{k-p,p} & 0_{k-p} & I_{k-p} - \frac{1}{k}J_{k-p} \end{pmatrix} \tag{3.3}$$

where I_p is a $p \times p$ identity matrix, J_p ($J_{m,n}$) is a $p \times p$ ($m \times n$) matrix in which all elements are 1, and 0_{k-p} is a $(k-p) \times (k-p)$ matrix in which all elements are 0. C_{d_0} matrix in (2.1) has positive eigenvalues 1 with frequency $2(k-p-1)$, 2 with frequency $(p-1)$, $\frac{p}{k}$, and $\frac{v}{k}$. Thus

$$\sum_{i=1}^{v-1} \frac{1}{z_{d_0 i}} = 2(k-p-1) + \frac{p-1}{2} + \frac{k}{p} + \frac{k}{v}. \tag{3.4}$$

Aside from the binary design in Figure 1, there are many non-binary designs in the class $D(v, b, k)$. We will use an average matrix to show that any non-binary design is A-inferior to the binary design.

For $\frac{v}{2} < k < v$ we have $r = \lfloor \frac{2k}{v} \rfloor = 1$. Therefore,we must have at least $2(k-p)$ treatments with just 1 replicate. Suppose now we have $2(k-p)+m$ treatments with just 1 replicate where $0 \leq m \leq p-1$. If there are $k-p-s$ of the treatments with one replicate in block one, where $-\frac{m}{2} \leq s \leq k-p$, then there must be $k-p+s+m$ of the treatments with one replicate in block two. Also we need $0 \leq s+m \leq p-1$ so that the design is connected. If $m = s = 0$ we get the binary design d_0. Every design in $D(v,2,k)$ is characterized by the integers p, s and m. In words, the integers m and s are:

$$
\begin{aligned}
m &= \text{the total excess in treatments with one replicate relative to } d_0. \\
s &= \text{the shortfall in treatments in block one with one replicate relative to } d_0.
\end{aligned}
$$

Note that a negative shortfall ($s < 0$) is actually an excess. The sign of s is not a consideration in the A- and D-optimality problems. Later it will be seen that $s < 0$ need not be considered for the E-optimality problem.

The following two lemmas are used in the proof for later theorems. The first lemma is a well-known result in elementary algebra.

Lemma 3.3. If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the n roots for an n^{th} order equation $P(\lambda) = 0$ where $P(\lambda)$ is defined as

$$P(\lambda) = a_n\lambda^n + a_{n-1}\lambda^{n-1} + \ldots + a_1\lambda + a_0, \tag{3.5}$$

then

$$
\begin{aligned}
&\lambda_1 + \lambda_2 + \ldots + \lambda_n = (-1)\tfrac{a_{n-1}}{a_n} \\
&\lambda_1\lambda_2 + \lambda_1\lambda_3 + \ldots + \lambda_{n-1}\lambda_n = (-1)^2\tfrac{a_{n-2}}{a_n} \\
&\vdots \\
&\lambda_1\lambda_2\ldots\lambda_n = (-1)^n\tfrac{a_0}{a_n}.
\end{aligned} \tag{3.6}
$$

Lemma 3.4. For $b = 2$ and $\frac{v}{2} < k < v$, the information matrix $C_{\overline{d}}$ obtained by averaging an information matrix C_d over the treatments with more than one replicate for any design $d \in D(v,b,k)$ is, for some values of ζ and η,

1. if $s \neq k-p$ then

$$C_{\overline{d}} = \begin{pmatrix} I_{k-p-s} - \frac{1}{k}J_{k-p-s} & 0_{k-p-s,k-p+s+m} & -\frac{p+s}{k(p-m)}J_{k-p-s,p-m} \\ 0_{k-p+s+m,k-p-s} & I_{k-p+s+m} - \frac{1}{k}J_{k-p+s+m} & -\frac{p-s-m}{k(p-m)}J_{k-p+s+m,p-m} \\ -\frac{p+s}{k(p-m)}J_{p-m,k-p-s} & -\frac{p-s-m}{k(p-m)}J_{p-m,k-p+s+m} & \zeta I_{p-m} + \eta J_{p-m} \end{pmatrix} \tag{3.7}$$

2. if $s = k-p$ then

$$C_{\overline{d}} = \begin{pmatrix} I_{2(k-p)+m} - \frac{1}{k}J_{2(k-p)+m} & -\frac{2p-k-m}{k(p-m)}J_{2(k-p)+m,p-m} \\ -\frac{2p-k-m}{k(p-m)}J_{p-m,2(k-p)+m} & \zeta I_{p-m} + \eta J_{p-m} \end{pmatrix} \tag{3.8}$$

In either case,

$$\zeta \leq \frac{2p-m}{p-m}. \tag{3.9}$$

Proof. If $s \neq k-p$ then obviously the average matrix $C_{\overline{d}}$ is of the following form:

$$C_{\overline{d}} = \begin{pmatrix} I_{k-p-s} - \frac{1}{k}J_{k-p-s} & 0_{k-p-s,k-p+s+m} & \gamma_1 J_{k-p-s,p-m} \\ 0_{k-p+s+m,k-p-s} & I_{k-p+s+m} - \frac{1}{k}J_{k-p+s+m} & \gamma_2 J_{k-p+s+m,p-m} \\ \gamma_1 J_{p-m,k-p-s} & \gamma_2 J_{p-m,k-p+s+m} & \zeta I_{p-m} + \eta J_{p-m} \end{pmatrix} \tag{3.10}$$

The row sum of $C_{\overline{d}}$ should be zero then,

$$\begin{aligned} \gamma_1 &= -\tfrac{p+s}{k(p-m)} \\ \gamma_2 &= -\tfrac{p-s-m}{k(p-m)} \\ \zeta + (p-m)\eta &= \tfrac{(p+s)(k-p-s)}{k(p-m)} + \tfrac{(p-s-m)(k-p+s+m)}{k(p-m)} \end{aligned} \tag{3.11}$$

For any design d, the average matrix $C_{\overline{d}}$ has the same trace as the original information matrix C_d. Denote the set of treatments with more than one replicate as Ω, which has $p-m$ treatments. We have

$$(p-m)(\zeta+\eta) = \sum_{i\in\Omega} r_{di} - \frac{1}{k}\sum_{i\in\Omega}\sum_{j=1}^{2} n_{dij}^2 = 2p-m-\frac{1}{k}\sum_{i\in\Omega}\sum_{j=1}^{2} n_{dij}^2. \tag{3.12}$$

Following the notations in chapter 1, n_{dij} is the number of occurences of the i^{th} treatment in the j^{th} block and r_{di} is the replicate number of the i^{th} treatment.

From (3.12) and the third equation in (3.11) one obtains

$$\begin{aligned}\sum_{i\in\Omega}\sum_{j=1}^{2} n_{dij}^2 &= k((2p-m)-(p-m)(\zeta+\eta))\\ &= k((2p-m)-(p-m-1)\zeta-(\zeta+(p-m)\eta))\\ &= k((2p-m)-(p-m-1)\zeta-\tfrac{(p+s)(k-p-s)}{k(p-m)}-\tfrac{(p-s-m)(k-p+s+m)}{k(p-m)}).\end{aligned} \tag{3.13}$$

If $\zeta > \frac{2p-m}{p-m}$, then we have

$$\begin{aligned}\sum_{i\in\Omega}\sum_{j=1}^{2} n_{dij}^2 &< k((2p-m)-(p-m-1)\tfrac{2p-m}{p-m}-\tfrac{(p+s)(k-p-s)}{k(p-m)}-\tfrac{(p-s-m)(k-p+s+m)}{k(p-m)})\\ &= p-m+\tfrac{2s(m+s)+p^2}{p-m}.\end{aligned} \tag{3.14}$$

One the other hand, since $\sum_{i\in\Omega} n_{di1} = p+s$ and $\sum_{i\in\Omega} n_{di2} = p-m-s$, we have

$$\begin{aligned}\sum_{i\in\Omega}\sum_{j=1}^{2} n_{dij}^2 &= \sum_{i\in\Omega} n_{di1}^2 + \sum_{i\in\Omega} n_{di2}^2\\ &\geq \tfrac{(\sum_{i\in\Omega} n_{di1})^2}{p-m} + \tfrac{(\sum_{i\in\Omega} n_{di2})^2}{p-m}\\ &= p-m+\tfrac{2s(m+s)+p^2}{p-m},\end{aligned} \tag{3.15}$$

which contradicts (3.15).

If $s = k-p$ then all the $2(k-p)+m$ treatments with just one replicate are in only one block . Thus we must have

$$2p \geq k+m+1 \tag{3.16}$$

in order that the design is connected. The average matrix $C_{\overline{d}}$ is of the following form:

$$C_{\overline{d}} = \begin{pmatrix} I_{2(k-p)+m} - \frac{1}{k}J_{2(k-p)+m} & \gamma J_{2(k-p)+m,p-m} \\ \gamma J_{p-m,2(k-p)+m} & \zeta I_{p-m} + \eta J_{p-m} \end{pmatrix} \tag{3.17}$$

Since the row sum of $C_{\overline{d}}$ is zero one can get:

$$\begin{aligned}\gamma &= -\tfrac{2p-k-m}{k(p-m)}\\ \zeta+(p-m)\eta &= \tfrac{(2p-k-m)(2(k-p)+m)}{k(p-m)}\end{aligned} \tag{3.18}$$

Following the same procedure (substitute $s = k - p$ into (3.14) and (3.15)), we can get the same conclusion: ζ must be less or equal to $\frac{2p-m}{p-m}$ when $s = k - p$. $\square$

Now we describe a technique which will be used repeatedly in the proofs for later theorems. For an information matrix in partitioned block form, we can find some eigenvalues very quickly by considering certain eigenvectors in the form of some treatment contrasts, after which the remaining unknown eigenvalues are the same as that of a non-symmetric matrix of small dimension.

We use the example of $C_{\overline{d}}$ in (3.7) to describe how to obtain the corresponding non-symmetric matrix by this technique. By considering orthogonal contrast vectors of treatments corresponding to the same diagonal block, one may quickly get $2(k-p)-3$ non-zero eigenvalues: 1 with frequency $2(k-p)+m-2$ and ζ with frequency $p-m-1$. Subtracting the corresponding spectral pieces for these $2(k-p)-3$ eigenvalues from the $C_{\overline{d}}$ matrix we get the remaining non-zero eigenvalues are the two non-zero eigenvalues of the following $v \times v$ matrix :

$$\begin{pmatrix} \frac{p+s}{k(k-p-s)} J_{k-p-s} & 0_{k-p-s,k-p+s+m} & \gamma_1 J_{k-p-s,p-m} \\ 0_{k-p+s+m,k-p-s} & \frac{p-s-m}{k(k-p+s+m)} J_{k-p+s+m} & \gamma_2 J_{k-p+s+m,p-m} \\ \gamma_1 J_{p-m,k-p-s} & \gamma_2 J_{p-m,k-p+s+m} & \frac{\zeta+\eta(p-m)}{p-m} J_{p-m} \end{pmatrix}$$

Notice (3.11), this matrix becomes:

$$\begin{pmatrix} \frac{p+s}{k(k-p-s)} J_{k-p-s} & 0_{k-p-s,k-p+s+m} & -\frac{p+s}{k(p-m)} J_{k-p-s,p-m} \\ 0_{k-p+s+m,k-p-s} & \frac{p-s-m}{k(k-p+s+m)} J_{k-p+s+m} & -\frac{p-s-m}{k(p-m)} J_{k-p+s+m,p-m} \\ -\frac{p+s}{k(p-m)} J_{p-m,k-p-s} & -\frac{p-s-m}{k(p-m)} J_{p-m,k-p+s+m} & \frac{(p+s)(k-p-s)+(p-s-m)(k-p+s+m)}{k(p-m)^2} J_{p-m} \end{pmatrix}$$

One may see that there are only two non-zero eigenvalues for the above matrix. And the corresponding eigenvectors to the two eigenvalues must be of the form

$$(c_1 \underline{1}'_{k-p-s}, c_2 \underline{1}'_{k-p+s+m}, c_3 \underline{1}'_{p-m})',$$

where c_1,c_2,c_3 satisfy the equations,

$$\begin{aligned}
\lambda c_1 &= \tfrac{(p+s)c_1}{k} - \tfrac{(p+s)c_3}{k} \\
\lambda c_2 &= \tfrac{(p-s-m)c_2}{k} - \tfrac{(p-s-m)c_3}{k} \\
\lambda c_3 &= -\tfrac{(p+s)(k-p-s)c_1}{k(p-m)} - \tfrac{(p-s-m)(k-p+s+m)c_2}{k(p-m)} + \tfrac{((p+s)(k-p-s)+(p-s-m)(k-p+s+m))c_3}{k(p-m)}.
\end{aligned} \tag{3.19}$$

and λ is any one of the two eigenvalues. But the equations (3.19) simply imply that the two eigenvalues are the non-zero eigenvalues of the following 3×3 matrix:

$$\widetilde{C}_{\overline{d}} = \begin{pmatrix} \frac{p+s}{k} & 0 & -\frac{p+s}{k} \\ 0 & \frac{p-m-s}{k} & -\frac{p-m-s}{k} \\ -\frac{(p+s)(k-p-s)}{k(p-m)} & -\frac{(p-s-m)(k-p+s+m)}{k(p-m)} & \frac{(p+s)(k-p-s)}{k(p-m)} + \frac{(p-s-m)(k-p+s+m)}{k(p-m)} \end{pmatrix} \tag{3.20}$$

Now we give the main result of this section.

Theorem 3.4. The binary design d_0 is uniquely A-optimal in $D(v, 2, k)$.

Proof. Suppose $s \neq k - p$. We use the average information matrix $C_{\overline{d}}$ in (3.7) for our proof. From the above discussion we know that the unknown non-zero eigenvalues of (3.7) are the two non-zero eigenvalues of the matrix (3.20).

On the other hand, the two non-zero eigenvalues λ_1 and λ_2 to $\widetilde{C}_{\overline{d}}$ are the roots of the equation

$$|\widetilde{C}_{\overline{d}} - \lambda I_3| = 0. \tag{3.21}$$

After some simplification we find λ_1 and λ_2 are the roots to the equation:

$$k^2(m-p)\lambda^2 - k(km - 2kp + mp + 2ms + 2s^2)\lambda + (2k-p)(m-p+s)(p+s) = 0 \tag{3.22}$$

By Lemma 3.3 one obtains

$$\frac{1}{\lambda_1} + \frac{1}{\lambda_2} = \frac{\lambda_1 + \lambda_2}{\lambda_1 \lambda_2} = \frac{k(km - 2kp + mp + 2ms + 2s^2)}{(2k-p)(m-p+s)(p+s)} \tag{3.23}$$

and

$$\sum_{i=1}^{v-1} \frac{1}{z_{\overline{d}i}} = 2(k-p) + m - 2 + \frac{(p-m-1)}{\zeta} + \frac{k(km - 2kp + mp + 2ms + 2s^2)}{(2k-p)(m-p+s)(p+s)}. \tag{3.24}$$

Notice (3.9), then

$$\sum_{i=1}^{v-1}\frac{1}{z_{\bar{d}i}} \geq 2(k-p)+m-2+\frac{(p-m-1)(p-m)}{2p-m}+\frac{k(km-2kp+mp+2ms+2s^2)}{(2k-p)(m-p+s)(p+s)}. \quad (3.25)$$

Using (3.25) − (3.4), after some simplification we have

$$\sum_{i=1}^{v-1}\frac{1}{z_{\bar{d}i}}-\sum_{i=1}^{v-1}\frac{1}{z_{d_0 i}} \geq \frac{m(p+1)}{4p-2m}+\frac{k(k-p)(2(s+\frac{m}{2})^2+m(p-\frac{m}{2}))}{(2k-p)p(p-m-s)(p+s)}. \quad (3.26)$$

It is easy to see that right side of (3.26) is always greater than 0 as long as s and m are not zero simultaneously.

If $s = k-p$, then we use the average matrix $C_{\bar{d}}$ in (3.8). In fact we can simply put $s = k-p$ into (3.26) to get the proof. □

3.4 D-optimal Designs

Theorem 3.5. The binary design d_0 is uniquely D-optimal in $D(v, 2, k)$.

Proof. For the binary design d_0 we have

$$\prod_{i=1}^{v-1} z_{d_0 i} = 2^{p-1}\frac{p(2k-p)}{k^2}. \quad (3.27)$$

We will be still using the average matrix technique to show that all other designs are D-inferior to d_0. It $s \neq k-p$, then we use the average matrix (3.7)

$$\prod_{i=1}^{v-1} z_{\bar{d}i} \leq \frac{(2k-p)(\frac{2p-m}{p-m})^{p-m}(p-m-s)(p+s)}{k^2(2p-m)}. \quad (3.28)$$

Note that we used fact that $\lambda_1\lambda_2 = (2k-p)(p-m-s)(p+s)/(k^2(p-m))$ from Lemma 3.3 applied to (3.22) to get (3.28).

Letting $ratio = (\prod_{i=1}^{v-1} z_{\bar{d}i})/(\prod_{i=1}^{v-1} z_{d_0 i})$, after some simplification for (3.28)/(3.27) one obtains

$$ratio \leq \frac{(\frac{2p-m}{p-m})^{p-m}(2(p-m-s)(p+s))}{2^p(2p-m)p}. \quad (3.29)$$

Now check the factor $\frac{(\frac{2p-m}{p-m})^{p-m}}{2^p}$. We will show it is no greater than 1 . If true then $ratio \leq 1$ because $\frac{2(p-m-s)(p+s)}{p(2p-m)} = \frac{p(2p-m)-(m+s)^2-m(p-m)}{p(2p-m)} \leq 1$. Let

$$W(m) = \frac{(\frac{2p-m}{p-m})^{p-m}}{2^p}. \tag{3.30}$$

Then

$$\frac{dW}{dm} = \frac{(\frac{2p-m}{p-m})^{p-m}(p-(2p-m)log(\frac{2p-m}{p-m}))}{2^p(2p-m)}. \tag{3.31}$$

We now show that $p-(2p-m)log(\frac{2p-m}{p-m}) < 0$. If it is true then $\frac{dW}{dm} < 0$ and the maximum of $W(m)$ is $W(0) = 1$ and $ratio \leq 1$. Let $m = \mu p$ where $0 \leq \mu \leq 1$ then $p-(2p-m)log(\frac{2p-m}{p-m}) = p(1-(2-\mu)log(\frac{-2+\mu}{-1+\mu}))$. In fact,

$$log(\frac{2-\mu}{1-\mu}) - \frac{1}{2-\mu} = (log(2) - \frac{1}{2}) + \sum_{j=1}^{\infty}(\frac{1}{j}(1-\frac{1}{2^j}) - (\frac{1}{2})^{j+1})\mu^j. \tag{3.32}$$

Obviously $log(2) - \frac{1}{2} > 0$. And $\frac{1}{j}(1-\frac{1}{2^j}) - (\frac{1}{2})^{j+1} = \frac{1}{j2^{j+1}}(2^{j+1}-j-2) > 0$ for any $j \geq 1$. So $log(\frac{2-\mu}{1-\mu}) - \frac{1}{2-\mu} > 0$ and $p-(2p-m)log(\frac{2p-m}{p-m}) < 0$.

Thus $ratio \leq 1$. The equality holds if and only if $m = s = 0$.

It $s = k - p$, then we use the average matrix (3.8). Simply put $s = k - p$ into (3.29) and we also get $ratio < 1$. □

3.5 E-optimal Designs

In this section we study the E-optimal incomplete block designs with $b = 2$. The class $D(v, 2, k)$ can be partitioned into two subclasses: one is the subclass $D_1(v, 2, k)$ in which all treatments have no more than two replicates, i.e., $r_{di} \in \{1, 2\}$ for $i = 1, 2, \ldots, v$; the other is the subclass $D_2(v, 2, k)$ in which some treatment has more than two replicates, i.e., some $r_{di} > 2$.

Lemma 3.5. Substitute real numbers $x = a$ and $x = b$ into $P(x)$ in (4). If $P(a)P(b) < 0$, then there is at least one root to the equation $P(x) = 0$ between (a, b).

Lemma 3.6. In the class $D_1(v,2,k)$, binary design d_0 is the unique E-optimal design if $\frac{v}{2} < k < \frac{5v}{6}$; non-binary design d^* is the unique E-optimal design if $\frac{5v}{6} < k < v$; the non-binary design d^* and the binary design d_0 are both E-optimal if $k = \frac{5v}{6}$ and no others designs can be E-optimal. The design d^* is of the pattern described in Figure 3.2.

Block 1	1	2	...	2p-k	2p-k+1	2p-k+1	2p-k+2	2p-k+2	...	2p-k+(k-p)=p	2p-k+(k-p)=p
Block 2	1	2	...	2p-k	p+1	p+2	p+3	p+4	...	2k-p-1	2k-p

Figure 3.2: Non-binary design d^*

Proof. For the binary design we have the smallest non-zero eigenvalue as

$$z_{d_0 1} = \frac{p}{k} \tag{3.33}$$

For later proof convenience, we denote $z_{d_0 1} = \frac{p}{k} = \alpha$.

Note that we need $p > \frac{k}{2}$, i.e., $k > \frac{2v}{3}$ so that the design d^* exists. The information matrix for the design d^* is

$$C_{d^*} = \begin{pmatrix} 2I_{2p-k} - \frac{2}{k}J_{2p-k} & -\frac{1}{k}J_{2p-k,2(k-p)} & -\frac{2}{k}J_{2p-k,k-p} \\ -\frac{1}{k}J_{2(k-p),2p-k} & I_{2(k-p)} - \frac{1}{k}J_{2(k-p)} & 0_{2(k-p),k-p} \\ -\frac{1}{k}J_{k-p,2p-k} & 0_{k-p,2(k-p)} & 2I_{k-p} - \frac{4}{k}J_{k-p} \end{pmatrix} \tag{3.34}$$

It is easy to get $2k-p-3$ non-zero eigenvalues of C_{d^*} are: 1 with frequency $2(k-p)-1$ and 2 with frequency $p-2$. Using the technique described in page 37 we have the left two eigenvalues are the non-zero eigenvalues of the matrix:

$$\widetilde{C}_{d^*} = \begin{pmatrix} \frac{4(k-p)}{k} & -\frac{2(k-p)}{k} & -\frac{2(k-p)}{k} \\ -\frac{2p-k}{k} & \frac{2p-k}{k} & 0 \\ -\frac{2(2p-k)}{k} & 0 & \frac{2(2p-k)}{k} \end{pmatrix} \tag{3.35}$$

The two non-zero eigenvalues λ_1 and λ_2 are the two non-zero roots of the equation:

$$|\widetilde{C}_{d^*} - \lambda I_3| = 0 \tag{3.36}$$

i.e., they are two roots of

$$F(\lambda) = k^2\lambda^2 - (k^2 + 2kp)\lambda - 4k^2 + 10kp - 4p^2 = 0. \tag{3.37}$$

Easy to check:

$$\begin{aligned} F(0) &= 2(2p-k)(2k-p) > 0 \\ F(\tfrac{p}{k}) &= (k-p)(5p-4k) \\ F(1) &= -4(k-p)^2 < 0 \\ F(2) &= 2(2p-k)(k-p) > 0 \end{aligned} \tag{3.38}$$

So one root is within the interval $(0,1)$ and the other is within $(1,2)$.

If $\alpha = \frac{p}{k} < \frac{4}{5}$ then $F(\frac{p}{k}) < 0$ and there is an eigenvalue for C_{d^*} smaller than α, therefore the resulted design is E-inferior to the design d_0.

If $\frac{p}{k} > \frac{4}{5}$ then solving equation (3.37) one obtains

$$\lambda_{1,2} = \frac{k + 2p \pm \sqrt{17k^2 - 36kp + 20p^2}}{2k}. \tag{3.39}$$

The smallest non-zero eigenvalue of C_{d^*} is the smaller of these two roots. Denote it by z_{d^*1} and notice $\frac{p}{k} = \alpha$ where $0 < \alpha < 1$, we have

$$z_{d^*1} = \frac{1}{2} + \alpha - \frac{1}{2}\sqrt{17 - 36\alpha + 20\alpha^2}. \tag{3.40}$$

When $\frac{4}{5} < \alpha < 1$, $\sqrt{17 - 36\alpha + 20\alpha^2} < 1$ and $z_{d^*1} > z_{d_01}$. If $\frac{p}{k} = \frac{4}{5}$ then $z_{d^*1} = z_{d_01} = \alpha$. Note that $\frac{p}{k} = \frac{4}{5}$ is equivalent to $k = \frac{5v}{6}$.

Every design in $D_1(v, 2, k)$ has the same numbers $2(k-p)$ and p of treatments with one and two replicates respectively. So the combinatorial structure of any design $d \in D_1(v, b, k)$ with $b = 2$ can be described as follows. In block one there are $k - p - s$ treatments with just one replicate, where $0 \leq s \leq k - p$, and $s + y$ non-binary treatments with two replicates where $y \geq 0$. In block two there are $k-p+s$ treatments with one replicate and y non-binary treatments with two replicates. The two blocks have in common $p-s-2y$ binary treatments with two replicates (see Figure 3.3).

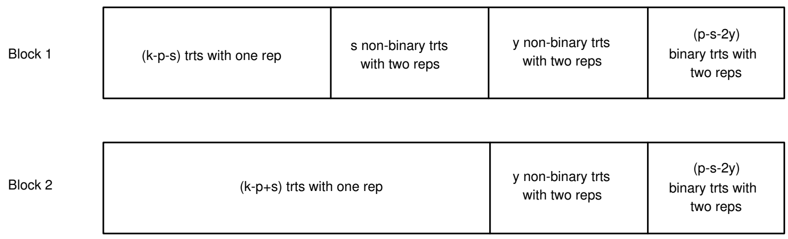

Figure 3.3: General Design Structure in $D_1(v, 2, k)$

Note that $s+2y < p$ so that the design is connected. If $s = y = 0$ we have the design d_0 and the design d^* is given by $s = k-p$ and $y = 0$. The general form of the information matrix C_d is:

$$\begin{pmatrix} I_{k-p+s} - \frac{1}{k}J_{k-p+s} & 0_{k-p+s,k-p-s} & 0_{k-p+s,s+y} & -\frac{2}{k}J_{k-p+s,y} & -\frac{1}{k}J_{k-p+s,p-s-2y} \\ 0_{k-p-s,k-p+s} & I_{k-p-s} - \frac{1}{k}J_{k-p-s} & -\frac{2}{k}J_{k-p-s,s+y} & 0_{k-p-s,y} & -\frac{1}{k}J_{k-p-s,p-s-2y} \\ 0_{s+y,k-p+s} & -\frac{2}{k}J_{s+y,k-p-s} & 2I_{s+y} - \frac{4}{k}J_{s+y} & 0_{s+y,y} & -\frac{2}{k}J_{s+y,p-s-2y} \\ -\frac{2}{k}J_{y,k-p+s} & 0_{y,k-p-s} & 0_{y,s+y} & 2I_y - \frac{4}{k}J_y & -\frac{2}{k}J_{y,p-s-2y} \\ -\frac{1}{k}J_{p-s-2y,k-p+s} & -\frac{1}{k}J_{p-s-2y,k-p-s} & -\frac{2}{k}J_{p-s-2y,s+y} & -\frac{2}{k}J_{p-s-2y,y} & 2I_{p-s-2y} - \frac{2}{k}J_{p-s-2y} \end{pmatrix}$$

Note that if $y = 0$ or $s = k-p$ the information matrix will collapse to fewer partitioned components.

We can get $2k-p-5$ non-zero eigenvalues of C_d very quickly: 1 with frequency $2(k-p)-2$ and 2 with frequency $p-3$. Using the same technique as on page 37 we have the remaining four non-zero eigenvalues are the nonzero eigenvalues of the following matrix:

$$\widetilde{C}_d = \begin{pmatrix} \frac{p-s}{k} & 0 & 0 & -\frac{2y}{k} & -\frac{p-s-2y}{k} \\ 0 & \frac{p+s}{k} & -\frac{2(s+y)}{k} & 0 & -\frac{p-s-2y}{k} \\ 0 & -\frac{2(k-p-s)}{k} & 2-\frac{4(s+y)}{k} & 0 & -\frac{2(p-s-2y)}{k} \\ -\frac{2(k-p+s)}{k} & 0 & 0 & \frac{2(k-2y)}{k} & -\frac{2(p-s-2y)}{k} \\ -\frac{k-p+s}{k} & -\frac{k-p-s}{k} & -\frac{2(s+y)}{k} & -\frac{2y}{k} & \frac{2(k-p+s+2y)}{k} \end{pmatrix} \quad (3.41)$$

The four non-zero eigenvalues are the four non-zero roots of the equation:

$$|\widetilde{C}_d - \lambda I_5| = 0 \quad (3.42)$$

i.e., they are the roots of

$$\widetilde{F_d}(\lambda) = (\lambda-2)(k^2\lambda^3 - 2k(2k-s-2y)\lambda^2 + (4k^2+2kp-p^2-6ks + 2ps - s^2 - 12ky + 4py)\lambda - 2(2k-p)(p-s-2y)) = 0. \quad (3.43)$$

One root is 2 and the other three are the roots to:

$$F_d(\lambda) = k^2\lambda^3 - 2k(2k-s-2y)\lambda^2 + (4k^2+2kp-p^2 - 6ks + 2ps - s^2 - 12ky + 4py)\lambda - 2(2k-p)(p-s-2y) = 0 \quad (3.44)$$

We need to check three cases.

Case I: $0 < s < k-p$ and $y = 0$. Then the matrix $\widetilde{C}_d$ collapses to a 4×4 partitioned matrix and $F_d(\lambda)$ becomes

$$F_{dI}(\lambda) = k^2\lambda^3 - 2k(2k-s)\lambda^2 + (4k^2+2kp-p^2-6ks+2ps-s^2)\lambda - 2(2k-p)(p-s) \quad (3.45)$$

It is easy to check

$$\begin{aligned} &F_{dI}(0) = -2(p-s)(2k-p) < 0 \\ &F_{dI}(\tfrac{p}{k}) = \tfrac{(4(k-p)^2-ps)s}{k} \\ &F_{dI}(1) = (k-p-s)(k-p+s) > 0 \\ &F_{dI}(\tfrac{2k-p}{k}) = -\tfrac{(2k-p)s^2}{k} < 0 \\ &F_{dI}(2) = 2s(p-s) > 0. \end{aligned} \quad (3.46)$$

So the three roots to the equation $F_{dI}(\lambda) = 0$ are within the intervals $(0, 1)$, $(1, \frac{2k-p}{k})$ and $(\frac{2k-p}{k}, 2)$, respectively. The smallest eigenvalue z_{dI_1} is within $(0, 1)$.

If $\frac{p}{k} \leq \frac{4}{5}$ then $F_{dI}(\frac{p}{k}) = \frac{(4(k-p)^2-ps)s}{k} > \frac{(4(k-p)^2-p(k-p))s}{k} = \frac{(k-p)(4k-5p)s}{k} \geq 0$ since $s < k-p$. So We have the smallest eigenvalue $z_{dI_1} < \frac{p}{k}$.

If $\frac{p}{k} > \frac{4}{5}$, let $s = k - p - l$ where $0 < l < k - p$. We introduce l here just for the simpler expression in later proof. The equation $F(\lambda) = 0$ in (3.37) has z_{d^*1} as a root and

$$\begin{aligned} F_{dI}(\lambda) &= k^2\lambda^3 - 2k(2k-s)\lambda^2 + (4k^2 + 2kp - p^2 - 6ks + 2ps - s^2)\lambda - 2(2k-p)(p-s) \\ &= (-1 - \frac{2l}{k} + \lambda)F(\lambda) + (-12kl + 22lp - \frac{8lp^2}{k} + (6kl - l^2 - 8lp)\lambda) \quad (3.47) \end{aligned}$$

Therefore,

$$F_{dI}(z_{d^*1}) = -12kl + 22lp - \frac{8lp^2}{k} + (6kl - l^2 - 8lp)z_{d^*1} \quad (3.48)$$

Notice $p = \alpha k$ and $z_{d^*1} = \frac{1}{2} + \alpha - \frac{1}{2}\sqrt{17 - 36\alpha + 20\alpha^2}$ we have,

$$F_{dI}(z_{d^*1}) = -l(l(\frac{1}{2} + \alpha - \frac{1}{2}\sqrt{17 - 36\alpha + 20\alpha^2}) - k(-3 + 4\alpha)(3 - 4\alpha + \sqrt{17 - 36\alpha + 20\alpha^2})) \quad (3.49)$$

Now we show that

$$\Theta = l(\frac{1}{2} + \alpha - \frac{1}{2}\sqrt{17 - 36\alpha + 20\alpha^2}) - k(-3 + 4\alpha)(3 - 4\alpha + \sqrt{17 - 36\alpha + 20\alpha^2}) < 0 \quad (3.50)$$

i.e., $F_{dI}(z_{d^*1}) > 0$. If true then there is an eigenvalue of C_d less than z_{d^*1} and the design d is E-inferior to d^*.

Noting that $l < (1 - \alpha)k$ and also $\frac{1}{2} + \alpha - \frac{1}{2}\sqrt{17 - 36\alpha + 20\alpha^2} > 0$ for $\frac{4}{5} < \alpha < 1$,

$$\begin{aligned} \Theta &< k(1 - \alpha)(\frac{1}{2} + \alpha - \frac{1}{2}\sqrt{17 - 36\alpha + 20\alpha^2}) \\ &\quad -k(-3 + 4\alpha)(3 - 4\alpha + \sqrt{17 - 36\alpha + 20\alpha^2}) \\ &= \frac{k}{2}(19 + 30\alpha^2 - 47\alpha - (7\alpha - 5)\sqrt{17 - 36\alpha + 20\alpha^2}) \end{aligned}$$

We now show that $(19 + 30\alpha^2 - 47\alpha) - (7\alpha - 5)\sqrt{17 - 36\alpha + 20\alpha^2} < 0$ so that $\Theta < 0$. Notice that $(7\alpha-5)\sqrt{17-36\alpha+20\alpha^2} > 0$ when $\alpha > \frac{4}{5}$. Then $\Theta < 0$ is implied by $T(\alpha) < 0$ where,

$$\begin{aligned} T(\alpha) &= (19+30\alpha^2-47\alpha)^2-((7\alpha-5)\sqrt{17-36\alpha+20\alpha^2})^2 \\ &= -8(\alpha-2)(\alpha-1)(2\alpha-1)(5\alpha-4) \end{aligned}$$

Easy to see that $T(\alpha) < 0$ for every $\alpha \in (\frac{4}{5}, 1)$ so that $\Theta < 0$ and thus $F_{dI}(z_{d^*1}) > 0$. The design d is E-inferior to d^* for $\frac{p}{k} > \frac{4}{5}$ in the second situation under case I.

Case II: $s = k - p$ and $y > 0$. Notice now $2p > k + 2y$ so that the design is connected. Then the matrix $\widetilde{C}_d$ collapses to a 4×4 partitioned matrix and $F_d(\lambda) = 0$ becomes:

$$\widetilde{F}_{dII}(\lambda) = (\lambda-2)(k^2\lambda^2-(k^2+2kp-4ky)\lambda-4k^2+10kp-4p^2-8ky+4py) = 0 \quad (3.51)$$

One root is 2, and the other two are the two roots to :

$$F_{dII}(\lambda) = k^2\lambda^2-(k^2+2kp-4ky)\lambda-4k^2+10kp-4p^2-8ky+4py = 0 \quad (3.52)$$

It is easy to check:

$$\begin{aligned} &F_{dII}(0) = 2(2k-p)(2p-k-2y) > 0 \\ &F_{dII}(\tfrac{p}{k}) = -(k-p)(4k-5p+8y) \\ &F_{dII}(1) = -4(k-p)(k-p+y) < 0 \\ &F_{dII}(2) = 2(2p-k)(k-p)+4py > 0. \end{aligned} \quad (3.53)$$

So the two roots are within the intervals $(0, 1)$ and $(1, 2)$ respectively. The smallest eigenvalue z_{dII_1} is within $(0, 1)$.

If $p \le \frac{4k}{5}$ then $F_{dII}(\frac{p}{k}) = -(k-p)(4k-5p+8y) < 0$. So we have the smallest eigenvalue $z_{dII_1} < \frac{p}{k}$.

If $p > \frac{4k}{5}$, notice the function $F(\lambda)$ in (3.37), and then $F_{dII}(\lambda)$ can be written

$$F_{dII}(\lambda) = F(\lambda) + 4y(-2k+p+k\lambda) \quad (3.54)$$

Therefore,

$$F_{dII}(z_{d^*1}) = 4y(-2k+p+kz_{d^*1}) \quad (3.55)$$

Since $z_{d^*1} < 1$, (3.55) < 0. Therefore, we must have an eigenvalue smaller than z_{d^*1}. The design d is E-inferior to d^* for $p > \frac{4k}{5}$ in the second situation under case II.

Case III: $s < k - p$ and $y > 0$. Now $F_{dIII}(\lambda) \equiv F_d(\lambda)$ satisfies

$$\begin{aligned} F_{dIII}(0) &= -2(p-s-2y)(2k-p) < 0 \\ F_{dIII}(\tfrac{p}{k}) &= \tfrac{4(k-p)^2(s+2y)-ps^2}{k} \\ F_{dIII}(1) &= (k-p-s)(k-p+s) > 0 \\ F_{dIII}(\tfrac{2k-p}{k}) &= -\tfrac{(2k-p)s^2}{k} < 0 \\ F_{dIII}(2) &= 2s(p-s) + 4py > 0 \end{aligned} \tag{3.56}$$

So the three roots are within interval $(0, 1)$, $(1, \frac{2k-p}{k})$ and $(\frac{2k-p}{k}, 2)$ respectively. The smallest positive eigenvalue z_{dIII_1} is within $(0, 1)$.

If $\frac{p}{k} \leq \frac{4}{5}$ then $F_{dIII}(\frac{p}{k}) = \frac{(4(k-p)^2-ps)s+8(k-p)^2y}{k} > \frac{(4(k-p)^2-p(k-p))s+8(k-p)^2y}{k} > 0$. So the smallest eigenvalue $z_{dIII_1} < \frac{p}{k}$.

If $\frac{p}{k} > \frac{4}{5}$, notice the function $F_{dI}(\lambda)$ in (3.45) and then,

$$F_{dIII}(\lambda) = F_{dI}(\lambda) + 4y[(2-\lambda)k - p](1-\lambda) \tag{3.57}$$

Therefore,

$$F_{dIII}(z_{dI_1}) = 4y[(2 - z_{dI_1})k - p](1 - z_{dI_1}) \tag{3.58}$$

Since $z_{dI_1} < 1$, $F_{dIII}(z_{dI_1}) > 0$. This means that we have an eigenvalue of C_{dIII} smaller than z_{dI_1} (so it is also smaller than $z_{d_1^*}$) for $p > \frac{4k}{5}$. The design d_{III} is E-inferior to d^* when $p > \frac{4k}{5}$, or equivalently, $k > \frac{5v}{6}$. □

Lemma 3.7. Any design in the class $D(v, 2, k)$ with at least $k - p + 1$ treatments with one replicate in both blocks is E-inferior to the binary design d_0.

Proof. Since both blocks have at least $k - p + 1$ treatments with one replicate, we can pick $k - p + 1$ treatments in block one as group 1 and $k - p + 1$ treatments in block two as group 2. The contrast vector $\underline{l}$ between the average of group 1 treatments and the average of group 2 treatments with contrast coefficients normalized gives $\underline{l}' C_d \underline{l} = \frac{p-1}{k} < \frac{p}{k}$. □

Lemma 3.8. (**Morgan and Reck (2003)**) Partition the C_d matrix as

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

where C_{d11} is a $t \times t$ submatrix and C_{d22} is a $(v-t) \times (v-t)$ submatrix, where $1 \leq t \leq v$. This partition is valid for any t treatments by permutation of rows and columns of the C_d matrix. Let $\underline{\omega}$ be any normalized vector (i.e., $\underline{\omega}^{'}\underline{\omega} = 1$), and write $x = \underline{\omega}^{'}\underline{1}$. Then

$$z_{d1} \leq \frac{v}{v-x^2}\underline{\omega}^{'}C_{d11}\underline{\omega} \tag{3.59}$$

One may refer to Morgan and Reck (2003) for a detailed proof.

Corollary 3.1. The smallest positive eigenvalue z_{d1} of C_d of a design $d \in D(v,b,k)$ is bounded by

$$z_{d1} \leq min(\frac{v}{v-1}C_{dii}, \frac{C_{dii}+C_{di'i'}-2C_{dii'}}{2}, \frac{v(C_{dii}+C_{di'i'}-2C_{dii'})}{2(v-2)}, \frac{v}{m(v-m)}\sum_{i,i'\in M}C_{dii'}) \tag{3.60}$$

where $C_{dii'}$ is the $(i,i^{'})th$ element of C_d; $i, i^{'} = 1, 2, \cdots, v$; $2 \leq m \leq v-1$ is an integer; and M is a subset of size m of the v treatments.

Proof. Following Lemma 3.8, taking $t = 1$ and $\underline{\omega} = 1$, we have $z_{d1} \leq \frac{v}{v-1}C_{dii}$; taking $t = 2$ and $\underline{\omega} = (\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})^{'}$, we have $z_{d1} \leq \frac{C_{dii}+C_{di'i'}-2C_{dii'}}{2}$; taking $t = 2$ and $\underline{\omega} = (\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})^{'}$, we have $z_{d1} \leq \frac{v(C_{dii}+C_{di'i'}-2C_{dii'})}{2(v-2)}$; taking $t = m$ and $\underline{\omega} = (\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}}, \cdots, \frac{1}{\sqrt{m}})^{'}$ we have $z_{d1} \leq \frac{v}{m(v-m)}\sum_{i,i'\in M}C_{dii'}$. □

M.Jacroux (1980a) first gave the results of corollary 3.1. Lemma 3.8 is an extended version his results.

Lemma 3.9. Any design in the class $D(v, 2, k)$ with more than $k - \frac{p}{2}$ treatments with one replicate in either of the blocks is E-inferior to the binary design d_0.

Proof. Suppose WLOG treatments $1, 2, \ldots, k-t$ have one replicate in one block in a design $d \in D(v, 2, k)$. Then by corollary 3.1,

$$z_{d1} \leq \frac{v}{(k-t)(v-k+t)} \sum_{i,i'=1}^{k-t} C_{dii'} = \frac{vt}{k(v-k+t)} = \frac{(2k-p)t}{(k-p+t)k}$$

If $\frac{(2k-p)t}{(k-p+t)k} < \frac{p}{k}$ then, the design d is E-inferior to the binary design d_0, i.e., $t < \frac{p}{2}$ □

Lemma 3.10. Any design in which some treatment has more than two replicates cannot be E-optimal in $D(v, 2, k)$, i.e., any design in $D_2(v, 2, k)$ cannot be E-optimal design in $D(v, 2, k)$.

A proof for this lemma is given in Appendix B. The average matrix technique, Lemma 3.5, Lemma 3.7 and Lemma 3.9 are used in the proof.

Theorem 3.6. In the class $D(v, 2, k)$, binary design d_0 is the unique E-optimal design if $\frac{v}{2} < k < \frac{5v}{6}$; non-binary design d^* is the unique E-optimal design if $\frac{5v}{6} < k < v$; the non-binary design d^* and the binary design d_0 are both E-optimal if $k = \frac{5v}{6}$ and no other design can be E-optimal. The design d^* is displayed in Figure 2.

Lemma 3.6 and Lemma 3.10 together imply Theorem 3.6.

Corollary 3.2. Denote the E- value (smallest positive eigenvalue of the information matrix) of the E-optimal designs in $D(v, 2, k)$ by EV. Then

$$EV = \begin{cases} 2 - \frac{v}{k} & \text{when } \frac{k}{v} \leq \frac{5}{6}; \\ \frac{5}{2} - \frac{v}{k} - \frac{1}{2}\sqrt{25 - \frac{44v}{k} + \frac{20v^2}{k^2}} & \text{when } \frac{k}{v} > \frac{5}{6}. \end{cases} \tag{3.61}$$

Corollary 3.3. EV is increasing in $\frac{k}{v}$, and for given v, it is also increasing in k.

Proof. Letting $\iota = \frac{k}{v}$, we have

$$\frac{\partial EV}{\partial \iota} = \begin{cases} \frac{1}{\iota^2} > 0 & \text{when } \iota \leq \frac{5}{6}; \\ \frac{10 - 11\iota + \sqrt{20 - 44\iota + 25\iota^2}}{\iota^2\sqrt{20 - 44\iota + 25\iota^2}} & \text{when } \frac{k}{v} > \frac{5}{6}. \end{cases} \tag{3.62}$$

when $\iota = \frac{k}{v} > \frac{5}{6}$, since $(\sqrt{20 - 44\iota + 25\iota^2})^2 - (10 - 11\iota)^2 = 16(1 - \iota)(6\iota - 5) > 0$, $\frac{\partial EV}{\partial \iota} > 0$.

For given v,

$$\frac{\partial EV}{\partial k} = \begin{cases} \frac{v}{k^2} > 0 & \text{when } \frac{k}{v} \leq \frac{5}{6}; \\ \frac{v(-11k+10v+\sqrt{25k^2-44kv+20v^2})}{k^3\sqrt{25k^2-44kv+20v^2}} & \text{when } \frac{k}{v} > \frac{5}{6}. \end{cases} \tag{3.63}$$

when $\frac{k}{v} > \frac{5}{6}$, since $(\sqrt{25k^2 - 44kv + 20v^2})^2 - (10v - 11k)^2 = 16(6k - 5v)(v - k) > 0$, $\frac{\partial EV}{\partial k} > 0$. □

We close this section with some examples of E-optimal designs.

Example 3.5.1. For $v = 13$ and $k = 11 > 5v/6$, the E-optimal design in the class $D(v, 2, k)$ is:

Block 1	1	2	...	7	8	8	9	9
Block 2	1	2	...	7	10	11	12	13

The E-value of this design is $EV \approx 0.835$.

Example 3.5.2. For $v = 9$ and $k = 7 < 5v/6$, the E-optimal design in the class $D(v, 2, k)$ is:

Block 1	1	2	...	5	6	7
Block 2	1	2	...	5	8	9

The E-value of this design is $EV = 5/7 \approx 0.714$.

Example 3.5.3. For $v = 12$ and $k = 10 = 5v/6$, there are two E-optimal designs:

Design 1:

Block 1	1	2	...	6	7	7	8	8
Block 2	1	2	...	6	9	10	11	12

Design 2:

Block 1	1	2	...	6	7	8	9	10
Block 2	1	2	...	6	7	8	11	12

The common E-value of the two designs is $EV = 2 - 6/5 = 0.8$.

3.6 Further Discussion in the class $D_1(v, 2, k)$

Theorem 3.7. In the class $D_1(v, 2, k)$, if $\frac{p}{k} = \frac{4}{5}$, d^* is the only non-binary design that is E-equal to binary design d_0 and all other non-binary designs are E-inferior to d_0 and d^*. If $\frac{p}{k} > \frac{4}{5}$, a necessary condition for a non-binary design to be E-superior to d_0 is $s \geq \lfloor \frac{4(k-p)^2}{p} \rfloor + 1$, that is, the range of s for a non-binary design to possibly be E-superior to d_0 is $[\lfloor \frac{4(k-p)^2}{p} \rfloor + 1, k - p]$. Furthermore, this necessary condition is also sufficient when $y = 0$. When $\frac{4(k-p)^2}{p}$ is an integer, $s = \frac{4(k-p)^2}{p}$, and $y = 0$, the corresponding designs are E-equal to d_0.

Proof. One may check $k - p \geq \lfloor \frac{4(k-p)^2}{p} \rfloor + 1$ if $\frac{p}{k} > \frac{4}{5}$.

If $s < \lfloor \frac{4(k-p)^2}{p} \rfloor$, then

$$\begin{aligned} F_{dI}(\frac{p}{k}) &= \frac{(4(k-p)^2 - ps)s}{k} > 0 \\ F_{dIII}(\frac{p}{k}) &= \frac{(4(k-p)^2 - ps)s + 8(k-p)^2 y}{k} > 0 \end{aligned}$$

and so designs corresponding to $s < \lfloor \frac{4(k-p)^2}{p} \rfloor$ are E- inferior to the binary design d_0 (see (3.47) and (3.57)).

If $\frac{4(k-p)^2}{p}$ is an integer and $s = \frac{4(k-p)^2}{p}$, we must have $\frac{4(k-p)^2}{p} \leq k - p$, or equivalently, $\frac{p}{k} \geq \frac{4}{5}$. Furthermore, if $y > 0$, the resulting designs are still E-inferior to the binary design d_0 by (3.56). If y=0, we need to discuss two cases:

a) $\frac{p}{k} = \frac{4}{5}$, then we have $s = 4(k-p)^2/p = k - p$. This is d^*.

b) $\frac{p}{k} > \frac{4}{5}$, the design has smallest eigenvalue $\frac{p}{k}$ thus we have found conditions for E-suboptimal non-binary designs that are E- equal to d_0.

This conclude the proof. □

Theorem 3.8. Among all non-binary designs that are E-superior to d_0 when $\frac{p}{k} > \frac{4}{5}$, the design with $s = \lfloor \frac{4(k-p)^2}{p} \rfloor + 1$ and $y = 0$ is A-best.

Proof. By (3.44) and Lemma 3.3, A-value for the general non-binary designs, denoted as A_{nb}, can be expressed as:

$$\begin{aligned} A_{nb} &= (2(k-p)-2) \times 1 + (p-2) \times \frac{1}{2} + \frac{4k^2 + 2kp - p^2 - 6ks + 2ps - s^2 - 12ky + 4py}{2(2k-p)(p-s-2y)} \\ &= \frac{1}{2(2k-p)(p-s-2y)}(4k^2 - 10kp + 8k^2 p + 5p^2 - 10kp^2 + 3p^3 + 6ks - 8k^2 s - 4ps \\ &\quad + 10kps - 3p^2 s - s^2 + 12ky - 16k^2 y - 8py + 20kpy - 6p^2 y) \end{aligned} \tag{3.64}$$

Check,

$$\begin{aligned} \frac{\partial A_{nb}}{\partial s} &= \frac{4k(k-p) + (p-s)^2 + 4sy}{2(2k-p)(p-s-2y)^2} > 0 \\ \frac{\partial A_{nb}}{\partial y} &= \frac{(2k-p-s)(2k-p+s)}{(2k-p)(p-s-2y)^2} > 0 \end{aligned}$$

Therefore, A_{nb} is an increasing function with respect to s and y respectively. And its smallest value takes place at $s = \lfloor \frac{4(k-p)^2}{p} \rfloor + 1$ and $y = 0$. □

Theorem 3.9. Among all non-binary designs that are E-superior to d_0 when $\frac{p}{k} > \frac{4}{5}$, the design with $s = \lfloor \frac{4(k-p)^2}{p} \rfloor + 1$ and $y = 0$ is D-best.

Proof. By (3.44) and Lemma 3.3, D-value for the general non-binary designs, denoted as D_{nb}, can be expressed as:

$$D_{nb} = (\frac{1}{2})^{p-2} \frac{k^2}{2(2k-p)(p-s-2y)} \tag{3.65}$$

Check,

$$\begin{aligned} \frac{\partial D_{nb}}{\partial s} &= \frac{2^{1-p}k^2}{(2k-p)(p-s-2y)^2} > 0 \\ \frac{\partial D_{nb}}{\partial y} &= \frac{2^{2-p}k^2}{(2k-p)(p-s-2y)^2} > 0 \end{aligned}$$

Therefore, D_{nb} is an increasing function with respect to s and y respectively. And its smallest value takes place at $s = \lfloor \frac{4(k-p)^2}{p} \rfloor + 1$ and $y = 0$. □

Theorem 3.10. Among all non-binary designs that are E-superior to d_0 when $\frac{p}{k} > \frac{4}{5}$, the smallest positive eigenvalue of the information matrix is increasing with respect to s and decreasing with respect to y.

Proof. The smallest positive eigenvalue is the smallest root to the equation $F_d(\lambda) = 0$. To show it is increasing with respect to s when $s \in [\lfloor \frac{4(k-p)^2}{p} \rfloor + 1, k-p]$, we only need to show that the smallest root for $s = x+1$ is greater than $s = x$, where x is an integer in $[\lfloor \frac{4(k-p)^2}{p} \rfloor + 1, k-p-1]$. Let $F_{x1}(\lambda) = F_d(\lambda)|_{s=x+1}$, $F_{x2}(\lambda) = F_d(\lambda)|_{s=x}$ and $F_{xd}(\lambda) = F_{x1}(\lambda) - F_{x2}(\lambda)$. One may check,

$$F_{xd}(\lambda) = 2k\lambda^2 - (1 + 6k - 2p + 2x)\lambda + 2(2k-p)$$

And

$$\begin{aligned} F_{xd}(0) &= 2(2k-p) > 0 \\ F_{xd}(\frac{p}{k}) &= \frac{4(k-p)^2 - 2px - p}{k} \\ &< \frac{4(k-p)^2 - 2p(4(k-p)^2/p) - p}{k} \\ &= -\frac{4(k-p)^2 + p}{k} < 0 \end{aligned}$$

Therefore, one root to $F_{xd}(\lambda) = 0$, denote it as λ_1, is less than $\frac{p}{k}$. Denote the other root as λ_2. By lemma 3.3,

$$\lambda_1 + \lambda_2 = \frac{1 + 6k - 2p + 2x}{2k}$$

We have,

$$\lambda_2 > \frac{1 + 6k - 2p + 2x}{2k} - \frac{p}{k} = \frac{1 + 6k - 4p + 2x}{2k} > 1$$

Suppose the E-value for $s = x+1$, denoted as z_{x1} is less than that for $s = x$, which is denoted as z_{x2}. By assumption of the theorem, both z_{x1} and z_{x2} are greater than $\frac{p}{k}$. Then we have,

$$\begin{aligned} F_{x1}(z_{x1}) &= 0 \\ F_{x2}(z_{x1}) &< 0 \\ F_{xd}(z_{x1}) &= F_{x1}(z_{x1}) - F_{x2}(z_{x1}) > 0 \end{aligned}$$

The second expression above holds because we know that if $F_{x2}(z_{x1}) > 0$ then $z_{x2} < z_{x1}$ since we know $F_{x2}(0) < 0$ by (3.46) and (3.56), which is against the assumption that $z_{x1} < z_{x2}$. So we must have $F_{x2}(z_{x1}) < 0$.

Then λ_2 must be in $(\frac{p}{k}, z_{x1})$. We know that $z_{x1} < 1$. Contradiction.

To show that E- value is decreasing with respect to y, we only need to show the E- value for $y = \rho + 1$ is greater than that for $y = \rho$, where ρ is an integer in $[0, \lceil (p-s)/2 \rceil - 1]$. Let $F_{y1}(\lambda) = F_d(\lambda)|_{y=\rho+1}$, $F_{y2}(\lambda) = F_d(\lambda)|_{y=\rho}$ and $F_{yd}(\lambda) = F_{y1}(\lambda) - F_{y2}(\lambda)$. One may check,

$$F_{yd}(\lambda) = 4(\lambda - 1)(-2k + p + k\lambda)$$

Two roots to $F_{yd} = 0$ are $\lambda_1 = 1$ and $\lambda_2 = (2k - p)/k > 1$. And

$$F_{yd}(0) = 4(2k - p) > 0$$

Suppose the E-value for $y = \rho + 1$, denoted as z_{y1} is greater than that for $y = \rho$, denoted as z_{y2}. Then we have,

$$\begin{aligned} F_{y1}(z_{y1}) &= 0 \\ F_{y2}(z_{y1}) &> 0 \\ F_{yd}(z_{y1}) &= F_{y1}(z_{y1}) - F_{y2}(z_{y1}) < 0 \end{aligned}$$

The second expression above holds because we know that if $F_{y2}(z_{y1}) < 0$ then $z_{y1} < z_{y2}$ since we know $F_{y2}(1) > 0$ by (3.56), which is against the assumption that $z_{y1} > z_{y2}$. So we must have $F_{y2}(z_{y1}) > 0$

Since $F_{yd}(0) > 0$, there must be a root to $F_{yd} = 0$ be in $(0, z_{y1})$. We know that $z_{y1} < 1$. Contradiction.

□

The proof of Theorem 3.10 has provided a new way to show Lemma 3.6.

Example 3.6.1. In the class $D(110, 2, 100)$, $p = 2k - v = 90$ and $\frac{p}{k} = 9/10 > \frac{4}{5}$. We know that d_0 is the A- and D-optimal design and d^* is the E-optimal design. In the subclass $D_1(110, 2, 100)$, the necessary condition for non-binary designs E-better than the binary design d_0 is

$$s \geq \lfloor \frac{4(100 - 90)^2}{90} \rfloor + 1 = 5$$

Suppose $y = 0$, the designs corresponding to $s \in \{5, 6, 7, 8, 9, 10\}$, are all E-better than d_0; when $s = k - p = 10$ we have the E-optimal d^*. Denote the designs in $D_1(110, 2, 100)$ with $s = 5, 6, 7, 8, 9$ as d_1, d_2, d_3, d_4 and d_5 respectively. Also use ">" to denote "better". We see that

$$\begin{aligned} &\text{A- and D-criteria}: \quad d_0 > d_1 > d_2 > d_3 > d_4 > d_5 > d^* \\ &\text{E-criterion}: \quad d^* > d_5 > d_4 > d_3 > d_2 > d_1 > d_0 \end{aligned}$$

It is interesting to notice that some designs, like d_1, d_2, d_3, d_4 and d_5, which are neither A-optimal nor E-optimal, are still good designs in the sense that they are E-better than the A-optimal design d_0 and A- and D-better than the E-optimal design d^* when $p > 4k/5$.

3.7 Discussion of ϕ_β-optimal designs in $D(v, 2, k)$

Definition 3.3. A design is said to be ϕ_β-optimal in $D(v, b, k)$ if it has the minimum value of $\phi_\beta(C_d)$ among all designs in $D(v, b, k)$, where

$$\phi_\beta(C_d) = (\sum_{i=1}^{v-1}(z_{di})^{-\beta})^{\frac{1}{\beta}} \tag{3.66}$$

Note that ϕ_β-optimality discussed in this section is equivalent to the ϕ_p-optimality introduced by Kiefer (1975), where $\phi_p(C_d) = (\sum_{i=1}^{v-1}(\frac{z_{di}}{v-1})^{-p})^{\frac{1}{p}}$. We simply dropped the constant term in ϕ_p to get ϕ_β. The reason we do not use the notation ϕ_p is that p has a special meaning in this chapter.

As pointed out by Shah and Sinha (1989), ϕ_β-optimality is a larger optimality class than A-, D- and E-optimality, i.e., ϕ_β-optimality $\supset$ A-, D- and E-optimality. In fact, A-optimality = ϕ_1-optimality, D-optimality = ϕ_0-optimality and E-optimality = ϕ_∞-optimality.

From previous sections we know that $\phi_\infty-$ (or E-) optimal designs may not be binary designs. It is a difficult task to find ϕ_β-optimal designs for other β except $\beta = 0$, 1 and ∞. But we will show that some other ϕ_β-optimal designs ($\beta < \infty$) must lie in the non-binary class. To see this we simply compare d^* to d_0.

Appendix E gives a Matlab program to compare d^* and d_0 in terms of ϕ_β when $k/v > 5/6$ and $4 \leq v \leq 100$. The program gives the value of $\widetilde{\beta}$ above which d^* is ϕ_β-better than d_0. Note that the returned value is an approximation to (a bit greater than) the root of $\phi_\beta(C_{d^*}) = \phi_\beta(C_{d_0})$. To see that, above $\widetilde{\beta}$, d^* is ϕ_β-better than d_0, one may simply plot $\phi_\beta(C_{d^*})$ and $\phi_\beta(C_{d_0})$ versus β. We omit the plots here. This program can also be used for

$k/v < 5/6$. In fact, we did not find any examples where d^* is ϕ_β-better than d_0 for any β in $(0, \infty)$ when $k/v < 5/6$.

It is interesting that the change of $\widetilde{\beta}$ over k for a given v is not monotone. Using the program in Appendix E, we found that for $v \le 24$, $\widetilde{\beta}$ is monotonely decreasing in k. This does not hold for $25 \le v \le 100$.

Example 3.7.1. With $v = 100$, for $k/v > 5/6$ we need $k \ge 84$. The following table gives $\widetilde{\beta}$ such that d^* is ϕ_β-better than d_0 for $\beta > \widetilde{\beta}$. $\widetilde{\beta}$ is decreasing when $84 \le k \le 94$, and then

k	$\widetilde{\beta}$	k	$\widetilde{\beta}$	k	$\widetilde{\beta}$	k	$\widetilde{\beta}$
84	9.771	85	7.316	86	6.253	87	5.628
88	5.213	89	4.923	90	4.714	91	4.566
92	4.465	93	4.405	94	4.384	95	4.405
96	4.474	97	4.614	98	4.872	99	5.421

Table 3.1: $\widetilde{\beta}$ for $v = 100$ and $84 \le k \le 99$

increasing when $94 \le k \le 99$.

Example 3.7.2. With $v = 24$, for $k/v > 5/6$ we need $k \ge 21$, the following table gives $\widetilde{\beta}$ such that d^* is ϕ_β-better than d_0 for $\beta > \widetilde{\beta}$. $\widetilde{\beta}$ is decreasing when $21 \le k \le 23$.

k	$\widetilde{\beta}$	k	$\widetilde{\beta}$	k	$\widetilde{\beta}$
21	5.401	22	4.494	23	4.459

Table 3.2: $\widetilde{\beta}$ for $v = 24$ and $21 \le k \le 23$

These examples show that the binary design d_0 is ϕ_β-better than the non-binary design d^* for only a relatively small set of β, and otherwise is inferior.

Chapter 4

Optimal Incomplete Binary Designs with Three Blocks

4.1 Summary

In this chapter we study the optimal incomplete block designs when there are three blocks of the same size. It turns out that a design d^* is E- and Type I-optimal in the class $D(v,3,k)$ when $k = 2v/3$. Denote the subclass of binary designs in $D(v,3,k)$ by $M(v,3,k)$. In $M(v,3,k)$, A-, D- and E-optimal designs are also identified when $k \neq 2v/3$. At the end of this chapter we discuss optimal designs for the entire class $D(v,3,k)$.

4.2 Optimal Designs in $D(v,3,k)$ when $k = \frac{2v}{3}$

Consider the class $D(v,3,k)$ with $k = \frac{2v}{3}$. We have $r = [\frac{3k}{v}] = 2$ and $p = bk - vr = 0$. It is obvious that the block size must be an even number. Let $k = 2m$ and $v = 3m$ where $m \geq 1$.

Consider a binary design d^* in which all the treatments have replication two.

$$\begin{array}{llllllllll} B_1: & 1 & 2 & \dots & m & m+1 & m+2 & \dots & 2m \\ B_2: & 1 & 2 & \dots & m & 2m+1 & 2m+2 & \dots & 3m \\ B_3: & m+1 & m+2 & \dots & 2m & 2m+1 & 2m+2 & \dots & 3m \end{array}$$

The design d^* is the only regular graph design in the class $D(v, 3, \frac{2v}{3})$. It can be seen that in d^*,

$$|B_1 \cap B_2| = |B_1 \cap B_3| = |B_2 \cap B_3| = m \tag{4.1}$$

where $|B_i \cap B_j|$ denote the intersection numbers for the three blocks. The information matrix of d^* is

$$C_{d^*} = \begin{pmatrix} 2I_m - \frac{1}{m}J_m & -\frac{1}{2m}J_m & -\frac{1}{2m}J_m \\ -\frac{1}{2m}J_m & 2I_m - \frac{1}{m}J_m & -\frac{1}{2m}J_m \\ -\frac{1}{2m}J_m & -\frac{1}{2m}J_m & 2I_m - \frac{1}{m}J_m \end{pmatrix} \tag{4.2}$$

One can get the $v-1$, i.e. $3m-1$, eigenvalues of C_{d^*} : 2 with multiplicity $3(m-1)$ and 3/2 with multiplicity 2. So the smallest eigenvalue for d^*, denoted as z_{d^*1}, is 3/2.

4.2.1 M-optimal Designs in the Equal-Replicate Subclass of $D(v, 3, 2v/3)$

For any row vector $\underline{x} = (x_1, x_2, \dots, x_n) \in \mathrm{R}^n$, let $(x_{(1)}, x_{(2)}, \dots, x_{(n)})$ denote the increasing reordering of $\underline{x}$, that is, it is the vector, obtained from $\underline{x}$ by permuting co-ordinate positions, such that $x_{(1)} \le x_{(2)} \le \dots \le x_{(n)}$. The next definition and theorem generalize material presented in section 3.2.

Definition 4.1. For any two row vectors $\underline{x}, \underline{y} \in \mathrm{R}^n$, $\underline{x}$ is said to be weakly majorized by $\underline{y}$ (in symbols, $\underline{x} \prec^w \underline{y}$) if

$$\sum_{i=1}^{l} x_{(i)} \ge \sum_{i=1}^{l} y_{(i)}, \quad l = 1, 2, \dots n. \tag{4.3}$$

We shall need the following theorem. See page 109 of Marshall and Olkin (1979) for a proof.

Theorem 4.1. $\underline{x} \prec^w \underline{y}$ if and only if

$$\sum_{i=1}^{n} f(x_i) \geq \sum_{i=1}^{n} f(y_i) \tag{4.4}$$

for every convex decreasing function $f : R^n \to R^n$.

Motivated by Theorem 4.1, B. Bagchi and S. Bagchi (2001) introduced the following.

Definition 4.2. A design d_1 is said to be better than another design d_2 in the sense of majorization (in short M- better) if

$$\underline{z}(C_{d_1}) \prec^w \underline{z}(C_{d_2}) \tag{4.5}$$

where $\underline{z}(C_d) = (z_{d,1}, z_{d,2}, \ldots, z_{d,v-1})$ is the vector of positive eigenvalues of the information matrix C_d.

Definition 4.3. A design $d^* \in D(v, b, k)$ is said to be optimal in the sense of majorization (in short, d^* is M- optimal in $D(v, b, k)$) if it is M- better than any other design in $D(v, b, k)$.

It can be shown that if d^* is M- better than d then d^* is better than d with respect to all the criteria of Type I- (B. Bagchi and S. Bagchi (2001)). In particular, M-optimality implies optimality with respect to all the usual criteria, including E-, A- and D-optimality.

Theorem 4.2. Design d^* is M- optimal in the equal-replicate subclass of $D(v, 3, 2v/3)$.

Proof. For any design d in the equal-replicate subclass in $D(v, 3, 2v/3)$, each treatment must have exactly two replicates. Consider the general combinatorial structure of such a design d.

In d, let $|B_1 \cap B_2| = s_1$, $|B_1 \cap B_3| = s_2$, and $|B_2 \cap B_3| = s_3$, where $s_1 + s_2 + s_3 \leq 3m$ and s_1, s_2, and s_3 are the block intersection numbers. Also let $t_1 = m - \frac{s_1+s_2}{2}$, $t_2 = m - \frac{s_1+s_3}{2}$ and $t_3 = m - \frac{s_2+s_3}{2}$. The integers t_1, t_2 and t_3 denote the number of treatments occurring twice in the each of the three blocks respectively. All designs (either binary or non-binary) in which all treatments have exactly two replicates are determined by the six integers s_1, s_2, s_3, t_1, t_2 and t_3. The information matrix for such a design d is

$$\begin{pmatrix} 2I_{t_1}-\frac{2}{m}J_{t_1} & 0 & 0 & -\frac{1}{m}J_{t_1,s_1} & -\frac{1}{m}J_{t_1,s_2} & 0 \\ 0 & 2I_{t_2}-\frac{2}{m}J_{t_2} & 0 & -\frac{1}{m}J_{t_2,s_1} & 0 & -\frac{1}{m}J_{t_2,s_3} \\ 0 & 0 & 2I_{t_3}-\frac{2}{m}J_{t_3} & 0 & -\frac{1}{m}J_{t_3,s_2} & -\frac{1}{m}J_{t_3,s_3} \\ -\frac{1}{m}J_{s_1,t_1} & -\frac{1}{m}J_{s_1,t_2} & 0 & 2I_{s_1}-\frac{1}{m}J_{s_1} & -\frac{1}{2m}J_{s_1,s_2} & -\frac{1}{2m}J_{s_1,s_3} \\ -\frac{1}{m}J_{s_2,t_1} & 0 & -\frac{1}{m}J_{s_2,t_3} & -\frac{1}{2m}J_{s_2,s_1} & 2I_{s_2}-\frac{1}{m}J_{s_2} & -\frac{1}{2m}J_{s_2,s_3} \\ 0 & -\frac{1}{m}J_{s_3,t_2} & -\frac{1}{m}J_{s_3,t_3} & -\frac{1}{2m}J_{s_3,s_1} & -\frac{1}{2m}J_{s_3,s_2} & 2I_{s_3}-\frac{1}{m}J_{s_3} \end{pmatrix}. \tag{4.6}$$

Its eigenvalues are 2 with multiplicity of $3(m-1)$, and the two roots to the equation:

$$4m^2{z_d}^2 - 4m(s_1+s_2+s_3)z_d + 3(s_1s_2+s_2s_3+s_1s_3) = 0 \tag{4.7}$$

The two roots are:

$$z_{d1} = \frac{s_1+s_2+s_3-\sqrt{1/2[(s_1-s_2)^2+(s_1-s_3)^2+(s_2-s_3)^2]}}{2m} \tag{4.8}$$

$$z_{d2} = \frac{s_1+s_2+s_3+\sqrt{1/2[(s_1-s_2)^2+(s_1-s_3)^2+(s_2-s_3)^2]}}{2m} \tag{4.9}$$

Since $s_1+s_2+s_3 \le 3m$,

$$z_{d1} \le \frac{3m-\sqrt{1/2[(s_1-s_2)^2+(s_1-s_3)^2+(s_2-s_3)^2]}}{2m} \le \frac{3}{2} = z_{d^*1}. \tag{4.10}$$

Now consider two cases.

Case I. Suppose $z_{d2} \le 2$. Then write the vector of eigenvalues $\underline{z}(C_d)$ with its elements in increasing order as

$$\underline{z}(C_d) = (z_{d1}, z_{d2}, 2, 2, \ldots, 2). \tag{4.11}$$

Also write the vector of eigenvalues $\underline{z}(C_{d^*})$ with its elements in increasing order as

$$\underline{z}(C_{d^*}) = (3/2, 3/2, 2, 2, \ldots, 2). \tag{4.12}$$

Since $tr(C_d) \le tr(C_{d^*})$, $z_{d1}+z_{d2} = (s_1+s_2+s_3)/m \le 3$ and so $\underline{z}(C_{d^*}) \prec^w \underline{z}(C_d)$.

Case II. Suppose $z_{d2} > 2$. Then write the vector of eigenvalues $\underset{\sim}{z}(C_d)$ with its elements in increasing order as

$$\underset{\sim}{z}(C_d) = (z_{d1}, 2, 2, \ldots, 2, z_{d2}). \tag{4.13}$$

Since $z_{d1} + z_{d2} = (s_1 + s_2 + s_3)/m \leq 3$, we must have $z_{d1} < 1$, and thus again $\underset{\sim}{z}(C_{d^*}) \prec^w \underset{\sim}{z}(C_d)$.

So d^* is M- better than any other design in the equal-replicate subclass in $D(v, 3, 2v/3)$, thus is M-optimal in this subclass. □

In the next two subsections we will show that d^* is E- and Type I-optimal in $D(v, 3, 2v/3)$. By Theorem 4.2, we only need to show that E- and Type I-optimal designs in $D(v, 3, \frac{2v}{3})$ must lie in the equal-replicate subclass.

4.2.2 E-optimal Designs

Theorem 4.3. Design d^* is E-optimal in $D(v, 3, \frac{2v}{3})$.

Proof. For a design $d \in D(v, 3, \frac{2v}{3})$, if some treatment has just one replicate, then the smallest eigenvalue of C_d is

$$z_{d1} \leq \frac{v}{v-1} C_{dii} = \frac{3m}{3m-1} \frac{2m-1}{2m} = \frac{6m-3}{6m-2} < 1 < \frac{3}{2} = z_{d^*1}. \tag{4.14}$$

Therefore, all the treatment must have exactly two replicates for E-optimal designs in $D(v, 3, \frac{2v}{3})$, and d^* is E-optimal in $D(v, 3, 2v/3)$ by Theorem 4.2. □

4.2.3 Type I-optimal Designs

Consider the Type I-optimality problems defined in chapter 1. If $f(x)$ satisfies the conditions in Definition 1.7, we want to find $x_1, x_2, \ldots, x_n$ to minimize

$$\sum_{i=1}^{n} f(x_i). \tag{4.15}$$

The following theorem is used to attack Type I-optimality problems in $D(v, 3, 2v/3)$.

Theorem 4.4. (Kunert (1985); Jacroux (1985)) The minimum value of the function given in (4.15) subject to constraints that

$$\begin{aligned} x_i &\geq 0 \text{ for } i = 1, 2, \ldots, n \\ \sum_i^n x_i &\leq C_1 \\ x_1 &\leq C_2 \text{ for some } C_2 \text{ satisfying } 0 < C_2 \leq C_1/(n-1) \end{aligned}$$

occurs when

$$\begin{aligned} x_1 &= C_2, \\ x_i &= \tfrac{C_1 - C_2}{n-1} \text{ for } i = 2, 3 \ldots, n. \end{aligned} \tag{4.16}$$

Theorem 4.5. Design d^* is Type I-optimal in $D(v, 3, \frac{2v}{3})$.

Proof. Since d^* is M-optimal in the equal-replicate subclass in $D(v, 3, \frac{2v}{3})$, it is also Type I-optimal in the equal-replicate subclass in $D(v, 3, \frac{2v}{3})$. We only need to show that Type I-optimal designs in $D(v, 3, \frac{2v}{3})$ cannot have some $r_i = 1$.

Suppose for design d there is some treatment with just one replicate. From the proof of Theorem 4.3, $z_{d1} \leq \frac{3m}{3m-1}\frac{2m-1}{2m} = \frac{6m-3}{6m-2} < 1$. And the $v-1$ eigenvalues of d satisfy the following constraints:

$$\begin{aligned} &(i)\ z_{d1} > 0; \\ &(ii)\ tr(C_d) \leq tr(C_{d^*}) = 3(2m-1) = C_1 \\ &(iii)\ z_{d1} \leq \tfrac{6m-3}{6m-2} = C_2 \end{aligned} \tag{4.17}$$

Consider a row $(1 \times (v-1))$ vector $\underline{z}(C_{\overline{d}})$, whose first element is C_2 and all other elements are $(C_1 - C_2)/(v-2)$, i.e.,

$$\underline{z}(C_{\overline{d}}) = (\frac{6m-3}{6m-2}, \frac{9(2m-1)^2}{2(3m-2)(3m-1)}, \frac{9(2m-1)^2}{2(3m-2)(3m-1)}, \ldots, \frac{9(2m-1)^2}{2(3m-2)(3m-1)}). \tag{4.18}$$

By Theorem 4.4, $\overline{d}$ (which may not be a real design) is as good as or better than d w.r.t. all Type I-criteria. Since

$$\sum_{i=1}^{l} z_{d^*,i} - \sum_{i=1}^{l} z_{\overline{d},i} = \frac{3m-l-2}{2(3m-2)(3m-1)} \geq 0 \tag{4.19}$$

where $1 \le l \le v-1 = 3m-2$, $\underline{z}(C_{d^*}) \prec^w \underline{z}(C_{\overline{d}})$ and consequently

$$\sum_{i=1}^{v-1} f(z_{d^*i}) \le \sum_{i=1}^{v-1} f(z_{\overline{d}i}) \le \sum_{i=1}^{v-1} f(z_{di}) \tag{4.20}$$

and d^* is Type I-optimal in $D(v,3,2v/3)$. □

Corollary 4.1. Design d^* is A-optimal and D-optimal in $D(v,3,\frac{2v}{3})$.

4.3 Optimal Designs in $M(v,3,k)$ when $k \neq 2v/3$

4.3.1 General Combinatorial Structure in $M(v,3,k)$ and Expressions of A- and D-values

For any design d in $M(v,3,k)$, we must have $r_i \in \{1,2,3\}$. So now let $|B_1 \cap B_2| = s_1 + t$, $|B_1 \cap B_3| = s_2 + t$, and $|B_2 \cap B_3| = s_3 + t$, where s_1, s_2 and s_3 are block intersection number for just those treatments with two replicates and t is the number of treatments occurring in all three blocks. Also let the number of treatments in block one with one replicate be x, the number of treatments in block two with one replicate be y, and the number of treatments in block three with one replicate is z. Note that since the block size is k, we have:

$$\begin{cases} t+x+y+z+s_1+s_2+s_3 = v \\ t+x+s_1+s_2 = k \\ t+y+s_1+s_3 = k \\ t+z+s_2+s_3 = k \end{cases} \tag{4.21}$$

By solving (4.21), one obtains:

$$\begin{cases} t = 3k-2v+x+y+z \\ s_1 = v-k-x-y \\ s_2 = v-k-x-z \\ s_3 = v-k-y-z \end{cases} \tag{4.22}$$

Note that x, y, z, s_1, s_2, s_3 and t are all non-negative integers and any design in $M(v,3,k)$ is determined by these seven integers. Thus by (4.22), all combinatorially distinct designs are determined by just x, y and z. WLOG we assume $x \leq y \leq z$. The information matrix of d is

$$C_d = \begin{pmatrix} 3I_t - \frac{3}{k}J_t & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{2}{k}J & -\frac{2}{k}J & -\frac{2}{k}J \\ -\frac{1}{k}J & I_x - \frac{1}{k}J_x & 0 & 0 & -\frac{1}{k}J & -\frac{1}{k}J & 0 \\ -\frac{1}{k}J & 0 & I_y - \frac{1}{k}J_y & 0 & -\frac{1}{k}J & 0 & -\frac{1}{k}J \\ -\frac{1}{k}J & 0 & 0 & I_z - \frac{1}{k}J_z & 0 & -\frac{1}{k}J & -\frac{1}{k}J \\ -\frac{2}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & 0 & 2I_{s_1} - \frac{2}{k}J_{s_1} & -\frac{1}{k}J & -\frac{1}{k}J \\ -\frac{2}{k}J & -\frac{1}{k}J & 0 & -\frac{1}{k}J & -\frac{1}{k}J & 2I_{s_2} - \frac{2}{k}J_{s_2} & -\frac{1}{k}J \\ -\frac{2}{k}J & 0 & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & -\frac{1}{k}J & 2I_{s_3} - \frac{2}{k}J_{s_3} \end{pmatrix}. \tag{4.23}$$

We can get $v-7$ positive eigenvalues of C_d quickly: 3 with frequency $3k-2v+x+y+z-1$, 1 with frequency $x+y+z-3$, and 2 with frequency $3(v-k-1)-2(x+y+z)$. The remaining six positive eigenvalues are the positive eigenvalues of the following reduced matrix:

$$\begin{pmatrix} 3-\frac{3t}{k} & -\frac{x}{k} & -\frac{y}{k} & -\frac{z}{k} & -\frac{2s_1}{k} & -\frac{2s_2}{k} & -\frac{2s_3}{k} \\ -\frac{t}{k} & 1-\frac{x}{k} & 0 & 0 & -\frac{s_1}{k} & -\frac{s_2}{k} & 0 \\ -\frac{t}{k} & 0 & 1-\frac{y}{k} & 0 & -\frac{s_1}{k} & 0 & -\frac{s_3}{k} \\ -\frac{t}{k} & 0 & 0 & 1-\frac{z}{k} & 0 & -\frac{s_2}{k} & -\frac{s_3}{k} \\ -\frac{2t}{k} & -\frac{x}{k} & -\frac{y}{k} & 0 & 2-\frac{2s_1}{k} & -\frac{s_2}{k} & -\frac{s_3}{k} \\ -\frac{2t}{k} & -\frac{x}{k} & 0 & -\frac{z}{k} & -\frac{s_1}{k} & 2-\frac{2s_2}{k} & -\frac{s_3}{k} \\ -\frac{2t}{k} & 0 & -\frac{y}{k} & -\frac{z}{k} & -\frac{s_1}{k} & -\frac{s_2}{k} & 2-\frac{2s_3}{k} \end{pmatrix}$$

Computing the characteristic polynomial of the above matrix, the six eigenvalues are the roots in z_d of the equation

$$l_0 + l_1 z_d + l_2 z_d^2 + l_3 z_d^3 + l_4 z_d^4 + l_5 z_d^5 + l_6 z_d^6 = 0 \tag{4.24}$$

where

$$\begin{aligned}
l_0 =& \quad 2v(9k^2 - 6kv + v^2 - (x^2 + y^2 + z^2 - xy - xz - yz)) \\
l_1 =& \quad -9k^3 - 60k^2v + 39kv^2 - 6v^3 + 6k^2x - 8kvx + 2v^2x + 3kx^2 + 4vx^2 + 6k^2y \\
& -8kvy + 2v^2y - 3kxy - 4vxy - x^2y + 3ky^2 + 4vy^2 - xy^2 + 6k^2z - 8kvz + 2v^2z \\
& -3kxz - 4vxz - x^2z - 3kyz - 4vyz + 6xyz - y^2z + 3kz^2 + 4vz^2 - xz^2 - yz^2 \\
l_2 =& \quad 33k^3 + 72k^2v - 45kv^2 + 6v^3 - 14k^2x + 18kvx - 4v^2x - 7kx^2 - 2vx^2 \\
& -14k^2y + 18kvy - 4v^2y + 3kxy + 4vxy + x^2y - 7ky^2 - 2vy^2 + xy^2 \\
& -14k^2z + 18kvz - 4v^2z + 3kxz + 4vxz + x^2z + 3kyz + 4vyz - 6xyz + y^2z \\
& -7kz^2 - 2vz^2 + xz^2 + yz^2 \\
l_3 =& \quad -46k^3 - 36k^2v + 21kv^2 - 2v^3 + 10k^2x - 12kvx + 2v^2x + 5kx^2 + 10k^2y \\
& -12kvy + 2v^2y - 2vxy + 5ky^2 + 10k^2z - 12kvz + 2v^2z - 2vxz - 2vyz \\
& +2xyz + 5kz^2 \\
l_4 =& \quad k(30k^2 + 6kv - 3v^2 - 2kx + 2vx - x^2 - 2ky + 2vy - y^2 - 2kz + 2vz - z^2) \\
l_5 =& \quad -9k^3 \\
l_6 =& \quad k^3.
\end{aligned} \tag{4.25}$$

By Lemma 3.3 the product of inverses of the six eigenvalues is

$$D_{dp} = \frac{l_6}{l_0} = \frac{k^3}{2v(9k^2 - 6kv + v^2 - (1/2[(x-y)^2 + (x-z)^2 + (y-z)^2]))} \tag{4.26}$$

so the D- value of design d is

$$D_d = \frac{k^3}{2v3^{3k-2v-1}2^{3(v-k-1)}} \frac{1}{9k^2 - 6kv + v^2 - (1/2[(x-y)^2 + (x-z)^2 + (y-z)^2])} (\frac{4}{3})^{x+y+z}. \tag{4.27}$$

Also we can get the sum of the inverse of the six eigenvalues by Lemma 3.3 as

$$\begin{aligned}
A_{dp} = -\tfrac{l_1}{l_0} =& \quad -(-9k^3 - 60k^2v + 39kv^2 - 6v^3 + 6k^2x - 8kvx + 2v^2x + 3kx^2 + 4vx^2 \\
& +6k^2y - 8kvy + 2v^2y - 3kxy - 4vxy - x^2y + 3ky^2 + 4vy^2 - xy^2 + 6k^2z \\
& -8kvz + 2v^2z - 3kxz - 4vxz - x^2z - 3kyz - 4vyz + 6xyz - y^2z + 3kz^2 \\
& +4vz^2 - xz^2 - yz^2)/(2v(9k^2 - 6kv + v^2 - x^2 + xy - y^2 + xz + yz - z^2))
\end{aligned} \tag{4.28}$$

so the A- value of design d is

$$\begin{aligned} A_d = \; & \tfrac{5v-3k-29+2(x+y+z)}{6} - (-9k^3 - 60k^2v + 39kv^2 - 6v^3 + 6k^2x - 8kvx + 2v^2x \\ & +3kx^2 + 4vx^2 + 6k^2y - 8kvy + 2v^2y - 3kxy - 4vxy - x^2y + 3ky^2 + 4vy^2 - xy^2 \\ & +6k^2z - 8kvz + 2v^2z - 3kxz - 4vxz - x^2z - 3kyz - 4vyz + 6xyz - y^2z + 3kz^2 \\ & +4vz^2 - xz^2 - yz^2)/(2v(9k^2 - 6kv + v^2 - x^2 + xy - y^2 + xz + yz - z^2)). \end{aligned} \tag{4.29}$$

Note that if any of x, y, z, t, s_1, s_2 and s_3 are zero, the matrix C_d (or the corresponding reduced matrix) will collapse to smaller dimensions. However, one may check that the expressions for D_d and A_d do not change.

4.3.2 D-optimal Designs in $M(v, 3, k)$ with $k \neq 2v/3$.

Before we discuss D- and A-optimal designs in $M(v, 3, k)$ with $k \neq 2v/3$, we give below a useful lemma, which will be repeatedly used in the proof of later theorems.

Lemma 4.1. The minimum of the symmetric function of non-negative integers x, y and z

$$g(x, y, z) = 1/2[(x-y)^2 + (x-z)^2 + (y-z)^2]$$

subject to $x + y + z = q$ and WLOG $x \leq y \leq z$ is as follows:

1) When $q = 3\theta$ where θ is a non-negative integer, (θ, θ, θ) is the minimum value point and the minimum value is zero.

2) When $q = 3\theta + 1$ where θ is a non-negative integer, $(\theta, \theta, \theta + 1)$ is the minimum value point and the minimum value is one.

3) When $q = 3\theta + 2$ where θ is a non-negative integer, $(\theta, \theta + 1, \theta + 1)$ is the minimum value point and the minimum value is one.

Theorem 4.6. D-optimal designs in $M(v, 3, k)$ for $k \neq 2v/3$ fall into three cases:

i) The design with $x = y = z = 0$ is uniquely D-optimal in $M(v, 3, k)$ when $k > 2v/3$.

ii) When $k = (v+2)/3$, connected designs in $M(v, 3, k)$ are minimally connected and the only two connected designs are D- equal;

iii) When $(v+2)/3 < k < 2v/3$ and

a) $2v - 3k = 3\theta$ where θ is a positive integer, then the design with $x = y = z = \theta$ is uniquely D-optimal;

b) $2v - 3k = 3\theta + 1$ where θ is a non-negative integer, then the design with $x = y = \theta$ and $z = \theta + 1$ is uniquely D-optimal;

c) $2v - 3k = 3\theta + 2$ where θ is a non-negative integer, then the design with $x = \theta$ and $y = z = \theta + 1$ is uniquely D-optimal.

Proof. From (4.27), the problem is to minimize

$$D_m = (\frac{4}{3})^{x+y+z} \frac{1}{(3k-v)^2 - g(x,y,z)} \tag{4.30}$$

where g is the function defined in Lemma 4.1. Note that we use D_m instead of D_d here after dropping the constant terms in D_d. It can be seen that D_m is an increasing function with respect to each of $x+y+z$ and $g(x, y, z)$. If we minimize these two factors simultaneously for some integer point (x, y, z), then the design corresponding to that (x, y, z) is the D-optimal design.

i) $k > \frac{2v}{3}$. The minimum values of $x + y + z$ and $g(x, y, z)$ are simultaneously achieved when $x = y = z = 0$. No other set of (x, y, z) does this. So the design with $x = y = z = 0$ is uniquely D-optimal.

ii) When $3k = v + 2$, the only two connected designs are the design with $x = y = z = k - 1$ and that with $x = k - 2$ and $y = z = k - 1$ (one may refer to chapter 2 to see why). It can be easily verified that both have the D- value $(v + 2)^3/(27v)$.

iii) When $3k > v + 2$ and $k < 2v/3$, $r = \lfloor \frac{3k}{v} \rfloor = 1$ and at least $2v - 3k$ treatments have exactly one replicate for any design in $M(v, 3, k)$, i.e., $x + y + z \geq 2v - 3k$.

a) $2v - 3k = 3\theta$ where θ is an positive integer. Then $x+y+z$ and $g(x,y,z)$ are simultaneously minimized if and only if $x = y = z = \theta$, and the corresponding design is D-optimal.

b) $2v - 3k = 3\theta + 1$ where θ is a non-negative integer. If $x+y+z$ achieves its minimum $3\theta+1$, there are no integer points (x,y,z) to make $g(x,y,z)$ zero. By lemma 4.1, the minimum of $g(x,y,z)$ is one, occurring at the point $(\theta, \theta, \theta + 1)$. If we want to make the $g(x,y,z)$ to be zero, we have to use different $x+y+z$, the smallest that can do this being $3\theta + 3$. In this case, $x = y = z = \theta + 1$. The smallest D_m value must be for either the design with $(x,y,z) = (\theta, \theta, \theta + 1)$ or the design with $(x,y,z) = (\theta + 1, \theta + 1, \theta + 1)$. Denoting the D_m values for these two designs by D_{m1} and D_{m2} respectively, by (4.30) we have,

$$D_{m1} = \frac{1}{(3k-v)^2 - 1}(\frac{4}{3})^{3\theta+1} \tag{4.31}$$

$$D_{m2} = \frac{1}{(3k-v)^2}(\frac{4}{3})^{3\theta+3} \tag{4.32}$$

By (4.31)/(4.32) we have,

$$\frac{D_{m1}}{D_{m2}} = \frac{9(3k-v)^2}{16[(3k-v)^2 - 1]}$$

Since $3k > v + 2$,

$$\frac{(3k-v)^2 - 1}{(3k-v)^2} = 1 - \frac{1}{(3k-v)^2} > \frac{3}{4}$$

we have

$$\frac{(3k-v)^2}{(3k-v)^2 - 1} < \frac{4}{3}$$

and thus

$$\frac{D_{m1}}{D_{m2}} = \frac{9(3k-v)^2}{16[(3k-v)^2 - 1]} < \frac{3}{4}.$$

We conclude $D_{m1} < D_{m2}$.

c) $2v - 3k = 3\theta + 2$ where θ is a non-negative integer. If $x+y+z$ achieves its minimum $3\theta+2$, there are no integer points (x,y,z) to make $g(x,y,z)$ zero. By lemma 4.1, the minimum of $g(x,y,z)$ subject to $x+y+z = 3\theta + 2$ is one, occurring at the point $(\theta, \theta + 1, \theta + 1)$. If we want $g(x,y,z)$ to be zero, we have to use different $x+y+z$, the smallest that can do so being

$3\theta+3$. In this case, $x = y = z = \theta+1$. The smallest D_m value must be for either the design with the $(x, y, z) = (\theta, \theta+1, \theta+1)$ or the design with the $(x, y, z) = (\theta+1, \theta+1, \theta+1)$. Denoting the D_m values corresponding to $(\theta, \theta+1, \theta+1)$ by D_{m3}, by (4.30) we have,

$$D_{m3} = \frac{1}{(3k-v)^2-1}(\frac{4}{3})^{3\theta+2}. \tag{4.33}$$

By (4.33)/(4.32) we also have for $3k > v+2$,

$$\frac{D_{m3}}{D_{m2}} = \frac{3(3k-v)^2}{4[(3k-v)^2-1]} < 1.$$

We conclude $D_{m3} < D_{m2}$. □

Example 4.3.1. For $M(12, 3, 10)$, $k = 10 > 2v/3 = 8$. By theorem 4.6 the unique D-optimal design has $x = y = z = 0$. By (4.22), $s_1 = s_2 = s_3 = v-k = 2$ and $t = 3k-2v = 6$. Then the D-optimal design is:

$B1:$	1	2	3	4	5	6	7	8	9	10
$B2:$	1	2	3	4	5	6	7	8	11	12
$B3:$	1	2	3	4	5	6	9	10	11	12

Example 4.3.2. For $M(28, 3, 10)$, $3k = v+2$. By theorem 4.6 the only two connected designs are D- equal. They are:

$B1:$	1	2	3	4	5	6	7	8	9	10
$B2:$	1	11	12	13	14	15	16	17	18	19
$B3:$	1	20	21	22	23	24	25	26	27	28

and

$B1:$	1	2	3	4	5	6	7	8	9	10
$B2:$	1	11	12	13	14	15	16	17	18	19
$B3:$	11	20	21	22	23	24	25	26	27	28

Example 4.3.3. For $M(16, 3, 10)$, $2v-3k = 2$. By theorem 4.6 the unique D-optimal design has $x = 0$ and $y = z = 1$. By (4.22), $s_1 = v-k-x-y = 5$, $s_2 = v-k-x-z = 5$,

$s_3 = v - k - y - z = 4$ and $t = 3k - 2v + x + y + z = 0$. Then the D-optimal design is:

$B1:$	1	2	3	4	5	6	7	8	9	10
$B2:$	1	2	3	4	5	11	12	13	14	15
$B3:$	11	12	13	14	16	6	7	8	9	10

Example 4.3.4. For $M(17, 3, 10)$, $2v - 3k = 4$. By theorem 4.6 the unique D-optimal design has $x = y = 1$ and $z = 2$. By (4.22), $s_1 = v - k - x - y = 5$, $s_2 = v - k - x - z = 4$, $s_3 = v - k - y - z = 4$ and $t = 3k - 2v + x + y + z = 0$. Then the D-optimal design is:

$B1:$	1	2	3	4	5	6	7	8	9	10
$B2:$	1	2	3	4	5	11	12	13	14	15
$B3:$	11	12	13	14	6	7	8	9	16	17

Example 4.3.5. For $M(18, 3, 10)$, $2v - 3k = 6$. By theorem 4.6 the unique D-optimal design has $x = y = z = 2$. By (4.22), $s_1 = v - k - x - y = 4$, $s_2 = v - k - x - z = 4$, $s_3 = v - k - y - z = 4$ and $t = 3k - 2v + x + y + z = 0$. Then the D-optimal design is:

$B1:$	1	2	3	4	5	6	7	8	13	14
$B2:$	1	2	3	4	9	10	11	12	15	16
$B3:$	5	6	7	8	9	10	11	12	17	18

4.3.3 A-optimal Designs in $M(v, 3, k)$ with $k \neq 2v/3$.

We need the following lemma for the proof of Theorem 4.7.

Lemma 4.2. The minimum of the symmetric function of non-negative integers x, y and z

$$h = x(y - z)^2 + y(x - z)^2 + z(x - y)^2$$

subject to $x + y + z = q$ and WLOG $x \leq y \leq z$ is as follows:

1) When $q = 3\theta$ where θ is a non-negative integer, (θ, θ, θ) and $(0, 0, 3\theta)$ are the two minimum value points of h and the minimum value is zero.

2) When $q = 3\theta+1$ where θ is a non-negative integer, then $(0, 0, 3\theta+1)$ is the minimum value point of h and the minimum value is zero. The second minimum value point is $(\theta, \theta, \theta + 1)$ and the corresponding value of h is 2θ.

3) When $q = 3\theta + 2$ where θ is a non-negative integer, $(0, 0, 3\theta + 2)$ is the minimum value point of h and the minimum value is zero. The second minimum value point is $(\theta, \theta+1, \theta+1)$ and the corresponding value of h is $2(\theta + 1)$.

Proof. 1) $q = 3\theta$. Obviously, $x(y - z)^2 + y(x - z)^2 + z(x - y)^2 \geq 0$ and the equality holds only for the two solutions (θ, θ, θ) and $(0, 0, 3\theta)$.

2) $q = 3\theta+1$. Clearly $z \geq \theta+1$. Let $z = \theta+1+\varepsilon$ where $\varepsilon \geq 0$ is an integer. When $z = \theta+1$ ($\varepsilon = 0$) and $x = y = \theta$, the value of h is 2θ, denoted by h_2. Consider three subcases:

2a) $y - x \geq 2$. Denote the corresponding h value by h_{21}. It can be seen $h_{21} > z(x - y)^2 \geq 4(\theta + 1) > h_2$.

2b) $y - x = 1$. Then $y = (2\theta - \varepsilon + 1)/2$, $x = (2\theta - \varepsilon - 1)/2$ and ε is odd. Denote the corresponding h value by h_{22}. If $\varepsilon \geq \theta$ then $h_{22} > z = 2\theta + 1 > h_2$. If $\varepsilon \leq \theta - 1$ then

$$h_{22} = (8 + 14\theta + 5\varepsilon + 24\theta\varepsilon - 12\varepsilon^2 + 18\theta\varepsilon^2 - 9\varepsilon^3)/4$$

and

$$h_{22} - h_2 = (\varepsilon + 1)(8 + 3(2\theta - \varepsilon) + 9\varepsilon(2\theta - \varepsilon))/4 > 0.$$

2c) $y = x$. We have $y = x = (2\theta - \varepsilon)/2$ and ε is even. If $y = x = 0$ ($\varepsilon = 2\theta$), the value of h is zero. If $y = x \neq 0$, then $\varepsilon \leq 2(\theta - 1)$. Denote the corresponding value of h by h_{23}. Then

$$h_{23} = (2\theta - \varepsilon)(3\varepsilon + 2)^2/4$$

and

$$h_{23} - h_2 = \varepsilon(-4 + 12(2\theta - \varepsilon) + 9\varepsilon^2(2\theta - \varepsilon))/4 > 0.$$

3) $q = 3\theta+2$. Clearly $z \geq \theta+1$. Let $z = \theta+1+\varepsilon$ where $\varepsilon \geq 0$ is an integer. When $z = \theta+1$

($\varepsilon = 0$), $x = \theta + 1$ and $y = \theta$, and the value of h is $2(\theta + 1)$, denoted by h_3. Now consider three subcases:

3a) $y - x \geq 2$. Denote the corresponding h value by h_{31}. It can be seen $h_{31} > z(x - y)^2 \geq 4(\theta + 1) > h_3$.

3b) $y - x = 1$. Then $y = (2\theta - \varepsilon + 2)/2$, $x = (2\theta - \varepsilon)/2$ and ε is even. Denote the corresponding h value by h_{32}. If $\varepsilon \geq \theta + 1$ then $h_{32} > z = 2(\theta + 1) = h_2$. If $\varepsilon \leq \theta$ then

$$h_{32} = (8 + 8\theta + 14\varepsilon + 12\theta\varepsilon + 3\varepsilon^2 + 18\theta\varepsilon^2 - 9\varepsilon^3)/4$$

and

$$h_{32} - h_3 = \varepsilon(14 + 12\theta + 3\varepsilon + \theta\varepsilon(2\theta - \varepsilon))/4 > 0.$$

3c) $y = x$. Then $y = x = (2\theta + 1 - \varepsilon)/2$ and ε is odd. If $y = x = 0$ ($\varepsilon = 2\theta + 1$), the value of h is zero. If $y = x \neq 0$, then we have $\varepsilon \leq 2\theta - 1$. Denote the corresponding value of h by h_{33}. Then

$$h_{33} = (1 + 2\theta - \varepsilon)(3\varepsilon + 1)^2/4$$

and

$$h_{33} - h_3 = (\varepsilon + 1)(-7 - 6\theta + 12\varepsilon + 18\varepsilon\theta - 9\varepsilon^2)/4.$$

If $1 \leq \varepsilon < \theta$, then $h_{32} - h_3 = (\varepsilon + 1)(-7 + 6\theta(\varepsilon - 1) + 12\varepsilon + 3\varepsilon(4\theta - 3\varepsilon))/4 > 0$. If $2\theta - 1 \geq \varepsilon \geq \theta$, $h_{32} - h_3 = (\varepsilon + 1)(-7 + 6(2\varepsilon - \theta) + 9\varepsilon(2\theta - \varepsilon))/4 > (\varepsilon + 1)(-7 + 9\varepsilon)/4 > 0$. So $h_{32} > h_3$ for $y = x \neq 0$.

□

Theorem 4.7. A-optimal designs in $M(v, 3, k)$ for $k \neq 2v/3$ fall into two cases:

i) The design with $x = y = z = 0$ is uniquely A-optimal if $k > 2v/3$.

ii) If $k < 2v/3$ and

a) $2v - 3k = 3\theta$ where θ is a positive integer, the design with $x = y = z = \theta$ is uniquely A-optimal;

b) $2v - 3k = 3\theta + 1$ where θ is a nonnegative integer, consider a judging polynomial

$$\Delta_1 = -9k - 9k^2 + 54k^3 + 7v + 18kv - 90k^2v - 54k^3v - v^2 + 42kv^2 + 54k^2v^2 - 6v^3 - 18kv^3 + 2v^4 \quad (4.34)$$

If $\Delta_1 > 0$ then the design with $x = y = z = \theta + 1$ is uniquely A-optimal; if $\Delta_1 < 0$ then the design with $x = y = \theta$ and $z = \theta + 1$ is uniquely A-optimal; and if $\Delta_1 = 0$ both of these designs are A-optimal.

c) $2v - 3k = 3\theta + 2$ where θ is a nonnegative integer, consider a judging polynomial

$$\Delta_2 = -9k^2 + 27k^3 + 2v + 15kv - 45k^2v - 27k^3v + 21kv^2 + 27k^2v^2 - 3v^3 - 9kv^3 + v^4 \quad (4.35)$$

If $\Delta_2 > 0$ then the design with $x = y = z = \theta + 1$ is uniquely A-optimal; if $\Delta_2 < 0$ then the design with $x = \theta$ and $y = z = \theta + 1$ is uniquely A-optimal; and if $\Delta_2 = 0$ both of these designs are A-optimal.

Proof. Rewrite the expression (4.29) as

$$A_d = \frac{p_{11} - p_{12}g}{6v(p_3 - g)} + \frac{(x + y + z)(p_{21} - p_{22}g)}{6v(p_3 - g)} + \frac{p_4}{6v(p_3 - g)} \quad (4.36)$$

where

$$\begin{aligned}
p_{11} &= (3k - v)(9k^2 - 24kv - 9k^2v + 11v^2 + 18kv^2 - 5v^3) \\
p_{12} &= 9k - 17v - 3kv + 5v^2 \\
p_{21} &= 2(3k - v)(3v - 3k + 3kv - v^2) \\
p_{22} &= 2v \\
p_3 &= (3k - v)^2 \\
p_4 &= 3[x(y - z)^2 + y(x - z)^2 + z(x - y)^2] = 3h \\
g &= 1/2[(x - y)^2 + (x - z)^2 + (y - z)^2]
\end{aligned}$$

First we show that both $(p_{11} - p_{12}g)/(p_3 - g)$ and $(p_{21} - p_{22}g)/(p_3 - g)$ are increasing function with respect to g. Since $\partial((p_{11} - p_{12}g)/(p_3 - g)) = (p_{11} - p_{12}p_3)/(p_3 - g)^2$ and

$\partial((p_{21}-p_{22}g)/(p_3-g))= (p_{21}-p_{22}p_3)/(p_3-g)^2$, we only indeed to show that $p_{11}-p_{12}p_3 > 0$ and $p_{21}-p_{22}p_3 > 0$. In fact,

$$\begin{aligned} p_{11}-p_{12}p_3 &= 6(3k-v)(6kv-3k^2-v^2) = 6(3k-v)(2vk+(3k-v)(v-k)) > 0 \\ p_{21}-p_{22}p_3 &= 6(v-k)(3k-v) > 0 \end{aligned}$$

Therefore, A_d is an increasing function with respect to each of g, h and $x+y+z$. If we minimize these three factors simultaneously for some integer point (x, y, z), then the corresponding design is A-optimal.

i) $k > \frac{2v}{3}$. The minimum values of $x+y+z$, g and h, which are all zero, are achieved simultaneously by $x = y = z = 0$. No other (x, y, z) cannot make the three factors simultaneously zero. So the design with $x = y = z = 0$ is uniquely A-optimal.

ii) $k < \frac{2v}{3}$. Then $r = \lfloor \frac{3k}{v} \rfloor = 1$ and at least $2v-3k$ treatments have exactly one replicate, i.e., $x+y+z \geq 2v-3k$. We need to discuss three subcases:

a) $2v-3k = 3\theta$, where θ is a positive integer. The smallest value of $x+y+z$, which is $2v-3k$, and the smallest values of g and h, which are both zero, are achieved by $x = y = z = \theta$. Therefore, the uniquely A-optimal design has $x = y = z = \theta$.

b) $2v-3k = 3\theta+1$, where θ is a non-negative integer. If $x = y = \theta$ and $z = \theta+1$ then $g = 1$ and $h = 2\theta$. This choice minimizes $x+y+z$ while g and h each attain their second smallest value. Relative to this choice, A_d is possibly smaller only if g or h attains its lower bound, in which case $x+y+z$ is larger than $3\theta+1$. Now $g = 0$ requires $x = y = z$, so the best candidate with smallest g is $x = y = z = \theta+1$, a choice which also makes $h = 0$. The lower bound for h is otherwise attained only if $x = y = 0$; subject to this constraint, both $x+y+z$ and g are minimized by $z = 3\theta+1$. Thus there are three competitor designs to be compared as shown here:

Situation	x	y	z	$x+y+z$	g	h
1	θ	θ	$\theta+1$	$3\theta+1$	1	2θ
2	$\theta+1$	$\theta+1$	$\theta+1$	$3\theta+3$	0	0
3	0	0	$3\theta+1$	$3\theta+1$	$(3\theta+1)^2$	0

Now we discuss A_d values for the three competitors.

b1) $x = y = \theta$ and $z = \theta + 1$. The corresponding A_d, denoted as A_{d11} is

$$\begin{aligned} A_{d11} = \ & (-2 - 15k + 81k^3 + 21v + 9kv - 189k^2v - 81k^3v - 9v^2 + 123kv^2 \\ & +135k^2v^2 - 23v^3 - 63kv^3 + 9v^4)/(6v(3k - v + 1)(3k - v - 1)) \end{aligned} \tag{4.37}$$

b2) $x = y = z = \theta + 1$. The corresponding A_d, denoted as A_{d12} is

$$A_{d12} = \frac{-12k + 27k^2 + 12v - 42kv - 27k^2v + 19v^2 + 36kv^2 - 9v^3}{6v(3k - v)} \tag{4.38}$$

b3) $x = y = 0$ and $z = 3\theta + 1$. Note that in this situation $z = 3\theta + 1 = 2v - 3k < k$ and thus $2k > v$. The corresponding A_d, denoted as A_{d13} is

$$A_{d13} = \frac{(v - k)(-8k + 5v + 6kv - 3v^2)}{2v(2k - v)} \tag{4.39}$$

First we show that $A_{d13} > A_{d11}$. Calculate,

$$A_{d13} - A_{d11} = \frac{(2v - 3k - 1)\Delta_{01}}{3v(3k - v + 1)(3k - v - 1)(2k - v)} \tag{4.40}$$

where

$$\Delta_{01} = -2k + 3k^2 - 9k^3 + v + 2kv - v^2 + 7kv^2 - 2v^3 \tag{4.41}$$

If $2v - 3k = 1$, A_{d13} and A_{d11} are identical. Consider $2v - 3k > 1$. To show $A_{d13} > A_{d11}$, it is sufficient to show that $\Delta_{01} > 0$.

Since $\partial\Delta_{01}/\partial v = 1 + 2k + 2v(k - 1) + 6v(2k - v) > 0$ and $v > 3k/2$,

$$\Delta_{01} > \Delta_{01}|_{v=3k/2} = \frac{k(15k - 2)}{4} > 0$$

It remains to compare A_{d11} and A_{d12}.

$$A_{d11} - A_{d12} = \frac{\Delta_1}{3v(3k-v+1)(3k-v-1)(3k-v)} \tag{4.42}$$

where Δ_1 is as defined in (4.34).

It can be seen that if $\Delta_1 > 0$ then $A_{d11} > A_{d12}$; if $\Delta_1 < 0$ then $A_{d11} < A_{d12}$; and if $\Delta_1 = 0$ then $A_{d11} = A_{d12}$.

c) $2v - 3k = 3\theta + 2$, where θ is a non-negtive integer. We give a similar discussion as in b). If $x = \theta$ and $y = z = \theta + 1$ then $g = 1$ and $L = 2\theta$. This choice minimizes $x + y + z$ while g and h each attain their second smallest value. Relative to this choice, A_d is possibly smaller only if g or h attains its lower bound, in which case $x + y + z$ is larger than $3\theta + 2$. Now $g = 0$ requires $x = y = z$, so the best candidate with smallest g is $x = y = z = \theta + 1$, a choice which also makes $h = 0$. The lower bound for h is otherwise attained only if $x = y = 0$; subject to this constraint, both $x + y + z$ and g are minimized by $z = 3\theta + 2$. Thus there are three competitor designs to be compared as shown here:

Situation	x	y	z	$x+y+z$	g	h
1	θ	$\theta+1$	$\theta+1$	$3\theta+2$	1	$2(\theta+1)$
2	$\theta+1$	$\theta+1$	$\theta+1$	$3\theta+3$	0	0
3	0	0	$3\theta+2$	$3\theta+2$	$(3\theta+2)^2$	0

Now we discuss A_d values for the three competitors.

c1) $x = \theta$ and $y = z = \theta + 1$. The corresponding A_d, denoted as A_{d21} is

$$\begin{aligned} A_{d21} = \; & (2 - 15k + 81k^3 + 21v + 9kv - 189k^2v - 81k^3v - 9v^2 + 123kv^2 \\ & +135k^2v^2 - 23v^3 - 63kv^3 + 9v^4)/(6v(3k-v+1)(3k-v-1)). \end{aligned} \tag{4.43}$$

c2) $x = y = z = \theta + 1$. The corresponding A_d, denoted as A_{d22} is

$$A_{d22} = \frac{(v-k)(2 - 9k + 7v + 9kv - 3v^2)}{2v(3k-v)}. \tag{4.44}$$

c3) $x = y = 0$ and $z = 3\theta + 2$. Note that in this situation $(2v-2)/3 \geq k > v/2$. The corresponding A_d, denoted as A_{d23}, has the same expression as given in the RHS of (4.39).

First we show that $A_{d23} > A_{d21}$. Calculate

$$A_{d23} - A_{d21} = \frac{(2v-3k+1)\Delta_{02}}{3v(3k-v+1)(3k-v-1)(2k-v)} \tag{4.45}$$

where

$$\Delta_{02} = -2k - 3k^2 - 9k^3 + v - 2kv + v^2 + 7kv^2 - 2v^3. \tag{4.46}$$

To show $A_{d23} > A_{d21}$, it is sufficient to show that $\Delta_{02} > 0$.

Since $\partial\Delta_{02}/\partial v = 1 + 2(v-k) + 6v(2k-v) + 2kv > 0$ and $v \geq 3k/2 + 1$,

$$\Delta_{02} \geq \Delta_{02}|_{v=3k/2+1} = \frac{3k(5k-2)}{4} > 0.$$

Then we only need to compare A_{d21} and A_{d22}. Calculate

$$A_{d21} - A_{d22} = \frac{\Delta_2}{3v(3k-v+1)(3k-v-1)(3k-v)} \tag{4.47}$$

where Δ_2 is given in (4.35).

It can be seen that if $\Delta_2 > 0$ then $A_{d21} > A_{d22}$; if $\Delta_2 < 0$ then $A_{d21} < A_{d22}$; and if $\Delta_2 = 0$ then $A_{d21} = A_{d22}$. □

Example 4.3.6. For $M(12, 3, 10)$, $k = 10 > 2v/3 = 8$. By Theorem 4.7 the uniquely A-optimal design has $x = y = z = 0$. By (4.22), $s_1 = s_2 = s_3 = v - k = 2$ and $t = 3k - 2v = 6$. The A-optimal design is:

$$\begin{array}{lcccccccccc} B1: & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ B2: & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 11 & 12 \\ B3: & 1 & 2 & 3 & 4 & 5 & 6 & 9 & 10 & 11 & 12 \end{array}$$

Example 4.3.7. For $M(17, 3, 10)$, $k < 2v/3$ and $2v - 3k = 4 = 3 \times 1 + 1$. Check $\Delta_1 = -9k - 9k^2 + 54k^3 + 7v + 18kv - 90k^2v - 54k^3v - v^2 + 42kv^2 + 54k^2v^2 - 6v^3 - 18kv^3 + 2v^4 =$

$-79896 < 0$. By Theorem 4.7 the uniquely A-optimal design has $x = y = 1$ and $z = 2$. By (4.22), $s_1 = v - k - x - y = 5$, $s_2 = v - k - x - z = 4$, $s_3 = v - k - y - z = 4$ and $t = 3k - 2v + x + y + z = 0$. The A-optimal design is:

$$\begin{array}{lcccccccccc} B1: & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ B2: & 1 & 2 & 3 & 4 & 5 & 11 & 12 & 13 & 14 & 15 \\ B3: & 11 & 12 & 13 & 14 & 6 & 7 & 8 & 9 & 16 & 17 \end{array}$$

Example 4.3.8. For $M(116, 3, 40)$, $k < 2v/3$ and $2v - 3k = 112 = 3 \times 37 + 1$. Check $\Delta_1 = -9k - 9k^2 + 54k^3 + 7v + 18kv - 90k^2v - 54k^3v - v^2 + 42kv^2 + 54k^2v^2 - 6v^3 - 18kv^3 + 2v^4 = 33972 > 0$. By Theorem 4.7 the uniquely A-optimal design has $x = y = z = 38$. By (4.22), $s_1 = s_2 = s_3 = 0$ and $t = 3k - 2v + x + y + z = 2$. The A-optimal design is:

$$\begin{array}{lccccccc} B1: & 1 & 2 & 3 & 4 & \ldots & 39 & 40 \\ B2: & 1 & 2 & 41 & 42 & \ldots & 77 & 78 \\ B3: & 1 & 2 & 79 & 80 & \ldots & 115 & 116 \end{array}$$

Example 4.3.8 shows that A-optimal design may not be as equally replicated as possible, at least in the binary class.

Example 4.3.9. For minimally connected design in $M(3k-2, 3, k)$, $k < 2v/3$ and $2v - 3k = 3(k-2) + 2$. Check $\Delta_2 = -9k^2 + 27k^3 + 2v + 15kv - 45k^2v - 27k^3v + 21kv^2 + 27k^2v^2 - 3v^3 - 9kv^3 + v^4 = 4(v-1)^2 > 0$. By Theorem 4.7 the uniquely A-optimal design has $x = y = z = k - 2 + 1 = k - 1$. Therefore, $s_1 = s_2 = s_3 = v - k - x - y = 0$, $t = 3k - 2v + x + y + z = 1$ and the A-optimal design is:

$$\begin{array}{lcccccc} B1: & 1 & 2 & 3 & \ldots & k-1 & k \\ B2: & 1 & k+1 & k+2 & \ldots & 2k-2 & 2k-1 \\ B3: & 1 & 2k & 2k+1 & \ldots & 3k-3 & 3k-2 \end{array}$$

The result shown in Example 4.3.9 is consistent with the known results for A-optimal minimally connected designs given by Mandal, Shah and Sinha (1991).

Example 4.3.10. For nearly minimally connected design in $M(3k-3,3,k)$, $k < 2v/3$ and $2v-3k = 3(k-2)$. By Theorem 4.7 the uniquely A-optimal design has $x = y = z = k-2$. Therefore, $s_1 = s_2 = s_3 = v-k-x-y = 1$, $t = 3k-2v+x+y+z = 0$ and the A-optimal design is:

$$\begin{array}{lcccccc} B1: & 1 & 2 & 4 & 5 & \dots & k & k+1 \\ B2: & 1 & 3 & k+2 & k+3 & \dots & 2k & 2k-1 \\ B3: & 2 & 3 & 2k & 2k+1 & \dots & 3k-4 & 3k-3 \end{array}$$

The result shown in Example 4.3.10 is consistent with the known results for A-optimal nearly minimally connected designs given by Krafft and Schaefer (1997).

4.3.4 Discussion of Δ_1 and Δ_2

In the previous section we found two judging polynomials involving k and v for A-optimal binary designs. In this section we discuss how Δ_1 and Δ_2 change in k for a given v. Studying this will give us some intuition about how A-optimal designs go from more to less combinatorial symmetry in terms of k.

The polynomials are useful only if $k < 2v/3$ and we need $k \geq (v+2)/3$ for the design to be connected. When $v = 3$, no feasible integer exists for k satisfying $k \in [(v+2)/3, 2v/3)$. When $v = 4$, there is only one feasible k, i.e., $k = 2$, and thus no need to discuss trends of Δ_1 and Δ_2. Therefore, the feasible k's in the two polynomials we will discuss are the integers within $[(v+2)/3, 2v/3)$ where $v \geq 5$.

Theorem 4.8. Both Δ_1 and Δ_2 are decreasing functions with respect to k and there is at most one integer root for each of the polynomials, where $k \in [(v+2)/3, 2v/3)$ and $v \geq 5$.

Proof. First we show that both Δ_1 and Δ_2 are decreasing functions with respect to k. In fact, by (4.34) and (4.35),

$$\begin{aligned} \frac{\partial \Delta_1}{\partial k} &= -3(6(3k-v)^2 v + 2(7v-9k)(3k-v) - 6(v-k) + 3) \\ &< -3(6v + 2(7v-9k)(3k-v) - 6(v-k) + 3) < 0. \end{aligned}$$

and

$$\begin{aligned} \frac{\partial \Delta_2}{\partial k} &= -3(3(3k-v)^2 v + (7v-9k)(3k-v) + 6k - 5v) \\ &< -3(3v + (7v-9k)(3k-v) + 6k - 5v) \\ &= -3((7v-9k)(3k-v) + 2(3k-v)) < 0. \end{aligned}$$

Next we show that there is a root with respect to k for given v for each of the two polynomials. Note that the root may not be an integer.

In fact,

$$\begin{aligned} \Delta_1|_{k=\frac{v+2}{3}} &= 2(2v^2 - 10v + 3) > 0 \\ \Delta_1|_{k=\frac{2v}{3}} &= -v(2v^3 + 2v^2 - 7v - 1) < 0 \\ \Delta_2|_{k=\frac{v+2}{3}} &= 4(v-1)^2 > 0 \\ \Delta_1|_{k=\frac{2v}{3}} &= -v(v^3 + v^2 - 6v - 2) < 0 \end{aligned}$$

□

For $v \leq 2000$, computer-based search found no feasible integer k to make $\Delta_1 = 0$ when $2v - 3k = 3\theta + 1$, or $\Delta_2 = 0$ when $2v - 3k = 3\theta + 2$ where θ is a non-negative integer. Consequently, we have not found two distinct, A-optimal designs.

4.3.5 E-optimal Designs in $M(v, 3, k)$ with $k \neq 2v/3$.

Theorem 4.9. E-optimal designs have $x = y = z = 0$ in $M(v, 3, k)$ when $k > \frac{2v}{3}$.

Proof. When $x = y = z = 0$, we have $s_1 = s_2 = s_3 = v - k$ and $t = 3k - 2v$. The information matrix for this design is

$$\begin{pmatrix} 3I_{3k-2v} - \frac{3}{k}J_{3k-2v} & -\frac{2}{k}J_{3k-2v,v-k} & -\frac{2}{k}J_{3k-2v,v-k} & -\frac{2}{k}J_{3k-2v,v-k} \\ -\frac{2}{k}J_{v-k,3k-2v} & 2I_{v-k} - \frac{2}{k}J_{v-k} & -\frac{1}{k}J_{v-k} & -\frac{1}{k}J_{v-k} \\ -\frac{2}{k}J_{v-k,3k-2v} & -\frac{1}{k}J_{v-k} & 2I_{v-k} - \frac{2}{k}J_{v-k} & -\frac{1}{k}J_{v-k} \\ -\frac{2}{k}J_{v-k,3k-2v} & -\frac{1}{k}J_{v-k} & -\frac{1}{k}J_{v-k} & 2I_{v-k} - \frac{2}{k}J_{v-k} \end{pmatrix}$$

The positive eigenvalues are: 3 with frequency of $3k-2v-1$, 2 with frequency of $3(v-k-1)$, $3-v/k$ with frequency 2, and $2v/k$ with frequency 1. Therefore, the smallest eigenvalues of the information matrix is $3-v/k$.

For any design d in which there is at least one treatment, say treatment 1, with only one replicate, by Lemma 3.8 the smallest positive eigenvalue of C_d satisfies

$$z_{d1} \leq \frac{v}{v-1} C_{d11} = \frac{v}{v-1}(1-\frac{1}{k}). \tag{4.48}$$

Since

$$\begin{aligned} \frac{v}{v-1}(1-\frac{1}{k})-(3-\frac{v}{k}) &= \frac{3k-2v-2kv+v^2}{k(v-1)} = \frac{3k-2v+v(-2k+v)}{k(v-1)} \\ &< \frac{3k-2v+v(-2k+\frac{3k}{2})}{k(v-1)} = \frac{3k-2v+v(-\frac{k}{2})}{k(v-1)} \\ &\leq \frac{3k-3v}{k(v-1)} < 0, \end{aligned}$$

we have $z_{d1} < 3-\frac{v}{k}$. □

The E-optimality problem in $M(v,3,k)$ with $k < 2v/3$ is a tough one due to the difficulty (perhaps impossibility) of finding an analytical expression for the smallest positive eigenvalue of the information matrix in (4.23). From above we know that this eigenvalue is the smallest root to the polynomial equation of order six given in (4.24). Therefore, we have used a computer program to find the E-optimal binary designs. In Appendix C, we give a MATLAB program for searching E-optimal designs in $M(v,3,k)$ when $k < 2v/3$. Here we only list the results (see Table 4.1) of E-optimal binary designs for $4 \leq v \leq 15$. They illustrate the following points:

1) In general, there is no consistent pattern for E-optimal designs in $M(v,3,k)$ when $k < 2v/3$. E-optimal designs can have all $r_i \in \{1,2\}$, or some $r_i \in \{1,2,3\}$, or some $r_i \in \{1,3\}$.

2) For minimally connected designs ($3k = v+2$), E-optimal designs have $x = y = z = k-1$, which is consistent with the known results for minimally connected designs given by Bapat and Dey (1991).

3) E-optimal designs in $M(v,3,k)$ when $k < 2v/3$ may not be unique. For example, we have two E-optimal designs in $M(5,3,3)$.

v	k	x	y	z	s_1	s_2	s_3	t
4	2	1	1	1	0	0	0	1
5	3	1	0	0	1	1	2	0
		1	1	1	0	0	0	2
6	3	1	1	1	1	1	1	0
7	3	2	2	2	0	0	0	1
	4	1	1	1	1	1	1	1
8	4	2	2	2	0	0	0	2
	5	1	0	0	2	2	3	0
9	4	2	2	2	1	1	1	0
	5	1	1	1	2	2	2	0
10	4	3	3	3	0	0	0	1
	5	2	2	2	1	1	1	1
	6	1	1	1	2	2	2	1
11	5	3	3	3	0	0	0	2
	6	2	2	2	1	1	1	2
	7	1	0	0	3	3	4	0
12	5	3	3	3	1	1	1	0
	6	2	2	2	2	2	2	0
	7	1	1	1	3	3	3	0
13	5	4	4	4	0	0	0	1
	6	3	3	3	1	1	1	1
	7	2	2	2	2	2	2	1
	8	1	1	1	3	3	3	1
14	6	4	4	4	0	0	0	2
	7	3	3	3	1	1	1	2
	8	2	2	2	2	2	2	2
	9	1	0	0	4	4	5	0
15	6	4	4	4	1	1	1	0
	7	3	3	3	2	2	2	0
	8	2	2	2	3	3	3	0
	9	1	1	1	4	4	4	0

Table 4.1: E-optimal designs in $M(v,3,k)$ with $k < 2v/3$ and $v \leq 15$

4.4 Discussion of the Optimality Problems in $D(v,3,k)$

In previous sections we focused on the optimal designs in the class $D(v,3,k)$ with $k = 2v/3$ and in the binary class $M(v,3,k)$ with $k \neq 2v/3$. In this section we give some discussion of optimal designs in the whole class $D(v,3,k)$ with $k \neq 2v/3$.

Are the A- (or the D-) optimal designs in $M(v,3,k)$ also the A- (or the D-) optimal ones in

$D(v,3,k)$? It is a conjecture that all A- and D-optimal designs must be binary. However, the proof of this conjecture, even in $D(v,3,k)$, remains a mystery. The techniques we know so far, like the theorems about Type I-optimality and the average matrix technique, seems not workable for proving that A- and D-optimal designs must be binary in $D(v,3,k)$. Among the reasons are:

i) Some A- (or D-)optimal designs in $M(v,3,k)$ are not regular graph designs or nearly balanced block designs, which means we can not always use theorems about Type I-optimality (see Jacroux (1985) and Morgan and Scrivastav (2001)). In fact we can use those theorems to make the searching range of A- (or D-) optimal designs smaller for only a few cases in $D(v,3,k)$ but still fail to give any optimality results. Therefore, those theorems are not effective.

ii) The average matrix technique is not workable for A- and D-optimality problems in $D(v,3,k)$, either. It is hard to choose suitable average matrices and it is impossible to use only one average matrix. Also in the optimality study with two blocks, we were able to find an upper bound for an eigenvalue of the average matrix. It will be hard to find such an upper bound for average matrices in $D(v,3,k)$ due to the increased number of parameters required.

For the E-optimality problem in $D(v,3,k)$, we still need to discuss two cases: $k > 2v/3$ and $k < 2v/3$. When $k > 2v/3$, by theorem 4.9 E-optimal designs must have all $r_i \geq 2$ therefore have at least $3(v-k)$ treatments with exactly two replicates each. Suppose the number of non-binary treatments with two replicates in three blocks are s_4, s_5 and s_6 respectively. We have $s_1 + s_2 + s_3 + s_4 + s_5 + s_6 \geq 3(v-k)$, where s_1, s_2 and s_3 are as in previous sections.

For $k > 2v/3$ we propose to use an average matrix, which averages all other treatments except $3(v-k)$ treatments with exactly two replicates each, to attach the E-optimality problem relating to the known best in $M(v,3,k)$. The average matrix is:

$$\begin{pmatrix} \omega I_{3k-2v} + \psi J_{3k-2v} & \xi_1 J & \xi_2 J & \xi_3 J & \xi_4 J & \xi_5 J & \xi_6 J \\ \xi_1 J & 2I_{s_1} - \frac{2}{k} J_{s_1} & -\frac{1}{k} J & -\frac{1}{k} J & -\frac{2}{k} J & 0 & 0 \\ \xi_2 J & -\frac{1}{k} J & 2I_{s_2} - \frac{2}{k} J_{s_2} & -\frac{1}{k} J & 0 & -\frac{2}{k} J & 0 \\ \xi_3 J & -\frac{1}{k} J & -\frac{1}{k} J & 2I_{s_3} - \frac{2}{k} J_{s_3} & 0 & 0 & -\frac{2}{k} J \\ \xi_4 J & -\frac{2}{k} J & 0 & 0 & 2I_{s_4} - \frac{4}{k} J_{s_4} & 0 & 0 \\ \xi_5 J & 0 & -\frac{2}{k} J & 0 & 0 & 2I_{s_5} - \frac{4}{k} J_{s_5} & 0 \\ \xi_6 J & 0 & 0 & -\frac{2}{k} J & 0 & 0 & 2I_{s_6} - \frac{4}{k} J_{s_6} \end{pmatrix}$$

where $s_1 + s_2 + s_3 + s_4 + s_5 + s_6 = 3(v - k)$, $\omega + \psi(3k - 2v)$, ξ_1, ξ_2, ξ_3, ξ_4, ξ_5 and ξ_6 are parameters that make the above matrix an information matrix, i.e., make the row and column sums of the matrix zero.

Using the technique described on page 38, one obtains the reduced average matrix

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & a_{16} & a_{17} \\ a_{21} & 2 - \frac{2s_1}{k} & -\frac{s_2}{k} & -\frac{s_3}{k} & -\frac{2s_4}{k} & 0 & 0 \\ a_{31} & -\frac{s_1}{k} & 2 - \frac{2s_2}{k} & -\frac{s_3}{k} & 0 & -\frac{2s_5}{k} & 0 \\ a_{41} & -\frac{s_1}{k} & -\frac{s_2}{k} & 2 - \frac{2s_3}{k} & 0 & 0 & -\frac{2s_6}{k} \\ a_{51} & -\frac{2s_1}{k} & 0 & 0 & 2 - \frac{4s_4}{k} & 0 & 0 \\ a_{61} & 0 & -\frac{2s_2}{k} & 0 & 0 & 2 - \frac{4s_5}{k} & 0 \\ a_{71} & 0 & 0 & -\frac{2s_3}{k} & 0 & 0 & 2 - \frac{4s_6}{k} \end{pmatrix} \tag{4.49}$$

where

$$\begin{aligned} a_{21} &= -2 + \tfrac{2s_1}{k} + \tfrac{s_2}{k} + \tfrac{s_3}{k} + \tfrac{2s_4}{k} & a_{12} &= \tfrac{a_{21}s_1}{3k-2v} \\ a_{31} &= \tfrac{s_1}{k} - 2 + \tfrac{2s_2}{k} + \tfrac{s_3}{k} + \tfrac{2s_5}{k} & a_{13} &= \tfrac{a_{231}s_2}{3k-2v} \\ a_{41} &= \tfrac{s_1}{k} + \tfrac{s_2}{k} - 2 + \tfrac{2s_3}{k} + \tfrac{2s_6}{k} & a_{14} &= \tfrac{a_{41}s_3}{3k-2v} \\ a_{51} &= \tfrac{2s_1}{k} - 2 + \tfrac{4s_4}{k} & a_{15} &= \tfrac{a_{51}s_4}{3k-2v} \\ a_{61} &= \tfrac{2s_2}{k} - 2 + \tfrac{4s_5}{k} & a_{16} &= \tfrac{a_{61}s_5}{3k-2v} \\ a_{71} &= \tfrac{2s_3}{k} - 2 + \tfrac{4s_6}{k} & a_{17} &= \tfrac{a_{71}s_6}{3k-2v} \\ a_{11} &= -(a_{12} + a_{13} + a_{14} + a_{15} + a_{16} + a_{17}) \end{aligned}$$

We know that the smallest positive eigenvalue of the information matrix of the E-optimal binary design with $x = y = z = 0$ is $3 - v/k$. If the smallest eigenvalue of (4.49) for any

$s_1 + s_2 + s_3 + s_4 + s_5 + s_6 = 3(v - k)$ is no greater than $3 - v/k$, we may conclude that the E-optimal binary design is also E-optimal in $D(v, 3, k)$.

The work is hard to carry on theoretically because the smallest positive eigenvalue of (4.49) is a root to a polynomial equation of sixth order. And it is apparently impossible to get an analytical expression for this eigenvalue. We resort to computer programming. We checked the smallest positive eigenvalue of the average matrices for $4 \leq v \leq 100$ and $k > 2v/3$ using a Matlab program (see Appendix D). Our results show that the average matrix technique can numerically show that the E-optimal binary designs are also E-optimal for $v \leq 9$. When $v \geq 10$, there are still some (but not all) settings that the average matrix technique can numerically show that the E-optimal binary designs are also E-optimal. We give two examples here. Readers may use the program in the Appendix D to get all results.

Example 4.4.1. The average matrix technique fails for $D(10, 3, 9)$ when $s_1 = s_2 = 0$, $s_3 = 3$ and $s_4 = s_5 = s_6 = 0$.

Example 4.4.2. The average matrix technique fails for $D(35, 3, 32)$ when $s_1 = s_2 = 0$, $s_3 = 8$, $s_4 = s_5 = 0$ and $s_6 = 1$.

We have not found any non-binary design that is E-better than the E-best binary design when $k > 2v/3$.

The E-optimality problem in $D(v, 3, k)$ when $k < 2v/3$ is even harder. E-optimal binary designs seem not to have a consistent pattern and have not yet been identified theoretically. The difficulty again arises from the impossibility of finding an analytical expression for the smallest positive eigenvalue of the information matrices.

Not surprisingly, we have computationally found that many non-binary designs are E- better than (or E- equal to) E-optimal binary designs when $k < 2v/3$. Below are some examples. Note that we have not shown any particular non-binary design to be E-optimal. The point is that E-optimal designs for some $D(v, 3, k)$ when $k < 2v/3$ must be non-binary.

Example 4.4.3. Consider $D(19, 3, 12)$. Using the MATLAB program we find the E-optimal design in $M(19,3,12)$,

$B1:$	1	2	3	4	5	6	7	8	9	10	11	17
$B2:$	1	2	3	4	5	6	12	13	14	15	16	18
$B3:$	1	7	8	9	10	11	12	13	14	15	16	19

The smallest positive eigenvalue of its information matrix is 0.86812.

Now consider the non-binary design:

$B1:$	1	2	3	4	5	6	7	8	16	16	17	17
$B2:$	1	2	3	4	9	10	11	12	13	14	15	18
$B3:$	5	6	7	8	9	10	11	12	13	14	15	19

The smallest positive eigenvalue of its information matrix is 0.86987.

Therefore, the non-binary design is E- better than the E-best binary design.

Example 4.4.4. Consider $D(29,3,19)$. Using the MATLAB program we find the E-optimal design in $M(29,3,19)$,

$B1:$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	29
$B2:$	1	2	3	4	5	6	7	8	9	19	20	21	22	23	24	25	26	27	28
$B3:$	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28

The smallest positive eigenvalue of its information matrix is 0.94737.

Now consider the non-binary design:

$B1:$	1	2	3	4	5	6	7	8	9	10	11	12	13	24	24	25	25	26	26
$B2:$	1	2	3	4	5	6	7	8	14	15	16	17	18	19	20	21	22	23	29
$B3:$	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	27	27	28	28

The smallest positive eigenvalue of its information matrix is 0.95227.

Therefore, the non-binary design is E- better than the E-best binary design.

Example 4.4.5. Consider $D(8, 3, 5)$. Using the MATLAB program we may get the E-optimal design in $M(8, 3, 5)$,

$$\begin{array}{llllll} B1: & 1 & 2 & 3 & 4 & 8 \\ B2: & 1 & 2 & 5 & 6 & 7 \\ B3: & 3 & 4 & 5 & 6 & 7 \end{array}$$

The smallest positive eigenvalue of its information matrix is 0.8.

Now consider the non-binary design:

$$\begin{array}{llllll} B1: & 1 & 2 & 3 & 4 & 8 \\ B2: & 1 & 2 & 5 & 6 & 6 \\ B3: & 3 & 4 & 5 & 7 & 7 \end{array}$$

The smallest positive eigenvalue of its information matrix is 0.8.

Therefore, the non-binary design is E- equal to the E-best binary design.

Chapter 5

Summary and Future Research

5.1 Summary

The goal of this research has been to discover optimal blocks designs within certain constrained, but important classes. Specifically, we have been working on problems where the amount of experimental material is limited. A paucity of blocks is not uncommon in practice, so we have studied the optimality problems for $b = 2$ and $b = 3$. For a given b, the minimal number of experimental units is provided by minimally connected designs, which we explored in chapter 1. Minimally connected designs are the block design analogue of saturated designs in the fractional factorial context.

We summarize our work in terms of techniques used and new results.

Techniques used for E-optimality problems and new results. Lemma 3.8 (Morgan and Reck 2003) gives a general method for bounding the smallest positive eigenvalue of an information matrix. This result may be taken as a projection theorem for the E-optimality problem. The word "projection" comes from the fact that any normalized treatment contrast is orthogonal to the overall mean treatment effect and any normalized treatment contrast variance can be used to bound the smallest positive eigenvalue of an information matrix.

When Lemma 3.8 and its corollaries (see chapter 3) cannot give a satisfying bound for smallest positive eigenvalue of an information matrix, we may use the average matrix and bound the smallest positive eigenvalue after deriving the characteristic polynomial of the averaged information matrix. In the study of optimal incomplete designs with two blocks, we successfully identified the E-optimal non-binary class using this technique.

Techniques used for A- and D-optimality problems and new results . We employed Theorem 4.4 (Kunert (1985) and Jacroux (1985)) to solve the type I optimality problem in $D(v, 3, k)$ when $k = 2v/3$. However, traditional results and theorems on type I optimality (see Cheng (1978), Jacroux (1985) and Morgan and Scrivastav (2001)) are not suitable for type I optimality problems when $k \neq 2v/3$. After deriving the general expression of the characteristic polynomial of information matrix and the general expressions of A- and D-values of any design in $M(v, 3, k)$, we successfully identified the A- and D-optimal designs in $M(v, 3, k)$ when $k \neq 2v/3$.

Average matrix is also a powerful technique for A- and D-optimality problems, as illustrated by our successful proof that binary designs must be A- and D-optimal incomplete designs in $D(v, 2, k)$.

A-optimal designs are those that minimize the average variance of elementary treatment contrasts. In some cases, we may use this fact to solve A-optimality problems. For minimally connect designs, there is only one unbiased estimate for any treatment contrast, no matter what is the variance structure of the observations. By comparing the average variance of elementary treatment contrasts, we successfully identified A-optimal, and also MV-optimal minimally connected block designs for spatially correlated data.

5.2 A Remark Regarding Two Famous Conjectures

In embarking on this dissertation we had entertained thoughts of debunking conjectures from Shah and Sinha (1989, p.60). We quote two of the conjectures here and give some discussion in view of our new results.

(1) "Binary (or generalized binary) designs form an essentially complete class."

In our study of optimal incomplete designs with two blocks, we found that E-optimality of binary designs in fact depends on the magnitude of k/v. When $k/v > 5/6$, E-optimal designs *must* lie in the non-binary class. In our study of optimal designs with three blocks, we also found that in some cases E-optimal designs must be non-binary when $k < 2v/3$. Therefore, the statement (1) is not correct, at least for E-optimal designs. As yet unknown is whether (1) is correct with respect to criteria that focus less on extreme behavior, such as A- and D-optimality, though we have determined many cases where binary designs are not ϕ_β-optimal for moderate β (see section 3.7). In our study, we have not found any non-binary designs to be A- and/or D-optimal. However, since we did find that A-optimal designs need not as balanced as possible and/or as equally replicated as possible in the binary class, we are now fairly convinced that combinatorial symmetry of designs need not be the deciding factor for the designs to be optimal or not. There might be non-binary designs that are A-optimal under certain circumstances, a question deserving further investigation.

(2) "When $k \geq 3$, an optimal design is necessarily (M,S)- optimal."

To understand this statement we need the definition of (M,S)-optimality.

Definition 5.1. A design d in $M(v,b,k)$ is (M,S)-optimal if its information matrix has minimum value of $\sum_{i=1}^{v-1} z_{di}^2$ among all possible designs in $M(v,b,k)$.

So the statement in fact says in binary classes, any optimal design should be one that minimizes $\sum_{i=1}^{v-1} z_{di}^2$. But is it true?

Morgan and Srivastav (2001) derived the expression of $tr(C_d^2)$ as follows. Since $tr(C_d^2) = \sum_{i=1}^{v-1} z_{di}^2$,

$$\sum_{i=1}^{v-1} z_{di}^2 = tr(C_d^2) = (\frac{k-1}{k})^2 \sum_{i=1}^{v} r_{di}^2 + \frac{2}{k^2} \sum \sum_{i<j} \lambda_{dij}^2. \tag{5.1}$$

It can be seen that a binary design is an (M,S)- optimal if it can minimize $\sum_{i=1}^{v} r_{di}^2$ and $\sum\sum_{i<j} \lambda_{dij}^2$ simultaneously, and a (M,S)- optimal design should be as balanced as possible and as equally replicated as possible.

But combinatorial symmetry need not to be the deciding factor for a design to be A-optimal. A-optimal minimally connected designs have one treatment with b replicates and all other treatments have only one replicate each. In the study of A-optimal designs in $M(v, 3, k)$ we found that A-optimal designs need not be as balanced as possible nor as equally replicated as possible under some circumstances.

Therefore, A-optimal designs need not be (M,S)- optimal. Statement (2) is not generally true. Here are two examples.

Example 5.2.1. A-optimal design d^* in $D(7, 3, 3)$ is not (M,S)- optimal, where d^* is given by

$$\begin{array}{lccc} B_1: & 1 & 2 & 3 \\ B_{l_1}: & 1 & 4 & 5 \\ B_{l_2}: & 1 & 6 & 7 \end{array}$$

It can be calculated that A-value of the design is 9.43 and by (5.1) that $\sum_{i=1}^{6} z_{d^*i}^2 = tr(C_{d^*}^2)$ is 8.67.

Consider a competing design d.

$$\begin{array}{lccc} B_1: & 1 & 2 & 3 \\ B_{l_1}: & 2 & 4 & 5 \\ B_{l_2}: & 4 & 6 & 7 \end{array}$$

It can be calculated that A-value of the design is 10.57 and by (5.1) that $\sum_{i=1}^{6} z_{di}^2 = tr(C_d^2)$ is 7.78. In fact, d is (M,S)- optimal since it can minimize $\sum_{i=1}^{7} r_{di}^2$ and $\sum\sum_{i<j} \lambda_{dij}^2$ simultaneously.

Example 5.2.2. For Example 4.3.8, we know in $M(116,3,40)$ A-optimal design d^* is:

$$\begin{array}{lcccccccc} B1: & 1 & 2 & 3 & 4 & \dots & 39 & 40 \\ B2: & 1 & 2 & 41 & 42 & \dots & 77 & 78 \\ B3: & 1 & 2 & 79 & 80 & \dots & 115 & 116 \end{array}$$

It can be calculated that A-value of the design is 151.85 and by (5.1) that $\sum_{i=1}^{115} z_{d^*i}^2 = tr(C_{d^*}^2)$ is 128.415.

Now consider a competing design d

$$\begin{array}{lcccccccc} B1: & 1 & 2 & 3 & 5 & \dots & 40 & 41 \\ B2: & 1 & 4 & 3 & 42 & \dots & 77 & 78 \\ B3: & 4 & 2 & 79 & 80 & \dots & 115 & 116 \end{array}$$

It can be calculated that A-value of the design is 153.31 and by (5.1) that $\sum_{i=1}^{115} z_{di}^2 = tr(C_d^2)$ is 124.608. In fact, d is (M,S)- optimal since it can minimize $\sum_{i=1}^{115} r_{di}^2$ and $\sum\sum_{i<j} \lambda_{dij}^2$ simultaneously.

5.3 Future Research

There are numerous open problems in the area of optimal block designs. In our research we have brought up new open problems in chapters two through four. They are not yet solved (or not fully solved) and thus stand as future research topics.

1. Is d^* the E-optimal design under all error structures considered in the class of minimally connected designs? We only give a sufficient condition for d^* to be E-optimal. The difficulty for the general structure (even for an AR model) is that we don't have an exact expression for the E-value, which at this time seems impossible because it requires finding roots to high order equations.

2. What are the binary E-optimal incomplete block designs in $D(v, 3, k)$? How about the optimality problems for the entire class $D(v, 3, k)$?

3. We successfully identified optimal incomplete block designs with two blocks. How about optimal designs with two blocks when $k > v$?

4. We have found that many E-optimal designs *must* be non-binary when $r = 1$. So are there any regular patterns for E-optimal designs for $r = 1$?

5. We have not found any A- and/or D-optimal designs to be non-binary. So is it true that "Binary (or generalized binary) designs form an essentially complete class for A- and D-optimality problems"?

Bibliography

[1] Bagchi, S. (1988), "A class of non binary unequally replicated E-optimal designs," *Metrika*, **35**, 1-12.

[2] Bagchi, B. and Bagchi S. (2001), "Optimality of partial geometric designs," *The Annals of Statistics*, **29**, **No. 2**, 577-594.

[3] Bapat, R. B. and Dey, A. (1991), "Optimal block designs with minimal number of observations," *Statistics and Probability letters*, **11**, 399-402.

[4] Birkes, D. and Dodge, Y. (1991), "Optimal $a \times b$ connected designs with $a + b$ observations," *Journal of Statistical Planning and Inference*, **28**, 49-59.

[5] Chakrabarti, M. C. (1963), "On the C-matrix in design of experiments," *Journal of Indian Statistical Society*, **1**, 8-23.

[6] Cheng, C.-S. (1978), "Optimality of certain asymmetrical experimental designs," *The Annals of Statistics*, **6**, 1239-1261.

[7] Cheng, C.-S. (1979), "Optimal incomplete block designs with four varieties," *Sankhya, Series B*, **41**, 1-14.

[8] Cheng, C.-S. (1980), "Some E-optimal block designs," *Journal of the Royal Statistical Society, Series B*, **42**, 199-204.

[9] Cheng, C.-S. and Constantine, G. M. (1981), "On the efficiency of regular generalized line graph designs," *Journal of Statistical Planning and Inference*, **15**, 1-10.

[10] Cheng, C.-S. and Wu, C. F (1981), "Nearly balanced incomplete block designs," *Biometrika*, **68**, 493-500.

[11] Cheng, C.-S. (1987), "An optimization problem with applications to optimal design theory," *The Annals of Statistics*, **15**, 712-723.

[12] Constantine, G. M. (1981), "Some E-opitmal block designs," *The Annals of Statistics*, **9**, 886-892.

[13] Constantine, G. M. (1982), "On the E-optimality of PBIB designs with a small number of blocks," *The Annals of Statistics*, **10**, 1027-1031.

[14] Constantine, G. M (1986), "On the optimality of block designs," *Annals of the Institute of Statistical Mathematics*, **38**, 161-174.

[15] Dey, A., Shah, K. R., and Das, A. (1995), "Optimal block designs with minimal and nearly minimal number of units," *Statisica Sinica*, **5**, 547-558.

[16] Haemers, W. H. (1980), *Eigenvalue Techniques in Design and Graph Theory*, Mathematical Center Tracts 121, Amsterdam.

[17] Hedayat, A. S., Jacroux, M., and Majumdar, D. (1988), "Optimal designs for comparing test treatments with controls (with discussion)," *Statistical Science*, **3**, 462-491.

[18] Hinklemann, K. and Kempthorne, O. (1994), *Design and Analysis of Experiments*, Volume 1, John Wiley and Sons, New York.

[19] Jacroux, M. A. (1980a), "On the E-optimality of regular graph designs," *Journal of the Royal statistical Society, Series B*, **42**, 205-209.

[20] Jacroux, M. A. (1980b), "On the determination and construction of E-optimal block designs with unequal number of replicates," *Biometrika*, **67**, 661-667.

[21] Jacroux, M. A. (1982), "Some E-optimal designs for the one-way and two-way elimination of heterogeneity," *Journal of the Royal Statistical Society, Series B*, **44**, 253-261.

[22] Jacroux, M. A. (1983a), "On the E-optimality of block designs," *Sankhya, Series B*, **45**, 351-361.

[23] Jacroux, M. A. (1983b), "Some minimum variance block designs for estimating treatment differences," *Journal of the Royal Statistical Society, Series B*, **45**, 70-76.

[24] Jacroux, M. A. (1985), "Some sufficient conditions for the Type 1 optimality of block designs," *Journal of Statistical Planning and Inference*, **11**, 385-398.

[25] John, J. A. and Mitchell, T. J. (1977), "Optimal incomplete block designs," *Journal of the Royal Statistical Society, Series B*, **39**, 39-43.

[26] John, J. A. and Williams, E. R. (1982), "Conjectures for incomplete block designs," *Journal of the Royal Statistical Society, Series B*, **44**, 221-225.

[27] Kiefer, J. (1958), "On the nonrandomized optimality and randomized optimality of symmetrical designs," *Annals of Mathematical Statistics*, **29**, 675-699.

[28] Kiefer, J. (1959), "Optimum experimental designs," *Journal of the Royal Statistical Society, Series B*, **21**,272-319.

[29] Kiefer, J. (1975), "Construction and optimality of generalized Youden designs," in *A Survey of Statistical Design and Linear Models* (J. N. Srivastava, editor). Amsterdam: North-Holland, 333-353.

[30] Krafft, O. and Schaefer, M. (1995), "A-optimal connected block designs with nearly minimal number of observations," *Journal of Statistical Planning and Inference*, **65**, 375-386.

[31] Mandal, N. K., Shah, K. R., and Sinha, B. K. (1991), "Uncertain resources and optimal designs: problems and perspectives," *Calcutta Statistical Association Bulletin*, **40**, 267-282.

[32] Marshall, A. W. and Olkin, I. (1979), *Inequalities: Theory of Majorization and Its Applications*, Academic Press.

[33] Mayer, C. D. (2000), *Matrix Analysis and Applied Linear Algebra*, SIAM.

[34] Morgan, J. P. and Chakravarti, I. M. (1988), "Block designs for first and second order neighbor correlations," *The Annals of Statistics*, **16** , 1206-1224.

[35] Morgan, J. P. and Reck, B (2003), "E-optimal design in irregular BIBD settings," Preprint.

[36] Morgan, J. P. (1997), "On pairs of Youden designs," *Journal of Statistical Planning and Inference*, **60**, 367-387.

[37] Morgan, J. P. and Scrivastav, S. K. (2000), "On the Type-1 optimality of nearly balanced incomplete block designs with small concurrence range," *Statistica Sinica*, **10**, 1091-1116.

[38] Parlett, B. N. (1980), *The Symmetric Eigenvalue Problem*, Prentice-Hall.

[39] Shah, K. R. (1960), "Optimality criteria for incomplete block designs," *Annals of Mathematical Statistics*, **31**, 791-794.

[40] Shah, K. R. and Sinha, B. K. (1989), *Theory of optimal designs*, Springer-Verlag, New York.

[41] Srivastav, S. K. and Morgan, J. P. (1998), "Optimality of designs with generalized group divisible structure," *Journal of Statistical Planning and Inference*, **71**, 313-330.

[42] Uddin, N. and Morgan, J. P. (1997), "Efficient block designs for settings with spatially correlated errors," *Biometrika*, **84**, 443-454.

Appendix A

Proofs for Corollaries 2.7 and 2.8

For simplicity of expressions, we will not include the term σ^2 in any variance-covariance matrix below since it does not affect the optimality comparisons. But we should keep in mind that the true variance-covariance matrices are those below times a factor σ^2.

Corollary 2.7 Design d^* is E-optimal when $k = 3$.

Proof. When $k = 3$, Σ^0 is:

$$\Sigma^0 = \begin{pmatrix} 1 & \rho_1 & \rho_2 \\ \rho_1 & 1 & \rho_1 \\ \rho_2 & \rho_1 & 1 \end{pmatrix} \tag{A.1}$$

Compute $(I - H_2)\Sigma^0(I - H_2')$ and delete its second row and second column. We have:

$$\Gamma_2 = \begin{pmatrix} 2 - 2\rho_1 & 1 - 2\rho_1 + \rho_2 \\ 1 - 2\rho_1 + \rho_2 & 2 - 2\rho_1 \end{pmatrix} \tag{A.2}$$

The eigenvalues of Γ_2 are $1 - \rho_2$ and $3 - 4\rho_1 + \rho_2$ and these two eigenvalues should be positive since Γ_2 is positive definite.

Compute $(I-H_1)\Sigma^0(I-H_1')$ and delete its first row and column. We have

$$\Gamma_1 = \begin{pmatrix} 2-2\rho_1 & 1-\rho_2 \\ 1-\rho_2 & 2-2\rho_2 \end{pmatrix}. \tag{A.3}$$

The largest non-zero eigenvalue of Γ_1 is $2-\rho_1-\rho_2+\sqrt{1+\rho_1^2-2\rho_2-2\rho_1\rho_2+2\rho_2^2}$.

For the matrix $\frac{\Gamma_1+\Gamma_2}{2}$, We have:

$$\frac{\Gamma_1+\Gamma_2}{2} = \begin{pmatrix} 2-2\rho_1 & 1-\rho_1 \\ 1-\rho_1 & 2-\rho_1-\rho_2 \end{pmatrix} \tag{A.4}$$

The largest non-zero eigenvalue of $\frac{\Gamma_1+\Gamma_2}{2}$ is $\frac{4-3\rho_1-\rho_2+\sqrt{4-8\rho_1+5\rho_1^2-2\rho_1\rho_2+\rho_2^2}}{2}$.

First show $\frac{\Gamma_1+\Gamma_2}{2}$ has smaller largest eigenvalue than Γ_1.

Compute

$$\begin{aligned} & \frac{4-3\rho_1-\rho_2+\sqrt{4-8\rho_1+5\rho_1^2-2\rho_1\rho_2+\rho_2^2}}{2} \\ - & \ (2-\rho_1-\rho_2+\sqrt{1+\rho_1^2-2\rho_2-2\rho_1\rho_2+2\rho_2^2}) \\ = & \ \frac{(\sqrt{4(1-\rho_1)^2+(\rho_1-\rho_2)^2}-\sqrt{4(1-\rho_2)^2+(\rho_1-\rho_2)^2})-(\rho_1-\rho_2)}{2} \leq 0 \end{aligned}$$

Then we show Γ_2 has smaller largest eigenvalue than $\frac{\Gamma_1+\Gamma_2}{2}$.

If $1-\rho_2$ is the largest eigenvalue of Γ_2 then compare $1-\rho_2$ with $\frac{4-3\rho_1-\rho_2+\sqrt{4-8\rho_1+5\rho_1^2-2\rho_1\rho_2+\rho_2^2}}{2}$.
Compute

$$\begin{aligned} & 1-\rho_2-\frac{4-3\rho_1-\rho_2+\sqrt{4-8\rho_1+5\rho_1^2-2\rho_1\rho_2+\rho_2^2}}{2} \\ = & \ \frac{-2+3\rho_1-\rho_2-\sqrt{4(1-\rho_1)^2+(\rho_1-\rho_2)^2}}{2} \\ \leq & \ \frac{-2+3\rho_1-\rho_2-(\rho_1-\rho_2)}{2} = -(1-\rho_1) < 0 \end{aligned}$$

If $3-4\rho_1+\rho_2 > 0$ is the largest eigenvalue of Γ_2 then compare $3-4\rho_1+\rho_2$ with

$\frac{4-3\rho_1-\rho_2+\sqrt{4-8\rho_1+5\rho_1^2-2\rho_1\rho_2+\rho_2^2}}{2}$.

Compute

$$\begin{aligned} & 3-4\rho_1+\rho_2-\frac{4-3\rho_1-\rho_2+\sqrt{4-8\rho_1+5\rho_1^2-2\rho_1\rho_2+\rho_2^2}}{2} \\ = & \frac{2-5\rho_1-3\rho_1)-\sqrt{4(1-\rho_1)^2+(\rho_1-\rho_2)^2}}{2} \\ \leq & \frac{2-5\rho_1+3\rho_2-2(1-\rho_1)}{2}=-\frac{3(\rho_1-\rho_2}{2}\leq 0 \end{aligned}$$

□

Corollary 2.8 Design d^* is E-optimal when $k=4$ and the covariance structure is defined as $\rho_s=\rho^s$ where $0<\rho<1$ and $s\geq 1$ is an integer.

Proof. Σ^0 is:

$$\Sigma^0=\begin{pmatrix} 1 & \rho & \rho^2 & \rho^3 \\ \rho & 1 & \rho & \rho^2 \\ \rho^2 & \rho & 1 & \rho \\ \rho^3 & \rho^2 & \rho & 1 \end{pmatrix} \tag{A.5}$$

First consider Γ_1.

Compute $(I-H_1)\Sigma^0(I-H_1')$ then delete its first row and column. We have:

$$\Gamma_1=\begin{pmatrix} 2-2\rho & 1-\rho^2 & 1-\rho+\rho^2-\rho^3 \\ 1-\rho^2 & 2-2\rho^2 & (1-\rho)(1+\rho)^2 \\ 1-\rho+\rho^2-\rho^3 & (1-\rho)(1+\rho)^2 & 2-2\rho^3 \end{pmatrix} \tag{A.6}$$

Three eigenvalues of Γ_1 are the three non-zero roots to the equation $|\Gamma_1-\lambda I|=0$, i.e., the three roots to the equation:

$$\begin{aligned} G_1(\lambda)= & -2(2-\rho)(1-\rho)^3(1+\rho)^2-(1-\rho)^2(1+\rho)(-9-\rho-2\rho^2+2\rho^3)\lambda \\ & +2(-1+\rho)(3+2\rho+\rho^2)\lambda^2+\lambda^3=0 \end{aligned} \tag{A.7}$$

Check:

$$
\begin{aligned}
G_1(0) &= -2(2-\rho)(1-\rho)^3(1+\rho)^2 < 0 \\
G_1(1-\rho) &= (1-\rho)^3\rho^2(1+2\rho-2\rho^2) > 0 \\
G_1(2-2\rho^2) &= -2(1-\rho)^3(1+\rho)^2(1+2\rho+2\rho^2+2\rho^3) < 0 \\
G_1(4) &= 2\rho(3+3\rho+18\rho^2+2\rho^3+11\rho^4-5\rho^5) > 0
\end{aligned}
\tag{A.8}
$$

So the three roots are within $(0, 1-\rho)$, $(1-\rho, 2-2\rho^2)$ and $(2-2\rho^2, 4)$ respectively. The largest eigenvalue of Γ_1, say z_{max1}, is within $(2-2\rho^2, 4)$.

Secondly, consider Γ_3. Compute $(I-H_3)\Sigma^0(I-H_3^{'})$ and delete its third row and column. we have:

$$
\Gamma_3 = \begin{pmatrix} 2-2\rho^2 & 1-\rho^2 & (1-\rho)^2(1+\rho) \\ 1-\rho^2 & 2-2\rho & (1-\rho)^2 \\ (1-\rho)^2(1+\rho) & (1-\rho)^2 & 2-2\rho \end{pmatrix}
\tag{A.9}
$$

Three non-zero eigenvalues of Γ_3 are the three non-zero roots to the equation $|\Gamma_3 - \lambda I| = 0$, i.e., the three roots to the equation:

$$
\begin{aligned}
G_3(\lambda = \quad & -2(2-\rho)(1-\rho)^3(1+\rho)^2 - (1-\rho)^2(1+\rho)(-9+\rho-\rho^2+\rho^3)\lambda \\
& +2(-1+\rho)(3+\rho)\lambda^2 + \lambda^3 = 0
\end{aligned}
\tag{A.10}
$$

Check:

$$
\begin{aligned}
G_3(0) &= -2(2-\rho)(1-\rho)^3(1+\rho)^2 < 0 \\
G_3(1-\rho) &= (2-\rho)(1-\rho)^3\rho^3 > 0 \\
G_3(2-2\rho^2) &= -2(1-\rho)^3(1+\rho)^2(1-\rho^2+\rho^3) < 0 \\
G_3(4) &= 2\rho(15+5\rho+10\rho^2-2\rho^3+7\rho^4-3\rho^5) > 0
\end{aligned}
\tag{A.11}
$$

So the three roots are within $(0, 1-\rho)$, $(1-\rho, 2-2\rho^2)$ and $(2-2\rho^2, 4)$ respectively. The largest eigenvalue of Γ_3 is within $(2-2\rho^2, 4)$.

Thirdly, Consider $\frac{\Gamma_1+\Gamma_3}{2}$. We have

$$
\frac{\Gamma_1+\Gamma_3}{2} = \begin{pmatrix} 2-\rho-\rho^2 & 1-\rho^2 & 1-\rho \\ 1-\rho^2 & 2-\rho-\rho^2 & \frac{2-\rho-\rho^3}{2} \\ 1-\rho & \frac{2-\rho-\rho^3}{2} & 2-\rho-\rho^3 \end{pmatrix}
\tag{A.12}
$$

Three non-zero eigenvalues of $\frac{\Gamma_1+\Gamma_3}{2}$ are the three non-zero roots to the equation $|\frac{\Gamma_1+\Gamma_3}{2} - \lambda I| = 0$, i.e., the three roots to the equation:

$$\begin{aligned} G(\lambda) = & -(-1+\rho)^3(1+\rho)(-16-8\rho-6\rho^2+3\rho^3+\rho^4)-(1-\rho)^2(-36-36\rho-19\rho^2 \\ & -6\rho^3+\rho^4)\lambda+4(-1+\rho)(6+3\rho+\rho^2)\lambda^2+4\lambda^3=0 \end{aligned} \tag{A.13}$$

Check:

$$\begin{aligned} G(0) &= -(-1+\rho)^3(1+\rho)(-16-8\rho-6\rho^2+3\rho^3+\rho^4)<0 \\ G(1-\rho) &= -(-1+\rho)^3(1+\rho)^3\rho^2>0 \\ G(2-2\rho^2) &= (-1+\rho)^3(1+\rho)(8+16\rho+\rho^3+\rho^4)<0 \\ G(4) &= \rho(72+70\rho+63\rho^2+19\rho^3+26\rho^4+8\rho^5-\rho^6-\rho^7)>0 \end{aligned} \tag{A.14}$$

So the three roots are within $(0, 1-\rho)$, $(1-\rho, 2-2\rho^2)$ and $(2-2\rho^2, 4)$ respectively. The largest eigenvalue of $\frac{\Gamma_1+\Gamma_3}{2}$, say, z_{max}, is within $(2-2\rho^2, 4)$ too.

Furthermore, one may check:

$$\begin{aligned} G_3(\lambda) = & \; G_1(\lambda)) + \lambda\rho(1-\rho^2)(2\lambda-(2-\rho)(1-\rho)(1+\rho)) \\ G_3(\lambda) = & \; \tfrac{G(\lambda)}{4} + \tfrac{\rho(1-\rho)}{4}[4\lambda^2(1+\rho)-(1-\rho)^2(1+\rho)\rho(-14+\rho(3+\rho)) \\ & -\lambda(1-\rho)^2(4+\rho(19+3\rho(2+\rho)))] \end{aligned} \tag{A.15}$$

For $z_{max1} \in (2-2\rho^2, 4)$, check:

$$\begin{aligned} G_3(z_{max1}) &= G_1(z_{max1}) + z_{max1}\rho(1-\rho^2)(2z_{max1}-(2-\rho)(1-\rho)(1+\rho)) \\ &> z_{max1}\rho(1-\rho^2)(2(2-2\rho^2)-(2-\rho)(1-\rho)(1+\rho)) \\ &= z_{max1}\rho(1-\rho^2)(1-\rho)(1+\rho)(2+\rho)>0 \end{aligned} \tag{A.16}$$

So the largest eigenvalue of Γ_3 is within $(2-2\rho^2, z_{max1})$. The largest eigenvalue of Γ_3 is smaller than that of Γ_1.

And for $z_{max} \in (2-2\rho^2, 4)$, check:

$$G_3(z_{max}) = \frac{G(z_{max})}{4} + R(z_{max}) \tag{A.17}$$

where

$$R(z_{max}) = \begin{array}{l} \frac{\rho(1-\rho)}{4}[4z_{max}^2(1+\rho)-(1-\rho)^2(1+\rho)\rho(-14+\rho(3+\rho)) \\ -z_{max}(1-\rho)^2(4+\rho(19+3\rho(2+\rho)))]. \end{array} \tag{A.18}$$

Differentiate $R(z_{max})$ with respect to z_{max}. We have:

$$\begin{aligned} \frac{\partial R(z_{max})}{\partial z_{max}} &= \frac{\rho}{4}[-8z_{max}(-1+\rho^2)-(-1+\rho)^2(4+\rho(19+3\rho(2+\rho)))] \\ &> \frac{\rho}{4}[-8(2-2\rho^2)(-1+\rho^2)-(-1+\rho)^2(4+\rho(19+3\rho(2+\rho)))] \\ &= \frac{1}{4}(1-\rho)^2\rho(12+13\rho+10\rho^2-3\rho^3)>0 \end{aligned} \tag{A.19}$$

So $R(z_{max})$ is an increasing function with respect to z_{max} when $z_{max} > 2-2\rho^2$. Check its value at $2-2\rho^2$:

$$R(2-2\rho^2) = \frac{1}{4}(1-\rho)^3\rho(8+16\rho+9\rho^2-6\rho^3-7\rho^4) > 0 \tag{A.20}$$

Therefore, $G_3(z_{max}) > 0$ for $z_{max} > 2-2\rho^2$

So the largest eigenvalue of Γ_3 is within $(2-2\rho^2, z_{max})$ and the largest eigenvalue of Γ_3 is smaller than that of $\frac{\Gamma_1+\Gamma_3}{2}$. □

Appendix B

A proof for Lemma 3.10

Lemma 3.10 Any design in which some treatment has more than two replicates cannot be E- optimal in $D(v, 2, k)$ with $v > k$.

Proof. Following the previous notations, this lemma says that E optimal designs cannot have $m \geq 1$. We resort to the average matrix technique to get the proof. Lemma 3.9 tells us $m + s \leq \frac{p}{2}$ and Lemma 3.7 tells us $s \geq 0$. For a design d in which some treatment has more than two replicates, we must have at least $p - 2m$ treatments with exactly two replicates. Suppose the number of these which occur only in block i is t_i, $i = 1, 2$. Then the number of the treatments with two replicates and occurring in both block in the design is at least $t_3 = p - 2m - t_1 - t_2$. Now we consider averaging over the other m treatments, all of those except a set of $p-2m$ treatments with exactly two replicates and the $2(k-p)+m$ treatments with exactly one replicate (see Figure B.1).

Then the average matrix becomes,

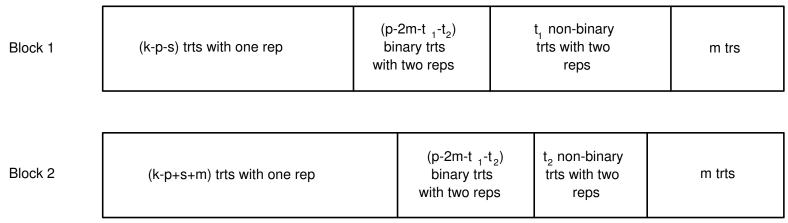

Figure B.1: Averaging Structure in $D(v, 2, k)$

$$\begin{pmatrix} \omega I_m + \psi J_m & \xi_1 J & \xi_2 J & \xi_3 J & \xi_4 J & \xi_5 J \\ \xi_1 J & 2I_{t_3} - \frac{2}{k} J_{t_3} & -\frac{2}{k} J & -\frac{2}{k} J & -\frac{1}{k} J & -\frac{1}{k} J \\ \xi_2 J & -\frac{2}{k} J & 2I_{t_1} - \frac{4}{k} J_{t_1} & 0 & -\frac{2}{k} J & 0 \\ \xi_3 J & -\frac{2}{k} J & 0 & 2I_{t_2} - \frac{4}{k} J_{t_2} & 0 & -\frac{2}{k} J \\ \xi_4 J & -\frac{1}{k} J & -\frac{2}{k} J & 0 & I_{k-p-s} - \frac{1}{k} J_{k-p-s} & 0 \\ \xi_5 J & -\frac{1}{k} J & 0 & -\frac{2}{k} J & 0 & I_{k-p+s+m} - \frac{1}{k} J_{k-p+s+m} \end{pmatrix}$$

where 0's are the matrices in which all elements are 0 with suitable dimensions and J's are the matrices in which all elements are 1 with suitable dimensions. ξ_1, ξ_2, ξ_3, ξ_4, ξ_5 and $\omega + m\psi$ are parameters decided by the fact the row and column sums of the above matrix are all zero. We will see later from the reduced average matrix that for E-optimality problem we do not need to know the values of ω and ψ individually. All that will be needed is $\omega + m\psi$, which is $-(p - s - m)/k$ as will be seen.

$2k - p - 6$ non-zero eigenvalues of the average matrix can be gotten immediately: 1 with frequency $2(k - p) + m - 2$, 2 with frequency $p - 2m - 3$, and ω with frequency $m - 1$. Using the technique described on page 37, one can get the remaining eigenvalues of the average matrix are those of the following reduced average matrix:

$$\overline{C}_{d,reduced} = \begin{pmatrix} a & -\frac{3t_3}{k} & -\frac{2t_1w_1}{km} & -\frac{2w_2t_2}{km} & -\frac{w_1(k-p-s)}{km} & -\frac{w_2(k-p+s+m)}{km} \\ -\frac{3m}{k} & \frac{2(k-t_3)}{k} & -\frac{2t_1}{k} & -\frac{2t_2}{k} & -\frac{k-p-s}{k} & -\frac{k-p+s+m}{k} \\ -\frac{2w_1}{k} & -\frac{2t_3}{k} & \frac{2k-4t_1}{k} & 0 & -\frac{2(k-p-s)}{k} & 0 \\ -\frac{2w_2}{k} & -\frac{2t_3}{k} & 0 & \frac{2k-4t_2}{k} & 0 & -\frac{2(k-p+s+m)}{k} \\ -\frac{w_1}{k} & -\frac{t_3}{k} & -\frac{2t_1}{k} & 0 & \frac{p+s}{k} & 0 \\ -\frac{w_2}{k} & -\frac{t_3}{k} & 0 & -\frac{2t_2}{k} & 0 & \frac{p-s-m}{k} \end{pmatrix} \quad \text{(B.1)}$$

where $a = \frac{3km-5m^2-2m(s+t_2-t_1)-2(s+t_2-t_1)^2}{km}$, $w_1 = s + 2m + t_2 - t_1$ and $w_2 = m - s - t_2 + t_1$. The parameters w_1 and w_2 are the numbers of plots taken by m treatments in block 1 and 2 respectively. They must be nonnegative and cannot be zero simultaneously. That is,

$$\begin{aligned} w_1 = s + 2m + t_2 - t_1 &\geq 0 \\ w_2 = m - s - t_2 + t_1 &\geq 0 \\ w_1 + w_2 &\neq 0 \end{aligned}$$

The average matrix will collapse to smaller dimensions if any of t_1, t_2, $p - 2m - t_1 - t_2$, $k - p - s$ are zero; all designs considered have $m \geq 1$. In the following, we first show that $G(0) > 0$ and there is always a positive eigenvalue less than one for the reduced average matrix. To do this we break the investigation into two cases, $s < k - p$ and $s = k - p$.

Case I. $s < k - p$. The smallest eigenvalue of the average matrix is one root to the equation

$G(\lambda) = 0$, where

$$\begin{aligned}
G(\lambda) \;=\;& -8km^2 + 12kmp + 4m^2p - 6mp^2 - 4kmt_1 + 2mpt_1 - 8kt_1^2 + 4pt_1^2 \\
& -8kms + 4mps + 16kt_1s - 8pt_1s - 8ks^2 + 4ps^2 - 20kmt_2 + 10mpt_2 \\
& +16kt_1t_2 - 8pt_1t_2 - 16kst_2 + 8pst_2 - 8kt_2^2 + 4pt_2^2 - 12k^2m\lambda \\
& +12km^2\lambda - 10kmp\lambda - 2m^2p\lambda + 5mp^2\lambda + 6kmt_1\lambda - 2m^2t_1\lambda \\
& -2mpt_1\lambda + 16kt_1^2\lambda - mt_1^2\lambda - 6pt_1^2\lambda + 16kms\lambda + 4m^2s\lambda \\
& +12pt_1s\lambda + 16ks^2\lambda + 4ms^2\lambda - 6ps^2\lambda + 38kmt_2\lambda - 2m^2t_2\lambda \\
& -6mps\lambda - 32kt_1s\lambda - 14mpt_2\lambda - 32kt_1t_2\lambda + 2mt_1t_2\lambda + 12pt_1t_2\lambda \\
& +32kst_2\lambda - 12pst_2\lambda + 16kt_2^2\lambda - mt_2^2\lambda - 6pt_2^2\lambda + 16k^2m\lambda^2 \\
& -8km^2\lambda^2 + 2kmp\lambda^2 - mp^2\lambda^2 - 2kmt_1\lambda^2 + 2m^2t_1\lambda^2 - 10kt_1^2\lambda^2 \\
& +mt_1^2\lambda^2 + 2pt_1^2\lambda^2 - 10kms\lambda^2 - 2m^2s\lambda^2 + 2mps\lambda^2 + 20kt_1s\lambda^2 \\
& -22kmt_2\lambda^2 + 2m^2t_2\lambda^2 + 4mpt_2\lambda^2 + 20kt_1t_2\lambda^2 - 2mt_1t_2\lambda^2 - 4pt_1t_2\lambda^2 \\
& -4pt_1s\lambda^2 - 10ks^2\lambda^2 - 2ms^2\lambda^2 + 2ps^2\lambda^2 - 20kst_2\lambda^2 + 4pst_2\lambda^2 \\
& -10kt_2^2\lambda^2 + mt_2^2\lambda^2 + 2pt_2^2\lambda^2 - 7k^2m\lambda^3 + 2km^2\lambda^3 + 2kt_1^2\lambda^3 + 2kms\lambda^3 \\
& -4kt_1s\lambda^3 + 2ks^2\lambda^3 + 4kmt_2\lambda^3 - 4kt_1t_2\lambda^3 + 4kst_2\lambda^3 + 2kt_2^2\lambda^3 + k^2m\lambda^4
\end{aligned}$$

is the characteristic polynomial of $(B.1)$ after removing factors λ and $\lambda - 2$. Now check:

$$\begin{aligned}
G(0) \;=\;& 2(2k-p)(-2m^2 + 3mp - mt_1 - 2t_1^2 - 2ms + 4t_1s - 2s^2 - 5mt_2 \\
& +4t_1t_2 - 4st_2 - 2t_2^2)
\end{aligned}$$

If $p = 2m + t_1 + t_2$, then $w_1w_2 > 0$, for otherwise, the design is disconnected. Substitute $p = 2m+t_1+t_2$ into the third term of G(0) to get $G(0) = 4(2k-p)(m+t_1-s-t_2)(2m-t_1+s+t_2) = 4(2k-p)w_1w_2 > 0$. If $p > 2m+t_1+t_2$, then $G(0) > 4(2k-p)(m+t_1-s-t_2)(2m-t_1+s+t_2) = 4(2k-p)w_1w_2 \geq 0$. Therefore, we will always have $G(0) > 0$.

Also check:

$$G(1) \;=\; -2m(k-p-s)(k-p+m+s) < 0$$

So there is a root of $G(\lambda) = 0$ between $(0, 1)$.

Case II. s=k-p. The reduced average matrix collapses into a 5×5 matrix.

$$\begin{pmatrix} a & -\frac{3t_3}{k} & -\frac{2t_1w_1}{km} & -\frac{2w_2t_2}{km} & -\frac{w_2(2(k-p)+m)}{km} \\ -\frac{3m}{k} & \frac{2(k-t_3)}{k} & -\frac{2t_1}{k} & -\frac{2t_2}{k} & -\frac{2(k-p)+m}{k} \\ -\frac{2w_1}{k} & -\frac{2t_3}{k} & \frac{2k-4t_1}{k} & 0 & 0 \\ -\frac{2w_2}{k} & -\frac{2t_3}{k} & 0 & \frac{2k-4t_2}{k} & -\frac{2(2(k-p)+m)}{k} \\ -\frac{w_2}{k} & -\frac{t_3}{k} & 0 & -\frac{2t_2}{k} & \frac{2p-k-m}{k} \end{pmatrix}$$

Two eigenvalues of this matrix are zero and 2. The smallest positive eigenvalue is the smallest root of the equation $Q(\lambda) = 0$, where

$$\begin{aligned} Q(\lambda) &= -8k^3 - 8k^2m - 8km^2 + 20k^2p + 24kmp + 4m^2p - 16kp^2 - 10mp^2 \\ &+4p^3 + 16k^2t_1 - 4kmt_1 - 24kpt_1 + 2mpt_1 + 8p^2t_1 - 8kt_1^2 + 4pt_1^2 \\ &-16k^2t_2 - 20kmt_2 + 24kpt_2 + 10mpt_2 - 8p^2t_2 + 16kt_1t_2 - 8pt_1t_2 \\ &-8kt_2^2 + 4pt_2^2 + 8k^3\lambda + 8km^2\lambda - 18k^2p\lambda - 16kmp\lambda - 2m^2p\lambda \\ &+12kp^2\lambda + 5mp^2\lambda - 2p^3\lambda - 16k^2t_1\lambda + 2kmt_1\lambda - 2m^2t_1\lambda + 20kpt_1\lambda \\ &-4p^2t_1\lambda + 8kt_1^2\lambda - mt_1^2\lambda - 2pt_1^2\lambda + 16k^2t_2\lambda + 18kmt_2\lambda - 2m^2t_2\lambda \\ &-20kpt_2\lambda - 4mpt_2\lambda + 4p^2t_2\lambda - 16kt_1t_2\lambda + 2mt_1t_2\lambda + 4pt_1t_2\lambda \\ &+8kt_2^2\lambda - mt_2^2\lambda - 2pt_2^2\lambda - 2k^3\lambda^2 + 4k^2m\lambda^2 - 2km^2\lambda^2 + 4k^2p\lambda^2 \\ &+2kmp\lambda^2 - 2kp^2\lambda^2 + 4k^2t_1\lambda^2 - 4kpt_1\lambda^2 - 2kt_1^2\lambda^2 - 4k^2t_2\lambda^2 \\ &-4kmt_2\lambda^2 + 4kpt_2\lambda^2 + 4kt_1t_2\lambda^2 - 2kt_2^2\lambda^2 - k^2m\lambda^3. \end{aligned}$$

Check

$$Q(0) = -2(2k-p)Q_1$$

where

$$\begin{aligned} Q_1 &= 2k^2 + 2km + 2m^2 - 4kp - 5mp + 2p^2 - 4kt_1 + mt_1 + 4pt_1 + 2t_1^2 + 4kt_2 \\ &+5mt_2 - 4pt_2 - 4t_1t_2 + 2t_2^2 \end{aligned}$$

and

$$Q(1) = -(2k - 2p + m)((k - p - t_1 + t_2)^2 + 2(k - p + t_1 + t_2)m) < 0.$$

Now we show that $Q(0) > 0$, i.e., $Q_1 < 0$. Q_1 is a quadratic function with respect to p and the coefficient of p^2 is $2 > 0$. If we can show that at two ending positions $p = 2m + t_1 + t_2$ and $p = k + 2m - t_1 + t_2$ its values are less than zero, we get the proof.

Check

$$\begin{aligned} Q_1|_{p=2m+t_1+t_2} &= 2(k - 2t_1)(k - 3m - 2t_1) \\ Q_1|_{p=k+2m-t_1+t_2} &= -3m(k - 2t_1) < 0. \end{aligned}$$

Note that when $p = 2m + t_1 + t_2$ and $s = k - p$, $k - 3m - 2t_1 = -w_2 < 0$. Therefore, there must be an eigenvalue in $(0, 1)$.

In fact,

$$G(\lambda)|_{s=k-p} = (1 - \lambda)Q(\lambda) \tag{B.2}$$

Therefore, for any $\lambda < 1$, $G(\lambda)|_{s=k-p}$ and $Q(\lambda)$ must be of the same sign.

Having established $G(0) > 0$ and existence of a root in $(0, 1)$, we will proceed as follows. First we will show that $G(z_{d_0 1}) < 0$ when $p \leq \frac{4k}{5}$, where $z_{d_0 1} = \frac{p}{k}$. If this is true then there is an eigenvalue for the average matrix less than $z_{d_0 1}$ when $p \leq 4k/5$. Then we will show that $G(z_{d^* 1}) < 0$ when $p > 4k/5$ where $z_{d^* 1} = \frac{p}{k} + \frac{1}{2} - \frac{1}{2}\sqrt{17\frac{p^2}{k^2} - 36\frac{p}{k} + 20}$. If this is true then there is an eigenvalue for the average matrix less than $z_{d^* 1}$ when $p > 4k/5$. Due to the discussion in previous paragraph, we use $s \leq k - p$ instead of separating $s < k - p$ and $s = k - p$. By $(B.2)$, $Q(z_{d_0 1}) < 0$ if $G(z_{d_0 1})|_{s=k-p} < 0$ and $Q(z_{d^* 1}) < 0$ if $G(z_{d^* 1}|_{s=k-p}) < 0$.

As will be seen below, the expression of $G(z_{d_0 1})$ or $G(z_{d^* 1})$ can be taken as a quadratic function of t_1 and t_2. The function will be shown to be concave and having no solutions to the equations $\partial G/\partial t_1 = 0$ and $\partial G/\partial t_2 = 0$. Therefore, its maximum value will be on the boundaries, i.e., on the lines $t_1 = 0$, $t_2 = 0$, $t_1 + t_2 = p - 2m$, $t_2 - t_1 = m - s$ or $t_1 - t_2 = s + 2m$

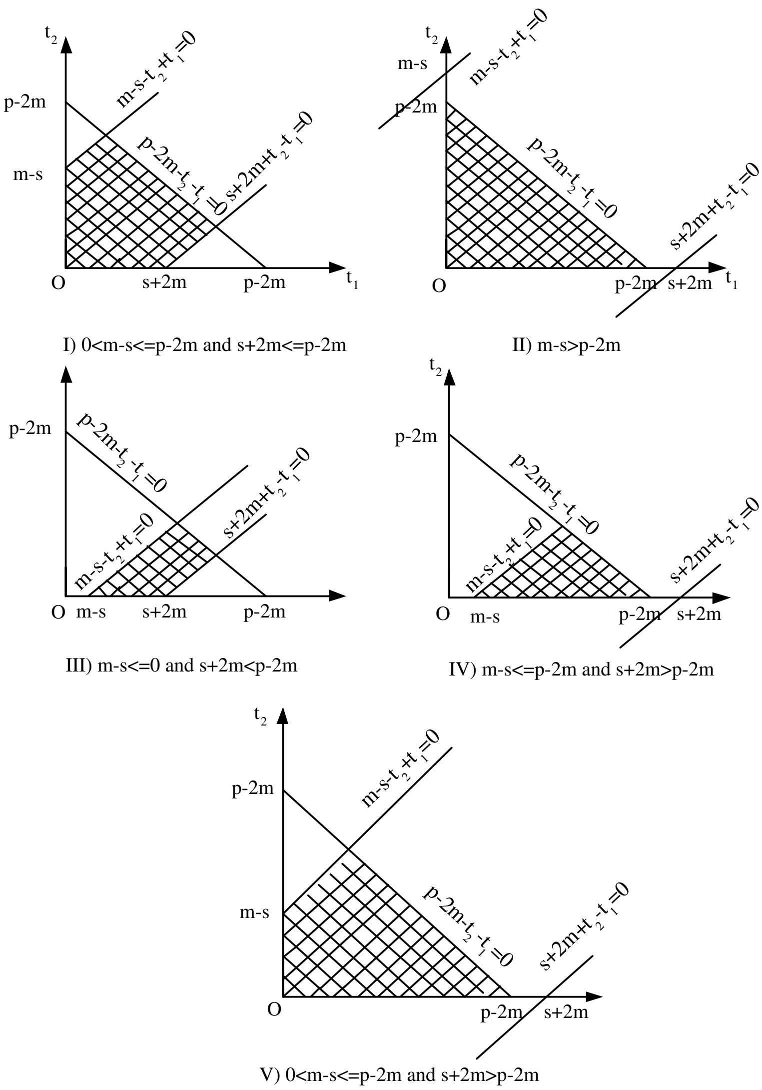

Figure B.2: Range for t_1 and t_2

(see Figure B.2). We will show that the values on the five lines are all smaller than zero. The fairly extensive technical details for this straightforward idea follow.

First check $G(p/k)$. One may use Mathematica to get the expression of $G(p/k)$, which is omitted here. Considered as a quadratic function of t_1 and t_2, check,

$$
\begin{aligned}
& \frac{\partial^2 G(p/k)}{\partial t_1^2} = \frac{\partial^2 G(p/k)}{\partial t_2^2} \\
= & -\frac{2(k-p)(4(k-p)(2k-p)+mp)}{k^2} \\
= & -\frac{\partial^2 G(p/k)}{\partial t_1 \partial t_2} = -\frac{\partial^2 G(p/k)}{\partial t_2 \partial t_1}
\end{aligned}
$$

Clearly the Hessian matrix is non-positive definite for every pair of t_1 and t_2 and the function is concave with respect to t_1 and t_2. If there is a solution (t_1, t_2) to the equations $\partial G(p/k)/\partial t_1 = 0$ and $\partial G(p/k)/\partial t_2 = 0$, the the solution is the maximum value point; if we cannot find such a solution, the maximum value of $G(p/k)$ must be on the boundaries.

Now we show that the solution does not exist.

Solve $\partial G(p/k)/\partial t_1 = 0$ and get a solution of t_1, call it t_{10},

$$
\begin{aligned}
t_{10} = (&-2k^2m + 2kmp - m^2p + 8k^2s - 12kps + 4p^2s + 8k^2t_2 \\
&- 12kpt + mpt + 4p^2t)/(8k^2 - 12kp + mp + 4p^2). \quad \text{(B.3)}
\end{aligned}
$$

Also solve $\partial G(p/k)/\partial t_2 = 0$ and get another expression for t_{10},

$$
\begin{aligned}
t_{10} = (&10k^2m - 14kmp + m^2p + 4mp^2 + 8k^2s - 12kps + 4p^2s + 8k^2t_2 \\
&- 12kpt_2 + mpt_2 + 4p^2t_2)/(8k^2 - 12kp + mp + 4p^2). \quad \text{(B.4)}
\end{aligned}
$$

Setting the difference of $(B.3)$ and $(B.4)$ to zero gives

$$
2m[(2(k-p)(3k-p) + mp] = 0.
$$

Obviously, this is impossible since $k > p$. Therefore, there are no solutions to the equations $\partial G(p/k)/\partial t_1 = 0$ and $\partial G(p/k)/\partial t_2 = 0$. The maximum value must be on the boundaries.

Now check the values of $G(p/k)$ on the boundary lines. This requires a bit of effort.

1a). $t_1 = 0$. Denote the value of $G(p/k)$ on it by G_1.

$$\begin{aligned} G_1 = G(p/k)|_{t_1=0} &= -\frac{1}{k^2}((k-p)(4(k-p)(2k-p)+mp)t_2^2 \\ &+2(k-p)(2m(5k-2p)(k-p)+4s(k-p)(2k-p)+m^2p)t_2 \\ &+2(2k-p)((2k^2-3kp+p^2-ps)m^2+s(2k^2-4kp+2p^2 \\ &-ps)m+2(k-p)^2s^2)) \end{aligned}$$

G_1 is a decreasing function with respect to t_2 because the coefficient of t_2^2 and the coefficient of t_2 are both less than zero. Therefore,

$$\begin{aligned} G_1 \leq G_1|_{t_2=0} &= -\frac{2(2k-p)}{k^2}((2k^2-3kp+p^2-ps)m^2 \\ &+s(2k^2-4kp+2p^2-ps)m+2(k-p)^2s^2) \end{aligned}$$

Since $s \leq k-p$ (keep in mind we relax the condition of s from $s < k-p$ to $s \leq k-p$ here) , $2k^2-3kp+p^2-ps \leq 2(k-p)^2 > 0$. If $2k^2-4kp+2p^2-ps > 0$, then $G_1 < 0$. If $2k^2-4kp+2p^2-ps < 0$, notice that when $t_1 = 0$, $w_2 = m-s-t_2 \geq 0$ and thus $m \geq s$, so for $p \leq \frac{4k}{5}$

$$\begin{aligned} &(2k^2-3kp+p^2-ps)m^2+s(2k^2-4kp+2p^2-ps)m \\ =\ & m((2k^2-3kp+p^2-ps)m+s(2k^2-4kp+2p^2-ps)) \\ \geq\ & m((2k^2-3kp+p^2-ps)s+s(2k^2-4kp+2p^2-ps)) \\ =\ & ms(4k^2-7kp+3p^2-2ps) \\ \geq\ & ms(4k-5p)(k-p) \geq 0 \end{aligned}$$

The last expression can be zero only if $s = k-p$ or $s = 0$. hen $s = k-p$, $2(k-p)^2s^2 > 0$. When $s = 0$, $m > s$. Therefore, we always have $G_1 \leq G_1|_{t_2=0} < 0$ when $p \leq 4k/5$.

1b). $t_2 = 0$. Denote the value of $G(p/k)$ on it by G_2.

$$\begin{aligned} G_2 &= -\frac{1}{k^2}(2(4k^3 - 8k^2p + 5kp^2 - p^3 + (k-p)pt_1 - 2kps + p^2s)m^2 \\ &\quad +(4k(k-p)^2t_1^2 + (k-p)pt_1 + 8k^3s - 20k^2ps + 16kp^2s \\ &\quad -4p^3s - 4kps^2 + 2p^2s^2)m + 4(k-p)^2(2k-p)(t_1-s)^2) \\ &\le -\frac{m}{k^2}(2(4k^3 - 8k^2p + 5kp^2 - p^3 + (k-p)pt_1 - 2kps + p^2s)m \\ &\quad 4k(k-p)^2t_1^2 + (k-p)pt_1 + 8k^3s - 20k^2ps + 16kp^2s \\ &\quad -4p^3s - 4kps^2 + 2p^2s^2) = G_{21} \end{aligned}$$

For G_{21}, if $m \ge s$, then $w_1 = m - s + t_1 \ge 0$ places no lower bound on t_1 and the achievable minimum value of t_1 is zero. We have

$$\begin{aligned} G_{21} &\le G_{21}|_{t_1=0} = -\frac{m}{k^2}(2(4k^3 - 8k^2p + 5kp^2 - p^3 - 2kps + p^2s)m \\ &\quad +8k^3s - 20k^2ps + 16kp^2s - 4p^3s - 4kps^2 + 2p^2s^2) \end{aligned}$$

since $s \le k - p$

$$4k^3 - 8k^2p + 5kp^2 - p^3 - 2kps + p^2s \ge 2(k-p)^2(2k-p) > 0$$

and

$$\begin{aligned} G_{21}|_{t_1=0} &\le -\frac{m}{k^2}(2(4k^3 - 8k^2p + 5kp^2 - p^3 - 2kps + p^2s)s \\ &\quad +8k^3s - 20k^2ps + 16kp^2s - 4p^3s - 4kps^2 + 2p^2s^2) \\ &= -\frac{2m(2k-p)s}{k^2}(4k^2 - 7kp + 3p^2 - 2ps) \\ &\le -\frac{2m(2k-p)s(4k-5p)(k-p)}{k^2}. \end{aligned}$$

It can be seen that $G_{21} \le 0$ if $p \le 4k/5$ and $m \ge s$. And $G_2 = G_{21}$ only if $t_1 = s$. However, when $t_1 = s = 0$, from $1a)$ $G_2 < 0$ for $p \le 4k/5$.

If $m < s$, then $w_1 \geq 0$ does restrict t_1 and the smallest achievable value of t_1 is $s - m$.

$$\begin{aligned} G_{21} &\leq -\frac{m}{k^2}(2(4k^3 - 8k^2p + 5kp^2 - p^3 + (k-p)p(s-m) - 2kps + p^2s)m \\ &\quad +4k(k-p)^2(s-m) + (k-p)p(s-m) + 8k^3s - 20k^2ps + 16kp^2s \\ &\quad -4p^3s - 4kps^2 + 2p^2s^2) \\ &= -\frac{m}{k^2}(m(-(k-p)pm + 2(2k^3 - 4k^2p + 3kp^2 - p^3 - 2kps + p^2s)) \\ &\quad +(3k-p)s(4(k-p)^2 - ps)). \end{aligned}$$

Since $m \leq p/2 - s$ by lemma (3.9), we have

$$\begin{aligned} G_{21} &\leq -\frac{m}{k^2}(m(-(k-p)p(p/2-s) + 2(2k^3 - 4k^2p + 3kp^2 - p^3 - 2kps + p^2s)) \\ &\quad +(3k-p)s(4(k-p)^2 - ps)) \\ &= -\frac{m}{k^2}(\frac{m}{2}(8k^3 - 16k^2p + 11kp^2 - 3p^3 - 6kps + 2p^2s) \\ &\quad +(3k-p)s(4(k-p)^2 - ps)) \\ &\leq -\frac{m}{k^2}(\frac{m}{2}(8k^3 - 16k^2p + 11kp^2 - 3p^3 - 6kp(k-p) + 2p^2(k-p)) \\ &\quad +(3k-p)(k-p)(4(k-p)^2 - p(k-p)) \\ &= -\frac{m}{k^2}(\frac{m}{2}(2k-p)(k-p)(4k-5p) + (3k-p)(k-p)^2(4k-5p)). \end{aligned}$$

It can be seen that if $m < s$ and $p \leq 4k/5$, $G_{21} \leq 0$. When $m < s$, $G_2 < G_{21} \leq 0$. In summary, G_2 will always be less than zero.

1c). $t_1 + t_2 = p - 2m$. Denote the value of $G(p/k)$ on this line by G_3. Substitute $t_2 = p - 2m - t_1$ to get an expression for G_3 as a quadratic function with respect to t_1. That is,

$$G_3 = -\frac{1}{k^2}(c_0 + c_1t_1 + c_2t_1^2)$$

where

$$c_2 = 4(k-p)(4(k-p)(2k-p) + mp) > 0.$$

Letting the solution of

$$\frac{\partial G_3}{\partial t_1} = 0$$

be t_{11}, then

$$\begin{aligned} t_{11} &= (-12k^2m + 8k^2p + 18kmp - 2m^2p - 12kp^2 - 5mp^2 + 4p^3 + 8k^2s \\ &\quad -12kps + 4p^2s)/(2(4(k-p)(2k-p) + mp)). \end{aligned}$$

Since $c_2 > 0$,

$$\begin{aligned} G_3 &\leq G_3|_{t_1=t_{11}} \\ &= -\frac{2m(2(k-p)(3k-p)+mp)L}{k^2[4(k-p)(2k-p)+mp]} \end{aligned}$$

where

$$\begin{aligned} L &= -12k^3m + 8k^3p + 32k^2mp - 2km^2p - 20k^2p^2 - 26kmp^2 + 2m^2p^2 \\ &\quad +16kp^3 + 6mp^3 - 4p^4 - 2kmps + mp^2s - 2kps^2 + p^2s^2. \end{aligned}$$

Need to show that $L > 0$ for $p \leq 4k/5$. It can be seen that L is a quadratic function with respect to m and its second order coefficient is $-2(k-p)p < 0$. So also check the values of L at $m = 0$ and $m = p/2 - s$.

$$\begin{aligned} L|_{m=0} &= (2k-p)p(2k-2p-s)(2k-2p+s) > 0 \\ L|_{m=p/2-s} &= \frac{1}{2}(4k^3p - 8k^2p^2 + 5kp^3 - p^4 + 24k^3s - 64k^2ps + 54kp^2s - 15p^3s \\ &\quad -4kps^2 + 4p^2s^2) \end{aligned}$$

$L|_{m=p/2-s}$ is a quadratic function with respect to s and its second order coefficient is $-4p(k-p) < 0$. Therefore, to show it is greater than zero, we need to show that it is greater than zero at $s = 0$ and $s = k - p$. In fact,

$$\begin{aligned} L|_{m=p/2-s,s=0} &= \frac{1}{2}(k-p)(2k-p)^2p > 0 \\ L|_{m=p/2-s,s=k-p} &= (k-p)^2(12k^2 - 20kp + 9p^2) = 3(4k-3p)(k-p) + kp > 0 \end{aligned}$$

1d). $t_2 = m - s + t_1$. Denote the value of $G(p/k)$ on this line by G_4.

$$\begin{aligned} G_4 &= -\frac{m}{k^2}(4(k-p)(6k^2 - 8kp + mp + 2p^2)t_1 + 36k^3m - 84k^2mp + 3km^2p \\ &+62kmp^2 - 3m^2p^2 - 14mp^3 - 12k^3s + 28k^2ps - 8kmps - 20kp^2s + 6mp^2s \\ &+4p^3s - 3kps^2 + p^2s^2). \end{aligned}$$

It can be seen that G_4 is an decreasing function with respect to t_1. If $m \geq s$ then the smallest value of t_1 is zero and we have shown in $1a$) that $G(p/k) < 0$ when $t_1 = 0$. If $m < s$ then the smallest value of t_1 is $s - m$ and $t_2 = 0$ when $t_1 = s - m$. We also have shown that $G(p/k) < 0$ when $t_2 = 0$. Therefore, $G_4 < 0$.

1e). $t_1 = 2m + s + t_2$. Denote the value of $G(p/k)$ on this line by G_5.

$$G_5 = -\frac{m}{k^2}(l_0t_2 + l_1m^2 + l_2m + l_3)$$

where

$$\begin{aligned} l_0 &= (4(k-p)(6k^2 - 8kp + 2p^2 + mp) > 0 \\ l_1 &= 8(k-p)p > 0 \\ l_2 &= 2((k-p)(24k^2 - 32kp + 9p^2) + (k-2p)ps) \\ l_3 &= (3k-p)s(4(k-p)^2 - ps) > (3k-p)s(4k-5p)(k-p) \geq 0. \end{aligned}$$

If $k \geq 2p$ then $l_2 > 0$ because $24k^2 - 32kp + 9p^2 = 3(8k-3p)(k-p) + kp > 0$ when $p \leq \frac{4k}{5}$. If $k < 2p$ then $l_2 > 2((k-p)(24k^2 - 32kp + 9p^2) + (k-2p)p(k-p)) = 2(24k - 7p)(k-p)^2 > 0$. Thus $G_5 < 0$ when $p \leq \frac{4k}{5}$.

Secondly, we check $G(z_{d*1})$. One may use Mathematica to get the expression of $G(z_{d*1})$. To make the expression simpler, we define $\delta = \sqrt{17 - 36\frac{p}{k} + 20\frac{p^2}{k^2}}$ and it can be seen that $0 < \delta < 1$ for $4/5 < p/k < 1$. Consider $G(z_{d*1})$ as a quadratic function of t_1 and t_2 and check,

$$\begin{aligned}
& \frac{\partial^2 G(z_{d*1})}{\partial t_1^2} = \frac{\partial^2 G(z_{d*1})}{\partial t_2^2} \\
= & -\frac{(k-2p+2\delta)(9k^2-18kp+8p^2+2mp+km(1-\delta)+6k\delta(k-p)+k^2\delta^2)}{2k^2} \\
= & -\frac{\partial^2 G(z_{d*1})}{\partial t_1 \partial t_2} = -\frac{\partial^2 G(z_{d*1})}{\partial t_2 \partial t_1}
\end{aligned}$$

To evaluate this expression we need to show $k - 2p + k\delta > 0$. The technique used to do this will be used repeatedly employed later to establish various inequalities involving k, p and δ. Substituting $\delta = \sqrt{17 - 36\frac{p}{k} + 20\frac{p^2}{k^2}}$ into $k - 2p + k\delta$ and setting $p = \alpha k$ gives $k - 2p + k\delta = k(1 - 2\alpha + \sqrt{17 - 36\alpha + 20\alpha^2})$. Plotting $1 - 2\alpha + \sqrt{17 - 36\alpha + 20\alpha^2}$ shows that it is always greater than zero for $\alpha \in (4/5, 1)$. It can be similarly shown that $9k^2 - 18kp + 8p^2 + 6k\delta(k - p) + k^2\delta^2 > 0$ for $p > 4/5k$.

Therefore, the Hessian matrix with respect to t_1 and t_2 for $G(z_{d^*1})$ is non-positive definite. Thus the function of $G(z_{d^*1})$ is concave with respect to t_1 and t_2. If there is a solution (t_1, t_2) to the equations $\partial G(z_{d^*1})/\partial t_1 = 0$ and $\partial G(z_{d^*1})/\partial t_2 = 0$, then the solution is the maximum value point; if we cannot find such a solution, the maximum value of $G(z_{d^*1})$ must be on the boundaries. Now we show that the solution does not exist.

Solve $\partial G(z_{d^*1})/\partial t_1 = 0$ and get a solution, call it t^*_{10},

$$\begin{aligned}
t^*_{10} = & (-3k^2m - km^2 + 4kmp - 2m^2p + 9k^2s - 18kps + 8p^2s + 9k^2t_2 + kmt_2 \\
& -18kpt_2 + 2mpt_2 + 8p^2t_2 - k^2m\delta + km^2\delta + 6k^2s\delta - 6kps\delta + 6k^2t_2\delta \\
& -kmt_2\delta - 6kpt_2\delta + k^2s\delta^2 + k^2t_2\delta^2)/(9k^2 + km - 18kp + 2mp + 8p^2 + 6k^2\delta \\
& -km\delta - 6kp\delta + k^2\delta^2).
\end{aligned}$$

Also solve $\partial G/\partial t_2 = 0$ and get another expression for t_{10}^*,

$$\begin{aligned} t_{10}^* &= (12k^2m + km^2 - 22kmp + 2m^2p + 8mp^2 + 9k^2s - 18kps + 8p^2s + 9k^2t_2 \\ &\quad +kmt_2 - 18kpt_2 + 2mpt_2 + 8p^2t_2 + 7k^2m\delta - km^2\delta - 6kmp\delta + 6k^2s\delta - 6kps\delta \\ &\quad +6k^2t_2\delta - kmt_2\delta - 6kpt_2\delta + k^2m\delta^2 + k^2s\delta^2 + k^2t_2\delta^2)/(9k^2 + km - 18kp \\ &\quad +2mp + 8p^2 + 6k^2\delta - km\delta - 6kp\delta + k^2\delta^2). \end{aligned}$$

Setting the numerators of the above equal, one gets

$$m(15k^2 - 26kp + 8p^2 + k^2\delta^2 + 2k\delta(4k - 3p) + 4mp + 2km(1 - \delta)) = 0.$$

One may verify using the technique described on the page 118 that $15k^2 - 26kp + 8p^2 + k^2\delta^2 + 2k\delta(4k - 3p) > 0$ for $p > 4k/5$. So the above equality is impossible and there are no solutions to the equations $\partial G(z_{d^*1})/\partial t_1 = 0$ and $\partial G(z_{d^*1})/\partial t_2 = 0$. The maximum value must be on the boundaries.

Now the truly tedious part begins. Check the values of $G(z_{d^*1})$ on the boundary lines.

2a). $t_1 = 0$. Denote the value of $G(z_{d^*1})$ on it by G_1^*.

$$\begin{aligned} G_1^* &= -\frac{1}{16k^2}(4(k - 2p + k\delta)(9k^2 + km - 18kp + 2mp + 8p^2 + 6k^2\delta - km\delta \\ &\quad -6kp\delta + k^2\delta^2)t_2^2 + 8(k - 2p + k\delta)((k + 2p - k\delta)m^2 + (3k - 4p \\ &\quad +k\delta)(4k - 2p + k\delta)m + s(3k - 4p + k\delta)(3k - 2p + k\delta))t_2 \\ &\quad +(3k - 2p + k\delta)L_r^*) \end{aligned}$$

where

$$\begin{aligned} L_r^* &= 4(5k^2 - 8kp + 4p^2 - 2ks - 4ps + 2k^2\delta - 4kp\delta + 2ks\delta + k^2\delta^2)m^2 \\ &\quad +4ms(3k^2 - 10kp + 8p^2 - 2ks - 4ps + 4k^2\delta - 6kp\delta + 2ks\delta + k^2\delta^2) \\ &\quad +4s^2(3k - 4p + k\delta)(k - 2p + k\delta) + km(1 - \delta)(3k - 4p \\ &\quad +k\delta)(5k - 2p + k\delta). \end{aligned}$$

One may verify that $3k - 4p + k\delta > 0$ for $p > 4k/5$ using the technique described on page 118. Therefore, the coefficient of t_2^2 (shown in the Hessian matrix) and the coefficient of t_2 in the expression of G_1^* are both less than zero. Thus we only need to show that $L_r^* > 0$.

Bound the coefficients of m^2 and m in the expression of L_r^* by setting $s = k - p$ as follows:

$$\begin{aligned} & 5k^2 - 8kp + 4p^2 - 2ks - 4ps + 2k^2\delta - 4kp\delta + 2ks\delta + k^2\delta^2 \\ > \ & (3k - 4p + k\delta)(k - 2p + k\delta) \end{aligned}$$

and

$$\begin{aligned} & 3k^2 - 10kp + 8p^2 - 2ks - 4ps + 4k^2\delta - 6kp\delta + 2ks\delta + k^2\delta^2 \\ > \ & -2(4p - 3k)(3k - 4p + k\delta) \\ = \ & -2(k - 2p + k\delta)(3k - 4p + k\delta) - 2(-4k + 6p - k\delta)(3k - 4p + k\delta). \end{aligned}$$

Therefore,

$$\begin{aligned} L_r^* \ > \ & 4(k - 2p + k\delta)(3k - 4p + k\delta)(m - s)^2 - 8ms(-4k + 6p \\ & -k\delta)(3k - 4p + k\delta) + km(1 - \delta)(3k - 4p + k\delta)(5k - 2p + k\delta). \end{aligned}$$

If $-4k + 6p - k\delta \leq 0$, $L_r^* > 0$. If $-4k + 6p - k\delta > 0$,

$$\begin{aligned} L_r^* \ > \ & m(-8(k - p)(-4k + 6p - k\delta)(3k - 4p + k\delta) \\ & +k(1 - \delta)(3k - 4p + k\delta)(5k - 2p + k\delta)) \\ = \ & 2m(3k - 4p + k\delta)(10k^2 - 23kp + 14p^2 + (2k - 3p)k\delta). \end{aligned}$$

Note that to get the last line above, one must replace $k^2\delta^2$ by $17k^2 - 36kp + 20p^2$. One may verify that $10k^2 - 23kp + 14p^2 + (2k - 3p)k\delta > 0$ using the technique described on page 118. Therefore, $L_r^* > 0$ and $G_1^* < 0$ for $p > 4k/5$.

2b). $t_2 = 0$. Denote the value of $G(z_{d^*1})$ on this line as G_2^*.

$$\begin{aligned} G_2^* \ = \ & -\frac{1}{16k^2}(c_1^* t_1^2 + c_2^* t_1 + c_3^*) \\ c_1^* \ = \ & 4(k - 2p + k\delta)(9k^2 - 18kp + 8p^2 + 6(k - p)k\delta + km(1 - \delta) + 2mp + k^2\delta^2) > 0. \end{aligned}$$

The maximum value of G_2^* is at some $t_1 = t_{11}^*$ if there is a solution $t_1 = t_{11}^*$ to $\partial G_2^*/\partial t_1 = 0$ when $0 \le t_1 \le p - 2m$ and $m - s + t_1 \ge 0$. Otherwise, the maximum value of G_2^* is on the boundary line $t_1 = 0$, $t_1 = p - 2m$, $t_1 = s - m$ or $t_1 = s + 2m$. Because sometimes, but not always, there is a proper solution t_1 to the equation $\partial G_2^*/\partial t_1 = 0$, we will consider all of these cases.

We have shown that if the maximum value is on the boundary line $t_1 = 0$, it must be less than zero. For $t_1 = p - 2m$, we will show this later in case $2c$.

For $t_1 = s - m$, we have $m < s$ since we have already disposed of $t_1 = 0$. We show the corresponding $G_2^* < 0$ next. Check

$$G_2^*|_{t_1=s-m} = -\frac{m}{16k^2}G_{21}^*$$

where

$$\begin{aligned} G_{21}^* &= 4(-k-2p+k\delta)(k-2p+k\delta)m^2 + 8m((-k-2p+k\delta)(3k-2p+k\delta)s \\ &\quad +9k^3 - 25k^2p + 28kp^2 - 12p^3 + 9k^3\delta - 24k^2p\delta + 16kp^2\delta + 5k^3\delta^2 \\ &\quad -7k^2p\delta^2 + k^3\delta^3) + (5k-2p+k\delta)(4(-k-2p+k\delta)s^2 + 4(3k-4p \\ &\quad +k\delta)(k-2p+k\delta)s + k(1-\delta)(3k-4p+k\delta)(3k-2p+k\delta). \end{aligned}$$

We need to show $G_{21}^* > 0$ for $m \in (0, s)$. It can be seen that it is a quadratic function with respect to m and the coefficient of m^2 is $4(-k-2p+k\delta)(k-2p+k\delta) < 0$. If $G_{21}^* \ge 0$ at $m = 0$ and $m = s$, then $G_{21}^* > 0$ for $m \in (0, s)$.

$$G_{21}^*|_{m=0} = (5k-2p+k\delta)G_{211}^*$$

where

$$\begin{aligned} G_{211}^* &= 4(-k-2p+k\delta)s^2 + 4(3k-4p+k\delta)(k-2p+k\delta)s \\ &\quad +k(1-\delta)(3k-4p+k\delta)(3k-2p+k\delta). \end{aligned}$$

Next we show that $G_{211}^* > 0$, which is a quadratic function with respect to s and the coefficient of s^2 is $4(-k-2p+k\delta) < 0$. So we need to check whether $G_{211}^* \ge 0$ holds at $s = 0$

and $s = k - p$.

$$\begin{aligned} G^*_{211}|_{s=0} &= k(1-\delta)(3k-4p+k\delta)(3k-2p+k\delta) > 0 \\ G^*_{211}|_{s=k-p} &= (k-2p+k\delta)(17k^2-36kp+20p^2-k^2\delta^2) = 0 \end{aligned}$$

This implies $G^*_{211} \geq 0$. Therefore, $G^*_{21}|_{m=0} \geq 0$.

When $m = s$, $t_1 = 0$. We have shown that in 2a) that the corresponding $G^*_1 < 0$.

For $t_1 = s + 2m$, we show the corresponding $G^*_2 < 0$ as below. Check

$$G^*_2|_{t_1=s+2m} = -\frac{m}{16k^2} G^*_{22}$$

where

$$\begin{aligned} G^*_{22} &= 4(-k-2p-k\delta)(5k-2p+k\delta)s^2 + 4(15k^3 - 56k^2p - 8kmp + 60kp^2 - 16mp^2 \\ &\quad -16p^3 + 23k^3\delta + 4k^2m\delta - 48k^2p\delta + 16kmp\delta + 20kp^2\delta + 9k^3\delta^2 \\ &\quad -4k^2m\delta^2 - 8k^2p\delta^2 + k^3\delta^3)s + 32(k+2p-k\delta)(k-2p+k\delta)m^2 \\ &\quad +4(63k^3 - 218k^2p + 236kp^2 - 72p^3 + 87k^3\delta - 192k^2p\delta + 92kp^2\delta \\ &\quad +37k^3\delta^3 - 38k^2p\delta^2 + 5k^3\delta^3)m + k(1-\delta)(3k-4p+k\delta)(3k-2p \\ &\quad +k\delta)(5k-2p+k\delta). \end{aligned}$$

Next we show that $G^*_{22} > 0$. And it can be seen that G^*_{22} is a quadratic function with respect to s and the coefficient of s^2 is $4(-k-2p-k\delta)(5k-2p+k\delta) < 0$. So we only need to show that $G^*_{22}|_{s=0} > 0$ and $G^*_{22}|_{s=k-p} > 0$. Check

$$\begin{aligned} G^*_{22}|_{s=0} &= 32(k+2p-k\delta)(k-2p+k\delta)m^2 + 4(63k^3 - 218k^2p + 236kp^2 \\ &\quad -72p^3 + 87k^3\delta - 192k^2p\delta + 92kp^2\delta + 37k^3\delta^2 - 38k^2p\delta^2 + 5k^3\delta^3)m \\ &\quad +k(1-\delta)(3k-4p+k\delta)(3k-2p+k\delta)(5k-2p+k\delta) > 0 \\ G^*_{22}|_{s=k-p} &= (k-2p+k\delta)(32(k+2p-k\delta)m^2 + 4(63k^2 - 100kp + 28p^2 + 28k^2\delta - 24kp\delta \\ &\quad +5k^2\delta^2)m + (5k-2p+k\delta)(17k^2-36kp+20p^2-k^2\delta^2)) > 0 \end{aligned}$$

Note that for the above deduction, we used the facts $17k^2 - 36kp + 20p^2 - k^2\delta^2 = 0$ and $63k^3 - 218k^2p + 236kp^2 - 72p^3 + 87k^3\delta - 192k^2p\delta + 92kp^2\delta + 37k^3\delta^3 - 38k^2p\delta^2 + 5k^3\delta^3 > 0$, and $63k^2 - 100kp + 28p^2 + 28k^2\delta - 24kp\delta + 5k^2\delta^2 > 0$, when $p > 4k/5$.

Case 2b) is completed if we can show that $G_2^* < 0$ when there is a solution $t_1 = t_{11}^*$ to $\partial G_2^*/\partial t_1 = 0$, satisfying $0 \le t_1 \le p - 2m$ and $m - s + t_1 \ge 0$.

Setting $\partial G_2^*/\partial t_1 = 0$ to get a solution t_{11}^* w.r.t. t_1,

$$\begin{aligned} t_{11}^* &= (-3k^2m - km^2 + 4mp - 2m^2p + 9k^2s - 18kps + 8p^2s - k^2m\delta + km^2\delta + 6k^2s\delta \\ &\quad -6kps\delta + k^2s\delta^2)/(9k^2 - 18kp + 8p^2 + 6(k-p)k\delta + km(1-\delta) + 2mp + k^2\delta^2). \end{aligned}$$

It can be seen that t_{11}^* may be negative. For $t_{11}^* \ge 0$, we need

$$s \ge \frac{3k^2m + km^2 - 4kmp + 2m^2p + k^2m\delta - km^2\delta}{9k^2 - 18kp + 8p^2 + 6k^2\delta - 6kp\delta + k^2\delta^2}.$$

Substituting t_{11}^* into G_2^*, we have

$$\begin{aligned} G_2^* &\le G_2^*|_{t_1 = t_{11}^*} \\ &= -\frac{m}{16k^2}(15k^2 + 2km - 26kp + 4mp + 8p^2 + 8k^2\delta - 2km\delta - 6kp\delta + k^2\delta^2)L_t^* \\ &\quad /(9k^2 - 18kp + 8p^2 + 6(k-p)k\delta + km(1-\delta) + 2mp + k^2\delta^2) \end{aligned}$$

where

$$\begin{aligned} L_t^* &= 27k^4 + 33k^3m - 2k^2m^2 - 72k^3p - 84k^2mp + 60k^2p^2 + 84kmp^2 + 8m^2p^2 \\ &\quad -16kp^3 - 32mp^3 + 36k^3s - 12k^2ms - 144k^2ps - 16kmps + 176kp^2s \\ &\quad +16mp^2s - 64p^3s - 12k^2s^2 - 16kps^2 + 16p^2s^2 + 29k^3m\delta + 24k^3p\delta \\ &\quad -72k^2mp\delta - 8km^2p\delta - 40k^2p^2\delta + 44kmp^2\delta + 16kp^3\delta + 60k^3s\delta + 8k^2ms\delta \\ &\quad +80kp^2s - 144k^2ps\delta - 16kmps\delta + 80kp^2s\delta + 8k^2s^2\delta - 16kps^2\delta - 18k^4\delta^2 \\ &\quad +15k^3m\delta^2 + 2k^2m^2\delta^2 + 40k^3p\delta^2 - 20k^2mp\delta^2 - 20k^2p^2\delta^2 + 28k^3s\delta^2 + 4k^2ms\delta^2 \\ &\quad -32k^2ps\delta^2 + 4k^2s^2\delta^2 - 8k^4\delta^3 + 3k^3m\delta^3 + 8k^3p\delta^3 + 4k^3s\delta^3 - k^4\delta^4. \end{aligned}$$

Since the other factors above, other than $-m/(16k^2)$, are positive, the problem now becomes to show that $L_t^* > 0$ given the conditions:

$$\begin{aligned} s &\geq f(m) = \frac{3k^2m + km^2 - 4kmp + 2m^2p + k^2m\delta - km^2\delta}{9k^2 - 18kp + 8p^2 + 6k^2\delta - 6kp\delta + k^2\delta^2} \\ m + s &\leq \frac{p}{2} \\ s &\leq k - p \\ m &> 0 \end{aligned}$$

We note that $f(m) > 0$ for $p/k \in (4/5, 1)$. The Figures B.3 and B.7 illustrated two possible situations. The range of s and m is defined by the area whose four vertices are $(0,0)$, $(0, k-p)$, $(m_1, k-p)$ or $(m_2, k-p)$, and (m_3, s_3). Here m_1 is the solution to $k - p = p/2 - m$, i.e., $m_1 = 3p/2 - k$; m_2 is the solution to $f(m) = k - p$; m_3 is the solution to $f(m) = p/2 - m$; and $s_3 = f(m_3)$. The two possibilities for the third coordinate correspond to $m_3 \geq m_1$ and $m_3 < m_1$, respectively (see Figure B.3 and B.7). Since $f(m) \geq 0$, m_3 cannot exceed $p/2$.

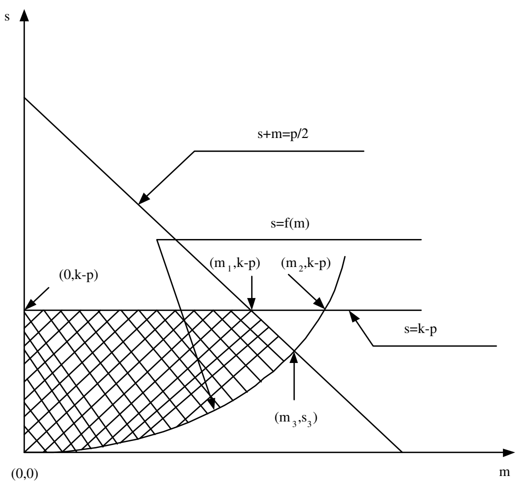

Figure B.3: Range of s and m under situation 1 for G_2^*

Situation 1: $m_3 \geq m_1$. One can obtain

$$\begin{aligned} m_3 &= (((24k^2 - 44kp + 16p^2 + 14k^2\delta - 12kp\delta + 2k^2\delta^2)^2 - 4(2k + 4p - 2k\delta)(-9k^2p \\ &\quad +18kp^2 - 8p^3 - 6k^2p\delta + 6kp^2\delta - k^2p\delta^2))^{1/2} - 24k^2 + 44kp - 16p^2 - 14k^2\delta \\ &\quad +12kp\delta - 2k^2\delta^2)/(2(2k + 4p - 2k\delta)). \end{aligned}$$

We need to find the appropriate range for k and p to satisfy $m_3 \geq m_1$. Let $\alpha = p/k$, substitute it into m_3 and m_1, then use Mathematica to solve the inequality of $m_3 \geq m_1$ in $\alpha \in (4/5, 1)$. We get $\alpha \in (4/5, 0.8276)$ approximately (the true right endpoint is a bit smaller).

Now take L_t^* as a quadratic function with respect to s and its second order term coefficient is $4(-k-2p+k\delta)(3k-2p+k\delta) < 0$. To show $L_t^* > 0$, we only need to verify that $L_t^*|_{s=k-p} > 0$ for $0 < m \leq m_1$, $L_t^*|_{s=p/2-m} > 0$ for $m_1 \leq m \leq m_3$ and $L_t^*|_{s=f(m)} > 0$ for $0 < m \leq m_3$.

First check $L_t^*|_{s=k-p}$,

$$L_t^*|_{s=k-p} = (k - 2p + k\delta)L_{t1}^*$$

where

$$\begin{aligned} L_{t1}^* &= m(2(-k - 2p + k\delta)m + (3k - 4p + k\delta)(7k - 6p + 3k\delta)) \\ &\geq m(2(-k - 2p + k\delta)m_1 + (3k - 4p + k\delta)(7k - 6p + 3k\delta)). \end{aligned}$$

Substitute $m_1 = 3/2p - k$ into the above expression and let $\alpha = p/k$, one may verify that $2(-k - 2p + k\delta)m_1 + (3k - 4p + k\delta)(7k - 6p + 3k\delta) = k^2 f_1(\alpha) > 0$ for $\alpha \in (4/5, 0.8276)$, where $f_1(\alpha) = 74 - 153\alpha + 78\alpha^2 + (14 - 15\alpha)\sqrt{17 - 36\alpha + 20\alpha^2} > 0$, if $\alpha \in (4/5, 0.8276)$. Figure B.4 is a plot for $f_1(\alpha)$ showing $\alpha = (109 + \sqrt{89})/132$ is the only root of $f_1(\alpha)$ for $\alpha \in (4/5, 1)$. Next check $L_t^*|_{s=p/2-m}$,

$$\begin{aligned} L_t^*|_{s=p/2-m} &= 2(k - 2p + k\delta)(-k - 2p + k\delta)m^2 + (-3k^3 + 66k^2p - 84kp^2 + 24p^3 \\ &\quad -31k^3\delta + 68k^2p\delta - 28kp^2\delta - 13k^3\delta^2 + 10k^2p\delta^2 - k^3\delta^3)m - (3k - 2p \\ &\quad +k\delta)(-9k^3 + 12k^2p + 13kp^2 - 14p^3 + 3k^3\delta - 20k^2p\delta + 19kp^2\delta + 5k^3\delta^2 \\ &\quad -8k^2p\delta^2 + k^3\delta^3). \end{aligned}$$

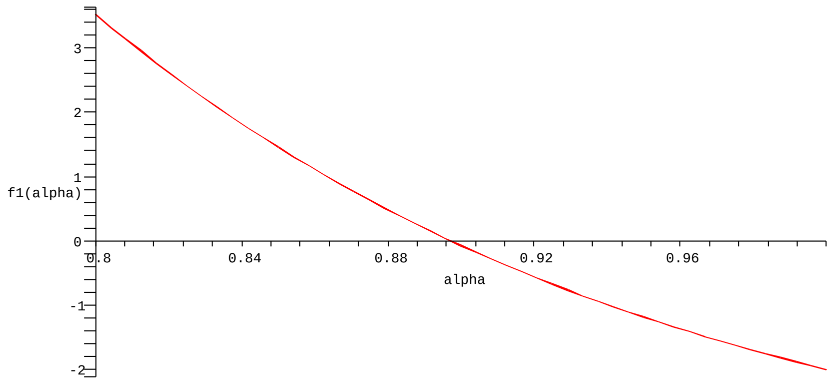

Figure B.4: Plot of $f_1(\alpha)$

This is a quadratic function with respect to m, so check its value at the two end points

$$\begin{aligned} L_t^*|_{s=p/2-m,m=3p/2-k} &= \frac{1}{2}(k-2p+k\delta)L_{t2}^* \\ L_{t2}^* &= 56k^3-125k^2p+93kp^2-26p^3+6k^3\delta-5kp^2\delta-12k^3\delta^2 \\ &\quad +13k^2p\delta^2-2k^3\delta^3 \end{aligned}$$

Substituting $p=\alpha k$ into L_{t2}^* yields $L_{t2}^*=k^3f_2(\alpha)>0$ if $\alpha\in(4/5,0.8276)$.

At $m=m_3$ the expression of $L_t^*|_{s=p/2-m}$ is messy so is omitted. It can be verified that $L_t^*|_{s=p/2-m,m=m_3}=k^4(3k-2p+k\delta)f_3(\alpha)/(2(k+2p-k\delta))$, where $f_3(\alpha)>0$ if $\alpha\in(4/5,0.8276)$. We omit the expression of $f_3(\alpha)$ since it is too long to write. The plot of this function is in Figure B.5, showing that $\alpha\approx 0.8368$ is an approximate, single root of $f_3(\alpha)$ when $\alpha\in(4/5,1)$. At last we check $L_t^*|_{s=f(m)}$.

$$\begin{aligned} L_t^*|_{s=f(m)} &= \frac{(9k^2-18kp+8p^2+k^2\delta^2+km(1-\delta)+6k(k-p)\delta+2mp)L_{t3}^*}{(3k-4p+k\delta)^2(3k-2p+k\delta)} \\ L_{t3}^* &= mL_{t4}^*+k(1-\delta)(3k-4p+k\delta)^2(3k-2p+k\delta)^2 \\ L_{t4}^* &= -4(k+2p-k\delta)^2m^2-8k(3k-4p+k\delta)(k+2p-k\delta)m+2(3k-4p \\ &\quad +k\delta)^2(7k^2-12kp+4p^2+6k^2\delta-4kp\delta+k^2\delta^2). \end{aligned}$$

We need to show that $L_{t3}^*>0$ for $0<m<m_3$ and $\alpha\in(4/5,0.8276)$. If $L_{t4}^*>0$, then

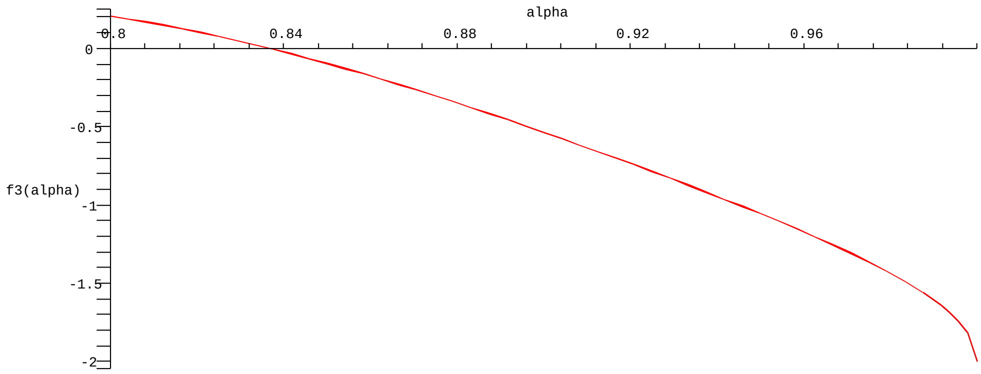

Figure B.5: Plot of $f_3(\alpha)$

$L^*_{t3} > 0$. If $L^*_{t4} < 0$, then

$$\begin{aligned} L^*_{t3} &> pL^*_{t4}/2 + k(1-\delta)(3k-4p+k\delta)^2(3k-2p+k\delta)^2 \\ &= -2p(k+2p-k\delta)^2m^2 - 4kp(3k-4p+k\delta)(k+2p-k\delta)m + p(3k-4p \\ &\quad +k\delta)^2(7k^2-12kp+4p^2+6k^2\delta-4kp\delta+k^2\delta^2) + k(1-\delta)(3k-4p \\ &\quad +k\delta)^2(3k-2p+k\delta)^2. \end{aligned}$$

The last expression is a quadratic function of m and the coefficient of m^2 is less than zero. To show this expression is always greater than zero, we only need to verify that it is greater than zero at $m = 0$ and $m = m_3$. It is easy to see that at $m = 0$, its value is

$$\begin{aligned} & p(3k-4p+k\delta)^2(7k^2-12kp+4p^2+6k^2\delta-4kp\delta+k^2\delta^2) \\ & +k(1-\delta)(3k-4p+k\delta)^2(3k-2p+k\delta)^2 \\ = \; & p(3k-4p+k\delta)^2(24(k-p)^2+2k\delta(3k-2p)) + k(1-\delta)(3k-4p \\ & +k\delta)^2(3k-2p+k\delta)^2 > 0. \end{aligned} \tag{B.5}$$

For $m = m_3$, the expression becomes messy. One may check that its value can be expressed as $(3k - 4p + k\delta)f_4(\alpha)$, though we omit the expression for $f_4(\alpha)$. The easiest way to verify $f_4(\alpha)$ is greater than zero for $\alpha \in (4/5, 0.8276)$ is to plot over $\alpha \in (4/5, 1)$. It can be seen in Figure B.6 that approximately $\alpha \approx 0.8314$ is the single root of $f_4(\alpha)$ when $\alpha \in (4/5, 1)$.

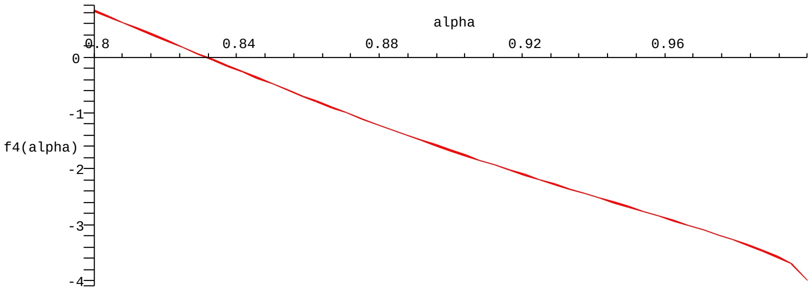

Figure B.6: Plot of $f_4(\alpha)$

Situation 2: $m_3 < m_1$. From the discussion in situation 1, we investigate $\alpha \in (0.8275, 1)$.

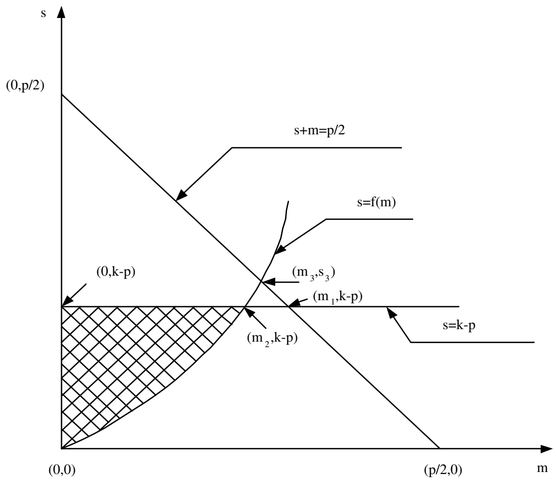

Figure B.7: Range of s and m under Situation 2 for G_2^*

One can obtain

$$\begin{aligned} m_2 \;=\; & (((-3k^2 + 4kp - k^2\delta)^2 + 4(k + 2p - k\delta)(9k^3 - 27k^2p + 26kp^2 - 8p^3 + 6k^3\delta \\ & -12k^2p\delta + 6kp^2\delta + k^3\delta^2 - k^2p\delta^2))^{1/2} - (3k^2 - 4kp + k^2\delta))/(2(k + 2p - k\delta)). \end{aligned}$$

Now taking L_t^* as a quadratic function with respect to s, its second order coefficient is $4(-k-2p+k\delta)(3k-2p+k\delta) < 0$. To show $L_t^* > 0$, we only need verify that $L_t^*|_{s=k-p} > 0$ and $L_t^*|_{s=f(m)} > 0$ for $0 < m < m_2$. Following the similar discussion in situation 1, we only need to verify that $L_{t1}^* > 0$ to show that $L_t^*|_{s=k-p} > 0$.

$$\begin{aligned} L_{t1}^* &= m(2(-k-2p+k\delta)m + (3k-4p+k\delta)(7k-6p+3k\delta)) \\ &\geq m(2(-k-2p+k\delta)m_2 + (3k-4p+k\delta)(7k-6p+3k\delta)). \end{aligned}$$

Substituting the expression m_2 and $p = \alpha k$ into $2(-k-2p+k\delta)m_2 + (3k-4p+k\delta)(7k-6p+3k\delta)$, one gets a function $k^2 f_5(\alpha)$. We omit the expression of $f_5(\alpha)$ here since it is too long to write. The plot in Figure B.8 shows that it is greater than zero for any $\alpha \in (4/5, 1)$.

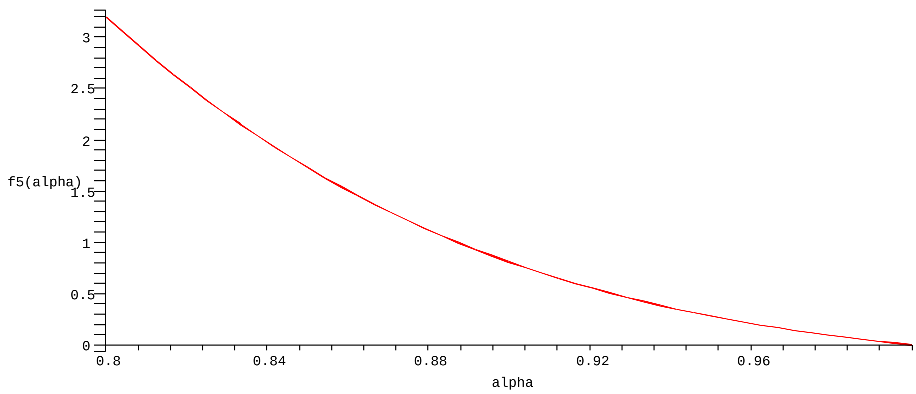

Figure B.8: Plot of $f_5(\alpha)$

To show $L_t^*|_{s=f(m)} > 0$, we need to verify that $L_{t3}^* > 0$ for $0 < m \leq m_2$ and $\alpha \in (0.8275, 1)$. If $L_{t4}^* > 0$, then $L_{t3}^* > 0$. If $L_{t4}^* < 0$, then

$$\begin{aligned} L_{t3}^* &> m_2 L_{t4}^* + k(1-\delta)(3k-4p+k\delta)^2(3k-2p+k\delta)^2 \\ &= m_2(-4(k+2p-k\delta)^2 m^2 - 8k(3k-4p+k\delta)(k+2p-k\delta)m + 2(3k-4p \\ &\quad +k\delta)^2(7k^2-12kp+4p^2+6k^2\delta-4kp\delta+k^2\delta^2)) + k(1-\delta)(3k-4p \\ &\quad +k\delta)^2(3k-2p+k\delta)^2. \end{aligned}$$

The last expression is a quadratic function of m and the coefficient of m^2 is less than zero. To show this expression is always greater than zero, we only need to verify that it is greater than zero at $m = 0$ and $m = m_2$. It is easy to see that at $m = 0$, its value is greater than zero as shown in (B.5). For $m = m_2$, the expression becomes messy. One may check that it can be expressed as $32(1-\alpha)^2 k^6 f_6(\alpha)/(k + 2p - k\delta)$ for another messy function of $f_6(\alpha)$. It can be seen that $f_6(\alpha) > 0$ for $\alpha \in (4/5, 1)$ in Figure B.9. The only root of $f_6(\alpha)$ in this interval is at $\alpha = 1$.

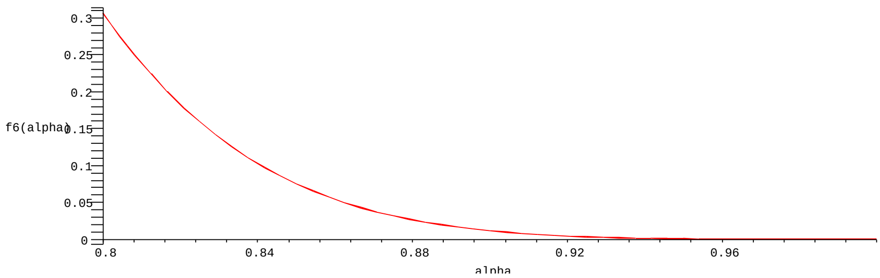

Figure B.9: Plot of $f_6(\alpha)$

2c) $t_1 + t_2 = p - 2m$. Simply substitute $t_2 = p - 2m - t_1$ into $G(z_{d^*1})$ and denote it as G_3^*.

$$G_3^* = -\frac{1}{16k^2}(c_1 t_1^2 + c_2 t_1 + c_3)$$

where

$$\begin{aligned} c_1 &= 16(k - 2p + k\delta)[9k^2 + km - 18kp + 2mp + 8p^2 + 6k^2\delta - km\delta \\ &\quad -6kp\delta + k^2\delta^2] > 0. \end{aligned}$$

Solve the equation $\partial G_3^*/\partial t_1 = 0$ and get solution t_{12}^*,

$$\begin{aligned} t_{12}^* &= (-27k^2m - 4km^2 + 18k^2p + 56kmp - 8m^2p - 36kp^2 - 20mp^2 + 16p^3 \\ &\quad +18k^2s - 36kps + 16p^2s - 18k^2m\delta + 4km^2\delta + 12k^2p\delta + 16kmp\delta \\ &\quad -12kp^2\delta + 12k^2s\delta - 12kps\delta - 3k^2m\delta^2 + 2k^2p\delta^2 + 2k^2s\delta^2) \\ &\quad /(4(9k^2 + km - 18kp + 2mp + 8p^2 + 6k^2\delta - km\delta - 6kp\delta + k^2\delta^2)). \end{aligned}$$

Substituting t_{12}^* into G_3^* and get a lower bound,

$$\begin{aligned} G_3^* &\leq \frac{1}{16k^2}(m(15k^2+2km-26kp+4mp+8p^2+8k^2\delta-2km\delta-6kp\delta \\ &\quad +k^2\delta^2)L_p^*))/(9k^2+km-18kp+2mp+8p^2+6k^2\delta-km\delta-6kp\delta+k^2\delta) \end{aligned}$$

where

$$\begin{aligned} L_p^* &= 8(k+2p-k\delta)(k-2p+k\delta)m^2+2(21k^3-112k^2p+148kp^2-48p^3 \\ &\quad +6k^2s+8kps-8p^2s+8kps\delta+49k^3\delta-120k^2p\delta+60kp^2\delta-4k^2s\delta \\ &\quad +23k^3\delta^2-24k^2p\delta^2-2k^2s\delta^2+3k^3\delta^3)m-(k+2p-k\delta)(3k-2p \\ &\quad +k\delta)(3k-4p-2s+k\delta)(3k-4p+2s+k\delta). \end{aligned}$$

Need to show that $L_p^* < 0$. Since it is a quadratic function with respect to m and the coefficient of the second order term is greater than zero, we only need to check the values of L_p^* at $m = 0$ and $m = p/2 - s$. If the values at the two endpoints are both less than zero, then $L_p^* < 0$. Check

$$\begin{aligned} L_p^*|_{m=0} &= -(k+2p-k\delta)(3k-2p+k\delta)(3k-4p-2s+k\delta)(3k-4p+2s+k\delta) \\ &< -(k+2p-k\delta)(3k-2p+k\delta)(k-2p+k\delta)(5k-6p+k\delta) < 0 \end{aligned}$$

and

$$\begin{aligned} L_p^*|_{m=p/2-s} &= 8(k+2p-k\delta)(k-2p+k\delta)s^2-2(21k^3-111k^2p+144kp^2 \\ &\quad -60p^3+49k^3\delta-118k^2p\delta+72kp^2\delta+23k^3\delta^3-27k^2p\delta^2+3k^3\delta^3)s \\ &\quad -(3k-2p+k\delta)(9k^3-13k^2p+4p^3-3k^3\delta+14k^2p\delta-12kp^2\delta \\ &\quad -5k^3\delta^2+7k^2p\delta^2-k^3\delta^3). \end{aligned}$$

Since this is a quadratic function with respect to s and its second order coefficient is positive, we can show it is less than zero if it is less than zero at $s = 0$ and $s = k - p$. Check

$$\begin{aligned}
L_p^*|_{m=p/2-s,s=0} &= -(3k-2p+k\delta)(9k^3-13k^2p+4p^3-3k^3\delta+14k^2p\delta-12kp^2\delta \\
&\quad -5k^3\delta^2+7k^2p\delta^2-k^3\delta^3)<0 \\
L_p^*|_{m=p/2-s,s=k-p} &= -(k-2p+k\delta)(61k^3-183k^2p+194kp^2-72p^3+37k^3\delta-74k^2p\delta \\
&\quad +38kp^2\delta-k^3\delta^2+k^2p\delta^2-k^3\delta^3)<0.
\end{aligned}$$

One may use the technique described on page 118 to verify that for $p > 4k/5$, $9k^3 - 13k^2p + 4p^3 - 3k^3\delta + 14k^2p\delta - 12kp^2\delta - 5k^3\delta^2 + 7k^2p\delta^2 - k^3\delta^3 > 0$, and $61k^3 - 183k^2p + 194kp^2 - 72p^3 + 37k^3\delta - 74k^2p\delta + 38kp^2\delta - k^3\delta^2 + k^2p\delta^2 - k^3\delta^3 > 0$.

2d) $m - s - t_2 + t_1 = 0$. The value of $G(z_{d^*1})$ on this boundary, call it G_4^*, is a linear function with respect to t_1, and the coefficient of t_1 is $-\frac{m}{2k^2}(k - 2p + k\delta)(15k^2 + 2km - 26kp + 4mp + 8p^2 + 8k^2\delta - 2km\delta - 6kp\delta + k^2\delta^2) < 0$. Therefore, G_4^* is a decreasing function with respect to t_1. If $m \geq s$, Its maximum value is at $t_1 = 0$ and we have already shown that for $t_1 = 0$, $G(z_{d^*1}) < 0$. If $m < s$, its maximum value is at $t_1 = s - m$ (i.e. $t_2 = 0$) and we have shown that for $t_2 = 0$, $G(z_{d^*1}) < 0$.

2e) Now check the value on $s + 2m + t_2 - t_1 = 0$, i.e., $t_1 = s + 2m + t_2$. One can get that this value of $G(z_{d^*1})$, call it G_5^*, is a linear function with respect to t_2. Because the linear coefficient is the same as that of t_1 in 2d), G_5^* is decreasing in t_2, so its maximum value is at $t_2 = 0$. And we have already shown that the value of $G(z_{d^*1})$ at $t_2 = 0$ is always greater than zero. □

Appendix C

A Matlab Program for Searching E-optimal Block Designs in $M(v, 3, k)$ when $k < 2v/3$

```
% This is a program for Searching E-optimal Block Designs
% in $M(v,3,k)$ when $k<2v/3$;
% for given v,  k is an integer between (v+2)/3 and 2v/3;
fid=fopen('b3sup.doc','w'); for v=4:100;
    for k=ceil((v+2)/3):ceil(2*v/3)-1;
        fprintf(fid,'v is %5d, k is %5d\n',v,k);
        number=0;
        Eopt=10^-12;
        Aopt=10^6;
        dopt=10^6;
        error=10^-12;
        Avalue=[];
        dvalue=[];
```

```
        Evalue=[];
        ta=[];
        sa1=[];
        sa2=[];
        sa3=[];
        xa=[];
        ya=[];
        za=[];
        i=0;
        for t=0:floor((3*k-v)/2);
            for s1=0:floor((3*k-v-2*t)/3);
                for s2=s1:floor((3*k-v-2*t-s1)/2);
                    s3=3*k-v-2*t-s1-s2;
                    x=k-t-s1-s2;
                    y=k-t-s1-s3;
                    z=k-t-s2-s3;
% some judgements whether a design is connected or not;
                    if (x<0 | y<0 |z<0 )
                        continue;
                    end;
                    if (x==k | y==k |z==k)
                        continue;
                    end;
                    i=i+1;
                    number=number+1;
                    ta(i)=t;
                    sa1(i)=s1;
                    sa2(i)=s2;
```

```
                    sa3(i)=s3;
                    xa(i)=x;
                    ya(i)=y;
                    za(i)=z;
% reduced information matrix;
                    cd=[3-3*t/k -2*s1/k -2*s2/k -2*s3/k -x/k -y/k -z/k;
                     -2*t/k 2-2*s1/k -s2/k -s3/k -x/k -y/k 0;
                     -2*t/k -s1/k 2-2*s2/k -s3/k -x/k 0 -z/k;
                     -2*t/k -s1/k -s2/k 2-2*s3/k 0 -y/k -z/k;
                        -t/k -s1/k -s2/k 0 1-x/k 0 0;
                        -t/k -s1/k 0 -s3/k 0 1-y/k 0;
                         -t/k 0 -s2/k -s3/k 0 0 1-z/k];
                    tn=t-1;
                    sn1=s1-1;
                    sn2=s2-1;
                    sn3=s3-1;
                    xn=x-1;
                    yn=y-1;
                    zn=z-1;
                    if(t==0)
                        tn=0;
                    end;
                    if(s1==0)
                      sn1=0;
                    end;
                    if(s2==0)
                        sn2=0;
                    end;
```

```
                    if(s3==0)
                        sn3=0;
                    end;
                    if(x==0)
                        xn=0;
                    end;
                    if(y==0)
                        yn=0;
                    end;
                    if(z==0)
                        zn=0;
                    end;

%find positive eigenvalues of reduced information matrix;
                    cdeig=eig(cd);
                    cdeig=cdeig(find(cdeig>error));
                    Evalue(i)=min(cdeig);
                    if (Evalue(i)-Eopt)>error
                        Eopt=Evalue(i);
                    end;
                end;
            end;
        end;
        fprintf(fid,'the number of designs compared is %5d\n',number);

%find E-optimal designs;
        num3=0;
        for j=1:number;
```

```
            temp=Evalue(j);
            if (abs(temp-Eopt)<error)
                num3=num3+1;
                fprintf(fid,'Eopt value is %12.5f\n', temp);
                fprintf(fid, 'te = %3d,se1= %3d, se2 = %3d,se3 = %3d,
                xe = %3d,ye= %3d, ze = %3d\n\n',...
                ta(j), sa1(j),sa2(j),sa3(j),
                xa(j),ya(j),za(j));
            end;
        end;
        if(num3>1)
            fprintf(fid, 'total number of E-optimal design ...
            is %5d\n\n', num3);
        end;
    end;
end; fclose(fid); fprintf('calculations completed');
```

Appendix D

A Matlab Program for E-optimality Problem in $D(v, 3, k)$ when $k > 2v/3$ Using Average Matrix Technique

```
% This is a program for E-optimality Problem
% in $D(v,3,k)$ when $k>2v/3$ Using Average Matrix Technique;
% for given v,  k is an integer between 2v/3 and v-1;
fid=fopen('averageresult.doc','w'); for v=4:80;
    for k=(floor(2*v/3)+1):(v-1);
eopt=3-v/k; p=3*(v-k); num=0; error=10^-8; for s1=0:p;
    for s2=0:(p-s1);
        for s3=0:(p-s1-s2);
            for s4=0:(p-s1-s2-s3);
                for s5=0:(p-s1-s2-s3-s4);
                    s6=p-s1-s2-s3-s4-s5;
                    w1=k-s1-s2-2*s4;
                    w2=k-s1-s3-2*s5;
```

```
                    w3=k-s2-s3-2*s6;
% some judgements whether a design is connected or not;
                    if ((s1+s2+2*s4>k)|(s1+s3+2*s5>k)|(s2+s3+2*s6>k))
                        continue;
                    end;
                    if (2*s4==k|2*s5==k|2*s6==k)
                        continue;
                    end;
                    if (s1==k|s2==k|s3==k)
                        continue;
                    end;
                    if (w1==0) & (w2==0) & (s1+2*s4==k) & (s1+2*s5==k)
                        continue;
                    end;

                    if (w1==0) & (w3==0) & (s2+2*s4==k) & (s2+2*s6==k)
                        continue;
                    end;

                    if (w2==0) & (w3==0) & (s3+2*s5==k) & (s3+2*s6==k)
                        continue;
                    end;

% get the reduced average matrix;
                    cd17=-(2-2*s1/k-s2/k-s3/k-2*s4/k-2*s5/k);
                    cd71=cd17*s1/(3*k-2*v);
                    cd27=-(2-2*s2/k-s1/k-s3/k-2*s4/k-2*s6/k);
                    cd72=cd27*s2/(3*k-2*v);
```

```
                    cd37=-(2-2*s3/k-s1/k-s2/k-2*s5/k-2*s6/k);
                    cd73=cd37*s3/(3*k-2*v);
                    cd47=-(2-4*s4/k-2*s1/k-2*s2/k);
                    cd74=cd47*s4/(3*k-2*v);
                    cd57=-(2-4*s5/k-2*s1/k-2*s3/k);
                    cd75=cd57*s5/(3*k-2*v);
                    cd67=-(2-4*s6/k-2*s2/k-2*s3/k);
                    cd76=cd67*s6/(3*k-2*v);
                    cd77=-(cd71+cd72+cd73+cd74+cd75+cd76);
                    if (cd17>0|cd27>0|cd37>0|cd47>0|cd57>0|cd67>0|cd77<0)
                        continue;
                    end;
                    cd=[2-2*s1/k -s2/k -s3/k -2*s4/k -2*s5/k 0 cd17;
                        -s1/k 2-2*s2/k -s3/k -2*s4/k 0 -2*s6/k cd27;
                        -s1/k -s2/k 2-2*s3/k 0 -2*s5/k -2*s6/k cd37;
                        -2*s1/k -2*s2/k 0 2-4*s4/k 0 0 cd47;
                        -2*s1/k 0 -2*s3/k 0 2-4*s5/k 0 cd57;
                        0 -2*s2/k -2*s3/k 0 0 2-4*s6/k cd67;
                        cd71 cd72 cd73 cd74 cd75 cd76 cd77];
% get the positive eigenvalues of reduced average matrix
% and the smallest one;
                    cdeig=eig(cd);
                    cdeig=cdeig(find(cdeig>error));
                    evalue=min(cdeig);
% check whether the average matrix technique works or not;
                    if (evalue-eopt)>error
                        num=num+1;
                        fprintf(fid,'v=%5d, k=%5d,
```

```
                        average technique failed\n', v, k);
                        fprintf(fid,'evalue=%12.5f,
                        eopt=%12.5f\n',evalue,eopt);
                        fprintf(fid, 's1=%3d,s2=%3d,s3=%3d,
                        s4=%3d,s5=%3d,s6=%3d\n',s1,s2,s3,s4,s5,s6);
                    end;
                end;
            end;
        end;
    end;
end;

if (num==0)
    fprintf(fid,'v=%d, k=%5d, average technique eliminated
    all other designs\n', v, k);
end;

end; end;

fclose(fid); fprintf('calculations completed');
```

Appendix E

A Matlab Program Comparing d^* to d_0 in Terms of ϕ_β-criterion for $k/v > 5/6$ in $D(v, 2, k)$

```
% This is a program to compare design d* and design d0 in terms of phi_p;
% for given v, the range of k is from 5v/6 to v-1;

fid=fopen('phi.doc','W'); for v=4:100;
    for k=floor(5*v/6)+1:v-1;
% find root such that \phi_p(C_{d*})=\phi_p(C_{d0});
        x=fzero(@phpd,10);
        fprintf(fid, '%5.0f %5.0f %10.5f \n', v, k, x);
    end;
end;

fclose(fid); fprintf('calculation completed');
```

```
%Define a function y=\phi_p(C_{d*})-\phi_p(C_{d0});
function y=phpd(x) v=evalin('base','v'); k=evalin('base','k');
y1=(2*k-2+2.^(-x).*(2*k-v-1)-2.*(2*k-v)+((2*k-v)/k).^(-x)...
+(v/k).^(-x)).^(1./x);
y2=(2*k-1+2.^(-x).*(2*k-v-2)-2*(2*k-v)+2.^x.*((k-sqrt(17*k^2...
-36*k*(2*k-v)+20*(2*k-v)^2)+2*(2*k-v))/k).^(-x)+2.^x.*((k...
+sqrt(17*k^2-36*k*(2*k-v)+20*(2*k-v)^2)+2*(2*k-v))/k).^(-x))^(1./x);
y=y1-y2;
```

Appendix F

Vita

The author, Bo Jin, was born on March 26, 1973 in Tianjin, P. R. China. He received his B.S. degree and M.S. degree in Naval Architecture and Ocean Engineering, in 1994 from Huazhong University of Science and Technology and in 1997 from Shanghai Jiao Tong University respectively. From 1997 and 1999 he worked in China State Shipbuilding Corporation as an engineering technician. In 2000 he began his studies in statistics in the Department of Statistics of Virginia Tech, where he received his M.S. degree in 2001 and Ph.D. degree in 2004.