AN ABSTRACT OF THE THESIS OF

Michael Allen Jacroux for the degree of DOCTOR OF PHILOSOPHY

in STATISTICS presented on August 3, 1976

Title: ON THE THEORY OF (M, S) OPTIMALITY IN INCOMPLETE BLOCK DESIGNS

Redacted for Privacy

Abstract approved: ______________________

Justus F. Seely

The problem considered is the determination of optimal incomplete block designs when the experimental material does not fit any of the usual textbook situations. The criterion used to determine an optimal design within a given class $\mathcal{D}$ of incomplete block designs is the (M, S) optimality criterion Let C denote the matrix of coefficients obtained in the reduced normal equations for estimating the treatment effects in a given incomplete block design. The (M, S) optimality criterion is to find within the class $\mathcal{D}$ the set of designs whose C-matrices have maximal trace, denoted by $\mathcal{M}\{\mathcal{D}\}$, and then to find within $\mathcal{M}\{\mathcal{D}\}$ those designs with minimum trace of C^2; such a design is said to be (M, S) optimal.

The classes of designs we consider are denoted by $\mathcal{D}[v;(r_i);b;k]$ and $\mathcal{D}[v;b;k]$. $\mathcal{D}[v;(r_i);b;k]$ consists of all incomplete block designs with v treatments arranged in b blocks of

size k such that treatment T_i is replicated r_i times and $\mathcal{D}[v;b;k]$ consists of all designs with v treatments arranged in b blocks of size k. The properties of (M,S) optimal designs within these classes is studied. Several lower bounds are established for trace of C^2 which help the experimenter to know when a design is optimal. Through the establishment of these lower bounds, several well known types of incomplete block designs are shown to be optimal. The question of how replications should be assigned to treatments for an (M,S) optimal design in $\mathcal{D}[v;b;k]$ is considered. Construction of optimal designs within the classes described above is also discussed.

On the Theory of (M,S) Optimality in Incomplete Block Designs

by

Michael Allen Jacroux

A THESIS

submitted to

Oregon State University

in partial fulfillment of
the requirements for the
degree of

Doctor of Philosophy

Completed July 1976

Commencement June 1977

APPROVED:

Redacted for Privacy

Associate Professor of Statistics
in charge of major

Redacted for Privacy

Head of Department of Statistics

Redacted for Privacy

Dean of Graduate School

Date thesis is presented August 3, 1976

Typed by Clover Redfern for Michael Allen Jacroux

ACKNOWLEDGMENT

The author wishes to express his deepest appreciation to Dr. Justus Seely who served as the author's major professor. Without his technical guidance, patience, and encouragement, this thesis would never have been written.

The author wishes to thank the many members of the Department of Statistics with whom he has had many valuable discussions. Special thanks go to Dr. David Thomas, Dr. David Birkes, and Dr. Roger Petersen.

Lastly the author acknowledges the financial support provided by a Department of Health, Education, and Welfare Biometry Traineeship during these studies.

TABLE OF CONTENTS

ON THE THEORY OF (M,S) OPTIMALITY IN INCOMPLETE BLOCK DESIGNS

I. INTRODUCTION

The general procedure in scientific research is to formulate a hypothesis and then to test it. The process of hypothesis testing usually necessitates the collection of observations relevant to the hypothesis. The observations are usually collected in some pattern or according to some experimental plan. By an experiment we mean the planning and collection of measurements or observations relevant to the testing of some hypothesis. The actual planned schedule for taking the observations is called the experimental design.

The pioneer in the theory of experimental design was the late Sir Ronald Fisher. He dominated the history of experimental design in the nineteen twenties and thirties. It was he who introduced the concept of randomization into statistics. Randomization is the principle upon which the application of statistical theory to the design of experiments is based.

Experimental designs in which treatments are randomly assigned over the experimental material are called randomized. All randomized designs are based upon the completely randomized design (CRD). The CRD is formed by dividing the experimental material into experimental units and then assigning the units to treatments at random. A treatment assigned to r of the units is said to be replicated r times. All other randomized designs can be derived from the CRD by placing restrictions upon the randomization procedure.

It is sometimes beneficial to partition the experimental material into blocks which are more homogeneous and randomly assign the treatments within each block. Such designs are called randomized block designs and are used in many fields of research. However, if the number of treatments is too large to preserve homogeneous conditions within complete blocks, or the size of the blocks is determined by the nature of the experiment, then incomplete block designs are used. A wide range of these designs is available for planning experiments in blocks of equal sizes but with a smaller number of experimental units than the total number of treatments. An experimenter who wants all the contrasts between treatments to be confounded with blocks to the same extent may use a balanced incomplete block design. A balanced incomplete block design may be constructed for any number of treatments which occur in blocks of equal size, but may require a large number of replicates. If the experimenter is willing to accept that some of the possible treatment contrasts are more confounded than others, one of the various partially balanced incomplete block designs listed in the standard works on experimental design may be used. Partially balanced incomplete block designs usually require a smaller number of replicates. However, the available lists of designs published in the literature have been restricted to balanced incomplete block designs and partially balanced incomplete block designs with two associate classes. Such lists may not include the number of treatments the experimenter is actually interested in or may supply him with plans that require too many replicates.

The high degree of symmetry in the pattern of balanced and partially balanced incomplete block designs is in many respects a desirable property. But the restriction of the designs to equal numbers of treatment replications and equal block sizes may be a serious practical obstacle in many experimental circumstances. Suppose for instance that the effects of a number of virus innoculations on mice are to be determined. It would be natural to use litters as blocks, but if the litters were of unequal sizes or one of the viruses was in short supply, an incomplete block design with differing block sizes and differing numbers of replications might need to be used.

The above mentioned restrictions as well as other possible restrictions in the use of balanced or partially balanced incomplete block designs give rise to the "make-shift" production of designs to deal with practical situations. Even though there may be severe limitations placed upon the construction of such designs, the experimenter usually has some freedom of choice and may therefore wish to know which of the possible designs is most desirable in the given circumstances. In certain cases there may exist known solutions, but in general the problem may be difficult to answer.

From the class of designs capable of achieving the experimenter's goals, a decision must be made as to what design to use. The decision is usually based on physical, economical, or statistical factors. The use of a statistical standard or criterion to choose a design is commonly known as the theory of optimal design. It will be the purpose of this thesis to study the application of the (M, S) optimality criterion to several classes of incomplete block designs. Properties of the (M, S) optimal designs within these classes and methods of construction will be discussed.

II. BACKGROUND AND DEFINITIONS

In this chapter, we introduce the terminology and notation which will be used throughout the remainder of this thesis.

Let $\Omega = \{T_1, \ldots, T_v\}$ denote a set of v treatments. Let there be $n = \sum_{i=1}^{b} k_i$ experimental units arranged in b blocks, denoted by B_j, $j = 1, \ldots, b$, with B_j containing k_j units. By an incomplete block design with parameters $v, r_1, \ldots, r_v, b, k_1, \ldots, k_b$ and incidence matrix N, we shall mean an allocation of the v treatments in Ω, one to each of the n experimental units, such that treatment T_i is replicated r_i times and the $v \times b$ matrix $N = (n_{ij})$ where n_{ij} denotes the number of experimental units in block B_j receiving treatment T_i. We shall denote such a block design by $D[v;r_1, \ldots, r_v;b;k_1, \ldots, k_b;N]$. If n_{ij} assumes only the values zero or one, the design is called binary. If n_{ij} assumes only the values zero, one, or two, the design is called ternary, etc. We shall sometimes use the notation $T_i \in B_j$ to indicate that treatment T_i occurs in block B_j, i.e., $n_{ij} \geq 1$.

A block design in which $r_i = r$ for each i is said to be equi-replicated and is denoted by $D[v;r;b;k_1, \ldots, k_b;N]$. A block design in which $k_j = k$ for each j is called proper and is denoted by $D[v;r_1, \ldots, r_v;b;k;N]$. Thus a proper equi-replicated block design is one for which $r_i = r$ for all i and $k_j = k$ for all j.

Such a design is denoted by $D[v;r;b;k;N]$.

In experimental design NN' is called the association matrix and $N'N$ the block characteristic matrix where N' denotes the transpose of N. The entries of NN' and $N'N$ shall be denoted by λ_{ij} and μ_{ij} respectively. Note that in binary designs, λ_{ij} indicates the number of blocks treatments T_i and T_j occur in together and μ_{ij} denotes the number of treatments that blocks B_i and B_j have in common.

The statistical model used throughout this thesis in the discussion of incomplete block designs is one with fixed block effects. The actual model used is the usual additive two-way model:

$$y_{ijk} = \mu + t_i + b_j + e_{ijk}$$

where

y_{ijk} = kth observed response of the ith treatment in the jth block

μ = the overall mean effect

t_i = the effect of treatment T_i

b_j = the effect of block B_j

and the e_{ijk}'s are random variables which are uncorrelated, have mean zero, and have constant variance σ^2. The normal equations for estimating the parameters are:

$$n\hat{\mu} + \sum_{i=1}^{v} r_i\hat{t}_i + \sum_{j=1}^{b} k_j\hat{b}_j = \sum\sum_{ij} y_{ij}$$

$$r_i\hat{\mu} + r_i\hat{t}_i + \sum_j n_{ij}\hat{b}_j = \sum_j y_{ij}\ , \quad i = 1,\ldots,v \qquad (2.1)$$

$$k_j\hat{\mu} + \sum_i n_{ij}\hat{t}_i + k_j\hat{b}_j = \sum_j y_{ij}\ , \quad j = 1,\ldots,b\ .$$

Let $\mathrm{diag}(a_1,\ldots,a_n)$ denote a matrix with entries a_i on the main diagonal and zeros elsewhere and let $R = \mathrm{diag}(r_1,\ldots,r_v)$ and $K = \mathrm{diag}(k_1,\ldots,k_b)$. From the normal equations, the reduced normal equations for estimating treatment contrasts are easily derived to be

$$C\hat{\underset{\sim}{t}} = Q \qquad (2.2)$$

where

$\hat{\underset{\sim}{t}}' = (\hat{t}_1,\ldots,\hat{t}_v)$ is any solution to (2.2)

$C = R - NK^{-1}N'$

$Q = T - NK^{-1}B$ (2.3)

T = column vector of treatment totals

B = column vector of block totals.

The matrix C defined in (2.3) is called the coefficient matrix of the design or the C-matrix.

A linear combination $\psi = \underset{\sim}{\ell}'\underset{\sim}{t} = \ell_1 t_1 + \ldots + \ell_v t_v$ of the treatment effects is said to be estimable if and only if there exists a linear combination $\underset{\sim}{c}'\underset{\sim}{Y}$ of the observations such that $E(\underset{\sim}{c}'\underset{\sim}{Y}) = \underset{\sim}{\ell}'\underset{\sim}{t}$. One can easily verify that $\underset{\sim}{\ell}'\underset{\sim}{t}$ is estimable with respect to a particular design if and only if $\underset{\sim}{\ell}$ is in the column space of the C-matrix of the design. A set of estimable functions $\underset{\sim}{\ell}_1'\underset{\sim}{t}, \ldots, \underset{\sim}{\ell}_m'\underset{\sim}{t}$ of the treatment effects is said to be linearly independent if the vectors $\underset{\sim}{\ell}_1, \ldots, \underset{\sim}{\ell}_m$ form a linearly independent set. For any estimable function $\underset{\sim}{\ell}'\underset{\sim}{t}$, the minimum variance linear unbiased estimator (B.L.U.E.) is $\underset{\sim}{\ell}'\hat{\underset{\sim}{t}}$ where $\hat{\underset{\sim}{t}}$ is any solution vector to (2.2).

If the goal of the experiment is to estimate treatment differences unbiasedly, or test the hypothesis that all treatment effects are the same, then the concept of connectedness plays an important role. An incomplete block design is said to be connected if its coefficient matrix has rank $v-1$. If a design is connected, then $\ell_1 t_1 + \ldots + \ell_v t_v$ is estimable if and only if $\ell_1 + \ldots + \ell_v = 0$, in which case the linear function $\underset{\sim}{\ell}'\underset{\sim}{t}$ is called a contrast. Elementary contrasts are those of the form $t_i - t_j$, and if a design is connected, all such contrasts are estimable.

The two most frequently studied types of incomplete block designs are the balanced and partially balanced designs. A proper equi-replicated binary incomplete block design in which each treatment occurs with every other treatment λ times is called a balanced incomplete block design (BIBD) and is denoted by BIBD[v;r;b;k;λ].

The characteristic property of the BIBD is that the variance of all best linear unbiased estimators for elementary contrasts is the same, i.e., $\mathrm{var}(\hat{t}_i - \hat{t}_j)$ is constant for all $i \neq j$. An alternative to the requirement of balance in a block design occurs in the usage of partially balanced incomplete block designs. For the definition of a partially balanced incomplete block design with m associate classes, denoted by PBIB(m), the reader is referred to John (1971). In a PBIB(m) design, all elementary treatment contrasts are not estimated with the same precision.

The dual of an incomplete block design is obtained by interchanging the roles of blocks and treatments. If N is the incidence matrix of an incomplete block design, then N' will be the incidence matrix of the dual design.

III. INTRODUCTION TO (M,S) OPTIMALITY

A design is said to be optimal within a specified class of designs if it is determined to be "best" by some well defined criterion. Many researchers have tried to characterize the optimal designs within a given class of incomplete block designs according to various criteria. This task is difficult in most situations. Many papers have been written on the subject of optimal design. Some of the most notable contributions to the theory have been made by Wald (1943), Ehrenfeld (1955), Kempthorne (1956), Masuyama (1957), Kshiragar (1958), Kiefer (1958, 1959, 1960, 1971, 1974), Shah (1960) and Takeuchi (1961).

Important aims in experimental design are to estimate treatment effects with maximum precision or to perform a test of a null hypothesis. These considerations lead to different criteria for choosing among the designs in a given class.

Consider a class $\mathcal{D}$ of connected incomplete block designs with v treatments. The three most well known and used optimality criteria to determine a best design in $\mathcal{D}$ are the A, D, and E optimality criteria. These criteria are defined in terms of functions of the nonzero eigenvalues of the C-matrices of the designs in $\mathcal{D}$. Let $\lambda_1, \ldots, \lambda_{v-1}$ be these nonzero eigenvalues. The A, D, and E optimality criteria are defined as follows:

A-optimality: minimize $\sum_i \lambda_i^{-1}$. This is equivalent to minimizing the average variance of all elementary treatment contrast estimates.

D-optimality: minimize $\prod_i \lambda_i^{-1}$. This is equivalent to minimizing the generalized variance of the estimates of any set of $v-1$ independent estimable functions of the treatment effects.

E-optimality: minimize the maximum λ_i^{-1}. This is equivalent to minimizing the maximum variance of the estimates of all normalized estimable functions of the treatment effects. [$\underset{\sim}{\lambda}'\underset{\sim}{t}$ is normalized if $\underset{\sim}{\lambda}'\underset{\sim}{\lambda} = 1$].

The three criteria mentioned so far are based on different considerations and need not necessarily agree in comparing two given designs. Which criterion should be adopted depends upon the aim in conducting the experiment. But most often the experimenter is interested in both the interval estimation of the treatment effects and the test of a null hypothesis.

We now set about defining the optimality criterion with which we will be concerned. It is easily seen that when a design D has a C-matrix with maximal $\operatorname{tr} C = \sum_{i=1}^{v-1} \lambda_i$ and all of its nonzero eigenvalues equal, then that design will be A, D, and E-optimal in $\mathcal{D}$. Rao (1958) has shown that for the C-matrix of a connected incomplete block design to have all of its nonzero eigenvalues equal, it must have the form $\alpha I_v + \beta J_v$ where I_v is the $v \times v$ identity matrix and J_v is that $v \times v$ matrix whose entries are all one. A design having a C-matrix of the form $\alpha I_v + \beta J_v$ is called variance balanced. When a design exists with a C-matrix of the form $\alpha I_v + \beta J_v$, it is easy to show that $\alpha = (\text{tr } C)/(v-1)$ and $\beta = -(\text{tr } C)/(v(v-1))$. So if there exists a variance balanced design $D \in \mathcal{D}$ whose C-matrix has maximal trace, then that design will be A, D, and E-optimal.

However, if in $\mathcal{D}$ there does not exist a variance balanced design with a C-matrix of maximal trace, it seems reasonable to find a design $D \in \mathcal{D}$ whose C-matrix has maximal trace and is close in some sense to the desired $\alpha I_v + \beta J_v$ form. We now define in what sense we want the optimal design to be close to the desired $\alpha I_v + \beta J_v$ form.

Let ζ = {all $v \times v$ symmetric matrices} and let $(\zeta, <,>)$ denote the finite dimensional inner product space consisting of ζ and $<A, B> = \text{tr } AB$ for $A, B \in \zeta$. Define a norm on ζ by $\|A\|^2 = <A, A>$ for $A \in \zeta$ and define the distance between $A, B \in \zeta$ to be $\|A-B\|^2 = <A-B, A-B>$. Note that this is simply an extension of the usual Euclidean norm to the set of $v \times v$ matrices.

As before, let $\mathcal{D}$ be a class of connected incomplete block designs. We would like to find that design $D \in \mathcal{D}$ whose C-matrix has maximal trace and such that $\| C - \alpha I_v - \beta J_v \|^2$ has a minimal value. Let $\mathcal{M}\{\mathcal{D}\}$ denote the set of designs in $\mathcal{D}$ with maximal trace. So we want to find $\bar{D} \in \mathcal{M}\{\mathcal{D}\}$ such that

$$\mathrm{tr}(\bar{C} - \alpha I_v - \beta J_v)^2 = \min_{D \in \mathcal{M}\{\mathcal{D}\}} \mathrm{tr}(C - \alpha I_v - \beta J_v)^2$$

But since for all $D \in \mathcal{M}\{\mathcal{D}\}$, $\mathrm{tr}\, C$ is constant and $CJ_v = 0$ (from 4.2.1) it is seen that we are simply looking for $D \in \mathcal{M}\{\mathcal{D}\}$ which has a minimal value for $\mathrm{tr}\, C^2$. So in finding a design $D \in \mathcal{M}\{\mathcal{D}\}$ which is "close" to balanced, we are finding a design in $\mathcal{D}$ which is approximately A, D, and E optimal.

Note also that $\mathrm{tr}\, C^2 = \sum_{i=1}^{v-1} \lambda_i^2$. Thus, since $\mathrm{tr}\, C$ is constant for all $D \in \mathcal{M}\{\mathcal{D}\}$, finding $D \in \mathcal{M}\{\mathcal{D}\}$ such that $\mathrm{tr}\, C^2$ is minimal is equivalent to finding $D \in \mathcal{M}\{\mathcal{D}\}$ such that $\sum_{i=1}^{v-1} (\lambda_i - \bar{\lambda})^2$ is minimal where $(v-1)\bar{\lambda} = \sum_{i=1}^{v-1} \lambda_i$. So in finding $D \in \mathcal{M}\{\mathcal{D}\}$ with minimal $\mathrm{tr}\, C^2$, we are finding $D \in \mathcal{D}$ whose average nonzero eigenvalue is as large as possible and whose individual eigenvalues are as close together as possible.

More generally, let $\mathcal{D}$ be an arbitrary class of designs with v treatments and b blocks and a fixed number of experimental units n. Let $\mathcal{M}\{\mathcal{D}\}$ be as defined above. We give the following definition.

Definition 3.1. $\bar{D} \epsilon \mathcal{D}$ is said to be (M, S) optimal if $\bar{D} \epsilon \mathcal{M}\{\mathcal{D}\}$ and $\text{tr } \bar{C}^2 \leq \text{tr } C^2$ for all $D \epsilon \mathcal{M}\{\mathcal{D}\}$. A design $\bar{D} \epsilon \mathcal{D}$ is said to be S-better than a design $D \epsilon \mathcal{D}$ if $\text{tr } \bar{C}^2 < \text{tr } C^2$.

The idea of minimizing $\text{tr } C^2$ originated with Shah (1960) who suggested its use in settings where tr C is constant for all designs in a given class $\mathcal{D}$. Shah's criterion was extended by Eccleston and Hedayat (1974) to the (M, S) optimality criterion given in Definition 3.1. The notation of Definition 3.1 was also used by Eccleston and Hedayat. However, the motivation and justification for usage of the (M, S) optimality criterion given above is different than that given by previous authors, and for that reason was included in this thesis.

A distinct advantage of the (M, S) optimality criterion over other criteria is its computational simplicity. Note that using the A, D, and E optimality criteria depends upon the knowledge of the actual eigenvalues of the C-matrices of the designs in $\mathcal{D}$, or the computation of various determinants for designs in $\mathcal{D}$. Hence it may be computationally difficult to find the optimum design in $\mathcal{D}$; particularly if the number of treatments is large or the class of designs $\mathcal{D}$ is large. The (M,S) optimality criterion on the other hand has a somewhat simple computational form since $\operatorname{tr} C^2$ is simply the sum of the squares of the elements of C.

Definition 3.2. Let $\mathcal{D}[v;(r_i);b;(k_j)]$ denote the class of incomplete block designs consisting of v treatments arranged in b blocks such that treatment T_i is replicated r_i times and block B_j contains k_j experimental units. Let $\mathcal{D}[v;b;(k_j)]$ denote the class of incomplete block designs with v treatments arranged in b blocks such that block B_j contains k_j experimental units.

Note that the difference between the two classes of designs defined above is that the r_i are fixed in $\mathcal{D}[v;(r_i);b;(k_j)]$ where as they are allowed to vary in $\mathcal{D}[v;b;(k_j)]$.

The classes of designs we will generally be concerned with are $\mathcal{D}[v;(r_i);b;(k_j)]$ where $k_j = k$ for all j, denoted by $\mathcal{D}[v;(r_i);b;k]$ and $\mathcal{D}[v;b;(k_j)]$ where $k_j = k$ for all j, denoted by $\mathcal{D}[v;b;k]$. In the following chapters, we shall give some of the properties and say something about the construction of (M,S) optimal designs in $\mathcal{D}[v;(r_i);b;k]$ and $\mathcal{D}[v;b;k]$.

IV. PRELIMINARY FACTS AND LEMMAS

In this chapter we shall give some facts and lemmas which will be referred to throughout the remainder of this thesis.

4.1. Facts Concerning Incidence Matrices

Let $D[v;r_1,\ldots,r_v;b;k_1,\ldots k_b;N]$ be an arbitrary binary incomplete design. Recall that N is the incidence matrix of the design. In this section, some simple results concerning $N = (n_{ij})$, $NN' = (\lambda_{ij})$, and $N'N = (\mu_{ij})$ will be given.

Lemma 4.1.1. Suppose $D[v;r_1,\ldots,r_v;b;k_1,\ldots,k_b;N]$ is an arbitrary binary incomplete block design, then

i) for fixed p, $\sum_q n_{pq} = r_p$

ii) for fixed q, $\sum_p n_{pq} = k_q$

iii) $\max[0, r_p+r_q-b] \leq \lambda_{pq} \leq \min[r_p, r_q]$

iv) $\max[0, k_p+k_q-v] \leq \mu_{pq} \leq \min[k_p, k_q]$

v) for fixed p, $\sum_{q\neq p} \lambda_{pq} = \sum_{T_p \in B_m} (k_m - 1)$

vi) $\sum\sum_{p \neq q} \lambda_{pq} = \sum_{m=1}^{b} k_m(k_m - 1)$

vii) for fixed p, $\sum_{q \neq p} \mu_{pq} = \sum_{T_m \in B_p} (r_m - 1)$

viii) $\sum\sum_{p \neq q} \mu_{pq} = \sum_{m=1}^{v} r_m(r_m - 1)$.

Pf. i) n_{pq} denotes the number of experimental units receiving treatment T_p in block B_q. Since treatment T_p is applied to r_p experimental units, it must be that $\sum_q n_{pq} = r_p$.

ii) Similar to i).

iii) Note that λ_{pq} represents the ordinary Euclidean vector inner product of the pth row of N with the qth row of N. Since there are only r_p ones in the pth row of N and r_q ones in the qth row of N, it is clear that the inner product between these two rows cannot exceed $\min\{r_p, r_q\}$. Also, λ_{pq} must be a nonnegative integer, but if $r_p + r_q > b$, then the least number of blocks that treatments T_p and T_q can occur in together is $r_p + r_q - b$, hence $\lambda_{pq} \geq \max\{0, r_p + r_q - b\}$. Hence we have the desired result.

iv) Similar to iii).

v) Note that for fixed p, T_p occurs in r_p blocks, and each block B_m containing T_p contains $k_m - 1$ other experimental units to which the remaining $v-1$ treatments can be assigned. Hence there are $\sum_{T_p \in B_m} (k_m - 1)$ experimental units in the r_p blocks containing T_p to which the remaining $v-1$ treatments can be assigned. Now λ_{pq} indicates the number of experimental units assigned to treatment T_q in blocks containing T_p, hence when p is fixed, it must be that $\sum_{q \neq p} \lambda_{pq} = \sum_{T_p \in B_m} (k_m - 1)$.

vi) $\sum\sum_{p \neq q} \lambda_{pq} = \sum_{p} \sum_{q \neq p} \lambda_{pq} = \sum_{p} \sum_{T_p \in B_m} (k_m - 1) = \sum_{m} k_m (k_m - 1)$

since there are k_m treatments in block B_m.

vii) Similar to v).

viii) Similar to vi).

<u>Corollary 4.1.2.</u> When $D[v; r_1, \ldots, r_v; b; k; N]$ is a proper binary incomplete block design, then

i) for fixed p, $\sum_{q \neq p} \lambda_{pq} = r_p (k-1)$

ii) $\sum\sum_{p \neq q} \lambda_{pq} = bk(k-1)$.

Lemma 4.1.3. Let $D[v;r_1,\ldots,r_v;b;k_1,\ldots,k_b;N]$ be a binary incomplete block design. If N is partitioned into N_1 and N_2 where N_1 consists of the first v_1 rows of N and N_2 consists of the remaining $v - v_1 = v_2$ rows of N and B_i^* represents that part of block B_i in the N_1 portion of N and B_i^{**} represents that part of block B_i in the N_2 portion of N, then

i) $2\sum_{p=1}^{v_1} \sum_{q>p}^{v_1} \lambda_{pq} = \sum_{i=1}^{b} k_i^*(k_i^*-1)$ where k_i^* is the number of experimental units assigned to B_i^*.

ii) $2\sum_{p=v_1+1}^{v} \sum_{q>p}^{v} \lambda_{pq} = \sum_{i=1}^{b} k_i^{**}(k_i^{**}-1)$ where k_i^{**} is the number of experimental units assigned to B_i^{**}.

iii) $2\sum_{p=1}^{v_1} \sum_{q=v_1+1}^{v} \lambda_{pq} = 2\sum_{i=1}^{b} k_i^*(k_i^{**})$.

Pf. i) Similar to the proof of 4.1.1 vi).

ii) Similar to the proof of 4.1.1 vi).

iii) $k_i^* + k_i^{**} = k_i$ and

$$2\sum_{p=1}^{v_1}\sum_{q=v_1+1}^{v}\lambda_{pq}$$

$$= 2\sum_{p=1}^{v}\sum_{q>p}^{v}\lambda_{pq} - 2\sum_{p=1}^{v_1}\sum_{q>p}^{v_1}\lambda_{pq} - 2\sum_{p=v_1+1}^{v}\sum_{q>p}^{v}\lambda_{pq}$$

$$= \sum_{i=1}^{b}(k_i^*+k_i^{**})(k_i^*+k_i^{**}-1) - \sum_{i=1}^{b}k_i^*(k_i^*-1) - \sum_{i=1}^{b}(k_i^{**})(k_i^{**}-1)$$

$$= 2\sum_{i=1}^{b}k_i^*(k_i^{**}) .$$

Note that this last lemma can be extended to further partitions of N in an obvious manner, i.e., by partitioning N_1 and N_2, etc.

4.2. Facts Concerning C-Matrices

In this section, several facts and lemmas concerning the coefficient matrices of designs will be given.

Let $\underline{N}(A)$ and $\underline{R}(A)$ denote the null space and column space respectively of an arbitrary matrix A. Let R^v denote Euclidean v-space. It is well-known that the C-matrix for any incomplete block design with v treatments has the following properties.

i) $C\underset{\sim}{1}_v = 0$ where $\underset{\sim}{1}_v$ is a $v \times 1$ vector of ones.

ii) $\underline{R}(C) \subseteq \underset{\sim}{1}_v^{\perp}$ where $\perp$ denotes the orthogonal complement. (4.2.1)

Let $\underline{r}(A)$ denote the rank of a matrix A. Let P denote the orthogonal projection on $\underline{R}(A)$ where A is some matrix. Then it can be shown that (Rao, (1973))

i) $\text{tr } P^2 = \text{tr } P = \underline{r}(A)$. (4.2.2)

Using (4.2.2), the following lemma can be proven.

Lemma 4.2.3. Suppose C is the coefficient matrix of an arbitrary incomplete block design and let P_c denote the orthogonal projection on $\underline{R}(C)$, then

$$\text{tr } C^2 \geq \frac{[\text{tr } C]^2}{\underline{r}(C)}$$

and equality holds if and only if $C = \gamma P_c$ for some scalar γ.

Pf. Let $(\zeta, <, >)$ denote the finite dimensional inner product space for $v \times v$ symmetric matrices introduced in Chapter III. Let P_c denote the orthogonal projection on $\underline{R}(C)$. By the Cauchy-Schwarz inequality and (4.2.2),

$$[\text{tr } C]^2 = [\text{tr}(P_c C)]^2 = |\langle C, P_c\rangle|^2 \leq \langle C, C\rangle\langle P_c, P_c\rangle$$

$$= (\text{tr } C^2)(\text{tr } P_c^2) = (\text{tr } C^2)(\underline{r}(C)) .$$

Also from the Cauchy-Schwarz inequality, we get equality if and only if $C = \gamma P_c$.

4.3. A Minimization Problem

In this section, a solution will be given to a minimization problem which occurs throughout the sequel. An application is also given.

Let $\underset{\sim}{x} = (x_1, \ldots, x_n)$. We wish to find the minimal value for

$$f(\underset{\sim}{x}) = \sum_{i=1}^{n} x_i^2 \qquad (4.3.1)$$

over the set of vectors F satisfying

i) the x_i are nonnegative integers

ii) $$g(\underset{\sim}{x}) = \sum_{i=1}^{n} x_i = c \qquad (4.3.2)$$

iii) $b_i \leq x_i \leq c_i, \quad i = 1, \ldots, n$

where c, b_i, and c_i are nonnegative integers for $i = 1, \ldots, n$.

Lemma 4.3.3. Let $\underset{\sim}{x} = (x_1, \ldots, x_n) \in F$. If there exists p and q such that 1) $x_p - x_q \geq 2$, 2) $b_p \leq x_p - 1$ and 3) $x_q + 1 \leq c_q$, then there exists $\underset{\sim}{y} \in F$ such that $f(\underset{\sim}{y}) < f(\underset{\sim}{x})$.

Pf. Suppose $\underset{\sim}{x} \in F$ and there are components x_p and x_q of $\underset{\sim}{x}$ satisfying conditions 1), 2), and 3) of the lemma. Let $\underset{\sim}{y} = (y_1, \ldots, y_n)$ where $y_p = x_p - 1$ and $y_q = x_q + 1$ and $y_k = x_k$ for $k \neq p$, $k \neq q$. Clearly $\underset{\sim}{y} \in F$ and

$$f(\underset{\sim}{y}) = \sum_{i=1}^{n} y_i^2 = \sum_{k \neq p,q} x_k^2 + (x_p - 1)^2 + (x_q + 1)^2 = f(\underset{\sim}{x}) + 2(x_q - x_p + 1).$$

But $x_p - x_q \geq 2$ and so $f(\underset{\sim}{y}) < f(\underset{\sim}{x})$ which implies the desired result.

Let G denote the set of vectors $\underset{\sim}{x} \in F$ having no components satisfying conditions 1), 2), and 3) of Lemma 4.3.3. By the lemma, we know that the set of vectors minimizing $f(\underset{\sim}{x})$ subject to the constraints must be contained in G. Let $\underset{\sim}{x}, \underset{\sim}{y} \in G$ and let $J = \{1, \ldots, n\}$ denote the subscripts of the components of $\underset{\sim}{x}$ and $\underset{\sim}{y}$. If possible, find $p, q \in J$ such that $x_p = y_q$ and $x_q = y_p$ and remove these subscripts from J. Repeat this procedure until no p and q exist for which $x_p = y_q$ and $x_q = y_p$. Let $\bar{J}$ denote the remaining set of subscripts and let $\underset{\sim}{\bar{x}}$ and $\underset{\sim}{\bar{y}}$ be those vectors whose components are the same as those of $\underset{\sim}{x}$ and $\underset{\sim}{y}$ and whose subscripts are in $\bar{J}$. Observe that if $\bar{J} = \phi$, then $f(\underset{\sim}{x}) = f(\underset{\sim}{y})$. Now suppose $\bar{J} \neq \phi$. Let $\bar{x}_u = \max\{\bar{x}_i\}$. If $\bar{x}_u < \bar{y}_u$, then since $\sum_{i \in \bar{J}} \bar{x}_i = \sum_{i \in \bar{J}} \bar{y}_i$, there exists $\bar{y}_v$ such that $\bar{x}_v > \bar{y}_v$. But then $\bar{y}_v < \bar{x}_v \leq \bar{x}_u < \bar{y}_u$ and we see that $\underset{\sim}{y}$ has components satisfying conditions 1), 2) and 3) of Lemma 4.3.3. But this is impossible since $\underset{\sim}{y} \in G$. If $\bar{x}_u > \bar{y}_u$ then since $\sum_{i \in \bar{J}} \bar{x}_i = \sum_{i \in \bar{J}} \bar{y}_i$, there exists $\bar{x}_v < \bar{y}_v$ such that $\bar{x}_u \neq \bar{y}_v$ or $\bar{x}_v \neq \bar{y}_u$. Without loss of generality, assume $\bar{x}_u \neq \bar{y}_v$. If $\bar{x}_u > \bar{y}_v$, then $\bar{x}_u > \bar{y}_v > \bar{x}_v$, and we see that $\underset{\sim}{x}$ has components satisfying conditions 1), 2) and 3) of Lemma 4.3.3. But this is a contradiction since $\underset{\sim}{x} \in G$, hence no such situation can occur. If $\bar{x}_u < \bar{y}_v$, then $\bar{y}_u < \bar{x}_u < \bar{y}_v$, and we again see that $\underset{\sim}{y}$ will have components satisfying the conditions of Lemma 4.3.3, a contradiction. Hence we see that $\bar{J}$ must be the empty set. Thus, all vectors in G give the same values for $f(\underset{\sim}{x})$, hence they are all optimal solutions.

<u>Theorem 4.3.4.</u> The set of vectors $\underset{\sim}{x}$ minimizing (4.3.1) subject to constraints (4.3.2) consists of those vectors $\underset{\sim}{x} \in F$ having no components x_p and x_q such that 1) $x_p - x_q \geq 2$, 2) $b_p \leq x_p - 1$, and 3) $x_q + 1 \leq c_q$.

Corollary 4.3.5. The minimal value for $f(\underset{\sim}{x}) = \sum_{i=1}^{n} x_i^2$ subject to the constraints that the x_i are nonnegative integers and $\sum_{i=1}^{n} x_i = c$ is achieved when $|x_i - x_j| \leq 1$ for all i, j.

Note that Theorem 4.3.4 characterizes the set of points which yield minimal values for $f(\underset{\sim}{x})$ subject to the constraints (4.3.2). The proof of Lemma 4.3.3 also yields a simple algorithm for finding this minimal value. If $\underset{\sim}{x}$ is any vector satisfying the given constraints, and if there exists components x_p and x_q of $\underset{\sim}{x}$ such that $x_p - x_q \geq 2$, $x_p - 1 \geq b_p$, and $x_q + 1 \leq c_q$, then by forming the vector $\underset{\sim}{y}$ where $y_p = x_p - 1$, $y_q = x_q + 1$, and $y_k = x_k$ for $k \neq p$, $k \neq q$, we have $f(\underset{\sim}{y}) < f(\underset{\sim}{x})$. By continuing this process until there does not exist components of the derived vector satisfying conditions 1), 2) and 3) of Lemma 4.3.3, the minimal value of f subject to the constraints will be achieved. Use of the algorithm is illustrated in the following example.

Example 4.3.6. In Lemma 4.3.3, let $n = 6$, $c = 33$, and let (8, 10), (6, 8), (0, 6), (0, 6), (0, 5) and (0, 4) represent ordered pairs (b_i, c_i), $i = 1, \ldots, 6$, such that $b_i \leq x_i \leq c_i$. Now $\underset{\sim}{x} = (9, 8, 5, 5, 3, 3)$ is a vector satisfying the constraints and $f(\underset{\sim}{x}) = 213$. Proceeding as outlined above, we obtain the following series of vectors and values of $f(\underset{\sim}{y})$.

y	f(y)
(8, 8, 5, 5, 3, 4)	203
(8, 7, 5, 5, 4, 4)	195
(8, 6, 5, 5, 5, 4)	191

So the minimal value for $f(\underset{\sim}{x})$ subject to the constraints is 191.

The algorithm given above for minimizing $f(\underset{\sim}{x})$ subject to the constraints will be referred to as algorithm (4. 3) for the remainder of the thesis.

As seen in Corollary 4. 3. 5, the minimal value for $\sum_{i=1}^{n} x_i^2$ subject to the constraints that the x_i are nonnegative and $\sum_{i=1}^{n} x_i = c$ is achieved when $|x_i - x_j| \leq 1$ for all i, j. An easy way to determine the actual minimal numerical value is the following. Let $r = [c/n]$ where $[\cdot]$ denotes the greatest integer function. Then write $c = nr + s = nr + s + sr - sr = (n-s)r + s(r+1)$. Hence s of the $x_i = r + 1$ and $n - s$ of the $x_i = r$. Note that this representation of c as the sum of nonnegative integers differing by one is unique, and that the minimal numerical value of $\sum_{i=1}^{n} x_i^2$ is $(n-s)r^2 + s(r+1)^2$.

The first step in applying the (M, S) optimality criterion to a class $\mathcal{D}$ of incomplete block designs is to determine $\mathcal{M}\{\mathcal{D}\}$. The next lemma offers a partial solution to this problem. Recall that $\mathcal{D}[v;(r_i);b;(k_j)]$ denotes that class of designs with fixed values for

r_i and k_j and $\mathcal{D}[v;b;(k_j)]$ denotes that class of incomplete block designs with fixed values for k_j only, i.e., the r_i are allowed to vary. Let $\mathcal{D}_1[v;b;(k_j)]$ denote that subclass of $\mathcal{D}[v;b;(k_j)]$ having incidence matrices $N = (n_{ij})$ such that $|n_{ij}-n_{i'j}| \leq 1$ for each j and all $i \neq i'$.

Lemma 4.3.7. a) $\mathcal{M}\{\mathcal{D}[v;b;(k_j)]\} = \mathcal{D}_1[v;b;(k_j)]$.

b) If $\mathcal{D}_1[v;b;(k_j)] \cap \mathcal{D}[v;(r_i);b;(k_j)] \neq \phi$, then

$$\mathcal{M}\{\mathcal{D}[v;(r_i);b;(k_j)]\} = \mathcal{D}_1[v;b;(k_j)] \cap \mathcal{D}[v;(r_i);b;(k_j)].$$

Pf. a) For each $D \in \mathcal{D}_1[v;b;(k_j)]$

i) $\operatorname{tr} C = \sum_{i=1}^{v} r_i - \sum_{j=1}^{b} k_j^{-1} \sum_{i=1}^{v} n_{ij}^2$

ii) $\sum_{i=1}^{v} n_{ij} = k_j$ for each fixed j.

iii) $|n_{ij}-n_{i'j}| \leq 1$ for each j and $i \neq i'$.

By applying Corollary 4.3.5, it is clear that $\mathcal{D}_1[v;b;(k_j)] \subseteq \mathcal{M}\{\mathcal{D}[v;b;(k_j)]\}$. Now observe for $D \in \mathcal{M}\{\mathcal{D}[v;b;(k_j)]\}$, that i) and ii) above must be satisfied. Furthermore, if $D \notin \mathcal{D}_1[v;b;k_j]$, it is easy to see using Corollary 4.3.5 that trC will not be maximal, hence we must have $D \in \mathcal{D}_1[v;b;(k_j)]$.

b) The proof is straight forward using (a) and the fact that $\mathcal{D}[v;(r_i);b;(k_j)] \subseteq \mathcal{D}[v;b;(k_j)]$.

<u>Corollary 4. 3. 8.</u> If $\mathcal{D}[v;(r_i);b;(k_j)]$ has the property that $|r_i - r_j| \leq 1$ for all i, j, then
$\mathcal{M}\{\mathcal{D}[v;(r_i);b;(k_j)]\} = \mathcal{D}[v;(r_i);b;(k_j)] \cap \mathcal{D}_1[v;b;(k_j)]$.

<u>Pf.</u> From Lemma 4. 3. 7, it must only be shown that

$$\mathcal{D}[v;(r_i);b;(k_j)] \cap \mathcal{D}_1[v;b;(k_j)] \neq \phi.$$

By Lemma 4. 3. 7 $\mathcal{D}_1[v;b;(k_j)] = \mathcal{M}\{\mathcal{D}[v;b;(k_j)]\}$. Let $D \in \mathcal{D}_1[v;b;(k_j)]$ and suppose $r_p - r_q \geq 2$ for some p and q. For some o, it must be true that $n_{po} = n_{qo} + 1$, otherwise $r_p \leq r_q$. For some such o, let D^* be a new design with incidence matrix N^* with $n^*_{po} = n_{qo}$ and $n^*_{qo} = n_{po}$ and $n^*_{uw} = n_{uw}$ for all other u, w. Clearly $D^* \in \mathcal{D}_1[v;b;(k_j)]$ and $r^*_p = r_p - 1$ and $r^*_q = r_q + 1$. Now

$$\text{tr } C - \text{tr } C^* = n^2_{po}/k_o + n^2_{po}/k_o - n^{*2}_{po}/k_o - n^{*2}_{qo}/k_o = 0,$$

hence $\text{tr } C = \text{tr } C^*$. Since this argument may be repeated whenever $r_p - r_q \geq 2$, it follows that there exists a design in $\mathcal{D}_1[v;b;(k_j)]$ with $|r_p - r_q| \leq 1$, and the result follows from the previous lemma.

4.4. A Maximization Problem

In this section, the solution is given for a maximization problem which occurs later on in this paper.

Let A be the set of vectors $\underset{\sim}{a} = (a_1, \ldots, a_s)$ and let B be the set of vectors $\underset{\sim}{b} = (b_1, \ldots, b_s)$ satisfying the following constraints:

i) a_i and b_i are integers for $i = 1, \ldots, s$

ii) $0 \leq a_i \leq c + p$ for $i = 1, \ldots, s$ and c and p are integers such that $c, p \geq 2$

iii) $0 \leq b_i \leq c$ for $i = 1, \ldots, s$ (4.4.1)

iv) $\sum_{i=1}^{s} a_i = (c+p)(k-1)$ where k is an integer and $k \geq 3$.

v) $\sum_{i=1}^{s} b_i = c(k-1)$.

vi) s is a fixed integer such that $k \leq s \leq (c+p)(k-1)$.

We wish to find $\max\limits_{\underset{\sim}{a} \in A} \max\limits_{\underset{\sim}{b} \in B} f_s(\underset{\sim}{a}, \underset{\sim}{b})$ where

$$f_s(\underset{\sim}{a}, \underset{\sim}{b}) = \sum_{i=1}^{s} a_i b_i - \sum_{i=1}^{s} a_i^2 .$$

Note that for fixed $\underset{\sim}{a} \in A$, $f_s(\underset{\sim}{a}, \underset{\sim}{b})$ is linear in each of the components of $\underset{\sim}{b}$. So for fixed $\underset{\sim}{a} \in A$, to find $\max_{\underset{\sim}{b} \in B} f_s(\underset{\sim}{a}, \underset{\sim}{b})$, select those a_i which are maximal and let the corresponding b_i assume the maximum value imposed by the constraints. But $0 \leq b_i \leq c$ and $\sum_{i=1}^{s} b_i = c(k-1)$, hence to find $\max_{\underset{\sim}{b} \in B} f_s(\underset{\sim}{a}, \underset{\sim}{b})$ for $\underset{\sim}{a} \in A$, pick those $k-1$ of the a_i which are maximal and let the corresponding $b_i = c$. Clearly, if $\underset{\sim}{a} \in A$, any vector derived by permuting the components of $\underset{\sim}{a}$ is in A. In particular, if $\underset{\sim}{a} \in A$, let $\hat{\underset{\sim}{a}}$ be that vector obtained from $\underset{\sim}{a}$ by permuting the components of $\underset{\sim}{a}$ such that $a_1 \geq a_2 \geq \ldots \geq a_s$ and let $\hat{A}$ be the set of all such ordered vectors. For $\underset{\sim}{a} \in A$

$$\max_{\underset{\sim}{b} \in B} f_s(\underset{\sim}{a}, \underset{\sim}{b}) = \max_{\underset{\sim}{b} \in B} f_s(\hat{\underset{\sim}{a}}, \underset{\sim}{b}) = c \sum_{i=1}^{k-1} \hat{a}_i - \sum_{i=1}^{s} \hat{a}_i^2 .$$

Let

$$g_s(\hat{\underset{\sim}{a}}) = c \sum_{i=1}^{k-1} \hat{a}_i - \sum_{i=1}^{s} \hat{a}_i^2$$

for all $\hat{\underset{\sim}{a}} \in \hat{A}$. Clearly maximizing $f_s(\underset{\sim}{a}, \underset{\sim}{b})$ over A and B is equivalent to maximizing $g_s(\hat{\underset{\sim}{a}})$ over $\hat{A}$.

Now let $\hat{A}$ be partitioned into equivalence class $\hat{A}_m$ according to the rule that $\hat{\underset{\sim}{a}} \in \hat{A}_m$ if and only if $\sum_{i=1}^{k-1} \hat{a}_i = m$. Note that for a given value of s, m will assume all values between $\max[0,(c+p)(2k-s-2)]$ and $(c+p)(k-1)$. Within the equivalence classes $\hat{A}_m$, we have by Corollary 4.3.5 that

$$\max_{\hat{\underset{\sim}{a}} \in \hat{A}_m} g_s(\hat{\underset{\sim}{a}}) = mc - \sum_{i=1}^{k-1} \hat{a}_i^2 - \sum_{i=k}^{s} \hat{a}_i^2$$

where $\hat{a}_1 \geq \cdots \geq \hat{a}_s$, $\hat{a}_1 - \hat{a}_{k-1} \leq 1$, and $\hat{a}_k - \hat{a}_s \leq 1$.

Since the maximal value of g_s achieved within each equivalence class of $\hat{A}$ is unique and since the vector which achieves the maximal value within each equivalence class is unique (by the ordering in $\hat{A}$), we may look for the set of vectors maximizing $g_s(\hat{\underset{\sim}{a}})$ among those vectors in $\hat{A}$ where $|\hat{a}_1 - \hat{a}_{k-1}| \leq 1$ and $|\hat{a}_k - \hat{a}_s| \leq 1$. Denote this latter set of vectors by $\bar{A}$. So finding the maximal value for g_s over $\hat{A}$ is equivalent to finding the maximal value for g_s over $\bar{A}$. Now let M denote the set of integers m such that there is $\bar{\underset{\sim}{a}} \in \bar{A}$ with $\sum_{i=1}^{k-1} \bar{a}_i = m$. Note that this relationship defines a one to one correspondence between vectors in $\bar{A}$ and integers in M. If we consider the function $h_s(m) = g_s(\bar{\underset{\sim}{a}})$ where $\bar{\underset{\sim}{a}}$ is that vector in $\bar{A}$ corresponding to m, then maximizing h_s over M is clearly equivalent to maximizing g_s over $\bar{A}$. Note that for $m \in M$ and the corresponding $\bar{\underset{\sim}{a}} \in \bar{A}$,

$$h_s(m) = g_s(\underset{\sim}{\bar{a}}) = cm - \sum_{i=1}^{k-1} \bar{a}_i^2 - \sum_{i=k}^{s} \bar{a}_i^2 ,$$

so

$$h_s(m+1) = c(m+1) - \sum_{\substack{i=1 \\ i \neq p}}^{k-1} \bar{a}_i^2 - (\bar{a}_p+1)^2 - \sum_{\substack{i=k \\ i \neq q}}^{s} (\bar{a}_i^2) - (\bar{a}_q-1)^2$$

$$= h_s(m) - 2\bar{a}_p + 2\bar{a}_q + c - 2$$

where $\bar{a}_p = \bar{a}_{k-1}$ and $\bar{a}_q = \bar{a}_k$. Hence

$$h_s(m+1) = h_s(m) - 2\bar{a}_{k-1} + 2\bar{a}_k + c - 2.$$

Similarly,

$$h_s(m-1) = h_s(m) + 2\bar{a}_1 - 2\bar{a}_s + c - 2.$$

Proposition 4.4.2. The property that $\bar{a}_1 - \bar{a}_s \leq (c+2)/2$ and $\bar{a}_{k-1} - \bar{a}_k \geq (c-2)/2$ characterizes all vectors $\underset{\sim}{\bar{a}} \in \bar{A}$ whose corresponding values of $m \in M$ maximize $h_s(m)$.

Pf. Observe that vectors satisfying the conditions in Proposition 4.4.2 exist since $k \leq s \leq (c+p)(k-1)$. Let $m \in M$ and let $\underset{\sim}{\bar{a}}$ be the corresponding vector in $\bar{A}$. From the paragraph preceding the proposition, we see that $h_s(m+1) > h_s(m)$ if and only if

$$h_s(m+1) - h_s(m) = 2\bar{a}_k - 2\bar{a}_{k-1} + c - 2 > 0$$

or

$$\bar{a}_{k-1} - \bar{a}_k < \frac{c-2}{2}$$

and $h_s(m-1) > h_s(m)$ if and only if

$$h_s(m-1) - h_s(m) = 2\bar{a}_1 - 2\bar{a}_s - c - 2 > 0$$

or

$$\bar{a}_1 - \bar{a}_s > \frac{c+2}{2}.$$

So for any value of m to yield a maximal value for h_s in M, the vector in $\bar{A}$ corresponding to it must have the property that $\bar{a}_{k-1} - \bar{a}_k \geq (c-2)/2$ and $\bar{a}_1 - \bar{a}_s \leq (c+2)/2$. To show that this property characterizes all vectors in $\bar{A}$ whose corresponding values of m maximize $h_s(m)$, let $\bar{\underset{\sim}{a}} \in \bar{A}$ have the property and let $m \in M$ be the corresponding integer. Consider $h_s(m+t)$ where t is a positive integer. If $\bar{\bar{\underset{\sim}{a}}}$ is that vector in $\bar{A}$ associated with $m+t$, since $m+t > m$, we must have $\bar{a}_{k-1} \leq \bar{\bar{a}}_{k-1}$ and $\bar{\bar{a}}_k \leq \bar{a}_k$, hence that $\bar{\bar{a}}_{k-1} - \bar{\bar{a}}_k \geq \bar{a}_{k-1} - \bar{a}_k \geq (c-2)/2$. From above, we see that this implies $h_s(m+t+1) \leq h_s(m+t)$, hence that $h_s(m) \geq h_s(m+t)$ for all positive integers t. Similarly, consider $h_s(m-t)$ for all positive integers t. If $\bar{\bar{\underset{\sim}{a}}}$ is that vector in $\bar{A}$ corresponding to $m-t$, we must have $\bar{\bar{a}}_1 \leq \bar{a}_1$ and $\bar{\bar{a}}_s \geq \bar{a}_s$, hence that

$\bar{\bar{a}}_1 - \bar{\bar{a}}_s \leq \bar{a}_1 - \bar{a}_s \leq (c+2)/2$. From above, we see that this implies $h_s(m-t) \geq h_s(m-t-1)$ for all t, hence that $h_s(m) \geq h_s(m-t)$ for all t.

Note that the characterization given in Proposition 4.4.2 gives an easy algorithm for determining the maximal value of $h_s(m)$. Let $\bar{\underset{\sim}{a}} \in \bar{A}$ be any vector for which $\bar{a}_1 - \bar{a}_s \leq 1$. Let $R_1 = (\bar{a}_1, \ldots, \bar{a}_{k-1})$ and $S_1 = (\bar{a}_k, \ldots, \bar{a}_s)$. Now simply go through the procedure of simultaneously adding one to the minimal value in R_1 and subtracting one from the maximal value in S_1 until a vector whose components satisfy Proposition 4.4.2 is found. The algorithm will be referred to as Algorithm (4.4) throughout the remainder of this paper. The following example will illustrate its use.

Example 4.4.3. Find the maximal value for $\sum_{i=1}^{6} a_i b_i - \sum_{i=1}^{6} a_i^2$ subject to the constraints that $\sum_{i=1}^{6} a_i = 8(2)$ and $\sum_{i=1}^{6} b_i = 6(2)$. Note that $s = 6$, $c = 6$, $p = 2$, and $k = 3$. Since $8(2) = 4(3) + 2(2)$, let $\bar{a}_1 = \bar{a}_2 = \bar{a}_3 = \bar{a}_4 = 3$ and $\bar{a}_5 = \bar{a}_6 = 2$. Using the algorithm, we obtain the following sequence of R_i and S_i.

$R_1 = (3,3) \qquad S_1 = (3,3,2,2)$

$R_2 = (4,3) \qquad S_2 = (3,2,2,2)$

$R_3 = (4,4) \qquad S_3 = (2,2,2,2)$

$R_4 = (5,4) \qquad S_4 = (2,2,2,1)$

$R_5 = (5,5) \qquad S_5 = (2,2,1,1)$

Note that all of the vectors $\bar{\underset{\sim}{a}}$ obtained at stages 3, 4, and 5 satisfy Proposition 4.4.2 and they all yield a maximal value for $f_s(\underset{\sim}{a},\underset{\sim}{b})$ of zero.

Lemma 4.4.4. Let k, c, and p be given positive integers. Let A_s and B_s be sets of vectors $\underset{\sim}{a} = (a_1, \ldots, a_s)$ and $\underset{\sim}{b} = (b_1, \ldots, b_s)$ where s, a_i, and b_i are integers satisfying the following constraints;

1) $k \leq s \leq (c+p)(k-1)$

2) $0 \leq a_i \leq (c+p)$ for $i = 1, \ldots, s$

3) $0 \leq b_i \leq c$ for $i = 1, \ldots, s$

4) $\sum_{i=1}^{s} a_i = (c+p)(k-1)$

5) $\sum_{i=1}^{s} b_i = c(k-1)$.

Let

$$f_s(\underset{\sim}{a}, \underset{\sim}{b}) = \sum_{i=1}^{s} a_i b_i - \sum_{i=1}^{s} a_i^2 .$$

i) If c is an even integer, then

$$\max_s \max_{\underset{\sim}{a} \in A_s} \max_{\underset{\sim}{b} \in B_s} f_s(\underset{\sim}{a}, \underset{\sim}{b}) = \frac{(k-1)(c^2 - 2c - 4p)}{4}$$

and ii) if c is an odd integer

$$\max_s \max_{\underset{\sim}{a} \in A_s} \max_{\underset{\sim}{b} \in B_s} f_s(\underset{\sim}{a}, \underset{\sim}{b}) = \frac{(k-1)[(c-1)^2 - 4p]}{4} .$$

Pf. For each fixed value of s, let $\bar{A}_s$ be the set of vectors $\underset{\sim}{\bar{a}} = (\bar{a}_1, \ldots, \bar{a}_s)$ defined previously in this section and let M_s denote the corresponding set of integers defined previously. Let $h_s(m)$ be that function defined on M_s where

$$h_s(m) = mc - \sum_{i=1}^{k-1} \bar{a}_i^2 - \sum_{i=k}^{s} \bar{a}_i^2$$

and $\underset{\sim}{\bar{a}} \in \bar{A}_s$ is the vector corresponding to $m \in M_s$.

Observe now that $M_s \subseteq M_{s+1}$ for all possible values of s and that for each fixed value of m, $\max_s h_s(m)$ will occur when for some value of s and $\underset{\sim}{\bar{a}} \in \bar{A}_s$ corresponding to m, $\sum_{i=k}^{s} \bar{a}_i^2$ is a minimum subject to the constraints that $0 \leq \bar{a}_i \leq c+p$, $\sum_{i=k}^{s} \bar{a}_i = (c+p)(k-1)$, and $k \leq s \leq (c+p)(k-1)$. It is easily seen that such a minimum will occur when $s = (c+p)(k-1)$. Note that the vector $\underset{\sim}{\bar{a}} \in \bar{A}_{(c+p)(k-1)}$ corresponding to m has the property that $\bar{a}_i = 0$ or 1 for $k \leq i \leq (c+p)(k-1)$ since $k-1 \leq m$ and $(c+p)(k-1)-m \leq (c+p)(k-1)-(k-1)$, hence for each $m \in M_{(c+p)(k-1)}$,

$$h_{(c+p)(k-1)}(m) = mc - \sum_{i=1}^{k-1} \bar{a}_i^2 - (c+p)(k-1) + m$$

where $\bar{a}_1 - \bar{a}_{k-1} \leq 1$ and $\sum_{i=1}^{k-1} \bar{a}_i = m$.

So now that value of m for which $h_{(c+p)(k-1)}(m)$ is maximal must be determined. Consider $m^* = (c/2)(k-1)$ when c is an even integer. Note that if $\underset{\sim}{a}^* \in \bar{A}_{(c+p)(k-1)}$ is the vector corresponding to m^*, then $a_1^* = \ldots = a_{k-1}^* = c/2$ and $a_k^* = 1$ and $a_{(c+p)(k-1)}^* = 0$ or 1 because $(c+p)(k-1)-m^* \leq (c+p)(k-1)-(k-1)$. The components of $\underset{\sim}{a}^*$ will clearly satisfy Proposition 4.4.2, hence this value of m yields a maximum for $h_{(c+p)(k-1)}(m)$ in $M_{(c+p)(k-1)}$ when c is an even integer. This maximal value is easily seen to be

$$\frac{(k-1)[c^2-2c-4p]}{r}.$$

When c is an odd integer, consider $m^* = ((c+1)/2)(k-1)$ in $M_{(c+p)(k-1)}$ and let $\underset{\sim}{a}^*$ be the corresponding vector in $\bar{A}_{(c+p)(k-1)}$. Note that $a_i^* = \ldots = a_{k-1}^* = (c+1)/2$ and $a_k^* = 1$ and $a_{(c+p)(k-1)}^* = 0$ or 1 because $(c+p)(k-1)-m^* \leq (c+p)(k-1)-(k-1)$. The components of $\underset{\sim}{a}^*$ will clearly satisfy Proposition 4.4.2, hence this value of m will yield a maximum for $h_{(c+p)(k-1)}(m)$ in $M_{(c+p)(k-1)}$ when c is an odd integer. The maximum value is easily seen to be

$$\frac{(k-1)[(c-1)^2-4p]}{4},$$

the desired result.

Proposition 4.4.4 will be of use in Chapter VI in determining an optimal property for the class of designs $\mathcal{D}[v;b;k]$.

Consider now constraints (4.4.1) for two different values of p, say $p_2 > p_1$. Let $\bar{A}_i$, $i = 1, 2$ be those sets of vectors $\bar{A}$ defined previously in this section for the two different sets of constraints and let M_i denote the corresponding sets of integers, i.e., $\underset{\sim}{\bar{a}} = (\bar{a}_1, \ldots, \bar{a}_s) \in \bar{A}_i$ if $\sum_{i=1}^{s} \bar{a}_i = (c+p_i)(k-1)$, $\bar{a}_1 \geq \ldots \geq \bar{a}_s$, $\bar{a}_1 - \bar{a}_{k-1} \leq 1$ and $\bar{a}_k - \bar{a}_s \leq 1$ and $m \in M_i$ if there is $\underset{\sim}{\bar{a}} \in \bar{A}_i$

such that $\sum_{i=1}^{k-1} \bar{a}_i = m$. Let $h_s^i(m)$, $i = 1, 2$ be that function defined previously on M_i, i.e.,

$$h_s^i(m) = mc - \sum_{i=1}^{k-1} \bar{a}_i^2 - \sum_{i=k}^{s} \bar{a}_i^2$$

where $m \in M_i$ and $\bar{\underset{\sim}{a}}$ is the vector in $\bar{A}_i$ corresponding to m.

Let $m \in M_1 \cap M_2$ and let $\bar{\underset{\sim}{c}}$ and $\bar{\underset{\sim}{d}}$ be the vectors in $\bar{A}_1$ and $\bar{A}_2$ corresponding to some such value of m. Since $p_2 > p_1$, $\sum_{i=k}^{s} \bar{c}_i < \sum_{i=k}^{s} \bar{d}_i$, and since $\bar{c}_k - \bar{c}_s$ and $d_k - d_s \leq 1$, we have $\bar{c}_i \leq \bar{d}_i$ for $i = 1, \ldots, s$, and so

$$\sum_{i=k}^{s} \bar{c}_i^2 < \sum_{i=k}^{s} \bar{d}_i^2 .$$

Also, since $\sum_{i=1}^{k-1} \bar{c}_i = \sum_{i=1}^{k-1} \bar{d}_i$, $\bar{c}_1 - \bar{c}_{k-1} \leq 1$ and $d_1 - d_{k-1} \leq 1$, we have $\bar{c}_i = \bar{d}_i$ for $i = 1, \ldots, k-1$, and so

$$mc - \sum_{i=1}^{k-1} \bar{c}_i^2 = mc - \sum_{i=1}^{k-1} \bar{d}_i^2 .$$

Now we have that

$$h_s^1(m) = mc - \sum_{i=1}^{k-1} \bar{c}_i^2 - \sum_{i=k}^{s} \bar{c}_i^2 > mc - \sum_{i=1}^{k-1} \bar{d}_i^2 - \sum_{i=k}^{s} \bar{d}_i^2 = h_s^2(m) .$$

So $h_s^1(m) > h_s^2(m)$ for all $m \in M_1 \cap M_2$.

Now consider $m_1 \in M_2$ but $m_1 \notin M_1$. Note that this implies $m_1 > (c+p_1)(k-1)$. Note also that

$$h_s^1[(c+p_1)(k-1)] = (c+p_1)(k-1)c - (k-1)(c+p_1)^2 .$$

Let $\bar{\underset{\sim}{d}}$ be the vector in $\bar{A}_2$ corresponding to m_1. Observe now that any polynomial of the form $gx-x^2$, $g > 0$, is decreasing for $x > g/2$. For $\bar{\underset{\sim}{d}}$, we have $\bar{d}_i \geq (c+p_1) > c/2$ for $1 \leq i \leq k-1$ and $\bar{d}_j > c+p_1$ for at least one value of j, $1 \leq j \leq k-1$, hence

$$h_s^2(m_1) = m_1 c - \sum_{i=1}^{k-1} \bar{d}_i^2 - \sum_{i=k}^{s} \bar{d}_i^2$$

$$= c \sum_{i=1}^{k-1} \bar{d}_i - \sum_{i=1}^{k-1} \bar{d}_i^2 - \sum_{i=k}^{s} \bar{d}_i^2$$

$$= \sum_{i=1}^{k-1} [c\bar{d}_i - \bar{d}_i^2] - \sum_{i=k}^{s} \bar{d}_i^2$$

$$\leq \sum_{i=1}^{k-1} [c\bar{d}_i - \bar{d}_i^2]$$

$$< (k-1)[c(c+p_1)-(c+p_1)^2]$$

$$= h_s^1[(c+p_1)(k-1)] .$$

Hence we see that for all values of m for which $h_s^2(m)$ is defined, there are values of h_s^1 which are larger, hence the maximal value for h_s^1 is larger than the maximal possible value for h_s^2. Since this argument can be repeated whenever $p_2 > p_1$, it follows that $\max_s h_s(m)$ decreases as p increases in constraints (4.4.1), hence that $\max_{\underset{\sim}{a} \epsilon A} \max_{\underset{\sim}{b} \epsilon B} f_s(\underset{\sim}{a}, \underset{\sim}{b})$ decreases as p increases in constraints (4.4.1).

Suppose now that $u \geq 1$ is an integer and that c is replaced by $c - u$ and p by $p + u$ in constraints (4.4.1). Let $\bar{A}_1$ and $\bar{A}_2$ denote the sets of vectors defined previously for constraints (4.4.1) and for constraints (4.4.1) when c is replaced by $c - u$ and p by $p + u$ respectively. Let M_1 and M_2 denote the corresponding sets of integers and let h_s^1 and h_s^2 denote the functions defined previously on M_1 and M_2. Note that for the two different sets of constraints, M_1 and M_2 contain the same integers. If m is any integer for which h_s^1 and h_s^2 are defined and if $\bar{\underset{\sim}{c}}$ and $\bar{\underset{\sim}{d}}$ are the corresponding vectors in $\bar{A}_1$ and $\bar{A}_2$, then

$$\sum_{i=1}^{k-1} \bar{c}_i = \sum_{i=1}^{k-1} \bar{d}_i$$

and

$$\sum_{i=k}^{s} \bar{c}_i = \sum_{i=1}^{s} \bar{d}_i$$

implies that $\bar{c}_i = \bar{d}_i$ for each i, hence that

$$h_s^1(m) = mc - \sum_{i=1}^{k-1} \bar{c}_i^2 - \sum_{i=k}^{s} \bar{c}_i^2$$

$$> m(c-u) - \sum_{i=1}^{k-1} \bar{d}_i^2 - \sum_{i=1}^{s} \bar{d}_i^2$$

$$= h_s^2(m) .$$

So for all values of $u > 0$,

$$\max_m h_s^1(m) > \max_m h_s^2(m) ,$$

hence we see that as c decreases and $c + p$ remains constant in constraints (4.4.1), $\max_{\underset{\sim}{a} \in A} \max_{\underset{\sim}{b} \in B} f_s(\underset{\sim}{a}, \underset{\sim}{b})$ will decrease.

Let $\bar{c}$ denote some fixed value of c in constraints (4.4.1) and let $\bar{p} = 2$. From the comments following Proposition 4.4.4, we see that if we simultaneously consider values of $c < \bar{c}$ and values of $p > \bar{p}$ in constraints 4.4.1, we will obtain smaller maximal values of $f_s(\underset{\sim}{a}, \underset{\sim}{b})$ than that obtained for $\bar{c} + \bar{p}$. This observation will prove useful in Chapter VI.

V. (M, S) OPTIMALITY IN $\mathcal{D}[v;(r_i)b;k]$

In this chapter, we consider the class of designs $\mathcal{D}[v;(r_i);b;k]$ defined in Chapter III where $r_i \leq b$ and $v > k$. For the rest of this chapter, this class of designs shall be denoted by $\mathcal{D}$.

5.1. Basic Lower Bounds

The first step in applying our optimality criterion is to determine $\mathcal{M}\{\mathcal{D}\}$, the set of designs in $\mathcal{D}$ having maximal trace. Since $v > k$ and $r_i \leq b$, there clearly exist binary designs in $\mathcal{D}$. Hence $\mathcal{D} \cap \mathcal{D}_1[v;b;k] \neq \phi$, and so by applying Lemma 4.3.7, the following statement can be made.

Theorem 5.1.1. $\mathcal{M}\{\mathcal{D}\}$ consists of all the binary designs in $\mathcal{D}$.

We now investigate the designs in $\mathcal{M}\{\mathcal{D}\}$ which have a minimal $\text{tr } C^2$. A natural question which arises is just how in fact can a design with minimal $\text{tr } C^2$ be recognized. One approach to answering the question would be to establish lower bounds for $\text{tr } C^2$ for designs in $\mathcal{M}\{\mathcal{D}\}$; and then try to find designs whose C-matrices have $\text{tr } C^2$ equal to one of the lower bounds. If such designs can be found, they will clearly be (M, S) optimal in $\mathcal{D}$. In what follows, several methods of establishing such lower bounds are discussed. We first give a fact recognized by Shah (1960) and which is implicit in the setting in which the (M, S) optimality criterion was introduced.

Theorem 5. 1. 2. If $\mathfrak{X}$ is an arbitrary class of incomplete block designs with v treatments such that $\operatorname{tr} C$ is constant for all $D \in \mathfrak{X}$, then any design in $\mathfrak{X}$ whose C-matrix has the form $\alpha I_v + \beta J_v$ will be (M, S) optimal in $\mathfrak{X}$.

Pf. Let M be the constant such that $\operatorname{tr} C = M$ for all $D \in \mathfrak{X}$. By using Lemma 4. 2. 3 and the fact that $\underline{r}(C) \leq v - 1$ for all $D \in \mathfrak{X}$, it is easily established that $\operatorname{tr} C^2 \geq M^2/(v-1)$ for all $D \in \mathfrak{X}$. Now let $\bar{D}$ denote any design in $\mathfrak{X}$ such that $\bar{C} = \alpha I_v + \beta J_v$. Because $\operatorname{tr}(\bar{C}) = M$ and because $\bar{C}\underset{\sim}{1}_v = 0$, it is seen that $\bar{C} = [M/(v-1)](I_v - v^{-1}J_v)$. But $\operatorname{tr} \bar{C}^2 = M^2/(v-1)$; so $\bar{D}$ must be (M, S) optimal in $\mathfrak{X}$.

From Theorem 5. 1. 2, any design D with a C-matrix of the form $\alpha I_v + \beta J_v$ will be (M, S) optimal in an arbitrary class of designs $\mathfrak{X}$ whenever $D \in \mathfrak{M}\{\mathfrak{X}\}$. For example, a balanced incomplete block design has a C-matrix of the form $\alpha I_v + \beta J_v$. Hence if there exists a BIBD in $\mathfrak{M}\{\mathfrak{X}\}$, then it will be (M, S) optimal in $\mathfrak{X}$.

Several lower bounds for $\operatorname{tr} C^2$ will now be developed for designs in $\mathcal{M}\{\mathcal{D}\}$. Some of the lower bounds will be easy to calculate while others will be computationally more difficult, though possibly more informative. Note that for any design in $\mathcal{M}\{\mathcal{D}\}$,

$$C = R - \frac{1}{k} NN'. \tag{5.1.3}$$

Hence

$$\begin{aligned} \operatorname{tr} C^2 &= \Big(\sum_i r_i^2\Big)\Big(1 - \frac{2}{k}\Big) + \frac{1}{k^2} \operatorname{tr}(NN')^2 \\ &= \Big(\sum_i r_i^2\Big)\Big(1 - \frac{1}{k}\Big)^2 + \frac{1}{k^2} \sum_{i \neq j}\sum \lambda_{ij}^2 . \end{aligned} \tag{5.1.4}$$

Also, since $\operatorname{tr}(NN')^2 = \operatorname{tr}(N'N)^2$,

$$\begin{aligned} \operatorname{tr} C^2 &= \Big(\sum_i r_i^2\Big)\Big(1 - \frac{2}{k}\Big) + \frac{1}{k^2} \operatorname{tr}(N'N)^2 \\ &= \Big(\sum_i r_i^2\Big)\Big(1 - \frac{2}{k}\Big) + b + \frac{1}{k^2} \sum_{i \neq j}\sum \mu_{ij}^2 . \end{aligned} \tag{5.1.5}$$

The first lower bounds for $\operatorname{tr} C^2$ will be established using expression (5.1.4). Since v, r_i, b, and k are fixed in $\mathcal{M}\{\mathcal{D}\}$, we see from (5.1.4) that finding a lower bound for $\operatorname{tr} C^2$ in $\mathcal{M}\{\mathcal{D}\}$ can be accomplished by simply finding a lower bound for

$tr(NN')^2$, or equivalently, for $\sum\sum_{i \neq j} \lambda_{ij}^2$. But a lower bound for this latter expression can easily be determined. To see this, let us note that the λ_{ij} are nonnegative integers and from Corollary 4.1.2 that $\sum\sum_{i \neq j} \lambda_{ij} = bk(k-1)$. Thus by solving the programming problem

$\min \sum\sum_{i \neq j} x_{ij}^2$ subject to the constraints that the x_{ij} are nonnegative integers such that $\sum\sum_{i \neq j} x_{ij} = bk(k-1)$, a lower bound will be determined for $\sum\sum_{i \neq j} \lambda_{ij}^2$ in $\mathcal{M}\{\mathcal{D}\}$. Now by using Corollary 4.3.5, we get the following result.

Theorem 5.1.6. For any design in $\mathcal{M}\{\mathcal{D}\}$

$$tr(NN')^2 \geq \sum_i r_i^2 + \sum\sum_{i \neq j} x_{ij}^2$$

where i) the x_{ij} are nonnegative integers, ii) $\sum\sum_{i \neq j} x_{ij} = bk(k-1)$, and iii) $|x_{ij} - x_{pq}| \leq 1$ for $i \neq j$, $p \neq q$.

Corollary 5.1.7. Any design $D \in \mathcal{M}\{\mathcal{D}\}$ having an incidence matrix N with the property that $|\lambda_{pq} - \lambda_{rs}| \leq 1$ for $p \neq q$, $r \neq s$, will be (M,S) optimal in $\mathcal{D}$.

Pf. Any design in $\mathcal{M}\{\mathcal{D}\}$ having the indicated property will meet the lower bound established in Theorem 5.1.6; hence it will be (M, S) optimal in $\mathcal{D}$.

Corollary 5.1.8. If $r_i = r$ for all i, and if in $\mathcal{M}\{\mathcal{D}\}$ there exists a PBIB(2) with $\lambda_2 = \lambda_1 + 1$, then that design will be (M, S) optimal in $\mathcal{D}$.

In deriving the lower bound for $tr(NN')^2$ given in Theorem 5.1.6, the most minimal linear constraints which the λ_{ij} must satisfy were used. When more stringent constraints are considered, lower bounds which are at least as good as the lower bound given in Theorem 5.1.6 are obtained; but the computational difficulty of calculating these lower bounds increases with the complexity of the constraints. Additional constraints will now be considered.

Recall from Corollary 4.1.2 that for fixed p, $\sum_{q \neq p} \lambda_{pq} = r_p(k-1)$. Thus by solving the programming problem $\min \sum\sum_{i \neq j} x_{ij}^2$ subject to the constraints that i) the x_{ij} are nonnegative integers and ii) for each fixed p, $\sum_{q \neq p} x_{pq} = r_p(k-1)$, a lower bound will be determined for $\sum\sum_{i \neq j} \lambda_{ij}^2$ in $\mathcal{M}\{\mathcal{D}\}$. For each p, let L_p denote the minimal value of $\sum_{q \neq p} x_{pq}^2$ subject to the relevant constraints. By

Corollary 4.3.5, L_p will be the value obtained when $|x_{pq}-x_{pr}| \leq 1$ for $q \neq p$, $r \neq p$. Now $L = \sum_i L_i$ gives a lower bound for $\sum\sum_{i \neq j} \lambda_{ij}^2$ in $\mathcal{M}\{\mathcal{D}\}$; hence we may state the following.

Theorem 5.1.9. For any design $D \in \mathcal{M}\{\mathcal{D}\}$,

$$\mathrm{tr}(NN')^2 \geq \sum_i r_i^2 + \sum\sum_{i \neq j} x_{ij}^2$$

where i) the x_{ij} are nonnegative integers, ii) for fixed p, $\sum_{q \neq p} x_{pq} = r_p(k-1)$, and iii) $|x_{pq}-x_{pr}| \leq 1$ for $q \neq p$, $r \neq p$.

Corollary 5.1.10. Any design $D \in \mathcal{M}\{\mathcal{D}\}$ having an incidence matrix N with the property that for each fixed value of p, $|\lambda_{pq}-\lambda_{pr}| \leq 1$, $q \neq p$, $r \neq p$, will be (M,S) optimal in $\mathcal{D}$.

Note that the lower bound given in Theorem 5.1.9 will always be at least as good as the lower bound given in Theorem 5.1.6. The following example is given to illustrate the computation of these lower bounds.

Example 5.1.11. Consider

$$\mathcal{M}\{\mathcal{D}[10; 5, 5, 4, 4, 4, 4, 4, 4, 4, 4; 14; 3]\}.$$

i) The lower bound given in Theorem 5.1.6 will first be calculated. We want to find the minimum for $\sum\sum_{i \neq j} x_{ij}^2$ subject to the constraints that the x_{ij} are nonnegative integers and that $\sum\sum_{i \neq j} x_{ij} = bk(k-1) = 84$. Now 84 can be represented uniquely as the sum of $v(v-1) = 10(9) = 90$ nonnegative integers such that $|x_{pq} - x_{rs}| \leq 1$ for $p \neq q$, $r \neq s$. Following the procedure outlined following Example 4.3.6, it is easily seen that

$$84 = 90(0) + 84 = 6(0) + 84(1).$$

Hence the lower bound for $tr(NN')^2$ given in Theorem 5.1.6 is

$$\sum_i r_i^2 + 6(0)^2 + 84(1)^2 = 262.$$

ii) The lower bound for $tr(NN')^2$ given in Theorem 5.1.9 will now be calculated. We want to find the minimum for $\sum\sum_{i \neq j} x_{ij}^2$ subject to the constraints that the x_{ij} are nonnegative integers and that for each fixed value of p, $\sum_{q \neq p} x_{pq} = r_p(k-1)$. For $p \leq 2$,

$$\sum_{q \neq p} x_{pq} = r_p(k-1) = 5(2) = 9(1) + 1 = 8(1) + 1(2);$$

hence L_p as defined in the proof of Theorem 5.1.9 is seen to be $8(1)^2 + 1(2)^2 = 12$. For $p \geq 3$,

$$\sum_{q \neq p} x_{pq} = r_p(k-1) = 4(2) = 9(0) + 8 = 1(0) + 8(1);$$

and L_p is seen to be $1(0)^2 + 8(1)^2$. Thus the lower bound for $tr(NN')^2$ given in Theorem 5.1.9 is

$$\sum_i r_i^2 + \sum_i L_i = 2(5)^2 + 8(4)^2 + 2(12) + 8(8) = 266\ .$$

The incidence matrix of a design achieving the lower bound established in ii) is given below:

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	B_{11}	B_{12}	B_{13}	B_{14}	
T_1	1	1	1	1	1										5
T_2				1	1	1	1	1							5
T_3	1							1	1	1					4
T_4		1					1		1		1				4
T_5			1			1			1			1			4
T_6				1						1		1	1		4
T_7					1					1	1			1	4
T_8	1						1					1		1	4
T_9		1				1							1	1	4
T_{10}			1					1			1		1		4
	3	3	3	3	3	3	3	3	3	3	3	3	3	3	

One final property possessed by the λ_{ij} which sometimes proves useful in the calculation of lower bounds for $\operatorname{tr} C^2$ in $\mathcal{M}\{\mathcal{D}\}$ is that for all i, j

$$\max[0, r_i + r_j - b] \le \lambda_{ij} \le \min[r_i, r_j] . \qquad \text{(Lemma 4.1.1)}$$

The following example illustrates the use of these new constraints in conjunction with those already given.

Example 5.1.12. Consider $\mathcal{M}\{\mathcal{D}[4; 5, 4, 2, 1; 6; 2]\}$.

i) The minimum for $\sum\sum_{i \ne j} x_{ij}^2$ subject to the constraints that the x_{ij} are nonnegative integers and $\sum\sum_{i \ne j} x_{ij} = bk(k-1) = 6(2) = 12$ is seen to occur when $x_{ij} = 1$ for all $i \ne j$. Hence the lower bound for $\operatorname{tr}(NN')^2$ given in Theorem 5.1.6 is $5^2 + 4^2 + 2^2 + 1^2 + 12(1)^2 = 58$.

ii) If L_p denotes the minimal value for $\sum_{q \ne p} x_{pq}$ subject to the constraints that the x_{pq} are nonnegative integers and $\sum_{q \ne p} x_{pq} = r_p(k-1)$, then it is easily seen that $L_1 = 9$, $L_2 = 6$, $L_3 = 2$, and $L_4 = 1$. Hence the lower bound for $\operatorname{tr}(NN')^2$ given in Theorem 5.1.9 is $\sum_i r_i^2 + \sum_i L_i = 5^2 + 4^2 + 2^2 + 1^2 + 9 + 6 + 2 + 1 = 64$.

iii) For each fixed value of p, let L_p denote the minimal value for $\sum_{q \neq p} x_{pq}^2$ subject to the constraints given in ii) above and $\max[0, r_p + r_q - b] \leq x_{pq} \leq \min[r_p, r_q]$. For $p = 1$, the actual constraints are $\sum_{q>1} x_{pq} = 5(1) = 5$, $3 \leq x_{12} \leq 4$, $1 \leq x_{13} \leq 2$, and $0 \leq x_{14} \leq 1$. Upon applying Algorithm (4.3), it is seen that $L_1 = 11$ and occurs when $x_{12} = 3$, $x_{13} = 1$, and $x_{14} = 1$. In a similar manner, it is easily seen that $L_2 = 10$, $L_3 = 2$, and $L_4 = 1$. Thus, an even better lower bound for $tr(NN')^2$ is obtained using the additional constraints. The actual lower bound is

$$\sum_i r_i^2 + L_1 + L_2 + L_3 + L_4 = 5^2 + 4^2 + 2^2 + 1^2 + 11 + 10 + 2 + 1 = 70.$$

The incidence matrix of a design satisfying the lower bound in iii) is given below:

	B_1	B_2	B_3	B_4	B_5	B_6	
T_1	1	1	1	1	1		5
T_2	1	1	1			1	4
T_3					1	1	2
T_4				1			1
	2	2	2	2	2	2	

A lower bound for $\operatorname{tr} C^2$ will now be determined using expression (5.1.5). Since v, r_i, b, and k are fixed in $\mathcal{M}\{\mathcal{D}\}$, it is seen from (5.1.5) that determining a lower bound for $\operatorname{tr} C^2$ in $\mathcal{M}\{\mathcal{D}\}$ is equivalent to determining a lower bound for $\operatorname{tr}(N'N)^2$ or $\sum\sum_{i \neq j} \mu_{ij}^2$. Note that the μ_{ij} must be nonnegative integers and from Lemma 4.1.1 that

$$\sum\sum_{i \neq j} \mu_{ij} = \sum_i r_i(r_i - 1).$$

Thus, proceeding in the same manner we did in establishing the lower bound in Theorem 5.1.6, we can again use Corollary 4.3.5 to obtain the following result.

<u>Theorem 5.1.13.</u> For any design in $\mathcal{M}\{\mathcal{D}\}$,

$$\operatorname{tr}(N'N)^2 \geq bk^2 + \sum\sum_{i \neq j} x_{ij}^2$$

where i) the x_{ij} are nonnegative integers, ii) $\sum\sum_{i \neq j} x_{ij} = \sum_i r_i(r_i - 1)$ and iii) $|x_{pq} - x_{rs}| \leq 1$ for $p \neq q$, $r \neq s$.

<u>Corollary 5.1.14.</u> Any design $D \in \mathcal{M}\{\mathcal{D}\}$ having an incidence matrix with the property that $|\mu_{pq} - \mu_{rs}| \leq 1$ for $p \neq q$, $r \neq s$, will be (M, S) optimal in $\mathcal{D}$.

For any design with incidence matrix N, $tr(NN')^2 = tr(N'N)^2$. However, the lower bounds determined for $tr(NN')^2$ and $tr(N'N)^2$ need not agree as the following example shows.

Example 5.1.15. Consider $\mathcal{M}\{\mathcal{D}[6; 3,3,3,3,2,2; 4; 4]\}$.

i) A lower bound will first be determined for $tr(NN')^2$ according to Theorem 5.1.6. Now $bk(k-1) = 48$ can be represented uniquely as the sum of nonnegative integers x_{ij} such that $|x_{pq} - x_{rs}| \leq 1$ for $p \neq q$, $r \neq s$. Following the procedure outlined following Example 4.3.6, it is easily seen that

$$48 = 30(1) + 18 = 12(1) + 18(2).$$

Hence the lower bound for $tr(NN')^2$ given in Theorem 5.1.6 is $\sum_{i=1}^{6} r_i^2 + 12(1)^2 + 18(2)^2 = 128$. With a little calculation, it can be seen that placing additional constraints upon the x_{ij} does not give a better bound for $tr(NN')^2$ for this example.

ii) A lower bound will now be determined for $tr(N'N)^2$ according to Theorem 5.1.13. Now $\sum_i r_i(r_i - 1) = 4(3)(2) + 2(2)(1) = 28$ has a unique representation as the sum of 12 nonnegative integers such that $|x_{pq} - x_{rs}| \leq 1$ for $p \neq q$, $r \neq s$. It is easily seen that

$$28 = 12(2) + 4 = 8(2) + 4(3).$$

Hence the lower bound for $tr(N'N)^2$ given in Theorem 5.1.13 is $bk^2 + 8(2)^2 + 4(3)^2 = 132$.

The techniques given so far for finding lower bounds for $tr(NN')^2$ and $tr(N'N)^2$ can also be used to show the nonexistence of certain designs with the property that $|\lambda_{pq}-\lambda_{rs}| \leq 1$ or $|\mu_{pq}-\mu_{rs}| \leq 1$ for $p \neq q$, $r \neq s$. This follows from the fact that any design in $\mathfrak{M}\{\mathcal{D}\}$ must have an incidence matrix with $tr(NN')^2 = tr(N'N)^2$ at least as large as any of the lower bounds established for $tr(NN')^2$ or $tr(N'N)^2$. Hence if the lower bound established in Theorem 5.1.13 for $tr(N'N)^2$ is larger than the lower bound established in Theorem 5.1.6 for $tr(NN')^2$, then there cannot exist a design in $\mathfrak{M}\{\mathcal{D}\}$ with $|\lambda_{pq}-\lambda_{rs}| \leq 1$ for $p \neq q$, $r \neq s$. A similar statement can be made if the lower bound established for $tr(N'N)^2$ is smaller than any of the lower bounds established for $tr(NN')^2$. We can state the following proposition.

<u>Proposition 5.1.16</u>. If in $\mathfrak{M}\{\mathcal{D}\}$, $r_i = r_j$ for all i, j and the lower bound established for $tr(N'N)^2$ in Theorem 5.1.13 is larger than the lower bound determined for $tr(NN')^2$ in Theorem 5.1.6, then there cannot exist a BIBD or a PBIB(2) with $\lambda_2 = \lambda_1 + 1$ in $\mathfrak{M}\{\mathcal{D}\}$.

<u>Example 5.1.17</u>. Consider $\mathcal{M}\{\mathcal{D}[10;2;4;5]\}$.

i) A lower bound for $\operatorname{tr}(NN')^2$ will first be determined.

Write

$$\sum\sum_{i \neq j} \lambda_{ij} = bk(k-1) = 4(5)(4) = 80$$

as $90(0) + 80 = 10(0) + 80(1)$. Hence the lower bound for $\operatorname{tr}(NN')^2$ given in Theorem 5.1.6 is $10(2)^2 + 10(0)^2 + 80(1)^2 = 120$.

ii) A lower bound for $\operatorname{tr}(N'N)^2$ will not be determined. Write

$$\sum\sum_{i \neq j} \mu_{ij} = \sum_i r_i(r_i - 1) = 10(2)(1)$$

as $12(1) + 8 = 4(1) + 8(2)$. Hence the lower bound for $\operatorname{tr}(N'N)^2$ given in Theorem 5.1.13 is $4(5)^2 + 4(1)^2 + 8(2)^2 = 136$.

Thus the lower bound established for $\operatorname{tr}(N'N)^2$ is larger than the lower bound established for $\operatorname{tr}(NN')^2$, and so Proposition 5.1.16 may be applied.

Let $[\cdot]$ denote the greatest integer function. For any value of p let $m_p = [r_p(k-1)/(v-1)]$. Now $r_p(k-1)$ can be written uniquely as the sum of $v-1$ nonnegative integers differing by at most one. This unique representation is given by

$$r_p(k-1) = (v-1)m_p + n_p = (v-1-n_p)m_p + n_p(m_p+1).$$

Proposition 5.1.18. Let m_p and n_p be as defined above. Then the following conditions are necessary for a binary design to exist whose incidence matrix has the property that for each fixed value of p, $|\lambda_{pq}-\lambda_{pr}| \leq 1$ for $q \neq p$, $r \neq p$.

i) $|m_p-m_q| \leq 1$ for all $p \neq q$.

ii) Let J_1 denote the set of subscripts of treatments having minimal values of m_p. If $p \in J_1$, then $v-n_p$ must be less than or equal to the number of subscripts in J_1.

iii) Let J_2 denote the set of subscripts of treatments having maximal values of m_p. If $p \in J_2$, then n_p must be less than or equal to the number of subscripts in J_2.

iv) Let J_2 be defined as in iii). Then $\sum_{p \in J_2} n_p$ cannot be odd.

v) Let J_1 be as defined in ii), then $\sum_{p \in J_1} (v-1-n_p)$ cannot be odd.

Pf. i) Suppose for all fixed values of i, $|\lambda_{ij}-\lambda_{i\ell}| \leq 1$ for $j \neq i$, $\ell \neq i$. Now suppose there exists p and q such that $m_p-m_q \geq 2$. From above, we see that since $|\lambda_{ps}-\lambda_{pt}| \leq 1$ for $s \neq p$, $s \neq t$, and $|\lambda_{qs}-\lambda_{qt}| \leq 1$ for $q \neq s$, $q \neq t$, we must have $\lambda_{ps} = m_p$ or m_p+1 for all $s \neq p$ and $\lambda_{qs} = m_q$ or m_q+1 for all $s \neq q$. But then λ_{pq} must simultaneously equal m_p or

m_p+1 and m_q or m_q+1, a contradiction since $m_p - m_q \geq 2$.

ii) Recalling i) let J_2 be defined as in iii) of the proposition. Assume that for each fixed value of i, $|\lambda_{ij} - \lambda_{i\ell}| \leq 1$ for $j \neq i$, $\ell \neq i$. Assume also that there exists $p \in J_1$ with $v - n_p$ greater than the number of subscripts in J_1. In order for $|\lambda_{pq} - \lambda_{pr}| \leq 1$ for $q \neq p$, $r \neq p$, we must have exactly $v-1-n_p$ of the λ_{pq}, $p \neq q$, equal to m_p. Since $v - n_p$ is larger than the number of subscripts in J_1, there must exist $s \in J_2$ such that $\lambda_{ps} = m_p$. But $m_s = m_p+1$ and in order for $|\lambda_{st} - \lambda_{su}| \leq 1$ for $t \neq s$, $u \neq s$, we must have $\lambda_{st} = m_s$ or m_s+1 for all $t \neq s$, a contradiction. Hence it must be that $v - n_p$ is not larger than the number of subscripts in J_1.

iii) Similar to ii).

iv) and v) are simple consequences of the fact that NN' is a symmetric matrix, that $\sum_{p \in J_2} n_p$ denotes the number of λ_{ij}, $i \neq j$, equal to the maximal value of m_p, and that $\sum_{p \in J_1} (v - n_p - 1)$ denotes the number of λ_{ij}, $i \neq j$, equal to the minimal value of m_p.

Example 5.1.19. Consider the class of designs $\mathcal{M}\{\mathcal{D}[6;5,4,4,4,4,3;6;4]\}$. Now $m_1 = [5(3)/5] = 3$ and $m_2 = [3(3)/5] = 1$, hence statement i) of the proposition is violated. So there cannot exist a design in $\mathcal{M}\{\mathcal{D}[6;5,4,4,4,4,3;6;4]\}$ with an incidence matrix having the property that for fixed p, $|\lambda_{pq}-\lambda_{pr}| \leq 1$ for $q \neq p$, $r \neq p$.

Example 5.1.20. Consider the class of designs $\mathcal{M}\{\mathcal{D}[5;4,4,4,3,3;6;3]\}$. Now $m_1 = m_2 = m_3 = 2$ and $m_4 = m_5 = 1$, hence $J_1 = \{4,5\}$ and $J_2 = \{1,2,3\}$. But

$$r_4(k-1) = 6 = (v-1)m_2 + n_4 = 4(1) + 2;$$

hence $v-n_4 = 3$ is larger than the number of subscripts in J_1 so statement ii) of the proposition is violated. Thus, there cannot exist a design in $\mathcal{M}\{\mathcal{D}[5;4,4,4,3,3;6;3]\}$ with an incidence matrix having the property that for fixed p, $|\lambda_{pq}-\lambda_{pr}| \leq 1$ for $q \neq p$, $r \neq p$.

Example 5.1.21. Consider the class of designs $\mathcal{M}\{\mathcal{D}[8;4,4,4,3,3,3,3,3;9;3]\}$. Now $m_i = 1$, $1 \leq i \leq 3$, and $m_i = 0$, $i \geq 4$, hence $J_1 = \{4,5,6,7,8\}$ and $J_2 = \{1,2,3\}$. But

$$r_p(k-1) = (v-1)m_p + n_p = 7(1) + 1 \quad \text{for} \quad p \in J_2,$$

hence $\sum_{p \in J_2} n_p = 3$ is odd and statement iv) of the proposition is violated. So there cannot exist a design in $\mathcal{M}\{\mathcal{D}[8;4,4,4,3,3,3,3,3,;9;3]\}$. having an incidence matrix with the property that for fixed p, $|\lambda_{pq} - \lambda_{pr}| \leq 1$ for $q \neq p$, $r \neq p$.

5.2. Another Lower Bound

Let $\mathcal{D} = \mathcal{D}[v;(r_i);b;k]$ be defined as in the previous section. Recall that finding a lower bound for $\text{tr } C^2$ in $\mathcal{M}\{\mathcal{D}\}$ is equivalent to finding a lower bound for $\text{tr}(NN')^2$ in $\mathcal{M}\{\mathcal{D}\}$. To this point, no use has been made of the fact that NN' is a symmetric matrix. The method given in this section for determining a lower bound for $\text{tr}(NN')^2$ takes advantage of this fact.

Let N be the incidence matrix of a typical design in $\mathcal{M}\{\mathcal{D}\}$ consisting of b blocks, each of size k, with v treatments such that treatment T_p is replicated r_p times. Without loss of generality, suppose $r_1 \geq r_2 \geq \cdots \geq r_v$. Now partition N into N_1 and N_2 where N_1 consists of the first v_1 rows of N and N_2 consists of the remaining $v - v_1 = v_2$ rows of N. So N_1 is a $v_1 \times b$ matrix and N_2 is a $v_2 \times b$ matrix. Note that the $\sum_{i=1}^{v_1} r_i = n_1$ experimental units assigned to $T_1, \ldots, T_{v_1}$ must occur in N_1, the $\sum_{i=v_1+1}^{v} r_i = n_2$ experimental units assigned to $T_{v_1+1}, \ldots, T_v$ must occur in N_2 and the k experimental units assigned to block B_i must be allocated between N_1 and N_2. Let B_i^* represent that part of block B_i contained in N_1, B_i^{**} that part of block B_i occurring in N_2, and let k_i^* and k_i^{**} represent the number of experimental units allocated to B_i^* and B_i^{**}. Then it must be the case that

$$\text{i)} \quad \sum_{i=1}^{b} k_i^* = n_1$$

$$\text{ii)} \quad \sum_{i=1}^{b} k_i^{**} = n_2 \qquad (5.2.1)$$

$$\text{iii)} \quad k_i^* + k_i^{**} = k \ .$$

Without loss of generality let us assume that $k_1^* \geq k_2^* \geq \cdots \geq k_b^*$. Let any particular ordered allocation of k_i^* to B_i^* be called an ordered configuration and denote any such configuration by $(k_1^*, \ldots, k_b^*)$.

Note that when N is partitioned as above,

$$tr(NN')^2 = tr(N_1N_1')^2 + tr(N_2N_2')^2 + 2\sum_{i=1}^{v_1}\sum_{v_1+1}^{v}\lambda_{ij}^2 .$$

Recall from Lemmas 4.1.1 and 4.1.3 that the entries in the three terms given in the expression above for $tr(NN')^2$ must satisfy

i) $2\sum_{i=1}^{v_1}\sum_{j>i}^{v_1}\lambda_{ij} = C_1$ where $C_1 = \sum_{i=1}^{b} k_i^*(k_i^*-1)$

ii) $2\sum_{i=v_1+1}^{v}\sum_{j>i}^{v}\lambda_{ij} = C_2$ where $C_2 = \sum_{i=1}^{b} k_i^{**}(k_i^{**}-1)$

iii) $2\sum_{i=1}^{v_1}\sum_{j=v_1+1}^{v}\lambda_{ij} = C_{12}$ where $C_{12} = 2\sum_{i=1}^{b} k_i^*(k_i^{**})$

iv) $\max[0, r_p+r_q-b] \le \lambda_{pq} \le \min[r_p, r_q]$.

Hence we see that for a given ordered configuration $(k_1^*, \ldots, k_b^*)$, a lower bound for $tr(NN')^2$ can be determined for any design whose incidence matrix has that configuration by solving the integer programming problem of minimizing

$$\sum_{i=1}^{v} r_i^2 + 2\sum_{i=1}^{v_1}\sum_{j>i}^{v_1} x_{ij}^2 + 2\sum_{i=v_1+1}^{v}\sum_{j>i}^{v} x_{ij}^2 + 2\sum_{i=1}^{v_1}\sum_{j=v_1+1}^{v} x_{ij}^2 \qquad (5.2.2)$$

subject to the constraints that

$$\text{i)}\quad 2\sum_{i=1}^{v_1}\sum_{j>i}^{v_1} x_{ij} = C_1$$

$$\text{ii)}\quad 2\sum_{i=v_1+1}^{v}\sum_{j>i}^{v} x_{ij} = C_2$$

(5. 2. 3)

$$\text{iii)}\quad 2\sum_{i=1}^{v_1}\sum_{j=v_1+1}^{v} x_{ij} = C_{12}$$

$$\text{iv)}\quad \max[0, r_p+r_q-b] \le x_{pq} \le \min[r_p, r_q].$$

For a design having a given ordered configuration, the actual minimal value is obtained by applying Algorithm (4. 3) to each of the terms in (5. 2. 2) subject to the relevant constraints in (5. 2. 3). Observe that if two distinct configurations yield the same values of C_1, C_2, and C_{12}, then the same minimal value for (5. 2. 2) subject to (5. 2. 3) will be obtained. Now observe that

$$\text{i)}\quad \sum_{i=1}^{v_1} r_i(k-1) = C_1 + (C_{12}/2)$$

(5. 2. 4)

$$\text{ii)}\quad \sum_{i=v_1+1}^{v} r_i(k-1) = C_2 + (C_{12}/2).$$

From (5.2.4), we see that when one of the values of C_1, C_2, or C_{12} is known, the remaining values are completely determined. Hence when two configurations yield the same value of C_1, they must also yield the same values for C_2 and C_{12} and the same minimal values for $tr(NN')^2$. So for a particular partition, to find a lower bound for $tr(NN')^2$, we must find those values of C_1, C_2, and C_{12} and those configurations giving these values of C_1, C_2, and C_{12} which yield the smallest possible minimal value for (5.2.2) subject to (5.2.3). A method will now be given for doing this.

Let $(k_1^*, \ldots, k_b^*)$ be any ordered configuration and let the values of C_1, C_2, and C_{12} given by this configuration be denoted by $\hat{C}_1$, $\hat{C}_2$, and $\hat{C}_{12}$. Now take any m and n such that $k_m^* \geq k_n^*$ and such that

$$\begin{aligned} &\text{i)}\ k_i^* > k_m^*, \quad i < m \\ &\text{ii)}\ k_i^* < k_n^*, \quad i > n \\ &\text{iii)}\ k_m^*+1 \leq \min[k, v_1] \\ &\text{iv)}\ k_n^{**}+1 \leq \min[k, v_2] \end{aligned} \qquad (5.2.5)$$

Form a new ordered configuration with k_m^* replaced by k_m^*+1 and k_n^* replaced by k_n^*-1 in the old ordered configuration. Let $p = k_m^* - k_n^*$. Then the values of C_1, C_2, and C_{12} that are given by the new ordered configuration are $\hat{C}_1+2p+2$, $\hat{C}_2+2p+2$, and $\hat{C}_{12}-4p-4$. Let any ordered pair of block sizes k_m^* and k_n^* satisfying (5.2.5) and such that $k_m^*-k_n^* = p$ be denoted by $(k_m^*, k_n^*)_p$. Note that for each distinct ordered pair $(k_m^*, k_n^*)_p$ of block sizes, a distinct ordered configuration can be generated from $(k_1^*, \ldots, k_b^*)$ in the manner described above. So there is a one to one correspondence between ordered pairs $(k_m^*, k_n^*)_p$ and distinct ordered configurations which can be generated from $(k_1^*, \ldots, k_b^*)$. Note also that the least amount by which $\hat{C}_1$ can be increased by forming a new configuration in this way is two and that this will occur when $p = 0$.

Observe that if in the above process of generating configurations from $(k_1^*, \ldots, k_b^*)$, there are ordered pairs of block sizes $(k_i^*, k_j^*)_{p_1}$ and $(k_i^*, k_m^*)_{p_2}$ satisfying (5.2.5) with $p_2 > p_1$, then that configuration formed from $(k_i^*, k_m^*)_{p_2}$ can be generated from the configuration formed from $(k_i^*, k_j^*)_{p_1}$. This is done by first forming the configuration with k_i^*+1 and k_j^*-1 giving $\hat{C}_1+2p_1+2$ and then from this configuration forming the one associated with the ordered pair $(k_h^*, k_m^*)_{p_2-p_1-1}$ satisfying (5.2.5) where $k_h^* = k_j^*-1$. A similar argument can be made for ordered pairs of the form $(k_i^*, k_j^*)_{p_1}$ and $(k_m^*, k_j^*)_{p_2}$, $p_2 > p_1$. It is also a simple matter to see that if there are ordered pairs of the form $(k_i^*, k_j^*)_{p_1}$ and $(k_m^*, k_n^*)_{p_2}$ with $p_2 \geq p_1 \geq 2$, then that configuration generated for $\hat{C}_1+2p_2+2$ using $(k_m^*, k_n^*)_{p_2}$ can be generated from a configuration giving $\hat{C}_1+2p_2-2p_1+4$. With this in mind, we give the following definition:

<u>Definition 5.2.6.</u> Let $(k_1^*, \ldots, k_b^*)$ denote some ordered configuration for a given partition. We shall say that a configuration which is derived from $(k_1^*, \ldots, k_b^*)$ using the ordered pair $(k_i^*, k_j^*)_p$ satisfying (5.2.5) is minimally derivable from $(k_1^*, \ldots, k_b^*)$ if there do not exist other ordered pairs satisfying (5.2.5) of the form

i) $(k_i^*, k_m^*)_q$, $q < p$

ii) $(k_m^*, k_j^*)_q$, $q < p$

iii) $(k_m^*, k_n^*)_q$, $p \geq q \geq 2$.

If $\hat{C}_1$ is some value of C_1 for which an ordered configuration exists, then it is easily seen that all ordered configurations giving $\hat{C}_1$ are minimally derivable from configurations associated with smaller values of C_1.

With these things in mind, let v_1 assume a particular value and let $(k_1^*, \ldots, k_b^*)$ be that unique ordered configuration where

$\sum_{i=1}^{b} k_i^* = n_1$ and $k_1^* - k_b^* \leq 1$. Using Corollary 4.3.5, it is seen that this configuration gives the minimal possible value for C_1 and C_2, hence the maximal possible value for C_{12}. Let $\bar{C}_1$, $\bar{C}_2$, and $\bar{C}_{12}$ denote the values of C_1, C_2, and C_{12} given by this configuration. Beginning with $\bar{C}_1$, apply Algorithm (4.3) to the problem of determining a minimal value for (5.2.2) subject to the constraints given in (5.2.3) for successively larger values of C_1 for which configurations exist. Those values of C_1 for which ordered configurations exist are determined by minimally deriving configurations from ordered configurations associated with smaller values of C_1. For instance, the set of ordered configurations giving the value of C_1 closest to $\bar{C}_1$ must be minimally derived from that configuration giving $\bar{C}_1$, etc.

For a fixed value of C_1, let x and y denote the minimal values of x_{pq} and x_{st} calculated using Algorithm (4.3) for the sum of squares associated with C_1 and C_2 respectively such that $x_{pq}+1$ and $x_{st}+1$ still satisfy the appropriate constraints, i.e., if $x = x_{pq}$ and $y = x_{st}$, then

$$\max[0, r_p+r_q-b] \leq x_{pq}+1 \leq \min[r_p, r_q]$$

and

$$\max[0, r_s+r_t-b] \leq x_{st}+1 \leq \min[r_s, r_t] .$$

Similarly, let $z_1 \geq z_2$ be the maximal values of the x_{ij} calculated for the sum of squares associated with C_{12} such that $z_1 - 1$ and $z_2 - 1$ still satisfy the constraints for the corresponding x_{ij}. In applying Algorithm (4.3), it is easily seen that the minimal value calculated for (5.2.2) subject to (5.2.3) for $C_1 + 2$ contains exactly the same values of x_{ij} as the minimal value obtained for C_1 except that x is replaced by $x+1$, y by $y+1$, and z_1 by $z_1 - 2$ if $z_1 - z_2 \geq 2$ and $z_1 - 2$ satisfies the constraints on the corresponding x_{ij}, otherwise z_1 is replaced by $z_1 - 1$ and z_2 is replaced by $z_2 - 1$. From this it is seen that when $z_1 - z_2 \geq 2$ and $z_1 - 2$ still satisfies the constraints on the corresponding x_{ij}, a smaller minimal value for (5.2.2) subject to (5.2.3) is obtained for $C_1 + 2$ if and only if $2z_1 > x+y+3$, a larger minimal value is obtained if and only if $2z_1 < x+y+3$, and no change occurs if and only if $2z_1 = x+y+3$. In all other cases, i.e., when $z_1 - z_2 \leq 1$ or when $z_1 - z_2 \geq 2$ and $z_1 - 2$ does not satisfy the constraints for the corresponding x_{ij}, a smaller minimal value for (5.2.2) subject to (5.2.3) is obtained for $C_1 + 2$ if and only if $z_1 + z_2 > x+y+2$, a larger minimal value is obtained if and only if $z_1 + z_2 < x+y+2$, and no change occurs if and only if $z_1 + z_2 = x+y+2$.

Let C_1^* be some value of C_1 such that one of the following conditions holds:

i) $\tilde{z}_1-\tilde{z}_2 > 1$, $\tilde{z}_1-2$ still satisfies the conditions for the corresponding x_{ij} and $2\tilde{z}_1 < \tilde{x}+\tilde{y}+3$

ii) $\tilde{z}_1-\tilde{z}_2 > 1$, $\tilde{z}_1-2$ does not satisfy the conditions for the corresponding x_{ij} and $\tilde{z}_1+\tilde{z}_2 < \tilde{x}+\tilde{y}+2$ (5.2.7)

iii) $\tilde{z}_1-\tilde{z}_2 \leq 1$ and $\tilde{z}_1+\tilde{z}_2 < \tilde{x}+\tilde{y}+2$.

where $\tilde{x}$, $\tilde{y}$, $\tilde{z}_1$, and $\tilde{z}_2$ are defined in the same manner as x, y, z_1, and z_2. Then for all values of $C_1 > \tilde{C}_1$, it is easily seen that

$$2z_1 \leq 2\tilde{z}_1 < \tilde{x}+\tilde{y}+3 \leq x+y+3$$

or

$$z_1+z_2 \leq \tilde{z}_1+\tilde{z}_2 < \tilde{x}+\tilde{y}+2 \leq x+y+2.$$

Hence all values of $C_1 > \tilde{C}_1$ will give larger values of (5.2.2) subject to (5.2.3) than $\tilde{C}_1$. So by beginning with $\bar{C}_1$ and determining lower bounds for successively larger values of C_1 until some $\tilde{C}_1$ for which any of conditions (5.2.7) hold, all values of C_1 yielding the smallest minimal value of (5.2.2) subject to (5.2.3) will be determined. The general procedure will be illustrated by the following examples.

<u>Example 5.2.8.</u> Consider the class of designs $\mathcal{M}\{\mathcal{D}[7;5,5,5,5,4,4,4;8;4]\}$ and let $v_1 = 4$. That ordered

configuration which minimizes C_1 when $v_1 = 4$ is $(3,3,3,3,2,2,2,2)$, and $\bar{C}_1 = 32$, $\bar{C}_2 = 8$, and $\bar{C}_{12} = 56$. Beginning with $\bar{C}_1$, we must now determine a minimal value for

$$\sum_{i=1}^{7} r_i^2 + 2\sum_{i=1}^{4}\sum_{j>i}^{4} x_{ij}^2 + 2\sum_{i=5}^{7}\sum_{j>i}^{7} x_{ij}^2 + 2\sum_{i=1}^{4}\sum_{j=5}^{7} x_{ij}^2 \qquad (5.2.9)$$

subject to the constraints that

$$\text{i)}\quad 2\sum_{i=1}^{4}\sum_{j>i}^{4} x_{ij} = C_1$$

$$\text{ii)}\quad 2\sum_{i=5}^{7}\sum_{j>i}^{7} x_{ij} = C_2$$

$$\text{iii)}\quad 2\sum_{i=1}^{4}\sum_{j=5}^{7} x_{ij} = C_{12} \qquad (5.2.10)$$

$$\text{iv)}\quad \max[0, r_p + r_q - b] \le x_{pq} \le \min[r_p, r_q] .$$

For $\bar{C}_1 = 32$, we see upon applying Algorithm (4.3) to each of the expressions in (5.2.9) subject to the relevant constraints in (5.2.10) that a minimal value is reached when $x_{ij} = 2$ or 3 for $1 \le i, j \le 4$, $i \neq j$; $x_{ij} = 1$ or 2 for $5 \le i, j \le 7$, $i \neq j$; and $x_{ij} = 2$ or 3 for $1 \le i \le 4$, $5 \le j \le 7$. Let x, y, z_1, and z_2 be defined as in the previous paragraph. For $C_1 = 32$, $x = 2$, $y = 1$, and $z_1 = z_2 = 3$. Since $z_1 - z_2 \leq 1$ and $z_1 + z_2 > x+y+2$, we see that a larger value of C_1 will yield a smaller value of (5.2.9) subject to (5.2.10). Hence we see that we must find the next value of C_1 for which configurations exist as well as the configurations yielding this value of C_1.

The set of ordered pairs of block sizes from (3, 3, 3, 3, 2, 2, 2, 2) which satisfy Definition 5.2.6 are $\{(k_1^*, k_4^*)_0, (k_5^*, k_8^*)_0\}$ and the configurations giving $C_1 = 34$ which are minimally derivable using these ordered pairs are easily seen to be (4, 3, 3, 2, 2, 2, 2, 2) and (3, 3, 3, 3, 3, 2, 2, 1). Observe that the ordered pair $(k_1^*, k_8^*)_1$ does not satisfy Definition 5.2.6, hence that configuration formed from this ordered pair is not minimally derivable from (3, 3, 3, 3, 2, 2, 2, 2). Thus we see that the next largest value of C_1 is 34.

When $C_1 = 34$, it is easily seen upon applying Algorithm (4.3) to each of the expressions in (5.2.9) subject to the relevant constraints in (5.2.10) that $x = 2$, $y = 1$, and $z_1 = z_2 = 3$. Hence $z_1 - z_2 \leq 1$ and $z_1 + z_2 > x+y+2$; so from (5.2.7), we see that a larger value of C_1 will give a smaller value of (5.2.9) subject to (5.2.10). Those ordered configurations which are minimally derivable from those configurations giving $C_1 = 34$ are given below as well as the ordered pairs of block sizes satisfying Definition 5.2.6 used to generate them.

Configuration	Ordered Pair	Derived Configuration	New Value of C_1
(4, 3, 3, 2, 2, 2, 2, 2)	$(k_2^*, k_3^*)_0$	(4, 4, 2, 2, 2, 2, 2, 2)	36
	$(k_4^*, k_5^*)_0$	(4, 3, 3, 3, 2, 2, 2, 1)	36
	$(k_1^*, k_3^*)_1$	(5, 3, 2, 2, 2, 2, 2, 2)	38
	$(k_2^*, k_8^*)_1$	(4, 4, 3, 2, 2, 2, 2, 1)	38
(3, 3, 3, 3, 3, 2, 2, 1)	$(k_1^*, k_5^*)_0$	(4, 3, 3, 3, 2, 2, 2, 1)	36
	$(k_6^*, k_7^*)_0$	(3, 3, 3, 3, 3, 3, 1, 1)	36
	$(k_1^*, k_7^*)_1$	(4, 3, 3, 3, 3, 2, 1, 1)	38
	$(k_6^*, k_8^*)_1$	(3, 3, 3, 3, 3, 3, 2, 0)	38

From above, we see that the next largest value of C_1 is 36.

When $C_1 = 36$ and Algorithm (4.3) is applied to (5.2.8) subject to (5.2.9), it is easily seen that $x = 2$, $y = 2$, and $z_1 = z_2 = 2$. Hence $z_1 - z_2 \leq 1$ and $z_1 + z_2 < x+y+2$; so from (5.2.7), we see that $C_1 = 38$ will give a larger minimal value for (5.2.8) subject to (5.2.9). Hence when $C_1 = 36$, $C_2 = 12$, and $C_{12} = 56$, we obtain a lower bound for $tr(NN')^2$ for $v_1 = 4$. The actual lower bound is easily seen to be 376. With a little calculation, it is also easy to see that none of the lower bounds obtained using the methods of Section 5.1 is as large as this.

Note that we do not only have a lower bound for

$tr(NN')^2$, but we have the set of ordered configurations which any design with $tr(NN')^2 = 376$ must possess when its incidence matrix is partitioned as in this example. From above, we see that those ordered configurations are $\{(4,4,2,2,2,2,2,2), (4,3,3,3,2,2,2,1), (3,3,3,3,3,3,1,1)\}$.

Example 5.2.10. Consider the class of designs $\mathcal{M}\{\mathcal{D}[5;5,5,4,3,1;6;3]\}$.

i) The lower bound for $tr(NN')^2$ given following Theorem 5.1.9 will first be determined. For a fixed value of i, let L_i denote the minimum of $\sum_{j \neq i} x_{ij}^2$ subject to the constraints that the x_{ij}, $i \neq j$, are nonnegative integers, $\max[0, r_i+r_j-b] \le x_{ij} \le \min[r_i, r_j]$, and $\sum_{j \neq i} x_{ij} = r_i(k-1)$. Upon applying Algorithm (4.3) to the problem of determining L_i subject to the relevant constraints, it is seen that $L_1 = 30$, $L_2 = 30$, $L_3 = 20$, $L_4 = 10$, and $L_5 = 2$. Hence a lower bound for $tr(NN')^2$ is $\sum_i r_i^2 + \sum_i L_i = 2(5)^2 + 4^2 + 3^2 + 1^2 + \sum_i L_i = 168$.

ii) The lower bound for $tr(N'N)^2$ given in Theorem 5.1.13 will now be determined. Note that

$$\sum\sum_{i \neq j} \mu_{ij} = \sum_i r_i(r_i - 1) = 58$$

Using Corollary 4.3.5, we see that the lower bound for $tr(N'N)^2$ given in Theorem 5.1.13 occurs when two of the x_{ij} are equal to one and the remaining x_{ij} equal two. The actual lower bound is $bk^2 + 2(1)^2 + 28(2)^2 = 168$.

iii) A lower bound will now be determined for $tr(NN')^2$ by the method given in this section for $v_1 = 4$. Note that the only possible ordered configuration is $(3,3,3,3,3,2)$, hence the only possible values for C_1, C_2, and $C_{12} = 2r_5(k-1)$ are 32, 0, and 4 respectively. Hence we must determine a lower bound for

$$\sum_{i=1}^{5} r_i^2 + 2\sum_{i=1}^{5}\sum_{j>i}^{5} x_{ij}^2$$

subject to the constraints that

i) The x_{ij} are nonnegative integers

ii) $\max[0, r_i+r_j-b] \leq x_{ij} \leq \min[r_i, r_j]$

iii) $2\sum_{i=1}^{4}\sum_{j>i}^{4} x_{ij} = 32$

iv) $2\sum_{i=1}^{4} x_{i5} = 4.$

By applying Algorithm (4.3), it is seen that a lower bound for $tr(NN')^2$ is attained when $\lambda_{35} = \lambda_{45} = 0$, $\lambda_{15} = \lambda_{25} = 1$, $\lambda_{14} = \lambda_{24} = 2$, $\lambda_{13} = \lambda_{23} = 3$, and $\lambda_{12} = 4$. The lower bound obtained for $tr(NN')^2$ is 172. Note that this lower bound is larger than those obtained in i) and ii) and the design whose incidence matrix is given below meets this lower bound; so it is (M, S) optimal.

	B_1	B_2	B_3	B_4	B_5	B_6	
T_1	1	1	1	1	1		5
T_2		1	1	1	1	1	5
T_3	1	1	1			1	4
T_4	1				1	1	3
T_5				1			1
	3	3	3	3	3	3	

VI. (M,S) OPTIMAL DESIGNS IN $\mathcal{D}[v;b;k]$

In this chapter, we consider the class of designs $\mathcal{D}[v;b;k]$. Recall that this class consists of all those designs having v treatments arranged in b blocks of size k, $v > k$. For simplicity, we shall simply denote this class of designs by $\mathcal{D}$ in the rest of this chapter. The essential difference between $\mathcal{D}$ and the class of designs $\mathcal{D}[v;(r_i);b;k]$ considered in the last chapter is that in the latter class of designs, the r_i are all fixed, while in $\mathcal{D}$ the r_i are allowed to vary. Clearly $\mathcal{D}$ contains that class of designs $\mathcal{D}[v;(r_i);b;k]$ for all possible (r_i).

The first step in applying our optimality criterion is to determine $\mathcal{M}\{\mathcal{D}\}$, the class of designs in $\mathcal{D}$ with maximal trace. From Lemma 4.3.7, $\mathcal{M}\{\mathcal{D}\} = \mathcal{D}_1[v;b;k]$. Since $v > k$, $\mathcal{D}_1[v;b;k]$ clearly consists of all the binary designs in $\mathcal{D}$. Hence we may state the following.

<u>Theorem 6.1.</u> $\mathcal{M}\{\mathcal{D}\}$ consists of all the binary designs in $\mathcal{D}$.

We must now find those designs in $\mathcal{M}\{\mathcal{D}\}$ which have minimal values for $\text{tr } C^2$. Since the r_i are allowed to vary in $\mathcal{D}$, a natural question which arises is just how in fact should the r_i be assigned to treatments in an (M,S) optimal design in $\mathcal{D}$. Since our goal is to find the design in $\mathcal{M}\{\mathcal{D}\}$ whose C-matrix is closest to the form $\alpha I_v + \beta J_v$, a "reasonable" answer would be to allocate replications to the various treatments as "equally" as possible, i.e., such that $|r_i - r_j| \leq 1$ for all i, j. A result will be given which partially affirms this answer.

If $D[v;(r_i);b;k;N]$ is a design in $\mathcal{D}$, then

$$C = \text{diag}[r_1, \ldots, r_v] - \frac{1}{k} NN' . \tag{6.2}$$

From (6.2), if $NN' = (\lambda_{ij})$ and $N'N = (\mu_{ij})$, we see that

$$\text{tr } C^2 = (1 - \frac{2}{k})(\sum_i r_i^2) + \frac{1}{k^2} \text{tr}(NN')^2$$

$$= (1 - \frac{1}{k})^2(\sum_i r_i^2) + \frac{1}{k^2} \sum\sum_{i \neq j} \lambda_{ij}^2 \tag{6.3}$$

or

$$\text{tr } C^2 = (1 - \frac{2}{k})(\sum_i r_i^2) + \frac{1}{k^2} \text{tr}(N'N)^2$$

$$= (1 - \frac{2}{k})(\sum_i r_i^2) + b + \frac{1}{k^2} \sum\sum_{i \neq j} \mu_{ij}^2 . \tag{6.4}$$

We wish to show that if D is a design in $\mathcal{M}\{\mathcal{D}\}$ with the property that $r_i - r_j > 1$ for some $i \neq j$, then there exists a design $\bar{D}$ in $\mathcal{M}\{\mathcal{D}\}$ which is S-better than D with the property that

$|\bar{r}_i - \bar{r}_j| \leq 1$. In order to show that $\bar{D}$ is S-better than D, it must be shown that $\text{tr } C^2 - \text{tr } \bar{C}^2 > 0$ where C and $\bar{C}$ are the coefficient matrices of D and $\bar{D}$ respectively. We will show that under certain conditions, there exists at least one replication of treatment T_i occurring in a block B_m not containing T_j which may be reassigned to treatment T_j within the same block to form a new design $\bar{D}$ which is S-better than D.

Without loss of generality, let D be a design in $\mathcal{M}\{\mathcal{D}\}$ for which $r_1 - r_2 \geq 2$, i.e., $r_1 = r_2 + p$ where p is a positive integer greater than one. Let $N = (n_{ij})$ be the incidence matrix of D and let $\bar{N} = (\bar{n}_{ij})$ be the incidence matrix of a design derived from D by reassigning a replication of T_1 to T_2 in some block B_m, i.e., $\bar{n}_{1m} = 0$, $\bar{n}_{2m} = 1$, and $\bar{n}_{ij} = n_{ij}$ for all other i.j. Let $\bar{N}\bar{N}' = (\bar{\lambda}_{ij})$. After a reassignment of treatment replications in some block B_m, we have:

$$\bar{\lambda}_{1j} = \lambda_{1j} - 1 \quad \text{for } T_j \text{ occurring in block } B_m$$

$$\bar{\lambda}_{2j} = \lambda_{2j} + 1 \quad \text{for } T_j \text{ occurring in block } B_m$$

$$\bar{\lambda}_{22} = \lambda_{22} + 1$$

$$\bar{\lambda}_{ij} = \lambda_{ij} \quad \text{for all other } i, j.$$

In order for the reassignment of treatment replications to make the design $\bar{D}$ S-better than D, it must satisfy the following:

$$\operatorname{tr} C^2 - \operatorname{tr} \bar{C}^2 = (1-\frac{1}{k})^2(\sum_i r_i^2) + \frac{1}{k^2}\sum\sum_{i\neq j}\lambda_{ij}^2$$

$$- (1-\frac{1}{k})^2(\sum_i \bar{r}_i^2) - \frac{1}{k^2}\sum\sum_{i\neq j}\bar{\lambda}_{ij}^2$$

$$= (1-\frac{1}{k})^2(r_1^2+r_2^2) + \frac{1}{k^2}\sum\sum_{i\neq j}\lambda_{ij}^2$$

$$- (1-\frac{1}{k})^2[(r_1-1)^2+(r_2+1)^2] - \frac{1}{k^2}\sum\sum_{i\neq j}\bar{\lambda}_{ij}^2$$

$$= (1-\frac{1}{k})^2(2r_1-2r_2-2) + \frac{2}{k^2}\sum_{\substack{T_j \in B_m \\ j>2}}\lambda_{1j}^2$$

$$+ \frac{2}{k^2}\sum_{\substack{T_j \in B_m \\ j>2}}\lambda_{2j}^2 - \frac{2}{k^2}\sum_{\substack{T_j \in B_m \\ j>2}}(\lambda_{1j}-1)^2$$

$$- \frac{2}{k^2}\sum_{\substack{T_j \in B_m \\ j>2}}(\lambda_{2j}+1)^2$$

$$= 2(1-\frac{1}{k})^2(p-1) - \frac{4(k-1)}{k^2} + \frac{4}{k^2}\sum_{\substack{T_j \in B_m \\ j>2}}\lambda_{1j}$$

$$- \frac{4}{k^2}\sum_{\substack{T_j \in B_m \\ j>2}}\lambda_{2j} \quad =$$

$$= \frac{2(k-1)(pk-p-k-1)}{k^2} + \frac{4}{k^2} \sum_{\substack{T_j \in B_m \\ j>2}} \lambda_{1j} - \frac{4}{k^2} \sum_{\substack{T_j \in B_m \\ j>2}} \lambda_{2j} > 0$$

which is equivalent to

$$(k-1)(pk-p-k-1) + 2 \sum_{\substack{T_j \in B_m \\ j>2}} \lambda_{1j} - 2 \sum_{\substack{T_j \in B_m \\ j>2}} \lambda_{2j} > 0 . \qquad (6.5)$$

If inequality (6. 5) holds for any replication reassignment of T_1 to T_2, then such a reassignment will make the design S-better.

As a special case, note that when $k = 2$ and $r_1 = r_2+p$, $p \geq 2$, there will always exist at least one $\lambda_{1j} > \lambda_{2j}$ since $\sum_{j \neq 1} \lambda_{1j} = r_1 > \sum_{j \neq 2} \lambda_{2j} = r_2$. If $\lambda_{1\ell} > \lambda_{2\ell}$, then there must exist a block B_m containing T_1 and T_ℓ but not T_2. If a replication reassignment is made from T_1 to T_2 within the block B_m, then inequality (6. 5) will be satisfied, and the design will be made S-better. So when $k = 2$, there always exists a treatment replication of T_1 which may be reassigned to T_2 to make the design S-better when $r_1 - r_2 \geq 2$.

More generally, let us assume that $k \geq 3$. For simplicity let us also assume that $\lambda_{12} = 0$. We wish to show that at least one of the r_1 replications for T_1 may be reassigned to T_2 to make the design S-better. If this is not the case then

$$\frac{k^2}{2}[\text{tr } C^2 - \text{tr } \overline{C}^2] = (k-1)(pk-p-k-1) + 2 \sum_{\substack{T_j \in B_m \\ j>2}} \lambda_{1j} - 2 \sum_{\substack{T_j \in B_m \\ j>2}} \lambda_{2j} \leq 0$$

for every block B_m containing T_1. Hence, summing over all blocks containing T_1, we get

$$(r_2+p)(k-1)(pk-p-k-1) + 2 \sum_{T_1 \in B_m} \sum_{\substack{T_j \in B_m \\ j>2}} \lambda_{1j} - 2 \sum_{T_1 \in B_m} \sum_{\substack{T_j \in B_m \\ j>2}} \lambda_{2j}$$

$$= (r_2+p)(k-1)(pk-p-k-1) + 2 \sum_{j>2} \lambda_{1j}^2 - 2 \sum_{j>2} \lambda_{1j}\lambda_{2j} \leq 0$$

or

$$\frac{(r_2+p)(k-1)(pk-p-k-1)}{2} \leq \sum_{j>2} \lambda_{1j}\lambda_{2j} - \sum_{j>2} \lambda_{1j}^2 . \tag{6.6}$$

So if it can be shown that an upper bound for the right hand side of (6.6) is less than $((r_2+p)(k-1)(pk-p-k-1))/2$, then it follows that there exists at least one replication of T_1 which may be reassigned to T_2 within a block to make the design S-better. Note that λ_{1j} and λ_{2j} must satisfy certain constraints, namely that all entries must be nonnegative integers, $0 \leq \lambda_{1j} \leq r_1$, $0 \leq \lambda_{2j} \leq r_2$, and since $\lambda_{12} = 0$, $\sum_{j>2} \lambda_{1j} = r_1(k-1)$ and $\sum_{j>2} \lambda_{2j} = r_2(k-1)$. By Lemma 4.4.4, we know that when r_2 is even

$\max \sum_{j>2} \lambda_{1j}\lambda_{2j} - \sum_{j>2} \lambda_{1j}^2$ subject to the constraints given above is $((k-1)(r_2^2-2r_2-4p))/4$, hence a reassignment of treatment replications can be made when

$$\frac{(k-1)(r_2^2-2r_2-4p)}{4} < \frac{(k-1)(r_2+p)(pk-p-k-1)}{2},$$

or equivalently, when

$$r_2^2 < 2p(r_2-1)(k-1) + 2p^2(k-1) - 2r_2k. \qquad (6.7)$$

Also from Lemma 4.4.4, we know that when r_2 is odd,

$$\max \sum_{j>2} \lambda_{1j}\lambda_{2j} - \sum_{j>2} \lambda_{1j}^2 = \frac{(k-1)}{4}[(r_2-1)^2-4p].$$

Hence a reassignment of treatment replications can be made when

$$\frac{(k-1)}{4}[(r_2-1)^2-4p] < \frac{(k-1)(r_2+p)(pk-p-k-1)}{2},$$

or equivalently, when

$$r_2^2+1 < 2p(r_2-1)(k-1) + 2p^2(k-1) - 2r_2k. \quad (6.8)$$

Note that if inequality (6.7) or (6.8) is satisfied for some value of p, then it will be satisfied for all larger values of p. In particular, when (6.7) or (6.8) is satisfied for $p = 2$, it will be satisfied for all larger values of p. When $p = 2$, (6.7) reduces to

$$r_2 < 2(k-1) \quad (6.9)$$

and (6.8) reduces to

$$(r_2+2)^2 < 2k(r_2+2) - 1. \quad (6.10)$$

Hence we have the following result.

Lemma 6.11. Consider a binary design with v treatments and b blocks of size k such that for T_i and T_j, $r_i-r_j \geq 2$, i.e., $r_i = r_j+p$. Let c denote the number of experimental units assigned to T_j which occur in blocks not containing T_i. Then if i) c is even and $c < 2(k-1)$ or ii) c is odd and $(c+2)^2 + 1 < 2k(c+2)$, then there exists a treatment replication of T_i which may be reassigned to T_j which will make the design S-better.

Pf. Without loss of generality, let $i = 1$ and $j = 2$. Note that in the paragraph preceding the lemma, it was assumed that

$\lambda_{12} = 0$. However, if $\lambda_{12} = z$, partition N into (N_1, N_2) where N_2 consists of the blocks where T_1 and T_2 occur together and N_1 consists of the remaining blocks. Then by applying the above proof to the N_1 portion of the incidence matrix, the proof goes through as before since the N_2 portion of the incidence matrix is irrelevant in the argument.

Note that according to Lemma 6.11, there does not necessarily have to exist a treatment replication of T_i which may be reassigned to T_j to make the design S-better when $r_i - r_j \geq 2$. The next example illustrates a situation in which such a reassignment cannot be made to make the design S-better.

Example 6.12. Consider the class of designs $\mathcal{D}[12;14;3]$, and a design whose incidence matrix has the form shown at the top of page 86.

Now for T_1 and T_2 we have that

$$\sum_{\substack{T_j \in B_m \\ j>2}} \lambda_{2j} - \sum_{\substack{T_j \in B_m \\ j>2}} \lambda_{1j} \leq \frac{(k-1)(k-3)}{2}$$

for $1 \leq m \leq 8$; hence no replication of T_1 may be reassigned to T_2 to make the design S-better (i.e., see (6.5)).

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	B_{11}	B_{12}	B_{13}	B_{14}	
T_1	1	1	1	1	1	1	1	1							8
T_2									1	1	1	1	1	1	6
T_3	1	1	1	1					1	1	1	1	1	1	10
T_4					1	1	1	1	1	1	1	1	1	1	10
T_5	1														1
T_6		1													1
T_7			1												1
T_8				1											1
T_9					1										1
T_{10}						1									1
T_{11}							1								1
T_{12}								1							1
	3	3	3	3	3	3	3	3	3	3	3	3	3	3	1

Note that Lemma 6.11 may be applied in any situation where $c < 2(k-1)$ or $(c+2)^2 + 1 < 2k(c+2)$ and it does not depend upon how many treatments v are in D. It is this lack of dependence on v which makes the result both general and at the same time inapplicable in some fairly obvious situations. In general, when the number of blocks is larger than the number of treatments, the lemma may not apply. The following example illustrates where the lemma is not applicable but where an argument similar to the one given in the proof of Lemma 6.11 justifies a replication reassignment.

Example 6.13. Consider $\mathcal{D} = \mathcal{D}[6; 14; 3]$ and $D \in \mathcal{M}\{\mathcal{D}\}$ with $r_1 = 8$ and $r_2 = 6$. We would like to show that a treatment replication of T_1 can be reassigned to T_2 to make the design S-better. Lemma 6.11 cannot be used to justify this reassignment in all cases since if $c \geq 4$, $c \geq 2(k-1) = 4$. To show that a treatment replication may always be reassigned from T_1 to treatment T_2 to make the design S-better, an argument similar to the one used to prove Lemma 6.11 can be applied, i.e., if

$$\max \sum_{j>2} \lambda_{1j}\lambda_{2j} - \sum_{j>2} \lambda_{1j}^2 < \frac{(r_2+p)(k-1)(pk-p-k-1)}{2},$$

then it will follow that there exists at least one replication of treatment T_1 which may be reassigned to treatment T_2 to make the design S-better. However, to apply this argument, the maximum value of $\sum_{j>2} \lambda_{1j}\lambda_{2j} - \sum_{j>2} \lambda_{1j}^2$ must be determined subject to the relevant constraints. As opposed to Lemma 6.11, this maximal value will depend on the specific number of treatments in the design. Algorithm (4.4) may be used to obtain this maximal value. The problem becomes equivalent to finding

$$\max \sum_{i=1}^{4} a_i b_i - \sum_{i=1}^{4} a_i^2$$

subject to the constraints that i) the a_i and b_i are integers, ii) $0 \le a_i \le 8$, iii) $0 \le b_i \le 6$, iv) $\sum_{i=1}^{4} a_i = 8(2) = 16$ and v) $\sum_{i=1}^{4} b_i = 6(2) = 12$. The maximal value as determined by Algorithm (4.4) is found to be

$$-8 < \frac{(r_2+p)(k-1)(pk-p-k-1)}{2} = 0 \ ;$$

hence a treatment replication may be reassigned from treatment T_1 to T_2 to make the design S-better.

Now let D be an arbitrary design in $\mathcal{M}\{\mathcal{D}\}$ which has $r_i > 7$ for some i. Since $bk = 14(3) = 6(7)$, it follows that there must exist $r_j < 7$, hence $r_i - r_j \ge 2$. Since a reassignment of treatment replications could be made whenever $r_i = 8$ and $r_j = 6$, it follows from the comments following Example 4.4.3 that a reassignment of treatment replications can be made to make D S-better whenever $r_i \ge 8$ and $r_j \le 6$. Hence it follows that an (M, S) optimal design in $\mathcal{D}[6;14;3]$ must have the property that $|r_i - r_j| \le 1$ for all i, j.

Many more individual situations not covered by Lemma 6.11 can be handled in the same way as Example 6.13. However, we now apply Lemma 6.11 to get a more general result concerning the parameters v, b, and k and the allocation of replications to treatments for an (M,S) optimal design in $\mathcal{D}$.

Theorem 6.14. i) An (M,S) optimal design in $\mathcal{D}[v;b;2]$ must have the property that $|r_i - r_j| \leq 1$ for all i, j.

ii) Let $[\cdot]$ denote the greatest integer function. If $k \geq 3$ and any of the following conditions hold, then the (M,S) optimal design in $\mathcal{D}[v;b;k]$ must have the property that $|r_i - r_j| \leq 1$ for all i, j.

a) $bk/v = r$ is an integer and $r \leq 2k-2$

b) bk/v is not an integer but $[bk/v] = r \leq 2k-3$

c) bk/v is an integer and $b - (bk/v) = b - r \leq 2k-2$

d) bk/v is not an integer and $b - [bk/v] = b - r \leq 2k-2$

Pf. i) Preceding Lemma 6.11, it was shown that when $k = 2$ and $r_i - r_j \geq 2$, it is always possible to reassign a treatment replication from T_i to T_j to make the design S-better.

ii) a) Suppose $bk/v = r$ is an integer and $r \leq 2k-2$ and suppose D is an arbitrary design in $\mathcal{M}\{\mathcal{D}\}$ with $r_i > r$ for some i. Since $vr = bk$ and $r_i > r$, there must exist T_j with $r_j < r$; hence $r_i - r_j \geq 2$. However, since $r \leq 2k-2$,

$r_j \leq 2k-3$, hence by applying Lemma 6.11, we see that there must exist a treatment replication of T_i which can be reassigned to T_j to make the design S-better. Since this argument can be repeated for any $r_i > r$, it follows that an (M,S) optimal design in $\mathcal{D}$ must have the property that $|r_i - r_j| \leq 1$ for all i, j.

b) Suppose $[bk/v] = r$ and $r \leq 2k-3$. Note that $bk = cr+d = (v-d)r + d(r+1)$ is a unique representation for bk as the sum of nonnegative integers differing by at most one. Suppose D is an arbitrary design in $\mathcal{M}\{\mathcal{D}\}$ with $r_i \neq r$ or $r+1$. If $r_i > r+1$, then there exists $r_j \leq r$, hence $r_i - r_j \geq 2$. However, since $r \leq 2k-3$, $r_j \leq 2k-3$, and by applying Lemma 6.11, we see that there must exist a treatment replication of T_i which can be reassigned to T_j to make the design S-better. Similarly, if $r_i < r$, there will exist $r_j \geq r+1$ such that a treatment replication of T_j may be reassigned to T_i to make the design S-better.

Since this argument can be repeated for any $r_p \neq r$ or $r+1$, it follows that an (M,S) optimal design in $\mathcal{D}$ must have the property that $|r_i - r_j| \leq 1$.

c) Suppose $bk/v = r$ is an integer and $b-r \leq 2k-2$. If D is a design in $\mathcal{M}\{\mathcal{D}\}$ with $r_i > r$, then there must exist T_j with $r_j < r$, hence $r_i - r_j \geq 2$. If c denotes the number of blocks containing T_j but not T_i, then $c \leq b - r_i < b - r \leq 2k-2$. Hence

$c \leq 2k-3$, and by applying Lemma 6.11, we see that there must exist a treatment replication of T_i which can be reassigned to T_j to make the design S-better. Since this argument can be repeated for any $r_p < r$, it follows that an (M,S) optimal design in $\mathcal{D}$ must have the property that $|r_i - r_j| \leq 1$ for all i, j.

d) Suppose bk/v is not an integer but $b - [bk/v] = b - r \leq 2k-2$ and suppose D is a design in $\mathcal{M}\{\mathcal{D}\}$ with $r_i \neq r$ or $r+1$. If $r_i > r+1$, then there must exist T_j with $r_j \leq r$, hence $r_i - r_j \geq 2$. If c denotes the number of blocks containing T_j but not T_i, then $c \leq b - r_i < b - r \leq 2k-2$. Hence $c \leq 2k-3$, and by applying Lemma 6.11, we see that a reassignment of a treatment replication from T_i to T_j can be made to make the design S-better. If $r_i < r$, then there must exist T_j with $r_j \geq r+1$. If c denotes the number of blocks containing T_i but not T_j, then $c \leq b - r_j < b - r \leq 2k-2$. Hence $c \leq 2k-3$ and by applying Lemma 6.11, we see that a reassignment of a treatment replication can be made to make the design S-better. Since this argument holds for any $r_p \neq r$ or $r+1$, the result follows.

Note that the above theorem takes care of many practical situations. In general, there must be many more blocks than treatments before the theorem does not apply. However, as seen in Example 6.13, in many classes of designs not covered by Theorem

6.14, it can be shown that an (M,S) optimal design must have the property that $|r_i - r_j| \leq 1$ for all i, j.

A natural conjecture stemming from the above discussion is than an (M,S) optimal design in $\mathcal{D}$ must always have the property that $|r_i - r_j| \leq 1$ for all i, j. A general result of this sort has eluded the author. It can be shown that whenever $v \leq 6$ or $v = k+2$, an (M,S) optimal design must have the equal allocation property, but for arbitrary $v \geq 7$ the question is still open except for the cases covered by Theorem 6.14.

As for the class of designs $\mathcal{D}[v;(r_i);b;k]$, the question arises of how to tell when a design is (M,S) optimal in $\mathcal{D}$. Again a reasonable answer seems to be to establish lower bounds for tr C^2 for designs in $\mathcal{M}\{\mathcal{D}\}$ and then find designs in $\mathcal{M}\{\mathcal{D}\}$ whose C-matrices have tr C^2 equal to one of the lower bounds established. Such designs will clearly be (M,S) optimal in $\mathcal{D}$. It has been shown for many classes of designs $\mathcal{D}$ that an (M,S) optimal design must have the property that $|r_i - r_j| \leq 1$ for all i, j. For these classes of designs, it is clear that applying the methods of the last chapter to establish lower bounds for tr C^2 for designs in $\mathcal{M}\{\mathcal{D}[v;(r_i);b;k]\}$ where $|r_i - r_j| \leq 1$ for all i, j will also establish lower bounds for tr C^2 for designs in $\mathcal{M}\{\mathcal{D}\}$. However, for those classes of designs where it is not known how replications should be assigned to treatments, lower bounds must be established taking into consideration the variation of the r_i.

From expression (6.3), we see that establishing a lower bound for $\operatorname{tr} C^2$ in $\mathcal{M}\{\mathcal{D}\}$ can be accomplished by simultaneously establishing a lower bound for $\sum_i r_i^2$ and $\sum\sum_{i \neq j} \lambda_{ij}^2$ in $\mathcal{M}\{\mathcal{D}\}$. By Lemma 4.1.1, we have that

$$\text{i)} \ \sum_i r_i = bk \quad \text{and} \quad \text{ii)} \ \sum\sum_{i \neq j} \lambda_{ij} = bk(k-1).$$

From above, we see that finding a lower bound for $\operatorname{tr} C^2$ in $\mathcal{M}\{\mathcal{D}\}$ can be accomplished by simultaneously solving the integer programming problems of

$$\text{i)} \ \min \sum_i m_i^2 \quad \text{and} \quad \text{ii)} \ \min \sum\sum_{i \neq j} x_{ij}^2 \tag{6.15}$$

subject to the constraints that

$$\text{i)} \ m_i \geq 0 \quad \text{and} \quad \text{ii)} \ \sum_i m_i = bk \tag{6.16}$$

$$\text{iii)} \ x_{ij} \geq 0 \ \text{for all} \ i \neq j \quad \text{and} \quad \text{iv)} \ \sum\sum_{i \neq j} x_{ij} = bk(k-1).$$

By applying Corollary 4.3.5 to each of the expressions appearing in (6.15) subject to the relevant constraints given in (6.16), we obtain the following result.

Theorem 6.17. If $D \in \mathcal{M}\{\mathcal{D}\}$, then

$$\operatorname{tr} C^2 \geq (1-\frac{1}{k})^2 (\sum_i m_i^2) + \frac{1}{k^2} \sum\sum_{i \neq j} x_{ij}^2$$

where i) the m_i are nonnegative integers, ii) $\sum_i m_i = bk$,

iii) $|m_i - m_j| \leq 1$, iv) the x_{ij} are nonnegative integers,

v) $\sum\sum_{i \neq j} x_{ij} = bk(k-1)$ and vi) $|x_{ij} - x_{pq}| \leq 1$ for all $i \neq j$, $p \neq q$.

Corollary 6.18. Any design $D \in \mathcal{M}\{\mathcal{D}\}$ having the property that $|r_i - r_j| \leq 1$ for all i, j and whose incidence matrix N has the property that $NN' = (\lambda_{ij})$ where $|\lambda_{ij} - \lambda_{pq}| \leq 1$ for $i \neq j$, $p \neq q$, will be (M, S) optimal in $\mathcal{D}$.

Corollary 6.19. If bk/v is an integer and if in $\mathcal{M}\{\mathcal{D}\}$ there exists a BIBD or a PBIB(2) with $\lambda_2 = \lambda_1 + 1$, then that design will be (M, S) optimal in $\mathcal{D}$.

From expression (6.1.4), we see that establishing a lower bound for $\operatorname{tr} C^2$ in $\mathcal{M}\{\mathcal{D}\}$ can also be accomplished by simultaneously establishing a lower bound for $\sum_i r_i^2$ and $\sum\sum_{i \neq j} \mu_{ij}^2$ in $\mathcal{M}\{\mathcal{D}\}$. By Lemma 4.1.1,

$$\text{i)}\ \sum_{i} r_i = bk \quad \text{and} \quad \text{ii)}\ \sum_{i \neq j}\sum \mu_{ij} = \sum_{i=1}^{v} r_i(r_i - 1) = \sum_{i=1}^{v} r_i^2 - bk$$

From the above, we see that a lower bound for $\operatorname{tr} C^2$ in $\mathcal{M}\{\mathcal{D}\}$ can be established by simultaneously solving the integer programming problems

$$\text{i)}\ \min \sum_{i=1}^{v} m_i^2 \quad \text{and} \quad \text{ii)}\ \min \sum_{i \neq j}\sum x_{ij}^2 \tag{6.20}$$

subject to the constraints that

$$\text{i)}\ m_i \geq 0 \quad \text{and} \quad \text{ii)}\ \sum_{i=1}^{v} m_i = bk$$

and (6.21)

$$\text{iii)}\ x_{ij} \geq 0 \ \text{ for all } i \neq j \quad \text{and} \quad \text{iv)}\ \sum_{i \neq j}\sum x_{ij} = \sum_{i} m_i^2 - bk .$$

However, it is easily seen that the minimum for $\sum_{i \neq j}\sum x_{ij}^2$ subject to the constraints that the x_{ij} are nonnegative integers and $\sum_{i \neq j}\sum x_{ij} = M$ increases as M increases. Hence simultaneously minimizing the terms in (6.20) subject to (6.21) is accomplished by first minimizing $\sum_i m_i^2$ subject to the relevant constraints in (6.21), and then minimizing $\sum\sum_{i \neq j} x_{ij}^2$. With this in mind and applying Corollary 4.3.5, we may state the following.

Theorem 6.22. For any design $D \in \mathcal{M}\{\mathcal{D}\}$,

$$\operatorname{tr} C^2 \geq (1 - \frac{2}{k})(\sum_i m_i^2) + b + \frac{1}{k^2} \sum\sum_{i \neq j} x_{ij}^2$$

where i) the m_i are nonnegative integers, ii) $\sum_i m_i = bk$, iii) $|m_i - m_j| \leq 1$ for all i, j, iv) the x_{ij} are nonnegative integers, v) $\sum\sum_{i \neq j} x_{ij} = \sum_{i=1}^{v} m_i(m_i - 1)$, and vi) $|x_{ij} - x_{pq}| \leq 1$ for $i \neq j$, $p \neq q$.

Corollary 6.23. Any design $D \in \mathcal{M}\{\mathcal{D}\}$ having the property that $|r_i - r_j| \leq 1$ for all i, j, and whose incidence matrix N has the property that $N'N = (\mu_{ij})$ where $|\mu_{ij} - \mu_{pq}| \leq 1$ for $i \neq j$, $p \neq q$, will be (M, S) optimal in $\mathcal{D}$.

VII. CONSTRUCTION OF (M,S) OPTIMAL DESIGNS

7.1. Complementary Designs

Let $D[v;r_1,\ldots,r_v;b;k_1,\ldots,k_b;N]$ denote a binary incomplete block design. We form the complementary design D^* by changing the zeros in N to ones and the ones to zeros. The new design is easily seen to have parameters

$$v^* = v, \quad r_i^* = b - r_i, \quad b^* = b, \quad k_j^* = v - k_j, \quad N^* = J - N \qquad (7.1.1)$$

where J is a $v \times b$ matrix of ones. Also, the association matrix for the new design is $N^*N^{*'} = (\lambda_{ij}^*)$ where $\lambda_{ij}^* = b + \lambda_{ij} - r_i - r_j$ for all i, j and the block characteristic matrix is $N^{*'}N^* = (\mu_{ij}^*)$ where $\mu_{ij}^* = v + \mu_{ij} - k_i - k_j$.

If $\mathfrak{X}$ denotes some class of binary incomplete block designs, let $\mathfrak{X}^*$ denote the class of complementary incomplete block designs.

<u>Theorem 7.1.2.</u> Consider $\mathcal{D} = \mathcal{D}[v;(r_i);b;k]$ where $r_i \leq b$ and $v > k$. If D is a design which is (M,S) optimal in $\mathcal{D}$, then D^* is (M,S) optimal in $\mathcal{D}[v;(b-r_i);b;v-k]$.

<u>Pf.</u> Note that $\mathcal{M}\{\mathcal{D}\}$ consists of all the binary designs in $\mathcal{D}$. Let $\mathcal{M}^*\{\mathcal{D}\}$ denote the class of designs which are complements of designs in $\mathcal{M}\{\mathcal{D}\}$. Now observe that

$\mathcal{M}^*\{\mathcal{D}\} = \mathcal{M}\{\mathcal{D}[v;(b-r_i);b;v-k]\}$ since both classes consist of the binary designs in $\mathcal{D}[v;(b-r_i);b;v-k]$. So finding a design in $\mathcal{D}[v;(b-r_i);b;v-k]$ which is (M, S) optimal in equivalent to finding a design in $\mathcal{M}^*\{\mathcal{D}\}$ with minimal $\operatorname{tr} C^{*2}$. Recall that for fixed r_i, finding a design in $\mathcal{M}^*\{\mathcal{D}\}$ with minimal $\operatorname{tr} C^{*2}$ is equivalent to finding a design with a minimal value for $\sum\sum_{i \neq j} \mu_{ij}^{*2}$. But for $D^* \epsilon \mathcal{M}^*\{\mathcal{D}\}$,

$$\sum_{i \neq j}\sum (\mu_{ij}^*)^2 = \sum_{i \neq j}\sum (v+\mu_{ij}-2k)^2$$

$$= b(b-1)v^2 + 2v\sum_i r_i(r_i-1) - 4b(b-1)vk + \sum_{i \neq j}\sum \mu_{ij}^2$$

$$- 4k\sum_{i \neq j}\sum \mu_{ij} + 4b(b-1)k^2$$

$$= c + \sum_{i \neq j}\sum \mu_{ij}^2$$

where c is constant because the r_i are fixed. From this last expression, we see that finding a minimal value for $\sum\sum_{i \neq j} (\mu_{ij}^*)^2$ in $\mathcal{M}^*\{\mathcal{D}\}$ is equivalent to finding a minimal value for $\sum\sum_{i \neq j} \mu_{ij}^2$ in $\mathcal{M}\{\mathcal{D}\}$, i.e., equivalent to finding a minimal value for $\operatorname{tr} C^2$ in

$\mathcal{M}\{\mathcal{D}\}$. Hence finding an (M, S) optimal design in $\mathcal{D}[v;(b-r_i);b;v-k]$ is equivalent to finding an (M, S) optimal design in $\mathcal{D}$.

<u>Theorem 7. 1. 3.</u> If a binary design $D(v;r_1,\ldots,r_v;b;k;N)$ has the property that $|\mu_{ij}-\mu_{\ell m}| \leq 1$ for $i \neq j$, $\ell \neq m$, then the complementary design has the property that $|\mu^*_{ij}-\mu^*_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$.

<u>Pf</u>. Simply observe that

$$|\mu^*_{ij}-\mu^*_{\ell m}| = |(b+\mu_{ij}-2k) - (b+\mu_{\ell m}-2k)| = |\mu_{ij}-\mu_{\ell m}| \leq 1$$

for all $i \neq j$, $\ell \neq m$.

<u>Corollary 7. 1. 4.</u> If a binary design $D(v;r_1,\ldots,r_v;b;k;N)$ in $\mathcal{D}[v;b;k]$ has the property that $|r_i-r_j| \leq 1$ and $|\mu_{pq}-\mu_{rs}| \leq 1$ for all $p \neq q$, $r \neq s$, then the complementary design D^* is (M, S) optimal in $\mathcal{D}[v;b;v-k]$.

<u>Pf</u>. The parameters of the complementary design are given in (7. 1. 1). Observe that $|r^*_i-r^*_j| = |(b-r_i)-(b-r_j)| = |r_i-r_j| \leq 1$ and by Theorem (7. 1. 3) $|\mu^*_{ij}-\mu^*_{\ell m}| \leq 1$ for $i \neq j$, $\ell \neq m$. Now, by applying Corollary 6. 18, we see that D^* is (M, S) optimal in $\mathcal{D}[v;b;v-k]$.

<u>Corollary 7.1.5.</u> If D is a binary design in $\mathcal{D}[v;b;k]$ with the property that $|r_i - r_j| \leq 1$ and $\lambda_{ij} \leq 1$ for all $i \neq j$, then D^* is (M, S) optimal in $\mathcal{D}[v;b;v-k]$.

<u>Pf.</u> Note that if $\lambda_{ij} \leq 1$, then no two treatments occur in more than one block together. Hence no two blocks can have more than one treatment in common. So $\mu_{ij} \leq 1$ for all $i \neq j$. Hence $|\mu_{ij} - \mu_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$, and the result follows from Corollary 7.1.4.

<u>Theorem 7.1.6.</u> Suppose D is a binary design in $\mathcal{D} = \mathcal{D}[v;b;k]$ which is (M, S) optimal and has the property that $|r_i - r_j| \leq 1$ for all i, j. If $v \geq 2k$, then D^* is (M, S) optimal in $\mathcal{D}[v;b;v-k]$.

<u>Pf.</u> Let $\mathcal{M}^*\{\mathcal{D}\}$ denote the class of designs which are complements of designs in $\mathcal{M}\{\mathcal{D}\}$. Observe that $\mathcal{M}\{\mathcal{D}[v;b;v-k]\} = \mathcal{M}^*\{\mathcal{D}\}$ since both classes consist of the binary designs in $\mathcal{D}[v;b;v-k]$. So finding an (M, S) optimal design in $\mathcal{D}[v;b;v-k]$ is equivalent to finding a design in $\mathcal{M}^*\{\mathcal{D}\}$ with minimal $\operatorname{tr} C^2$. For any design $D^* \in \mathcal{M}^*\{\mathcal{D}\}$,

$$\mathrm{tr}\, C^{*2} = (1 - \frac{2}{k^*}) \sum_{i=1}^{v} r_i^{*2} + b^* + \frac{1}{k^{*2}} \sum\sum_{i \neq j} \mu_{ij}^{*2}$$

$$= \frac{(v-k)(v-k-2)}{(v-k)^2} \sum_{i=1}^{v} (b-r_i)^2 + b + \frac{1}{(v-k)^2} \sum\sum_{i \neq j} (v+\mu_{ij}-2k)^2$$

$$= (\text{constant}) + [\frac{v(v-2k)}{(v-k)^2}] \sum_{i=1}^{v} r_i^2 + \frac{1}{(v-k)^2} \left[k(k-2) \sum_{i=1}^{v} r_i^2 + \sum\sum_{i \neq j} \mu_{ij}^2 \right]$$

$$= (\text{constant}) + [\frac{v(v-2k)}{(v-k)^2}] \sum_{i=1}^{v} r_i^2 + \frac{k^2}{(v-k)^2} [\mathrm{tr}\, C^2 - b].$$

From this last expression, we see that when $v \geq 2k$, $\mathrm{tr}\, C^{*2}$ is minimal when $\sum_{i=1}^{v} r_i^2$ is minimal and when $\mathrm{tr}\, C^2$ is minimal in $\mathcal{M}(\mathcal{D})$.

Theorem 7.1.7. Suppose D is a binary design in $\mathcal{D}[v;b;k]$ such that $|r_i - r_j| \leq 1$ for all i, j, and suppose D^* is (M,S) optimal in $\mathcal{D}[v;b;v-k]$. If $v \leq 2k$, then D is (M,S) optimal in $\mathcal{D}[v;b;k]$.

Pf. Similar to Theorem 7.1.6.

It will be shown in the next example that S-betterness is not necessarily preserved in $\mathcal{D}[v;b;k]$ under the operation of complementation.

Example 7.1.8. Consider $\mathcal{D}[7;5;3]$. Let D_1 and D_2 be given by the following incidence matrices.

	B_1	B_2	B_3	B_4	B_5	
T_1	1	1	1			3
T_2		1		1	1	3
T_3	1			1		2
T_4	1				1	2
T_5		1	1			2
T_6				1	1	2
T_7			1			1
	3	3	3	3	3	

	B_1	B_2	B_3	B_4	B_5	
T_1	1	1	1			3
T_2	1	1				2
T_3	1	1				2
T_4			1	1		2
T_5				1	1	2
T_6				1	1	2
T_7			1		1	2
	3	3	3	3	3	

Now $\text{tr } C_1^2 = 19\ 1/3$ and $\text{tr } C_2^2 = 19\ 7/9$, hence $\text{tr } C_1^2 < \text{tr } C_2^2$. If we take complements of D_1 and D_2, then designs D_1^* and D_2^* are obtained where $\text{tr } C_1^{*2} = 40\ 1/4$ and $\text{tr } C_2^{*2} = 39\ 5/8$, hence $\text{tr } C_1^{*2} > \text{tr } C_2^{*2}$. So "S-betterness" is not necessarily preserved under complementation in $\mathcal{D}[v;b;k]$.

Corollary 7.1.9. If the parameters in $\mathcal{D}[v;b;k]$ satisfy any of the conditions in Theorem 6.14 and $v \geq 2k$, then the complement of an (M, S) optimal design in $\mathcal{D}[v;b;k]$ will be (M, S) optimal in $\mathcal{D}[v;b;v-k]$.

Pf. If the parameters in $\mathcal{D}[v;b;k]$ satisfy any of the conditions in Theorem 6.14, then an (M,S) optimal design in $\mathcal{D}[v;b;k]$ must have the property that $|r_i - r_j| \leq 1$ for all i, j. The result then follows from Theorem 7.1.6.

Corollary 7.1.10. If the parameters in $\mathcal{D}[v;r;v-k]$ satisfy any of the conditions in Theorem 6.14 and $v \leq 2k$, then the complement of an (M, S) optimal design in $\mathcal{D}[v;b;v-k]$ will be (M, S) optimal in $\mathcal{D}[v;b;k]$.

Pf. Similar to that of Corollary 7.1.9.

While it is not yet known whether the complement of an (M, S) optimal design in $\mathcal{D}[v;b;k]$ is always (M, S) optimal in $\mathcal{D}[v;b;v-k]$, such a conjecture appears extremely reasonable. If it could be proven that an (M, S) optimal design in $\mathcal{D}[v;b;k]$ always has the property that $|r_i - r_j| \leq 1$, then the conjecture would easily be affirmed by what has been proven here.

Clearly the operation of complementation is not an actual method of construction, but it can be useful in that it may be easier to construct the complement of the desired (M, S) optimal design rather than the actual needed design. As an example, consider the construction of the (M,S) optimal design in $\mathcal{D}[v;b;k]$ where $v = k+1$. Since $v \leq 2k$, if an (M,S) optimal design in the trivial class of designs $\mathcal{D}[v;b;1]$ has the property that $|r_i - r_j| \leq 1$ for all i,j, then by Theorem 7.1.7, its complement will be (M,S) optimal in $\mathcal{D}[v;b;k]$ where $v = k+1$. But for any design in $\mathcal{D}[v;b;1]$, C is the zero matrix, hence every design in $\mathcal{D}[v;b;1]$ is trivially (M,S) optimal. Therefore, we must simply find a design in $\mathcal{D}[v;b;1]$ with $|r_i - r_j| \leq 1$ for all i,j. But such a design can always be found in $\mathcal{D}[v;b;1]$ since the design having an incidence matrix $N = (n_{pq})$ with $n_{pq} = 1$ for $p = 1,\ldots,v$, and

$$(1-r_p) + \sum_{i=1}^{p} r_i \leq q \leq \sum_{i=1}^{p} r_i, \quad \text{and} \quad n_{pq} = 0 \text{ elsewhere has this}$$

property. Hence Theorem 7.1.7 is applicable, and the (M,S) optimal design in $\mathcal{D}[v;b;k]$ where $v = k+1$ is the complement of the design in $\mathcal{D}[v;b;1]$ described above.

<u>Example 7.1.11</u>. Suppose we wish to find an (M,S) optimal design in $\mathcal{D}[6;10;5]$. Let us construct the (M,S) optimal design in $\mathcal{D}[6;10;1]$. This is simply any design in $\mathcal{D}[6;10;1]$ with $|r_i - r_j| \leq 1$. The incidence matrix of the design described above having this property is given below.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	
T_1	1	1									2
T_2			1	1							2
T_3					1	1					2
T_4							1	1			2
T_5									1		1
T_6										1	1
	1	1	1	1	1	1	1	1	1	1	

The complement of the above design is (M, S) optimal in $\mathcal{D}[6;10;5]$.

7.2. (M, S) Optimal Designs in $\mathcal{D}[v;b;2]$

In experimental work, particularly in some fields of biology, blocks of size two are of fairly frequent occurrence. For example, an experimenter may have blocks consisting of twins, or halves of plants, or halves of leaves. Since experiments with blocks of size two are of importance, we now restrict ourselves to the construction of (M, S) optimal designs in $\mathcal{D}[v;b;2]$.

Recall from Theorem 6.14 that the (M, S) optimal design in $\mathcal{D}[v;b;2]$ must have the property that $|r_i - r_j| \leq 1$. In addition to this, the following theorem can be stated.

Theorem 7.2.1. An (M,S) optimal design $D \in \mathcal{D}[v;b;2]$ with incidence matrix N can always be constructed such that $|r_i - r_j| \leq 1$ for all i, j and such that $NN' = (\lambda_{ij})$ where $|\lambda_{ij} - \lambda_{pq}| \leq 1$ for all $i \neq j$, $p \neq q$.

Pf. From Theorem 6.14, the (M,S) optimal design in $\mathcal{D} = \mathcal{D}[v;b;2]$ must have the property that $|r_i - r_j| \leq 1$ for all i, j. Let $\lambda = [2b/v(v-1)]$ where $[\cdot]$ denotes the greatest integer function. To obtain the desired association matrix, we must have $\lambda_{ij} = \lambda$ or $\lambda+1$ for all $i \neq j$. Let $D \in \mathcal{D}$ be such that $|r_i - r_j| \leq 1$ for all i, j. Let N be the incidence matrix of D and let $NN' = (\lambda_{ij})$. Suppose for some $i \neq j$, $\lambda_{ij} > \lambda+1$. Without loss of generality, suppose $\lambda_{12} > \lambda+1$. Since $2b = \sum_i r_i$ and $|r_i - r_j| \leq 1$ for all i, j, we must have that $\lambda \leq r_1/(v-1) \leq \lambda+1$. So there must exist a nonnegative integer a_1 such that

$$r_1 = (v-1-a_1)\lambda + a_1(\lambda+1) = \sum_{j \geq 2} \lambda_{1j} .$$

Since $\lambda_{12} > \lambda+1$, there must exist T_m such that $\lambda_{1m} \leq \lambda$; so $\lambda_{12} - \lambda_{1m} \geq 2$. Since $|r_2 - r_m| \leq 1$ and $r_m = \sum_{i \neq m} \lambda_{im}$, we must also have that $\sum_{\substack{j \geq 2 \\ j \neq m}} \lambda_{mj} > \sum_{j > 2} \lambda_{2j}$.

Hence for some treatment T_p, $\lambda_{mp} > \lambda_{2p}$. Now assign a replication of treatment T_2 occurring in a block containing T_1 to T_m and a replication of treatment T_m occurring in a block containing T_p to treatment T_2. Since $k = 2$, the new design $\bar{D}$ has incidence matrix $\bar{N}$ with $\bar{N}\bar{N}' = (\bar{\lambda}_{ij})$ where

$$\bar{\lambda}_{12} = \lambda_{12} - 1 \qquad \bar{\lambda}_{2p} = \lambda_{2p} + 1$$
$$\bar{\lambda}_{1m} = \lambda_{1m} + 1 \qquad \bar{\lambda}_{mp} = \lambda_{mp} - 1$$

and $\bar{\lambda}_{ij} = \lambda_{ij}$ for all other i, j. Now

$$\begin{aligned} & tr(NN')^2 - tr(\bar{N}\bar{N}')^2 \\ &= 2(\lambda_{12}^2 + \lambda_{1m}^2 + \lambda_{2p}^2 + \lambda_{mp}^2) - (\bar{\lambda}_{12}^2 + \bar{\lambda}_{1m}^2 + \bar{\lambda}_{2p}^2 + \bar{\lambda}_{mp}^2) \\ &= 4(\lambda_{12} - \lambda_{1m}) + 4(\lambda_{mp} - \lambda_{2p}) - 8 > 0 \end{aligned}$$

since $\lambda_{12} - \lambda_{1m} \geq 2$ and $\lambda_{mp} > \lambda_{2p}$. So $tr(\bar{N}\bar{N}')^2 < tr(NN')^2$. A similar interchange can be made to reduce $tr(NN')^2$ when there exists $\lambda_{ij} < \lambda$ for some $i \neq j$. So by beginning with an arbitrary design $D \in \mathcal{D}$ with incidence matrix N, we can make interchanges as described above to reduce $tr(NN')^2$ whenever $\lambda_{ij} \neq \lambda$ or $\lambda + 1$ for some $i \neq j$. Since there are only finitely many designs in $\mathcal{D}$, we will eventually obtain a design $\tilde{D}$ having incidence matrix $\tilde{N}$ such that $\tilde{N}\tilde{N}' = (\tilde{\lambda}_{ij})$ where $|\tilde{\lambda}_{ij} - \tilde{\lambda}_{pq}| \leq 1$ for all $i \neq j$, $p \neq q$.

We shall now give an easy process by which the (M, S) optimal design in $\mathcal{D}[v;b;2]$ may be constructed.

In the first stage of the construction process, we assign T_1 to experimental units occurring in the first r_1 blocks of the design, i.e., $n_{1m} = 1$ for $1 \leq m \leq r_1$. Beginning with T_2, we then sequentially assign treatments to the experimental units remaining in blocks $B_1, \ldots, B_{r_1}$, i.e., T_2 is assigned to the experimental unit remaining in B_1, T_3 is assigned to the experimental unit remaining in B_2, etc. If $r_1 > v-1$, then T_v is assigned to the experimental unit remaining in B_{v-1}, T_2 is assigned to the experimental unit remaining in B_v, and the process of assigning succeeding treatments to succeeding blocks is continued until treatments have been assigned to all of the experimental units occurring in blocks $B_1, \ldots, B_{r_1}$. The following examples illustrate how a typical incidence matrix might look after the first stage of the construction process, depending on whether $r_1 \leq v-1$ or $r_1 > v-1$.

Example 7.2.2. Consider $\mathcal{D}[6;10;2]$. After the first stage, the design we are constructing for this class of designs has the following form (note that $r_1 \leq v-1$).

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	
T_1	1	1	1	1							4
T_2	1										4
T_3		1									3
T_4			1								3
T_5				1							3
T_6											3
	2	2	2	2	2	2	2	2	2	2	

<u>Example 7.2.3.</u> Consider $\mathcal{D}[5;13;2]$. After the first stage, the design being constructed for this class of designs has an incidence matrix with the following form (note that $r_1 > v-1$).

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	B_{11}	B_{12}	B_{13}	
T_1	1	1	1	1	1	1								6
T_2	1				1									5
T_3		1				1								5
T_4			1											5
T_5				1										5
	2	2	2	2	2	2	2	2	2	2	2	2	2	

Note that after the first stage of the construction process, $|\lambda_{1\ell}-\lambda_{1m}| \leq 1$ for $\ell, m > 1$. Note also that for $i \geq 2$, there are $r_i-\lambda_{1i}$ replications of treatment T_i which have not yet been assigned to blocks and which must occur in blocks $B_{r_1+1}, \ldots, B_b$.

We start the second stage of the construction process by taking the $r_2-\lambda_{12}$ replications of T_2 which have not yet been assigned to blocks and assign T_2 to experimental units occurring in blocks $B_{r_1+1}, \ldots, B_{r_1+r_2-\lambda_{12}}$, i.e., $n_{2m} = 1$ for $r_1+1 \leq m \leq r_1+r_2-\lambda_{12}$. We now sequentially assign treatments to experimental units remaining in blocks $B_{r_1+1}, \ldots, B_{r_1+r_2-\lambda_{12}}$ beginning with the treatment after which the sequential assignment of treatments to succeeding blocks ended in stage one, i.e., if the sequential assignment of treatments to succeeding blocks ended in stage one with T_s being assigned to B_{r_1}, then the procedure is begun in stage two by assigning treatment T_{s+1} or T_3 to the experimental unit remaining in B_{r_1+1} depending upon whether $s = v$ or 2, and then T_{s+2} or T_4 is assigned to B_{r_1+2}, etc. After the second stage of the procedure, the incidence matrix of the design being constructed may look as in the following examples.

Example 7.2.2. (Cont.) After the second stage of the procedure, the incidence matrix of the design being constructed has the following form.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	
T_1	1	1	1	1							4
T_2	1				1	1	1				4
T_3		1				1					3
T_4			1				1				3
T_5				1							3
T_6					1						3
	2	2	2	2	2	2	2	2	2	2	

<u>Example 7.2.3.</u> (Cont.) After the second stage of the procedure, the incidence matrix of the design being constructed has the following form.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	B_{11}	B_{12}	B_{13}	
T_1	1	1	1	1	1	1								6
T_2	1				1		1	1	1					5
T_3		1				1			1					5
T_4			1				1							5
T_5				1				1						5
	2	2	2	2	2	2	2	2	2	2	2	2	2	

We now repeat the procedure for each succeeding treatment until the design is complete, i.e., at the pth stage of the construction process, we take the $r_p - \sum_{i=1}^{p-1} \lambda_{ip}$ replications of treatment T_p which have not been assigned to blocks in the previous $p-1$ stages, and assign T_p to experimental units in blocks B_m, $\sum_{i=1}^{p-1} r_i - \sum_{i=1}^{p-1} \sum_{j>i}^{p-1} \lambda_{ij} + 1 \leq m \leq \sum_{i=1}^{p} r_i - \sum_{i=1}^{p} \sum_{j>i}^{p} \lambda_{ij}$. We then sequentially assign treatments to the experimental units remaining in the blocks to which T_p was assigned beginning with the treatment after which the sequential assignment of treatments to succeeding blocks ended in stage $p-1$. Note that each stage may be identified with a particular row of the incidence matrix in which that particular stage begins, i.e., stage p begins in row p of N.

Example 7.2.2. (Cont.) Following the above design procedure we obtain a design in $\mathcal{D}[6;10;2]$ with the following incidence matrix.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	
T_1	1	1	1	1							4
T_2	1				1	1	1				4
T_3		1				1		1			3
T_4			1				1		1		3
T_5				1				1		1	3
T_6					1				1	1	3
	2	2	2	2	2	2	2	2	2	2	

Example 7.2.3. (Cont.) Following the above design procedure, we obtain a design in $\mathcal{D}[5;13;2]$ with the following incidence matrix.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	B_{11}	B_{12}	B_{13}	
T_1	1	1	1	1	1	1								6
T_2	1				1		1	1	1					5
T_3		1				1			1	1	1			5
T_4			1				1			1		1	1	5
T_5				1				1			1	1	1	5
	2	2	2	2	2	2	2	2	2	2	2	2	2	

From Theorem 7.2.1 and this construction process, we can easily determine the (M,S) optimal design in $\mathcal{D}[v;b;k]$ where $v = k+2$ as the following result shows.

Corollary 7.2.4. The (M,S) optimal design in $\mathcal{D}[v;b;k]$ where $v = k+2$ is the complement of the (M,S) optimal design in $\mathcal{D}[v;b;2]$.

Pf. Since $v = k+2$ and $v = k+2 \leq 2k$ for all $k \geq 2$, Theorem 7.1.7 is applicable and the result follows.

Example 7.2.5. If we take the complement of the design obtained in Example 7.2.2, the (M,S) optimal design in $\mathcal{D}[6;10;4]$ will be determined and it has the following incidence matrix.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	
T_1					1	1	1	1	1	1	6
T_2		1	1	1				1	1	1	6
T_3	1		1	1	1		1		1	1	7
T_4	1	1		1	1	1		1		1	7
T_5	1	1	1		1	1	1		1		7
T_6	1	1	1	1		1	1	1			7
	4	4	4	4	4	4	4	4	4	4	

Note that as a result of Theorem 7.2.1 and Corollary 7.2.4, we know that the (M,S) optimal design in $\mathcal{D}[v;b;k]$ when $v = k+2$ must always have the property that $|r_i - r_j| \leq 1$ for all i,j.

7.3. Constructing (M,S) Optimal Designs from Known Optimal Designs

The concept of a dual incomplete block design will be used several times in this section. Recall from Chapter II that if $D[v;r_1,\ldots,r_v;b;k_1,\ldots,k_b;N]$ is a binary incomplete block design, then the dual design is that design obtained by interchanging the roles of blocks and treatments. If $\overline{N}$ is the incidence matrix of the dual design, then $\overline{N} = N'$.

A linked block design with parameters v, b, r, k and μ is defined to be a binary incomplete block design with v treatments arranged in b blocks of size k where each treatment is replicated r times and any two blocks have exactly μ treatments in common. Clearly, the dual of a linked block design is a BIBD. We shall now discuss several methods of obtaining (M,S) optimal designs from linked block designs.

i) Suppose from a linked block design with parameters v, b, r, k and μ, we eliminate m treatments such that no two of the eliminated treatments occur in the same block. Then the blocks break up into two groups, the first of which consists of those blocks from which a treatment was eliminated and the last group consists of those blocks from which no treatment was eliminated.

Clearly any block from which a treatment was eliminated will have $\mu-1$ treatments in common with blocks from which the same treatment was eliminated and μ treatments in common with all other blocks. The blocks from which no treatment was eliminated will have μ treatments in common with all other blocks. Thus, after the elimination of treatments, we will have a block design with $v-m$ treatments, mr blocks of size $k-1$, $b-mr$ blocks of size k, and with an incidence matrix N such that $N'N = (\mu_{ij})$ where $\mu_{ij} = \mu$ or $\mu-1$ for all $i \neq j$. If $\bar{D}$ denotes the dual of this latter design, then $\bar{v} = b$, $\bar{r}_i = k$ or $k-1$, $\bar{b} = v-m$, $\bar{k} = r$, and $\bar{N}\bar{N}' = (\bar{\lambda}_{ij})$ where $\bar{\lambda}_{ij} = \mu$ or $\mu-1$ for all $i \neq j$. Note that $\bar{D}$ is (M,S) optimal in $\mathcal{D}[\bar{v};\bar{b};\bar{k}]$. An example will now be given to illustrate this construction technique.

Example 7.3.1. Consider the symmetrical BIBD with $\lambda = 2$, $v = b = 7$ and $r = k = 4$. The design is given by the following incidence matrix.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	
T_1		1	1	1		1		4
T_2			1	1	1		1	4
T_3	1			1	1	1		4
T_4		1			1	1	1	4
T_5	1		1			1	1	4
T_6	1	1		1			1	4
T_7	1	1	1		1			4
	4	4	4	4	4	4	4	

When we eliminate treatment T_1 and take the dual, we get the following (M, S) optimal design in $\mathcal{D}[7;6;4]$.

	B_1	B_2	B_3	B_4	B_5	B_6	
T_1		1		1	1	1	4
T_2			1		1	1	3
T_3	1			1		1	3
T_4	1	1			1		3
T_5	1	1	1			1	4
T_6		1	1	1			3
T_7	1		1	1	1		4
	4	4	4	4	4	4	

ii) Suppose now we take a set of m treatments in a linked block design, no two of which occur in the same block, and replace each treatment in the set by a group of two treatments occurring in the same blocks as the original treatment. Upon adding these treatments, we get a block design with $v+m$ treatments, mr blocks of size $k+1$, $b-mr$ blocks of size k, and an incidence matrix N such that $N'N = (\mu_{ij})$ where $\mu_{ij} = \mu$ or $\mu+1$. If $\bar{D}$ denotes the dual of this latter design, then $\bar{v} = b$, $\bar{r}_i = k$ or $k+1$, $\bar{b} = v+m$, $\bar{k} = r$, and $\bar{N}\bar{N}' = (\bar{\lambda}_{ij})$ where $\bar{\lambda}_{ij} = \mu$ or $\mu+1$. Clearly this latter design will be (M, S) optimal in $\mathcal{D}[\bar{v};\bar{b};\bar{k}]$.

<u>Example 7.3.2</u>. Suppose in Example 7.3.1, instead of eliminating treatment T_1, we replace it with two treatments each occurring in the same block as T_1. When this is done, and when the dual of the constructed design is taken, we get an (M, S) optimal design in $\mathcal{D}[7;8;4]$ with the following incidence matrix.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	
T_1				1		1	1	1	4
T_2	1	1			1		1	1	5
T_3	1	1	1			1		1	5
T_4	1	1	1	1			1		5
T_5			1	1	1			1	4
T_6	1	1		1	1	1			5
T_7			1		1	1	1		4
	4	4	4	4	4	4	4	4	

We shall now devise some methods for constructing (M,S) optimal designs from designs which are already known to exist. As an example, it was shown in an earlier chapter that if a balanced incomplete block design or a PBIB(2) with $\lambda_2 = \lambda_1 + 1$ exists in $\mathcal{D}[v;b;k]$, then that design will be (M,S) optimal in $\mathcal{D}[v;b;k]$. If possible, we would like to use those known and tabulated designs which are (M,S) optimal to derive (M,S) optimal designs with different parameters. To this end, we have the following result.

Theorem 7.3.3. Let D be an (M,S) optimal binary design in $\mathcal{D}[v;(r_i);b;k]$ whose incidence matrix N has the property that $|\mu_{ij} - \mu_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$. Then any combination of distinct columns of N will give the incidence matrix of an (M,S) optimal design in $\mathcal{D}[v;(\hat{r}_i);m;k]$ where m represents the number of distinct columns in the new design and $\hat{r}_i$ the number of replications of T_i.

Pf. Simply observe that any combination of distinct columns of N still has the property that $|\mu_{ij} - \mu_{\ell m}| \leq 1$ for $i \neq j$, $\ell \neq m$, hence from Corollary 5.1.14, the design is (M,S) optimal.

Recall the definition of a linked design given earlier in this section. We now extend this definition to a partially linked incomplete block design. A partially linked incomplete block design with m associate classes is a binary design consisting of an arrangement of v treatments, each replicated r times, contained in b blocks of size k such that the dual design is a PBIB(m). We shall denote such a design by PLIB(m).

Let N be the v x b incidence matrix of a linked incomplete block design or a PLIB(2) with the property that $\mu_{ij} = \mu$ or $\mu+1$. Clearly these designs will be (M, S) optimal in $\mathcal{D}[v;b;k]$; hence by Theorem 7.3.3 by taking any combination of m distinct columns of N, we will still have an (M, S) optimal design in $\mathcal{D}[v;(\hat{r}_i);m;k]$. However, such a design may not be (M, S) optimal in the larger class of designs $\mathcal{D}[v;m;k]$, since it may not have the property that $|\hat{r}_i - \hat{r}_j| \leq 1$ for all i, j. However, if N_1 is the v x m incidence matrix derived from $N = (N_1, N_2)$ by eliminating N_2 and has the property that $|\hat{r}_i - \hat{r}_j| \leq 1$, then N_1 will be the incidence matrix of an (M, S) optimal design in $\mathcal{D}[v;m;k]$. Note that N_2 will also be the incidence matrix of an (M, S) optimal design in $\mathcal{D}[v;b-m;k]$. Note also that any single column may be eliminated from N or any two columns i and j can be eliminated from N if $\mu_{ij} = \max[0, 2k-v]$ and still have an (M, S) optimal design in $\mathcal{D}[v;b-1;k]$ and $\mathcal{D}[v;b-2;k]$ respectively.

In general, suppose we are looking for an (M, S) optimal design in $\mathcal{D}[v;(r_i);b;k]$ or $\mathcal{D}[v;b;k]$ where bk/v is not an integer. Keep v and k fixed and find the smallest positive r' and b' > b such that vr' = b'k. If there exists an (M, S) optimal design in $\mathcal{D}[v;b';k]$ with an incidence matrix N such that $|\mu_{ij}-\mu_{\ell m}| \leq 1$ for $i \neq j$, $\ell \neq m$ then by taking any b columns of N having the proper parameters, we will have the incidence matrix of an (M,S) optimal design in $\mathcal{D}[v;(r_i);b;k]$ or $\mathcal{D}[v;b;k]$.

Since the construction of incomplete block designs where bk/v is an integer has been studied extensively, many designs having the property that $|\lambda_{ij}-\lambda_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$ have been catalogued and published. So if we are looking for a design in $\mathcal{D}[v;b';k]$ with the property that $|\mu_{ij}-\mu_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$, it may simply be a matter of finding the dual of the desired design in some published catalogue of designs. An example will illustrate the technique.

Example 7.3.4. Suppose we are looking for an (M,S) optimal design in $\mathcal{D}[9;5;6]$. The smallest possible integers such that $vr' = b'k$ are $b' = 6$ and $r' = 4$; so we are seeking a design in $\mathcal{D}[9;6;6]$ with the property that $|\mu_{ij}-\mu_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$, or equivalently, a design in $\mathcal{D}[6;9;4]$ with the property that $|\lambda_{ij}-\lambda_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$. Using the Tables of Partially Balanced Designs with Two Associate Classes we see that a PBIB(2) design in $\mathcal{D}[6;9;4]$ exists with the property that $\lambda_2 = \lambda_1+1$. This design is given by

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	
T_1	1	1	1	1	1	1				6
T_2	1		1	1		1	1		1	6
T_3	1	1	1				1	1	1	6
T_4	1	1		1	1		1	1		6
T_5				1	1	1	1	1	1	6
T_6		1	1		1	1		1	1	6
	4	4	4	4	4	4	4	4	4	

Clearly, if we eliminate any row in the above design and take the dual, we will have a design which is (M,S) optimal in $\mathcal{D}[9; 5; 6]$. The final design is given below.

	B_1	B_2	B_3	B_4	B_5	
T_1	1	1	1	1		4
T_2	1		1	1		3
T_3	1	1	1			3
T_4	1	1		1	1	4
T_5	1			1	1	3
T_6	1	1			1	3
T_7		1	1	1	1	4
T_8			1	1	1	3
T_9		1	1		1	3
	6	6	6	6	6	

7.4. Patchwork Techniques

For $i = 1, \ldots, t$, let $D_i[v_i; r_1, \ldots, r_{v_i}; b_i; k_{b_i}; N_i]$ be an incomplete block design defined on Ω_i. Let $D = \bigcup_{i=1}^{t} D_i$ denote the design obtained by combining all the D_i, i.e., D is that design defined on $\Omega = \bigcup_{i=1}^{t} \Omega_i$ consisting of the $b = \sum_{i=1}^{t} b_i$ blocks contained in $D_1, D_2, \ldots, D_t$. An interesting and practically useful problem is to find necessary and sufficient conditions on the D_i which will make D an (M,S) optimal design. The solution to this problem is in general unknown and appears to be very difficult. However, we now give some techniques for combining designs so as to yield (M,S) optimal designs.

i) Let $\bar{D} = D[v; \bar{r}_1, \ldots, \bar{r}_v; \bar{b}; k; \bar{N}]$ denote a binary incomplete block design defined on Ω such that $\bar{N}\,\bar{N}' = (\bar{\lambda}_{ij})$ has all of its off diagonal elements equal. Let $\hat{D} = D[v; \hat{r}_1, \ldots, \hat{r}_v; \hat{b}; k; \hat{N}]$ be a binary incomplete block design also defined on Ω with $\hat{N}\hat{N}' = (\hat{\lambda}_{ij})$ where $|\hat{\lambda}_{ij} - \hat{\lambda}_{pq}| \leq 1$ for all $i \neq j$, $p \neq q$. Let $D = \bar{D} \cup \hat{D}$ denote the design defined on Ω whose incidence matrix N is given by $(\bar{N}, \hat{N})$. Note that D is binary and that $NN' = (\lambda_{ij})$ where $\lambda_{ij} = \bar{\lambda}_{ij} + \hat{\lambda}_{ij}$ for all $i \neq j$. Hence

$$|\lambda_{ij}-\lambda_{pq}| = |(\bar{\lambda}_{ij}+\hat{\lambda}_{ij}) - (\bar{\lambda}_{pq}+\hat{\lambda}_{pq})| = |\hat{\lambda}_{ij}-\hat{\lambda}_{pq}| \leq 1$$

for all $i \neq j$, $p \neq q$. By Theorem 5.1.1 and Corollary 5.1.7, D will be (M, S) optimal in $\mathcal{D}[v;(\bar{r}_i+\hat{r}_i);\bar{b}+\hat{b};k]$. If D also has the property that $|(\bar{r}_i+\hat{r}_i)-(\bar{r}_j+\hat{r}_j)| \leq 1$ for all $i \neq j$, then by Corollary 6.18, D will be (M, S) optimal in $\mathcal{D}[v;\bar{b}+\hat{b};k]$.

Example 7.4.1. Let D denote the BIBD with $\lambda = 1$ whose incidence matrix N is given below.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	
T_1	1	1		1				3
T_2		1	1		1			3
T_3			1	1		1		3
T_4				1	1		1	3
T_5	1				1	1		3
T_6		1				1	1	3
T_7	1		1				1	3
	3	3	3	3	3	3	3	

Let D_i denote that design whose incidence matrix consists of the first i columns given below, $1 \leq i \leq 5$.

	B_1	B_2	B_3	B_4	B_5
T_1	1		1		
T_2	1			1	
T_3	1				1
T_4		1	1		
T_5		1		1	
T_6		1			1
T_7			1	1	1
	3	3	3	3	3

All of the designs $D = D \cup D_i$ will be (M, S) optimal in $\mathcal{D}[7;7+i;3]$ for $i = 1, \ldots, 5$.

ii) Let $D = D[v;r_1, \ldots, r_v;b;k;N]$ be a binary incomplete block design defined on Ω with $\lambda_{ij} = x$ or $x+1$ for all $i \neq j$. If there exists a set G consisting of $m \geq k$ treatments in Ω such that $\lambda_{ij} = x$ for all $T_i, T_j \in G$, then a block containing any k of the treatments in G may be added to D and the resulting design $\bar{D}$ will be (M, S) optimal in the class $\mathcal{D}$ of designs with $b+1$ blocks of size k and fixed replication sizes to which $\bar{D}$ belongs.

To see that $\bar{D}$ is optimal in $\mathcal{D}$, note first that $\bar{D}$ is a binary design. Note also that if $\bar{N}$ is the incidence matrix for $\bar{D}$, then $\bar{N}\bar{N}' = (\bar{\lambda}_{ij})$ where $\bar{\lambda}_{ij} = \lambda_{ij}$ if either T_i or T_j

does not occur in block $b+1$, and $\bar{\lambda}_{ij} = \lambda_{ij}+1$ if both T_i and T_j occur in block $b+1$. Hence $\bar{\lambda}_{ij} = x$ or $x+1$ for all $i \neq j$, so by Theorem 5.1.1 and Corollary 5.1.7, $\bar{D}$ will be (M,S) optimal in $\mathcal{D}$.

Note that this process of adding blocks to a design D may be continued as long as there exists a set G of treatments in Ω satisfying the necessary conditions.

<u>Example 7.4.2.</u> Let $D[9;3;9;3;N]$ be the PBIB(2) with $\lambda_1 = 0$ and $\lambda_2 = 1$ whose incidence matrix is given below.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	
T_1	1			1			1			3
T_2	1				1			1		3
T_3	1					1			1	3
T_4		1			1				1	3
T_5			1	1				1		3
T_6		1		1				1		3
T_7			1			1			1	3
T_8		1				1	1			3
T_9			1		1		1			3
	3	3	3	3	3	3	3	3	3	

Note that $\lambda_{14} = \lambda_{17} = \lambda_{47} = 0$. Hence a column B_{10} containing treatments T_1, T_4, and T_7 may be added to the above design, and the resulting design will be (M, S) optimal in $\mathcal{D}[9;4,3,3,4,3,3,4,3,3;10;3]$.

iii) Let $\bar{D} = D[\bar{v};\bar{r}_1,\ldots,\bar{r}_{\bar{v}};b;\bar{k};\bar{N}]$ be a binary incomplete block design defined on $\bar{\Omega}$ with $\bar{N}'\bar{N} = (\bar{\mu}_{ij})$ where $\bar{\mu}_{ij} = \mu$ for all $i \neq j$. Let $\hat{D} = D[\hat{v};\hat{r}_1,\ldots,\hat{r}_{\hat{v}};b;\hat{k};\hat{N}]$ be a binary incomplete block design defined on $\hat{\Omega}$ with $\bar{\Omega} \cap \hat{\Omega} = \phi$ and with $\hat{N}'\hat{N} = (\hat{\mu}_{ij})$ where $|\hat{\mu}_{ij} - \hat{\mu}_{pq}| \leq 1$ for all $i \neq j$, $p \neq q$. Let D denote the design defined on $\bar{\Omega} \cup \hat{\Omega}$ whose incidence matrix N is given by $\binom{\bar{N}}{\hat{N}}$.

Note that D is binary and that $N'N = (\mu_{ij})$ where $\mu_{ij} = \bar{\mu}_{ij} + \hat{\mu}_{ij}$ for all $i \neq j$. Hence

$$|\mu_{ij} - \mu_{pq}| + |\bar{\mu}_{ij} + \hat{\mu}_{ij} - (\bar{\mu}_{pq} + \hat{\mu}_{pq})| = |\hat{\mu}_{ij} - \hat{\mu}_{pq}| \leq 1$$

for all $i \neq j$, $p \neq q$. By Theorem 5.1.1 and Corollary 5.1.14, D will be (M, S) optimal in $\mathcal{D}[\bar{v}+\hat{v};(r_i);b;\bar{k}+\hat{k}]$ where $r_i = \bar{r}_i$, $1 \leq i \leq \bar{v}$, $r_i = \hat{r}_i$, $\bar{v}+1 \leq i \leq \bar{v}+\hat{v}$.

iv) Let $\bar{D} = D[\bar{v};\bar{r}_1,\ldots,\bar{r}_{\bar{v}};b;\bar{k};\bar{N}]$ be a binary incomplete block design defined on $\bar{\Omega}$ with $\bar{N}'\bar{N} = (\bar{\mu}_{ij})$ and which is (M, S) optimal in $\mathcal{D}[\bar{v};(\bar{r}_i);b;\bar{k}]$. Let $\hat{D} = D[\hat{v};\hat{r}_1,\ldots,\hat{r}_{\hat{v}};b;\hat{k};\hat{N}]$ denote a complete binary randomized block design defined on $\hat{\Omega}$ with $\bar{\Omega} \cap \hat{\Omega} = \phi$, i.e., $\hat{r}_i = b$ for all i and $\hat{N}'\hat{N} = (\hat{\mu}_{ij})$ where

$\hat{\mu}_{ij} = \hat{k}$ for all $i \neq j$. Now let D denote the design defined on $\bar{\Omega} \cup \hat{\Omega}$ whose incidence matrix N is equal to $\binom{\bar{N}}{\hat{N}}$.

Note that D is a binary design hence it will have maximal $\operatorname{tr} C$ in $\mathcal{D} = \mathcal{D}[\bar{v}+\hat{v};(r_i);b;\bar{k}+\hat{k}]$ where $r_i = \bar{r}_i$ for $1 \leq i \leq \bar{v}$ and $r_i = \hat{r}_i$ for $\bar{v}+1 \leq i \leq \bar{v}+\hat{v}$. Note also that if the incidence $\tilde{N}$ of any design $\tilde{D} \in \mathcal{M}\{\mathcal{D}\}$ is partitioned as in the previous paragraph, i.e., $\tilde{N} = \binom{N_1}{N_2}$ where N_1 and N_2 have the same row and column sums as the incidence matrices for $\bar{D}$ and $\hat{D}$ above, then it is easily seen

$$\operatorname{tr}(\tilde{N}\tilde{N}')^2 = \operatorname{tr}(N_1 N_1')^2 + M$$

where M is a constant for all designs in $\mathcal{M}\{\mathcal{D}\}$. From this last expression, we see that finding an (M,S) optimal design in $\mathcal{D}$ is equivalent to finding an (M,S) optimal design in $\mathcal{D}[\bar{v},(\bar{r}_i);b;\bar{k}]$. So D as defined above will be (M,S) optimal in $\mathcal{D}$.

7.5. A Heuristic Approach to the Construction of (M,S) Optimal Designs

While a direct method of constructing (M,S) optimal designs is not given in this section, the procedure described can be of great value to the experimenter in constructing optimal designs in situations where the previously given methods of construction are not applicable.

Let $\mathcal{D} = \mathcal{D}[v;(r_i);b;k]$. In Chapter V, various methods were given for determining lower bounds for $\operatorname{tr}(NN')^2$ for designs in the class $\mathcal{M}\{\mathcal{D}\}$. If a design exists having an incidence matrix with $\operatorname{tr}(NN')^2$ equal to one of the lower bounds established, we would like to use the information gained in the establishment of the lower bound to aid in the construction of the design.

Let N be the incidence matrix of a typical design in $\mathcal{M}\{\mathcal{D}\}$ where $r_1 \geq r_2 \geq \cdots \geq r_v$. Now partition N into N_1 and N_2 where N_1 consists of the first v_1 rows of N and N_2 consists of the remaining $v-v_1$ rows of N. Note that the $\sum_{i=1}^{v_1} r_i = n_1$ replications assigned to $T_1, \ldots, T_{v_1}$ must occur in N_1, the $\sum_{i=v_1+1}^{v} r_i = n_2$ replications assigned to $T_{v_1+1}, \ldots, T_v$ must occur in N_2, and the k experimental units assigned to block B_i must be allocated between N_1 and N_2. Let us use the same notation and terminology as in Section 5.2. Recall that if $(k_1^*, \ldots, k_b^*)$ denotes any particular ordered configuration, then a minimal value for $\operatorname{tr}(NN')^2$ can be determined for any design whose incidence matrix has that ordered configuration. This minimal value is determined by solving the integer programming problem of minimizing (5.2.2) subject to the constraints given in (5.2.3).

In Section 5.2, a method was given for determining those values of C_1 yielding a lower bound for $tr(NN')^2$ in $\mathcal{M}\{\mathcal{D}\}$ and for finding those configurations yielding these values of C_1 for a given partition of N. If the process of determining a lower bound for $tr(NN')^2$ and determining those configurations yielding the lower bound is carried on for each possible partition of N, a great deal of information about the incidence matrix of a design with $tr(NN')^2$ equal to the lower bounds established is obtained. We would now like to use this information to construct an (M, S) optimal design for $\mathcal{D}$. Several examples will be given on how to do this.

Before proceeding, we shall give several facts which will prove useful later. Let $\bar{v}_1 > \hat{v}_1$ represent two different partitions of an incidence matrix N of a particular design $D \epsilon \mathcal{M}\{\mathcal{D}\}$ and let $\{\bar{k}_1^*, \ldots, \bar{k}_b^*\}$ and $\{\hat{k}_1^*, \ldots, \hat{k}_b^*\}$ represent the actual unordered configurations of the incidence matrix of the design for these two partitions of N. If $\bar{C}_1$ and $\hat{C}_1$ are the values of C_1 given by these configurations respectively, then by a proof analogous to that given for Lemma 4.1.3, it can be shown that

$$\bar{C}_1 - \hat{C}_1 = 2\sum_{i=1}^{\hat{v}_1}\sum_{j=\hat{v}_1+1}^{\bar{v}_1}\lambda_{ij} + 2\sum_{i=\hat{v}_1+1}^{\bar{v}_1}\sum_{j>i}^{\bar{v}_1}\lambda_{ij}$$

$$= 2\sum_{i=1}^{b}(\bar{k}_i^* - \hat{k}_i^*)(\hat{k}_i^*) + 2\sum_{i=1}^{b}(\bar{k}_i^* - \hat{k}_i^*)(\bar{k}_i^* - \hat{k}_i^* - 1). \qquad (7.5.1)$$

In particular, when $\bar{v}_1 = \hat{v}_1 + 1$,

$$\bar{C}_1 - \hat{C}_1 = 2\sum_{i=1}^{\hat{v}_1}\lambda_{i\bar{v}_1} = 2\sum_{T_{\bar{v}_1}\in B_m}\hat{k}_m^*. \qquad (7.5.2)$$

Note also that for any design D when $\bar{v}_1 = \hat{v}_1 + 1$, the values of $\bar{k}_i^*$ in $\{\bar{k}_1^*, \ldots, \bar{k}_b^*\}$ must be obtainable from the values in $\{\hat{k}_1^*, \ldots, \hat{k}_b^*\}$ by adding one to exactly $r_{\bar{v}_1}$ of the $\hat{k}_i^*$.

From this point on, if $v_1 = s$, let C_1^s, C_2^s, and C_{12}^s denote the values of C_1, C_2, and C_{12} which are given by the configuration under consideration.

Example 7.5.3. Suppose we wish to find an (M,S) optimal design in $\mathcal{D} = \mathcal{D}[6;5,5,5,4,4,4;9;3]$. The values of C_1^s, C_2^s, and C_{12}^s yielding lower bounds for $tr(NN')^2$ for the various partitions of N as determined using the methods of Section 5.2 are given below.

The various ordered configurations yielding these lower bounds are also given.

s	C_1^s	C_2^s	C_{12}^s	LB	Configurations
1	0	34	20	225	(1, 1, 1, 1, 1, 0, 0, 0, 0)
2	4	18	36	225	(2, 2, 1, 1, 1, 1, 1, 1, 0)
3	12	6	36	225	(2, 2, 2, 2, 2, 2, 1, 1, 1)
4	24	2	28	225	(3, 3, 2, 2, 2, 2, 2, 2, 1)
5	30	0	16	225	(3, 3, 3, 3, 3, 2, 2, 2, 2)

It is seen in using Algorithm (4.3) to calculate the lower bounds for the various partitions that for a design to have an incidence matrix with $tr(NN')^2 = 225$, it must be the case that $\lambda_{ij} = 1$ or 2 for all $i \neq j$. Now observe that for each value of s, we have the somewhat unusual situation that there are unique values of C_1^s giving the lower bounds for $tr(NN')^2$ and unique ordered configurations giving these values of C_1^s. So in order for any design to have an incidence matrix with $tr(NN')^2$ equal to the lower bound established, it must have the ordered configuration given above for each different partition.

Note that when $s = 3$, for any design in $\mathcal{M}\{\mathcal{D}\}$

i) $C_1^3 = 2(\lambda_{12}+\lambda_{13}+\lambda_{23})$

ii) $C_2^3 = 2(\lambda_{45}+\lambda_{46}+\lambda_{56})$

iii) $C_{12}^3 = 2 \sum_{i=1}^{3} \sum_{j=4}^{6} \lambda_{ij}$.

So for any design to have an incidence matrix with $|\lambda_{ij} - \lambda_{\ell m}| \leq 1$ for $i \neq j$, $\ell \neq m$, it must have $C_1^3 = 12$, $C_2^3 = 6$, and $C_{12}^3 = 36$. Hence it must have

i) $\lambda_{12} = \lambda_{13} = \lambda_{23} = 2$

ii) $\lambda_{45} = \lambda_{46} = \lambda_{56} = 1$

iii) $\lambda_{ij} = 2, \quad i \leq 3, \ j > 3$.

Using this information, we shall set about constructing an (M, S) optimal design in $\mathcal{D}$.

Since $C_1^2 = 4$ and $\lambda_{12} = 2$, it is easily seen that the first two rows of any design having $tr(NN')^2 = 225$ must have the following form.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	
T_1	1	1	1	1	1					5
T_2	1	1				1	1	1		5
	2	2	1	1	1	1	1	1	0	

For $s = 3$, the incidence matrix must have an ordered configuration of the form (2, 2, 2, 2, 2, 2, 1, 1, 1). Using (7.5.2), since $C_1^3 - C_1^2 = 8$, treatment T_3 should be assigned to experimental units in blocks such that $\sum_{T_3 \epsilon B_m} k_m^* = 4$ where the k_m^* are taken from the unordered configuration given above for $s = 2$ and in such a way that $\lambda_{12} = \lambda_{13} = 2$. The three rows given below satisfy these properties.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	
T_1	1	1	1	1	1					5
T_2	1	1				1	1	1		5
T_3			1	1		1	1		1	5
	2	2	2	2	1	2	2	1	1	

For $s = 4$, the incidence matrix must have an ordered configuration of the form $(3, 3, 2, 2, 2, 2, 2, 2, 1)$. Using (7.5.2), since $C_1^4 - C_1^3 = 12$, treatment T_4 must be assigned to experimental units in blocks in such a way that $\sum_{T_4 \epsilon B_m} k_m^* = 6$ where the k_m^* are taken from the unordered configuration given above for $s = 3$ and in such a way that $\lambda_{14} = \lambda_{24} = \lambda_{34} = 2$. The four rows given below satisfy these properties.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	
T_1	1	1	1	1	1					5
T_2	1	1				1	1	1		5
T_3			1	1		1	1		1	5
T_4	1				1	1			1	4
	3	2	2	2	2	3	2	1	2	

Continuing in this manner, we get the following design.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	
T_1	1	1	1	1	1					5
T_2	1	1				1	1	1		5
T_3			1	1		1	1		1	5
T_4	1				1	1			1	4
T_5		1		1				1	1	4
T_6			1		1		1	1		4
	3	3	3	3	3	3	3	3	3	

Note that the design is (M, S) optimal since $|\lambda_{ij} - \lambda_{\ell m}| \leq 1$ for $i \neq j$, $\ell \neq m$.

For Example 7.5.3, any (M, S) optimal design having an incidence matrix with $tr(NN')^2 = 225$ had to possess the particular ordered configurations given for each value of s. Hence in this sense, the

(M,S) optimal design in $\mathcal{D}[6;5,5,5,4,4,4;9;3]$ was completely determined.

Several more examples will now be given on how to use the information collected from the establishment of the various lower bounds in the construction of optimal designs.

Example 7.5.4. Consider the class of designs $\mathcal{D} = \mathcal{D}[7;6,6,6,6,6,5,5;10;4]$. The values of C_1^s, C_2^s, and C_{12}^s yielding lower bounds for $tr(NN')^2$ for the various partitions of N as determined using the methods of Section 5.2 are given below. The various ordered configurations yielding those lower bounds are also given.

s	C_1^s	C_2^s	C_{12}^s	LB	Configurations
2	6	54	60	578	(2, 2, 2, 1, 1, 1, 1, 1, 1, 0)
3	18	30	72	578	(3, 2, 2, 2, 2, 2, 2, 1, 1, 1)
					(2, 2, 2, 2, 2, 2, 2, 2, 2, 0)
4	36	12	72	578	(3, 3, 3, 3, 2, 2, 2, 2, 2, 2)
5	62	2	56	586	(4, 3, 3, 3, 3, 3, 3, 3, 3, 2)
	64	4	52		(4, 4, 3, 3, 3, 3, 3, 3, 2, 2)
6	90	0	30	578	(4, 4, 4, 4, 4, 4, 3, 3, 3, 3)

Note that the lower bound established for $tr(NN')^2$ in $\mathcal{M}\{\mathcal{D}\}$ when $s = 5$ is 586 and there are two values of C_1^5 giving this lower bound. When $C_1^5 = 62$, it is seen in using Algorithm (4. 3) to calculate the lower bound, that any design whose incidence matrix has $tr(NN')^2 = 586$ must have $\lambda_{ij} = 3$ or 4 for $1 \leq i \neq j \leq 5$, $\lambda_{67} = 1$, and $\lambda_{ij} = 2$ or 3 for all other $i \neq j$. When $C_1^5 = 64$, any design whose incidence matrix has $tr(NN')^2 = 586$ must have $\lambda_{ij} = 3$ or 4 for $1 \leq i \neq j \leq 5$, $\lambda_{67} = 2$, and $\lambda_{ij} = 2$ for all other $i \neq j$. When a situation such as this occurs, one can only choose a particular configuration giving the lower bound and use this as a base from which to start constructing the design.

We will now construct an (M,S) optimal design using that ordered configuration associated with $C_1^5 = 62$ as a base configuration. Since $C_1^5 = 62 = 2 \sum_{i=1}^{5} \sum_{j>i}^{5} \lambda_{ij}$, the set of λ_{ij} minimizing $2 \sum_{i=1}^{5} \sum_{j>i}^{5} \lambda_{ij}^2$ subject to the usual constraints is seen from Algorithm (4. 3) to consist of one λ_{ij} equal to four, and nine of the λ_{ij} equal to three. Without loss of generality, assume that $\lambda_{45} = 4$, hence $\lambda_{ij} = 3$ for all other $i,j \leq 5$, $i \neq j$. Making this assumption, it is easily seen using (7. 5. 2) that any design having an incidence matrix with the λ_{ij} equal to the above, must have $C_1^2 = 6$, $C_1^3 = 18$, $C_1^4 = 36$, and $C_1^5 = 62$. The configurations associated with these values of s and C_1^s are given below.

s	C_1^s	Configurations
2	6	(2, 2, 2, 1, 1, 1, 1, 1, 1, 0)
3	18	(3, 2, 2, 2, 2, 2, 2, 1, 1, 1)
		(2, 2, 2, 2, 2, 2, 2, 2, 2, 0)
4	36	(3, 3, 3, 3, 2, 2, 2, 2, 2, 2)
5	62	(4, 3, 3, 3, 3, 3, 3, 3, 3, 2)

Note that there are two possible ordered configurations associated with $C_1^3 = 18$. However, for any design to have an incidence matrix with λ_{ij} equal to the above, it must have an ordered configuration of the form (3, 3, 3, 3, 2, 2, 2, 2, 2, 2) when $s = 4$. This configuration must be obtainable from the configuration given for $s = 3$ by adding one to r_4 of the k_i^* in the configuration given for $s = 3$. This will clearly be impossible if for $s = 3$, the incidence matrix has an ordered configuration of the form (2, 2, 2, 2, 2, 2, 2, 2, 2, 0). Hence any design having an incidence matrix with λ_{ij} equal to the above must have an ordered configuration of the form (3, 2, 2, 2, 2, 2, 2, 1, 1, 1) when $s = 3$. Using this information we now set about the construction process.

Clearly when $s = 2$ and $C_1^2 = 6$, the first two rows of the design must have the following form.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	
T_1	1	1	1	1	1	1					6
T_2	1	1	1				1	1	1		6
	2	2	2	1	1	1	1	1	1	0	

For $s = 3$, the incidence matrix must have an ordered configuration of the form $(3, 2, 2, 2, 2, 2, 2, 1, 1, 1)$. Using (7.5.2) since $C_1^3 - C_1^2 = 12$, treatment T_3 should be assigned to experimental units in blocks in such a way that $\sum_{T_3 \epsilon B_m} k_m^* = 6$ where the k_m^* are taken from the unordered configuration given above for $s = 2$ and in such a way that $\lambda_{13} = \lambda_{23} = 3$. The three rows given below satisfy these properties.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	
T_1	1	1	1	1	1	1					6
T_2	1	1	1				1	1	1		6
T_3	1			1	1		1	1		1	6
	3	2	2	2	2	1	2	2	1	1	

For $s = 4$, the incidence matrix of a design with λ_{ij} equal to the above must have an ordered configuration of the form $(3, 3, 3, 3, 2, 2, 2, 2, 2, 2)$. Using (7.5.2), since $C_1^4 - C_1^3 = 18$, treatment T_4 should be assigned to experimental units in blocks in such a way that $\sum_{T_4 \epsilon B_m} k_m^* = 9$ where the k_m^* are taken from the unordered configuration given above for $s = 3$ and in such a way that $\lambda_{14} = \lambda_{24} = \lambda_{34} = 3$. The four rows given below possess these properties.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	
T_1	1	1	1	1	1	1					6
T_2	1	1	1				1	1	1		6
T_3	1			1	1		1	1		1	6
T_4		1		1		1	1		1	1	6
	3	3	2	3	2	2	3	2	2	2	

For $s = 5$, the incidence matrix of a design with λ_{ij} equal to the above must have an ordered configuration of the form (4, 3, 3, 3, 3, 3, 3, 3, 3, 2). Using (7.5.2), since $C_1^5 - C_1^4 = 26$, T_5 should be assigned to experimental units in blocks in such a way that

$\sum_{T_5 \epsilon B_m} k_m^* = 13$ where the k_m^* are taken from the unordered configuration given above for $s = 4$ and in such a way that $\lambda_{15} = \lambda_{25} = \lambda_{35} = 3$ and $\lambda_{45} = 4$. The five rows given below possess these properties.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	
T_1	1	1	1	1	1	1					6
T_2	1	1	1				1	1	1		6
T_3	1			1	1		1	1		1	6
T_4		1		1		1	1		1	1	6
T_5			1	1		1		1	1	1	6
	3	3	3	4	2	3	3	3	3	3	

Note that at this point, the remaining portion of the design is practically determined. All that remains is to assign treatments T_6 and T_7 to experimental units in blocks in such a way that $\lambda_{67} = 1$ and λ_{i6} and λ_{i7} equal two or three for all $i \leq 5$. The optimal design which is finally derived is given by the following incidence matrix.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	
T_1	1	1	1	1	1	1					6
T_2	1	1	1				1	1	1		6
T_3	1			1	1		1	1		1	6
T_4		1		1		1	1		1	1	6
T_5			1	1		1		1	1	1	6
T_6	1	1			1			1	1		5
T_7			1		1	1	1			1	5
	4	4	4	4	4	4	4	4	4	4	

One more example will be given to illustrate that even with a knowledge of the various lower bounds and of the configurations yielding these lower bounds for the various partitions, an (M,S) optimal design whose incidence matrix has $tr(NN')^2$ equal to one of the lower bounds established may be difficult or impossible to construct.

Example 7.5.10. Consider the class of designs $\mathcal{D}[7;4,4,4,4,4,4,3;9;3]$. The values of C_1^s, C_2^s, and C_{12}^s yielding lower bounds for $tr(NN')^2$ for the various partitions of N as determined using the methods of Section 5.2 are given on the following page. The various ordered configurations yielding these lower bounds are also given.

Notice that there are many more configurations yielding lower bounds for the various partitions in this example than in previous examples. In using Algorithm (4.3) to calculate these lower bounds, it is easily seen that for a design to have an incidence matrix N with $tr(NN')^2$ equal to the lower bounds established, it must have $NN' = (\lambda_{ij})$ where $\lambda_{ij} = 1$ or 2 for all $i \neq j$. When so many configurations yield lower bounds for the various partitions, one can simply choose one value of C_1 which has some "nice" property and then use a configuration yielding this value of C_1 as a base for the construction process as in the previous example.

s	C_1^s	C_2^s	C_{12}^s	LB	Configurations
2	2	14	38	183	(2, 1, 1, 1, 1, 1, 1, 0, 0)
	4	16	34		(2, 2, 1, 1, 1, 1, 0, 0, 0)
3	6	12	36	183	(2, 2, 2, 1, 1, 1, 1, 1, 1)
	8	14	32		(3, 2, 1, 1, 1, 1, 1, 1, 1)
					(2, 2, 2, 2, 1, 1, 1, 1, 0)
	10	16	28		(3, 2, 2, 1, 1, 1, 1, 1, 0)
					(2, 2, 2, 2, 2, 1, 1, 0, 0)
	12	18	24		(3, 3, 1, 1, 1, 1, 1, 1, 0)
					(3, 2, 2, 2, 1, 1, 1, 1, 0)
					(2, 2, 2, 2, 2, 2, 0, 0, 0)
4	16	6	32	183	(3, 2, 2, 2, 2, 2, 1, 1, 1)
					(2, 2, 2, 2, 2, 2, 2, 2, 0)
	18	18	28		(3, 3, 2, 2, 2, 1, 1, 1, 1)
					(3, 2, 2, 2, 2, 2, 2, 1, 0)
	20	10	24		(3, 3, 3, 2, 1, 1, 1, 1, 1)
					(3, 3, 2, 2, 2, 2, 1, 1, 0)
5	28	2	24	183	(3, 3, 3, 2, 2, 2, 2, 2, 1)
	30	4	20		(3, 3, 3, 3, 2, 2, 2, 1, 1)
6	42	6	12	183	(3, 3, 3, 3, 3, 3, 2, 2, 2)

Note that when $s = 3$, $C_1^3 = 6$ yields a lower bound for $tr(NN')^2$. The "nice" properties of this particular value of C_1^3 are i) that there is a unique configuration giving the value of C_1^3 and ii) that any design having an incidence matrix with this ordered configuration and with $tr(NN')^2 = 183$ must have $\lambda_{12} = \lambda_{13} = \lambda_{23} = 1$ and $\lambda_{ij} = 1$ for $j > i$, $i \geq 4$. (This is easily seen when the lower bound for $C_1^3 = 6$ is calculated using Algorithm (4.3).) We shall now use this information to construct an (M, S) optimal design in $\mathcal{D}$.

From the basic configuration, we know that $C_2^3 = 12$ and that for an incidence matrix to have this configuration and $tr(NN')^2 = 183$ it must have $\lambda_{45} = \lambda_{46} = \lambda_{47} = 1$. But $r_4(k-1) = 8 = \sum_{i \neq 4} \lambda_{i4}$, so from (7.5.2) we have

$$\lambda_{14} + \lambda_{24} + \lambda_{34} = \frac{C_1^4 - C_1^3}{2} = 5.$$

So $C_1^4 = C_1^3 + 10 = 16$. Similarly, it can be seen that for an incidence matrix to have an ordered configuration of the form $(2, 2, 2, 1, 1, 1, 1, 1, 1)$ for $s = 3$ and $tr(NN')^2$ equal to the lower bound established, those configurations for $s = 5, 6$ must give values of $C_1^5 = 28$ and $C_1^6 = 42$. The configurations yielding these values of C_1^s are given below.

s	C_1^s	Configurations
3	6	(2, 2, 2, 1, 1, 1, 1, 1, 1)
4	16	(3, 2, 2, 2, 2, 2, 1, 1, 1)
		(2, 2, 2, 2, 2, 2, 2, 2, 1)
5	28	(3, 3, 3, 3, 2, 2, 2, 1, 1)
6	42	(3, 3, 3, 3, 3, 3, 2, 2, 2)

Note that when $s = 4$, there are two possible ordered configurations associated with $C_1^4 = 16$. However, for $s = 5$ there is a unique configuration given and it must clearly be obtainable from the configuration given for $s = 4$ by adding one to r_5 of the k_i^* occurring in the configuration given for $s = 4$. This will clearly be impossible if for $s = 4$, the incidence matrix has an ordered configuration of the form (2, 2, 2, 2, 2, 2, 2, 2, 1). Hence any design having an incidence matrix with $tr(NN')^2$ equal to the lower bound established and configuration (2, 2, 2, 1, 1, 1, 1, 1, 1) for $s = 3$ must have an ordered configuration of the form (3, 2, 2, 2, 2, 2, 1, 1, 1) for $s = 4$.

We know that for any incidence matrix to have the basic configuration given for $s = 3$ and $tr(NN')^2 = 183$, it must have $\lambda_{12} = \lambda_{13} = \lambda_{23} = 1$. Using this information, it is easily seen that the first three rows of the incidence matrix must have the following form.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	
T_1	1	1	1	1						4
T_2	1				1	1	1			4
T_3		1			1			1	1	4
	2	2	1	1	2	1	1	1	1	

For $s = 4$, the incidence matrix must have an ordered configuration of the form $(3, 2, 2, 2, 2, 2, 1, 1, 1)$. Using (7.5.2), since $C_1^4 - C_1^3 = 10$, T_4 should be assigned to experimental units in blocks in such a way that $\sum_{T_4 \epsilon B_m} k_m^* = 5$ where the k_m^* are taken from the actual unordered configuration given above for $s = 3$. Also from (7.5.2), in order for $|\lambda_{ij} - \lambda_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$, we must have two of the λ_{i4} equal to two and one of the λ_{i4} equal to one for $i \leq 3$. The four rows given below have these properties.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	
T_1	1	1	1	1						4
T_2	1				1	1	1			4
T_3		1			1			1	1	4
T_4	1		1			1		1		4
	3	2	2	1	2	2	1	2	1	

For $s = 5$, the incidence matrix must have an ordered configuration of the form $(3, 3, 3, 2, 2, 2, 2, 2, 1)$. Using (7.5.2), since $C_1^5 - C_1^4 = 12$, T_5 should be assigned to experimental units in blocks in such a way that $\sum_{T_5 \in B_m} k_m^* = 6$ where the k_m^* are taken from the actual unordered configuration given above for $s = 4$. Also from (7.5.2), in order for $|\lambda_{ij} - \lambda_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$, we must have two of the λ_{i5} equal to two and two of the λ_{i5} equal to one for $i \leq 4$. The five rows given below possess these properties.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	
T_1	1	1	1	1						4
T_2	1				1	1	1			4
T_3		1			1			1	1	4
T_4	1		1			1		1		4
T_5			1		1		1		1	4
	3	2	3	1	3	2	2	2	2	

Continuing in this manner, we finally derive the design whose incidence matrix is given below.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	
T_1	1	1	1	1						4
T_2	1				1	1	1			4
T_3		1			1			1	1	4
T_4	1		1			1		1		4
T_5			1		1		1		1	4
T_6		1	1				1	1		4
T_7			1		1			1		3
	3	3	3	3	3	3	3	3	3	

From this example, it is seen that constructing an (M,S) optimal design may not be easy even with the use of the information concerning lower bounds and configurations. In general, if one can start with a configuration having some "nice" properties, such as almost all of the λ_{ij} in one part of the partition having one value, then the construction is somewhat easier.

There are several things the experimenter should be aware of in using the information made available to him in this section to construct (M,S) optimal designs. The simple fact that for each value of s it is possible to find values of C_1^s, C_2^s and C_{12}^s which give lower bounds having the property that $\lambda_{ij} = m$ or $m+1$ for all $i \neq j$ does not guarantee that such a design will exist, it is simply a good indicator that such a design will exist. (A counter example is found in the class of designs $\mathcal{D}[9;5,5,5,5,4,4,4,4,4;10;4]$.) In fact, the construction of the designs in this section presupposes the existence of designs having incidence matrices attaining the lower bounds established for the different partitions. However, if that lower bound determined for $tr(N'N)^2$ given in Theorem 5.1.13 is larger than any of the lower bounds established for the various partitions of N, then no design whose incidence matrix has $tr(NN')^2$ equal to the lower bounds calculated by the method of Section 5.2 will exist and the construction technique given in this section will be of little use.

VIII. MISCELLANEOUS RESULTS

8.1. (M, S) Optimality and Connectedness

In this section, the relationship between connectedness and (M, S) optimality is examined in some of the classes of designs we have been considering.

Recall that an incomplete block design with v treatments is said to be connected if its coefficient matrix has rank $(v-1)$. We now present an alternative characterization of connectedness which was given by Eccleston and Hedayat (1974).

i) A design D is connected if and only if its incidence matrix N cannot be partitioned after any permutation of rows and columns into the form $\text{diag}(N_1, \ldots, N_a)$, $1 < a \leq v$ where the N_i are the incidence matrices of connected subsets of treatments.

Theorem 8.1.1. Consider the class of designs $\mathcal{D} = \mathcal{D}[v;(r_i);b;k]$ where $b \geq 2$ and $r_i \geq 2$ for each i. If $D \in \mathcal{M}\{\mathcal{D}\}$ is a disconnected design with incidence matrix N, then there exists a connected design $\bar{D} \in \mathcal{M}\{\mathcal{D}\}$ with incidence matrix $\bar{N}$ such that $\text{tr}(NN')^2 \geq \text{tr}(\bar{N}\,\bar{N}')^2$.

Pf. Suppose $D \in \mathcal{M}\{\mathcal{D}\}$ is disconnected. Then the incidence matrix N can be partitioned as in i) above. Suppose $a = 2$. Birkes, Dodge, and Seely (1972) have proven that if $\hat{N}$ is the $\hat{v} \times \hat{b}$

incidence matrix of a connected binary incomplete block design and if there are more than $\hat{v}+\hat{b}-1$ observations, then there exists at least one observation which may be removed from $\hat{D}$ and the design will still be connected. Since $r_i \geq 2$ for each i and since N_1 and N_2 are the incidence matrices of connected subsets of treatments in D, there will exist observations which can be removed from N_1 and N_2 such that the resulting incidence matrices will still be connected. Suppose an observation of treatment T_f in block B_u may be removed and suppose an observation of treatment T_g in block B_w may be removed such that the resulting incidence matrices $\overline{N}_1$ and $\overline{N}_2$ are still connected. Now assign the replication of T_f occurring in block B_u to block T_g and the replication of T_g occurring in block B_w to T_f. After the interchange of replication assignments, we have a new design $\overline{D}$ with incidence matrix $\overline{N}$. Now because $\overline{N}_1$ and $\overline{N}_2$ are connected and because $\overline{n}_{fw} = 1$, it is easy to see that $\overline{N}$ cannot be partitioned as in i) above. Hence $\overline{D}$ is a connected design. Furthermore, $\overline{N}\,\overline{N}' = (\overline{\lambda}_{ij})$ where

$$\overline{\lambda}_{f\ell} \leq \lambda_{f\ell} - 1 \quad \text{for } T_\ell \text{ occurring in } B_u, \ \ell \neq f$$

$$\overline{\lambda}_{f\ell} \geq 1 \quad \text{for } T_\ell \text{ occurring in } B_w, \ \ell \neq g$$

$$\overline{\lambda}_{g\ell} \leq \lambda_{g\ell} - 1 \quad \text{for } T_\ell \text{ occurring in } B_w, \ \ell \neq g$$

$$\overline{\lambda}_{g\ell} \geq 1 \quad \text{for } T_\ell \text{ occurring in } B_u, \ \ell \neq f.$$

Thus

$$\operatorname{tr}(NN')^2 - \operatorname{tr}(\bar{N}\bar{N}')^2 = 2 \sum_{\substack{T_\ell \in B_u \\ \ell \neq f}} [\lambda_{f\ell}^2 - \bar{\lambda}_{f\ell}^2] + 2 \sum_{\substack{T_\ell \in B_w \\ \ell \neq g}} [0 - \bar{\lambda}_{f\ell}^2]$$

$$+ 2 \sum_{\substack{T_\ell \in B_w \\ \ell \neq g}} [\lambda_{g\ell}^2 - \bar{\lambda}_{g\ell}^2] + 2 \sum_{\substack{T_\ell \in B_u \\ \ell \neq f}} [0 - \bar{\lambda}_{g\ell}^2]$$

$$\geq 2 \sum_{\substack{T_\ell \in B_u \\ \ell \neq f}} [\lambda_{f\ell} - (\lambda_{f\ell} - 1)^2] - 2 \sum_{\substack{T_\ell \in B_w \\ \ell \neq g}} 1$$

$$+ 2 \sum_{\substack{T_\ell \in B_w \\ \ell \neq g}} [\lambda_{g\ell}^2 - (\lambda_{g\ell} - 1)^2] + 2 \sum_{\substack{T_\ell \in B_u \\ \ell \neq f}} 1$$

$$= 4 \sum_{\substack{T_\ell \in B_u \\ \ell \neq f}} \lambda_{f\ell} + 4 \sum_{\substack{T_\ell \in B_w \\ \ell \neq g}} \lambda_{g\ell} - 8(k-1) \geq 0$$

as we were to show. Now if $a > 2$, the argument can be repeated for all pairs of connected subsets, and the result follows.

Corollary 8.1.2. If $\mathcal{D}$ is as in Theorem 8.1.1, then there exists an (M, S) optimal design in $\mathcal{D}$ which is connected.

The following is an example of a design which is (M,S) optimal in $\mathcal{D}[v;(r_i);b;k]$, but which is not connected.

Example 8.1.3. Consider the class of incomplete block designs $\mathcal{D} = \mathcal{D}[6;2;6;2]$. Then the design with the following incidence matrix is (M,S) optimal in $\mathcal{D}$ since $\lambda_{ij} = 0$ or 1 for all $i \neq j$, but it is clearly not connected by i) of this section.

	B_1	B_2	B_3	B_4	B_5	B_6	
T_1	1	1					2
T_2	1		1				2
T_3		1	1				2
T_4				1	1		2
T_5				1		1	2
T_6					1	1	2
	2	2	2	2	2	2	

However, by interchanging the replications of treatments T_3 and T_4 occurring in blocks B_3 and B_4 respectively, a design is obtained which is connected and is still (M,S) optimal in $\mathcal{D}$.

Corollary 8.1.4. Consider the class of designs $\mathcal{D}[v;b;k]$. If the parameters b, k, and v satisfy any of the conditions of Theorem 6.14 and if $[bk/v] \geq 2$, then there exists an (M,S) optimal design in $\mathcal{D}[v;b;k]$ which is connected.

Pf. If b, k, and v satisfy any of the conditions of Theorem 6.14, then the (M,S) optimal design must be contained in the class of designs $\mathcal{D}[v;(r_i);b;k]$ where $|r_i - r_j| \leq 1$ for all i,j. Since $[bk/v] \geq 2$, $r_i \geq 2$ for all i, and the conditions of Corollary 8.1.2 are satisfied.

Theorem 8.1.5. Let $\mathcal{D}[v;(r_i);b;k]$ be a class of designs with $r_i \leq b$ for each i and $r_p(k-1) \geq v-1$ for some p. Then if $D \in \mathcal{M}\{\mathcal{D}\}$ is disconnected, then there exists a connected design $\bar{D} \in \mathcal{M}\{\mathcal{D}\}$ which is S-better than D.

Pf. Suppose $D \in \mathcal{M}\{\mathcal{D}\}$ is disconnected and has incidence matrix N. Then N can be partitioned as in i) given at the beginning of this section where $N_1, \ldots, N_a$ are the incidence matrices of connected subsets of treatments. Note that D must be a binary design. Without loss of generality suppose $r_1(k-1) \geq (v-1)$. Now if N_1 is an m x n matrix then $\lambda_{ij} = 0$ for $1 \leq i \leq m$, $m < j \leq v$. Since $r_1(k-1) \geq (v-1)$ and $\sum_{j>1}^{m} \lambda_{1j} = r_1(k-1)$, there must exist $\lambda_{1p} \geq 2$ for some $2 \leq p \leq m$. Denote one of the blocks in which T_1 and T_p occur together by B_u. Now choose any block B_w, $w \geq n+1$ and any treatment T_q occurring in block B_w and assign the treatment replication of T_1 occurring in block

B_u to B_w and the treatment replication of T_q occurring in B_w to B_u. After the interchange of replication assignments, we have a new design $\bar{D}$ with incidence matrix $\bar{N}$ and $\bar{N}\bar{N}' = (\bar{\lambda}_{ij})$. As in the proof of Theorem 8. 1. 1, using $1 = f$ and $q = g$, we see that

$$\operatorname{tr}(NN')^2 - \operatorname{tr}(\bar{N}\bar{N}')^2 \geq 4 \sum_{\substack{T_\ell \in B_u \\ \ell \neq 1}} \lambda_{1k} + 4 \sum_{\substack{T_\ell \in B_w \\ \ell \neq q}} \lambda_{q\ell} - 8(k-1) > 0$$

since $\lambda_{1p} \geq 2$ and $\lambda_{1\ell} \geq 1$ for $T_\ell \in B_u$ and $\lambda_{q\ell} \geq 1$ for $T_\ell \in B_w$. Now if the new design is not connected, by permuting the $i \geq 2$ rows and columns of the new design, $\bar{N}$ can be partitioned in the same manner as N. Note that after the partitioning, there will still exist $\bar{\lambda}_{1\ell} \geq 2$ for some ℓ. Now we can repeat the argument given above for reducing $\operatorname{tr}(\bar{N}\bar{N}')^2$. This procedure may be followed until a connected design is obtained or until $\bar{\lambda}_{1j} \geq 1$ for all $j > 1$. Note that any design for which $\bar{\lambda}_{1j} \geq 1$ for all $j \geq 2$ cannot be partitioned as in i) given at the beginning of this section, hence it will be connected, and the result follows.

<u>Corollary 8. 1. 6.</u> Let $\mathcal{D}[v;(r_i);b;k]$ be a class of designs with $r_i \leq b$ for each i and $r_p(k-1) \geq v-1$ for some p. Then the (M,S) optimal design in $\mathcal{M}\{\mathcal{D}\}$ must be connected.

Corollary 8.1.7. Consider the class of designs $\mathcal{D}[v;b;k]$. If i) $bk/v = r$ is an integer and $r(k-1) \geq v-1$ or ii) bk/v is not an integer and $\{[bk/v]+1\}(k-1) \geq v-1$, then an (M,S) optimal design in $\mathcal{D}[v;b;k]$ must be connected.

Pf. An (M,S) optimal design in $\mathcal{D}[v;b;k]$ must be binary, hence it must be contained in one of the classes $\mathcal{D}[v;(r_i);b;k]$ satisfying the conditions of Corollary 8.1.6. Since bk has a unique representation as the sum of nonnegative integers differing by one, any class of designs $\mathcal{D}[v;(r_i);b;k]$ contained in $\mathcal{D}[v;b;k]$ must have at least one r_p such that $r_p(k-1) \geq (v-1)$, and the result follows.

For further results on the relationship between the (M,S) optimality criterion and connectedness, the reader should see Eccleston and Hedayat (1974).

8.2. (M,S) Optimality and the Estimation of Block Effects

Using the two way classification model given in Chapter II, we shall now investigate how the application of the (M,S) optimality criterion to the estimation of the treatment parameters in the model effects the estimation of the block parameters in the model. We shall consider the class of designs $\mathcal{D} = \mathcal{D}[v;(r_i);b;k]$ where $r_i \leq b$ and $v > k$.

The reduced normal equations for estimating the block effects $\underset{\sim}{b}' = (b_1, \ldots, b_b)$ for any design $D \in \mathcal{D}$ are given by

$$F\hat{\underset{\sim}{b}} = G \qquad (8.2.1)$$

where

$$F = kI_b - N' \operatorname{diag}(r_1^{-1}, \ldots, r_v^{-1})N \qquad (8.2.2)$$

$$G = B - N' \operatorname{diag}(r_1^{-1}, \ldots, r_v^{-1})T$$

and N, B and T are the same as defined in (2.1.3). Let

$$\mathcal{M}_F\{\mathcal{D}\} = \{D \in \mathcal{D}: \text{ tr } F \text{ is maximal}\}.$$

<u>Definition 8.2.3.</u> $\bar{D} \in \mathcal{D}$ is said to be (M,S) optimal for estimating $\underset{\sim}{b}$ if $\bar{D} \in \mathcal{M}_F\{\mathcal{D}\}$ and $\text{tr } \bar{F}^2 \leq \text{tr } F^2$ for all $D \in \mathcal{M}_F(\mathcal{D})$. $\bar{D} \in \mathcal{D}$ is said to be S-better than $D \in \mathcal{D}$ for estimating $\underset{\sim}{b}$ if $\text{tr } \bar{F}^2 \leq \text{tr } F^2$.

<u>Lemma 8.2.4.</u> $\mathcal{M}_F\{\mathcal{D}\} = \mathcal{M}\{\mathcal{D}\} = \{$all binary designs in $\mathcal{D}\}$.

<u>Pf.</u> From (8.2.2), we see that for any design $D \in \mathcal{D}$,

$$\text{tr } F = bk - \sum_i r_i^{-1} \sum_j n_{ij}^2 .$$

Using this expression, a proof similar to that given for Theorem 5.1.1

will yield the desired conclusion.

From (8.2.2), for $D \in \mathcal{D}$

$$\operatorname{tr} F^2 = bk^2 + v(1-2k) + \sum_i r_i^{-2} \sum_{j \neq i} \lambda_{ij}^2 \tag{8.2.6}$$

From (8.2.6), we see that finding a lower bound for $\operatorname{tr} F^2$ in $\mathcal{M}_F\{\mathcal{D}\}$ is equivalent to finding a lower bound for

$$\sum_{i=1}^{v} r_i^{-2} \sum_{j \neq i}^{v} \lambda_{ij}^2 \tag{8.2.7}$$

in $\mathcal{M}_F\{\mathcal{D}\}$. But by Corollary 4.1.2, for each fixed value of i,

$$\sum_{j \neq i} \lambda_{ij} = r_i(k-1) . \tag{8.2.8}$$

From (8.2.7) and (8.2.8), we see that if we solve the integer programming problem of minimizing

$$\sum_{i=1}^{v} r_i^{-2} \sum_{j \neq i} x_{ij}^2$$

subject to the constraints that i) the x_{ij} are nonnegative integers and ii) for each fixed value of i, $\sum_{j\neq i} x_{ij} = r_i(k-1)$, then we will obtain a lower bound for $\operatorname{tr} F^2$ in $\mathcal{M}_F\{\mathcal{D}\}$. By Corollary 4.3.5, we immediately get the following.

Theorem 8.2.9. For any design $D \in \mathcal{M}_F\{\mathcal{D}\}$ with incidence matrix N,

$$\operatorname{tr} F^2 \geq bk^2 + v(1-2k) + \sum_i r_i^{-2} \sum_{j\neq i} x_{ij}^2$$

where i) the x_{ij} are nonnegative integers, ii) for fixed values of p, $\sum_{q\neq p} x_{pq} = r_p(k-1)$ and iii) $|x_{pq}-x_{pr}| \leq 1$ for $p \neq q$, $p \neq r$.

Corollary 8.2.10. Any design $D \in \mathcal{M}\{\mathcal{D}\}$ such that for each fixed value of p, $|\lambda_{pq}-\lambda_{pr}| \leq 1$ for $q \neq p$, $r \neq p$, will be (M,S) optimal in $\mathcal{D}$ for estimating both $\underset{\sim}{t}$ and $\underset{\sim}{b}$.

Note that if the rolls of blocks and treatments are interchanged in $\mathcal{D}$, i.e., we consider the class of designs $\tilde{\mathcal{D}}$ which are duals to designs in $\mathcal{D}$; we get the following corollary.

Corollary 8.2.11. Let $\tilde{\mathcal{D}}$ denote the class of designs which are duals to designs in $\mathcal{D}$. Then any $\tilde{D} \in \mathcal{M}\{\tilde{\mathcal{D}}\}$ such that for each fixed value of p, $|\tilde{\mu}_{pq}-\tilde{\mu}_{pr}| \leq 1$ for $q \neq p$, $r \neq p$, will be (M,S) optimal for estimating $\tilde{\underset{\sim}{b}}$ and $\tilde{\underset{\sim}{t}}$.

The following is an example of a design which is (M,S) optimal in $\mathcal{D}$ for estimating $\underset{\sim}{t}$ but not (M,S) optimal for estimating $\underset{\sim}{b}$.

Example 8.2.12. Consider the class of designs $\mathcal{D} = \mathcal{D}[5;6,5,4,4,2;7;3]$ which is considered in Example 8.3.2. Consider also the two designs $D \in \mathcal{D}$ and $\bar{D} \in \mathcal{D}$ which are considered in that example. Now D was (M,S) optimal in $\mathcal{D}$ for estimating $\underset{\sim}{t}$. If F and $\bar{F}$ denote the matrices which are obtained for estimating $\underset{\sim}{b}$ from D and $\bar{D}$ respectively; then it is easily seen that $\mathrm{tr}\ F^2 = 44.25555$ and $\mathrm{tr}\ \bar{F}^2 = 43.99167$. Hence D is not (M,S) optimal in $\mathcal{D}$ for estimating $\underset{\sim}{b}$.

Note that if blocks are considered as a factor with b levels and treatments are considered as a factor with v levels in Corollaries 8.2.10 and 8.2.11, then any design whose incidence matrix satisfies either of the corollaries will be (M,S) optimal for estimating the levels of both factors.

We now restrict attention to the case where $r_i = r \leq b$ for all i. For any design in this class,

$$\mathrm{tr}\ C^2 = vr^2(1 - \frac{1}{k})^2 + \frac{1}{k^2}\mathrm{tr}(NN')^2 \qquad (8.2.13)$$

and

$$\mathrm{tr}\ F^2 = bk^2(1 - \frac{1}{r})^2 + \frac{1}{r^2}\mathrm{tr}(N'N)^2. \qquad (8.2.14)$$

From expressions (8.2.13) and (8.2.14), it is clear that any design which minimizes $\text{tr } C^2$ in $\mathcal{M}\{\mathcal{D}\}$ will also minimize $\text{tr}(NN')^2$ and any design which minimizes $\text{tr } F^2$ in $\mathcal{M}\{\mathcal{D}\} = \mathcal{M}_F\{\mathcal{D}\}$ will also minimize $\text{tr}(N'N)^2$. Hence we may state the following.

Theorem 8.2.15. Any design in $\mathcal{D} = \mathcal{D}[v;(r_i);b;k]$ where $r_i = r \leq b$ for all i and $v > k$ which is (M,S) optimal in $\mathcal{D}$ for estimating $\underset{\sim}{t}$ will also be (M,S) optimal for estimating $\underset{\sim}{b}$.

8.3. (M,S) Optimality and Other Optimality Criteria

In this section, we will draw some comparisons between the (M,S) optimality criterion and the A, D, and E optimality criteria which were introduced in Chapter III.

Consider any class $\mathcal{D}$ of connected binary incomplete block designs with three treatments such that tr C = (constant) for all $D \in \mathcal{D}$. Let $\lambda_1 \geq \lambda_2$ denote the nonzero eigenvalues of a C-matrix of a design in $\mathcal{D}$. Suppose $\bar{D}$ is (M,S) optimal in $\mathcal{D}$, i.e., $\bar{\lambda}_1^2 + \bar{\lambda}_2^2 \leq \lambda_1^2 + \lambda_2^2$ for all $D \in \mathcal{D}$. Since
$\text{tr } \bar{C} = \bar{\lambda}_1 + \bar{\lambda}_2 = \lambda_1 + \lambda_2 = \text{tr } C$ for all $D \in \mathcal{D}$,

$$(\text{tr } \bar{C})^2 = \bar{\lambda}_1^2 + \bar{\lambda}_2^2 + 2\bar{\lambda}_1\bar{\lambda}_2 = \lambda_1^2 + \lambda_2^2 + 2\lambda_1\lambda_2 = (\text{tr } C)^2$$

for all $D \in \mathcal{D}$; and since $\bar{D}$ is (M,S) optimal in $\mathcal{D}$,

$\bar{\lambda}_1\bar{\lambda}_2 \geq \lambda_1\lambda_2$ for all $D \in \mathcal{D}$, hence $\bar{D}$ is also D-optimal in $\mathcal{D}$. Now since $\bar{D}$ is D-optimal,

$$\frac{1}{\bar{\lambda}_1} + \frac{1}{\bar{\lambda}_2} = \frac{\bar{\lambda}_1 + \bar{\lambda}_2}{\bar{\lambda}_1\bar{\lambda}_2} = \frac{\text{tr } C}{\bar{\lambda}_1\bar{\lambda}_2} = \frac{(\text{constant})}{\bar{\lambda}_1\bar{\lambda}_2} ,$$

hence $\bar{D}$ is also A-optimal in $\mathcal{D}$. Finally, it is easily shown that if $\bar{\lambda}_1 + \bar{\lambda}_2 = \lambda_1 + \lambda_2$ and $\bar{\lambda}_1^2 + \bar{\lambda}_2^2 \leq \lambda_1^2 + \lambda_2^2$, then $\lambda_1 \geq \bar{\lambda}_1 \geq \bar{\lambda}_2 \geq \lambda_2$; hence $\bar{\lambda}_2$ is maximal in $\mathcal{D}$ and $\bar{D}$ is also E-optimal in $\mathcal{D}$.

Proposition 8.3.1. For any class $\mathcal{D}$ of designs as defined in the previous paragraph, any design which is (M, S) optimal in $\mathcal{D}$ will also be A, D, and E optimal in $\mathcal{D}$.

General results concerning the relationship between the (M, S) optimality criterion and the A, D, and E optimality criteria for classes of designs with more than three treatments appear difficult to obtain. However, Takeuchi (1961) was able to show that if in any class $\mathcal{D}$ of connected binary designs contained in $\mathcal{D}[v;r;b;k]$ there exists a group divisible PBIB(2) with $|\lambda_{ij} - \lambda_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$, then that design will be A and E optimal in $\mathcal{D}$. Such designs are also (M, S) optimal.

Mitchell (1971) ran a computer search for small D-optimal designs. In the classes of designs $\mathcal{D}[v;r;b;k]$ which he considered, the D-optimal design (or its dual), turned out to be either a BIBD or a PBIB(2) with $|\lambda_{ij}-\lambda_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$. Such designs are also (M,S) optimal.

However, to conclude that (M,S) optimal designs are always A, D, and E optimal is not true as the following example shows.

Example 8.3.2. Consider the class of designs $\mathcal{D}[5;6,5,4,4,2;7;3]$. By considering the class of complementary designs [as in Section 7.1], it is easily seen that an (M,S) optimal design D for this class is given by the following incidence matrix.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	
T_1	1	1	1	1	1	1		6
T_2	1	1			1	1	1	5
T_3	1		1		1		1	4
T_4			1	1		1	1	4
T_5		1		1				2
	3	3	3	3	3	3	3	

The C-matrix for this design is

$$\frac{1}{3}\begin{bmatrix} 12 & -4 & -3 & -3 & -2 \\ -4 & 10 & -3 & -2 & -1 \\ -3 & -3 & 8 & -2 & 0 \\ -3 & -2 & -2 & 8 & -1 \\ -2 & -1 & 0 & -1 & 4 \end{bmatrix}$$

Let $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ denote the nonzero eigenvalues of this matrix, then

i) $\lambda_1 = 5.1577 \quad \lambda_2 = 3.9811 \quad \lambda_3 = 3.3039 \quad \lambda_4 = 1.5593$

ii) $\sum_{i=1}^{4} 1/\lambda_i = 1/5.1557 + 1/3.9811 + 1/3.3039 + 1/1.5593 = 1.3891$

iii) $\prod_{i=1}^{4} \lambda_i = (5.1557)(3.9811)(3.3039)(1.5593) = 105.74$

iv) $\text{tr } C^2 = \sum_{i=1}^{4} \lambda_i^2 = (5.1557)^2 + (3.9811)^2 + (3.3039)^2 + (1.5593)^2$

$= 55.778$.

Now consider the design $\bar{D}$ in $\mathcal{D}[5;6,5,4,4,2;7;3]$ given by the following incidence matrix.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	
T_1		1	1	1	1	1	1	6
T_2	1		1	1	1	1		5
T_3		1	1	1			1	4
T_4	1				1	1	1	4
T_5	1	1						2
	3	3	3	3	3	3	3	

The C-matrix for this design is given by

$$\frac{1}{3}\begin{bmatrix} 12 & -4 & -4 & -3 & -1 \\ -4 & 16 & -2 & -3 & -1 \\ -4 & -2 & 8 & -1 & -1 \\ -3 & -3 & -1 & 8 & -1 \\ -1 & -1 & -1 & -1 & 4 \end{bmatrix}$$

Let $\bar{\lambda}_1 \geq \bar{\lambda}_2 \geq \bar{\lambda}_3 \geq \bar{\lambda}_4$ denote the nonzero eigenvalues for this matrix, then

i) $\bar{\lambda}_1 = 5.2827 \quad \bar{\lambda}_2 = 4.1091 \quad \bar{\lambda}_3 = 2.9415 \quad \bar{\lambda}_4 = 1.6667$

ii) $\sum_{i=1}^{4} 1/\bar{\lambda}_i = 1/5.2827 + 1/4.1091 + 1/2.9415 + 1/1.6667 = 1.3725$

iii) $\prod_{i=1}^{4} \bar{\lambda}_i = (5.2827)(4.1091)(2.9415)(1.6667) = 106.42$

iv) $\text{tr}\,\bar{C}^2 = (5.2827)^2 + (4.1091)^2 + (2.9415)^2 + (1.6667)^2$

$= 56.2219.$

So

i) $\bar{\lambda}_4 = 1.667 > \lambda_4 = 1.5591$

ii) $\sum_{i=1}^{4} 1/\bar{\lambda}_i = 1.3725 < \sum_{i=1}^{4} 1/\lambda_i = 1.3891$

iii) $\prod_{i=1}^{4} \bar{\lambda}_i = 106.42 > \prod_{i=1}^{4} \lambda_i = 105.74$

iv) $\operatorname{tr} \bar{C}^2 = \sum_{i=1}^{4} \lambda_i^2 = 506/9 > \operatorname{tr} C^2 = \sum_{i=1}^{4} \lambda_i^2 = 502/9$.

So $\bar{D}$ is A, D, and E "better" than D, in $\mathcal{D}[5;6,5,4,4,2;7;3]$ but D is (M, S) optimal in $\mathcal{D}[5;6,5,4,4,2;7;3]$.

IX. SUMMARY

The problem we have considered in this thesis is the determination of optimal incomplete block designs when the experimental material does not fit any of the usual text book situations. The criterion used to determine an optimal design within a given class $\mathcal{D}$ of incomplete block designs is the (M, S) optimality criterion. This criterion is to find within the class $\mathcal{D}$ the set of designs whose C-matrices have maximal trace, denoted by $\mathcal{M}\{\mathcal{D}\}$, and then to find within $\mathcal{M}\{\mathcal{D}\}$ those designs with minimum trace of C^2; such a design is said to be (M, S) optimal.

Chapters II and III are basically introductory. Chapter II is used to introduce the notation and terminology which are used throughout the thesis. In Chapter III, the (M, S) optimality criterion is introduced. The reasons for using the (M, S) optimality criterion to determine optimal incomplete block designs are i) designs which are (M, S) optimal also tend to be A, D, and E optimal since they have C-matrices which are close to the ideal $\alpha I_v + \beta J_v$ form and ii) its computational simplicity.

In Chapter IV, several facts and lemmas used later on in the thesis are given. In Sections 4.3 and 4.4, the solutions are given for two integer programming problems which occur naturally with the (M, S) optimality criterion.

The class $\mathcal{D} = \mathcal{D}[v;(r_i);b;k]$ of incomplete block designs where $r_i \leq b$ is studied in Chapter V. This class consists of all designs with v treatments arranged in b blocks of size k such that treatment T_i is replicated r_i times. $\mathcal{M}\{\mathcal{D}\}$ consists of all the binary designs in $\mathcal{D}$. It is shown that finding a design in $\mathcal{M}\{\mathcal{D}\}$ with a minimal $\text{tr } C^2$ is equivalent to finding a design in $\mathcal{M}\{\mathcal{D}\}$ with a minimal $\text{tr}(NN')^2$ and $\text{tr}(N'N)^2$. Using the results of Section 4.2, several lower bounds are established for $\text{tr}(NN')^2$ and $\text{tr}(N'N)^2$ for designs in $\mathcal{M}\{\mathcal{D}\}$ to help the experimenter know when a design is optimal. Through the establishment of these lower bounds, several well known standard types of designs are shown to be (M,S) optimal. In particular, any design whose association matrix or block characteristic matrix has the property that $|\lambda_{ij}-\lambda_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$ or $|\mu_{ij}-\mu_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$, will be (M,S) optimal. In this chapter it is also shown how lower bounds for $\text{tr } C^2$ can be used to show the nonexistence of certain PBIB(2)'s with $\lambda_2 = \lambda_1+1$. In Section (5.2), a lower bound is developed which is dependent upon partitioning the incidence matrix of a typical binary design in $\mathcal{D}$. In determining this lower bound, the set of ordered configurations which any design must have whose incidence matrix has $\text{tr}(NN')^2$ equal to the lower bound established are also determined. It is shown in Chapter VII how these configurations can sometimes be used to help the experimenter construct an (M, S) optimal design in $\mathcal{D}$.

In Chapter VI, the class $\mathcal{D} = \mathcal{D}[v;b;k]$ of incomplete block designs is studied. This class consists of all designs with v treatments arranged in b blocks of size k. The class $\mathcal{M}\{\mathcal{D}\}$ consists of all the binary designs in $\mathcal{D}$. Since the r_i are allowed to vary in $\mathcal{D}$, the first question considered is how replications should be assigned to treatments in an (M, S) optimal design. It is shown that in most cases, the (M, S) optimal design in $\mathcal{D}$ must have the property that $|r_i - r_j| \leq 1$ for all $i \neq j$. Using the results of Chapter IV, several lower bounds are established for $tr(NN')^2$ and $tr(N'N)^2$ for designs in $\mathcal{M}\{\mathcal{D}\}$. In establishing these lower bounds it is seen that any binary design with $|r_i - r_j| \leq 1$ for all i, j and whose incidence matrix has the property that $|\lambda_{ij} - \lambda_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$, or $|\mu_{ij} - \mu_{\ell m}| \leq 1$ for all $i \neq j$, $\ell \neq m$, will be (M, S) optimal in $\mathcal{D}[v;b;k]$.

Several methods of constructing (M, S) optimal designs in $\mathcal{D}[v;b;k]$ and $\mathcal{D}[v;(r_i);b;k]$ are presented in Chapter VII. In Section 7.1, several results concerning complementary incomplete block designs are given. Basically, it is shown that the complement of an (M, S) optimal design in $\mathcal{D}[v;(r_i);b;k]$ will be (M, S) optimal in $\mathcal{D}[v;(b-r_i);b;v-k]$ and under certain conditions, the complement of an (M, S) optimal design in $\mathcal{D}[v;b;k]$ will be

(M, S) optimal in $\mathcal{D}[v;b;v-k]$. In Section 7.2, a method is given for constructing an (M, S) optimal design in $\mathcal{D}[v;b;2]$. Using this construction process and the results of Section 7.1, the (M, S) optimal design in $\mathcal{D}[v;b;k]$ where $v = k+2$ is also easily obtained. Section 7.3 is used to show how (M, S) optimal designs may be constructed from known (M, S) optimal designs. In Section 7.4, several different methods of combining incomplete block designs to obtain (M, S) optimal block designs are discussed. A heuristic approach to the construction of (M, S) optimal designs is given in Section 7.5. The approach is based upon the technique given in Section 5.2 for determining lower bounds for $tr(NN')^2$ in $\mathcal{M}\{\mathcal{D}[v;(r_i);b;k]\}$ and for determining the various configurations yielding these lower bounds. The construction process presupposes the existence of a binary design in $\mathcal{D}[v;(r_i);b;k]$ whose incidence matrix has $tr(NN')^2$ equal to the lower bounds established by the method of Section 5.2.

Chapter VIII contains miscellaneous results. It is shown in Section 8.1 that for most classes of designs $\mathcal{D}[v;(r_i);b;k]$ and $\mathcal{D}[v;b;k]$, the (M, S) optimal design must be connected. In Section 8.2 it is shown that many designs which are (M, S) optimal for estimating treatment effects are also (M, S) optimal for estimating block effects. Section 8.3 is used to show that for many classes of designs, the (M, S) optimal design tends to be A, D, and E optimal. However, an example is given which shows this is not always the case.

BIBLIOGRAPHY

Birkes, D., Dodge, Y., Hartmann, N., and Seely, J. [1972], Estimability and analysis for additive two-way classification models with missing observations. Oregon State University. Dept. of Statistics, Technical Report No. 30.

Bose, R.C., Clatworthy, W.H., and Shrikhande, S.S. [1954], Tables of partially balanced incomplete block designs with 2-associate classes, Institute of Statistics, University of North Carolina.

Chakrabarti, M.C. [1963], On the C-matrix in the design of experiments. Journal of the Indian Statistical Association 1:8-23.

Corsten, L.A. [1962], Balanced block designs with two different number of replicated. Biometrics 18:499-520.

Connor, W.S., Clatworthy, W.H. [1954], Some theorems for partially balanced designs. The Annals of Mathematical Statistics 25:100-113.

Ehrenfeld, S. [1953], On the efficiency of experimental designs. The Annals of Mathematical Statistics 26:247-258.

Federov, V.V. [1972], The theory of optimal design. New York, Academic Press.

John, P.W. [1971], Statistical design and analysis of experiments. New York, The Macmillan Company.

Kempthorne, O. [1953], A class of experimental designs using blocks of two plots. The Annals of Statistics 24:76-80.

Kempthorne, O. [1956], On the efficiency factor of an incomplete block design. The Annals of Mathematical Statistics 26:846-849.

Kempthorne, O. [1953], The design and analysis of experiments. New York, Wiley and Sons.

Kiefer, J. [1958], On the nonrandomized optimality and randomized non-optimality of symmetrical designs. The Annals of Mathematical Statistics 29:675-699.

Kiefer, J. [1959], Optimum experimental designs (with discussion). Journal of the Royal Statistical Society, Series B 1:272-319.

Kiefer, J. [1960], Optimum experimental designs (abstract). Annals of Mathematical Statistics 31:245.

Kiefer, J. [1971], The role of symmetry and approximation in exact design optimality. Statistical Decision Theory and Related Topics. New York. Academic Press, pp. 109-118.

Kiefer, J. [1974], General equivalence theory of optimum designs (approximate theory), The Annals of Statistics 2:849-879.

Kiefer, J. [1975], Balanced block designs and generalized youden squares, I. construction (patchwork). The Annals of Statistics 3:109-118.

Kshirsagar, A. M. [1958], A note on incomplete block designs. The Annals of Mathematical Statistics 29:907-910.

Masuyama, M. [1957], On the optimality of balanced incomplete block designs. Reports on Statistics and Applied Research, J. U. S. E. 5:4-8.

Mitchell, T. J. [1971], Computer construction of small "D-optimal" incomplete block designs. Bulletin of the International Statistical Institute. Proceedings of the 39th session 45:199-204.

Mote, V. L. [1958], On a minimax property of balanced incomplete block designs. The Annals of Mathematical Statistics 29:910-914.

Pearce, S. C. [1964], Experimenting with blocks of natural size. Biometrics 20:699-706.

Pearce, S. C. [1970], The efficiency of block designs in general. Biometrika 57:339-346.

Rao, C. R. [1973], Linear statistical inference and its applications. New York, John Wiley and Sons.

Rao, V. R. [1958], A note on balanced designs. The Annals of Mathematical Statistics 29:290-294.

Shah, B.V. [1959], A generalization of PBIB designs. The Annals of Mathematical Statistics 30:1041-1050.

Shah, K.R. [1960], Optimality criteria for incomplete block designs. The Annals of Mathematical Statistics 31:791-794.

Shah, K.R., Raghavarao, D., and Khatri, C.G. [1976], Optimality of two and three factor design. The Annals of Statistics 4:409-413.

Takeuchi, K. [1961], On the optimality of certain types of PBIB designs. Reports on Statistics and Applied Research 8:140-145.

Tocher, K.D. [1952], The design and analysis of block experiments. Journal of the Royal Statistical Society, Series B 14:45-91.

Wald, A.L. [1943], On the efficient design of statistical investigations. The Annals of Mathematical Statistics 26:247-255.