University of Southampton

Faculty of Mathematical Studies

Mathematics

Block Designs for Comparing Dual with Single Treatments

by

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In memory of my mother

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Praise be to Allah, Lord of the worlds;
The beneficient, the merciful;
Owner of the Day of judgement.
Thee (alone) we worship;
Thee (alone) we ask for help.
Shows us the straight path.

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UNIVERSITY OF SOUTHAMPTON

ABSTRACT

FACULTY OF MATHEMATICAL STUDIES

MATHEMATICS

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Block Designs for Comparing Dual with Single Treatments.

by: Abbas Gerami

This investigation concerns the design of experiments whose purpose is to compare the joint effects of two factors A and B at n and m levels respectively with the effect of the individual factor. The experiments are subject to the constraint that one particular treatment combination cannot be used. An example is a medical trial to investigate the joint effects of two drugs, each of which is either absent or given at a number of predefined dose levels, in which it is unethical to administer a double placebo. This type of clinical trial has practical application in the quest for treatments of acute conditions, such as severe hypertension when the improvement produced by a single drug might be inadequate. The aim of this investigation is to find efficient designs in the sense of having small variance for the estimators of the contrasts of interest.

The criterion employed for design choice is the A-criterion. The methods used include finding a lower bound on the total of the variances of the estimators of the contrasts and identifying a class of designs containing many efficient designs.

For m=n=2, the problem is a special case of the test treatments versus a control problem, for which series of A-optimal and near A-optimal designs are already available. These known results are used to find series of new A-optimal and near A-optimal designs to fill the gaps in a practical range of parameter values. For any n and m=2, the class of PBDS designs is identified and shown to contain very efficient designs. Methods of constructing such designs are developed and overall A-optimal and efficient designs are tabulated.

For n and m both greater than 2, a generalization of the PBDS class is developed and shown to include highly efficient designs by comparison with the bound and, for small experiments, computer generated designs.

Further issues on which results are given include the design of completely randomized experiments, efficient designs for estimating certain contrasts more accurately than others and the estimation of factorial effects. Finally, a method is developed of identifying designs efficient for estimating specific contrasts, $C\underline{\tau}$, through linking the structure of the intra-block information matrix to the structure of $C'C$.

Contents

Chapter 1

INTRODUCTION

1.1 Description of the Problem:

In factorial experiments there are cases where we want to compare the effect of combinations of two or more treatment factors when it is not possible to include all treatment combinations in the experiment. An example is a medical trial to investigate the joint effect of two drugs , each of which is either absent or given at a number of predefined dose levels, in which it is unethical to administer a double placebo.

Suppose A and B are two treatment factors : A with n levels labelled 0,1,2,...., n-1, and B with m levels labelled 0,1,2,....,m-1 . Each treatment combination is denoted by ij, where i and j are the levels of A and B respectively, and is called a **single** treatment if i=0 or j=0; otherwise it is called a **dual** treatment. We assume treatment 00 cannot be employed. Hence there are t=mn-1 treatments in the experiment. The objective of the experiment is to compare the effects of having both A and B at levels with non-zero labels with the effects of having only one of the factors at a non-zero labelled level. More specifically we require efficient estimation of the following contrasts, which we shall call **dual versus single** contrasts:

$$\tau_{ij} - \tau_{i0} \tag{1.1}$$

and

$$\tau_{ij} - \tau_{0j} \tag{1.2}$$

for i=1,2,...,n-1, and j=1,2,...,m-1, where τ_{ij} denotes the effect of treatment combination ij.

We can view the problem as comparing each of the (n-1)(m-1) dual treatments with two single treatments. Contrasts (1.1) and (1.2) respectively compare the dual treatments with treatments having A alone at a non-zero labelled level, and with treatments having B alone at a non-zero labelled level. In the example of the medical trial, the contrasts can be used to examine if there is greater efficacy when two drugs are given rather than one. This type of clinical trial is important in the quest for treatment of acute conditions, such as severe hypertension, when the improvement produced by a single drug might be inadequate.

The problem addressed in the first six chapters of this thesis is how to arrange the treatment combinations in block designs, so that the set of contrasts defined in (1.1) and (1.2) can be efficiently estimated. In practice the blocks might be groups of patients in the same age-range or having the same sex.

Bounds on the total of the variances of the contrasts of interest are established and used to assess the performance of the designs. A particular class of designs is investigated and the most efficient designs in the class are found. Necessary conditions for a design to be A-optimal are established. In Chapter 7 two additional problems are examined. Firstly, a general factorial experiment is considered in which one of the treatment combinations is not observed and some higher order interactions can be assumed negligible. The estimators with minimum loss of information on a set of factorial contrasts of interest are found. Secondly, a link is found between the structure of the intra-block information matrix of the class of designs containing highly efficient designs and the structure of another matrix obtained by premultiplying the matrix of the contrasts of interest with its transpose. Finally, conclusions are given and ideas for further work are described.

In the first chapter, the general analysis of block designs is studied, and criteria for design selection are described. For the special case when both factors have two levels, the dual-versus-single design problem reduces to the test treatment versus a control design problem. A brief review therefore will be given of optimal and near optimal designs available in the literature for the test treatment versus a control problem. New optimal and near optimal designs will then be listed for this case, which cover parameter values of practical interest for which designs are not currently available.

1.2 Block Designs:

In this section the analysis for a general block design for estimating the dual versus single treatment contrasts is summarized.

1.2.1 General Theory:

Consider an experiment involving t treatments and b blocks each of size k . The treatment structure is assumed to be two factors , one at n and one at m levels. The treatment effects will be held in a $t \times 1$ column vector. Let $y_{ij\ell h}$, denote the observation when the ijth treatment is applied to unit h of the ℓth block. The following linear model with no treatment block interactions will be assumed:

$$y_{ij\ell h} = \mu + \tau_{ij} + \beta_\ell + e_{ij\ell h}, \tag{1.3}$$

where $i = 0, 1, 2, \ldots, n-1$, $j = 0, 1, 2, \ldots, m-1$, excluding ij=00 ; $\ell = 1, 2, \ldots, b$, and h=1,2,..., $n_{ij\ell}$. Here $e_{ij\ell h}$'s are assumed to be uncorrelated random variables with zero means and common variances σ^2. Throughout this thesis without loss of generality we assume, for simplicity that $\sigma^2 = 1$. The unknown constants μ, τ_{ij} and β_ℓ represent the general mean, the effect of treatment ij, and the effect of block ℓ respectively; $n_{ij\ell}$ denotes the number of times that the ijth treatment is applied in the ℓth block.

In this thesis we shall concentrate on the intra-block analysis of the experiment in which treatment comparisons are estimated within blocks only, i.e. the estimates of all contrasts in the treatment effects are expressible in terms of comparisons between observations in the same block. If the blocks can be regarded as a random sample from some population, then estimates of treatment comparisons may also be available from between block differences, giving rise to an inter-block analysis. Where information is available from both between and within blocks, the intra- and inter-block estimates can be combined to provide overall estimates of treatment comparisons.

Throughout this thesis the following ordering of treatments will be adopted:

$$\tau_{01}, \tau_{02}, \ldots, \tau_{0q}, \tau_{10}, \tau_{20}, \ldots, \tau_{p0}, \tau_{11}, \tau_{12}, \ldots, \tau_{1q}, \tau_{21}, \tau_{22}, \ldots, \tau_{2q},$$
$$\ldots, \ldots, \tau_{p1}, \tau_{p2}, \ldots, \tau_{pq}, \tag{1.4}$$

where t=mn-1, p=n-1, and q=m-1.

We put the ordering of treatments in a $t \times 1$ column vector $\underline{\tau}$. Let N=$(n_{ij\ell})$ denote the **incidence** matrix; where the rows of N follow the same ordering. Then NN' is called the **concurrence** matrix, where N' denotes the transpose of N. A block design is called **binary** if each treatment appears at most once in each block. Let $r_{ij} = \sum_{\ell=1}^{b} n_{ij\ell}$, the number of times the ijth treatment is replicated in the entire design, and $\underline{r} = (r_{ij})$, be the vector of treatment replications. Then the reduced normal equations after eliminating the block parameters are:

$$A\underline{\hat{\tau}} = \underline{Q}, \tag{1.5}$$

where $\underline{l}'\underline{\hat{\tau}}$ is the **Best Linear Unbiased Estimator (BLUE)** of $\underline{l}'\underline{\tau}$, $\underline{Q} = \underline{T} - (1/k)N\underline{B}$, is the vector of treatment totals adjusted for blocks, $\underline{B}$ is the vector of block totals and

$$A = r^{\delta} - (1/k)NN' \tag{1.6}$$

is called the **information** matrix or **intra-block** matrix; r^{δ} is a diagonal matrix with the entry r_{ij}, and $\underline{T}$ is the vector of treatment totals . We shall refer to A as the **A-matrix.** The A-matrix is singular because A$\underline{1} = \underline{0}$, and R(A)$\leq$t-1. Therefore there is no unique solution to the reduced normal equations $A\underline{\hat{\tau}} = \underline{Q}$. In general these equations have a solution $\underline{\hat{\tau}} = \Omega\underline{Q}$, for any generalized inverse(g-inverse), Ω of A. The value of $\underline{\hat{\tau}}$ depends on the particular g-inverse used.

The general solution to $A\underline{\hat{\tau}} = \underline{Q}$ is

$$\underline{\hat{\tau}} = \Omega\underline{Q} + (\Omega A - I)\underline{Z}, \tag{1.7}$$

where $\underline{Z}$ is any arbitrary vector, and Ω is a g-inverse of A. Any linear combinations of the treatment parameters $\underline{\tau}$ can be expressed as $C\underline{\tau}$ and estimated by:

$$C\underline{\hat{\tau}} = C\Omega\underline{Q} + C(\Omega A - I)\underline{Z}, \tag{1.8}$$

for arbitrary $\underline{Z}$.

$C\underline{\tau}$ is **estimable**, i.e. $C\underline{\hat{\tau}}$ is unique, if and only if $C(\Omega A - I)\underline{Z} = \underline{0}$ for all $\underline{Z}$, i.e. $C\Omega A = C$, and it is a contrast if $C\underline{1} = \underline{0}$. A contrast is **elementary** if it has only two non-zero elements, -1 and 1. If a design has all elementary contrasts estimable, the design is **connected** and this is possible if and only if R(A)=t-1. A matrix C is a **contrast** matrix if $C\underline{\tau}$ has rows which are contrasts, i.e. $C\underline{1} = \underline{0}$.

For any connected design $C\underline{\hat{\tau}} = C\Omega\underline{Q}$ is a unique estimator of $C\underline{\tau}$ with $V(C\underline{\hat{\tau}}) = \sigma^2 C\Omega C'$ if and only if C is a contrast matrix, where $V(C\underline{\hat{\tau}})$ stands for the variance-covariance matrix of $C\hat{\underline{\tau}}$. In this case $C\hat{\underline{\tau}} = C\Omega\underline{Q}$ and $C\Omega C'$ are invariant for any choice of Ω. Throughout this thesis, unless explicity stated to the contrary, we consider only designs which are connected. In addition all designs considered are **proper**, that is all their blocks have the same size, say k units.

The A-matrix is **symmetric** and hence has a complete set of **orthonormalized eigenvectors** $\underline{\xi}_0, \underline{\xi}_1, \ldots, \underline{\xi}_{t-1}$, say. Thus:

$$\begin{aligned} \underline{\xi}_i'\underline{\xi}_i &= 1, \\ \underline{\xi}_i'\underline{\xi}_j &= 0 (i \neq j). \end{aligned} \tag{1.9}$$

The eigenvectors are unique if and only if the eigenvalues of the A-matrix are distinct. Denote the eigenvalues $\lambda_0 = 0, \lambda_1, \ldots, \lambda_{t-1}$. Since $A\underline{1} = \underline{0}$, one eigenvector of A is $\underline{\xi}_0 = t^{(-1/2)}\underline{1}$ with corresponding eigenvalue 0. Since the design is connected, all the other t-1 eigenvalues are non-zero and positive. The matrix A can be expressed in **canonical** form:

$$A = \sum_{i=1}^{t-1} \lambda_i \underline{\xi}_i \underline{\xi}_i', \tag{1.10}$$

and has a g-inverse:

$$\Omega = \sum_{i=1}^{t-1} \lambda_i^{-1} \underline{\xi}_i \underline{\xi}_i', \tag{1.11}$$

which is called the **Moore Penrose** g-inverse. Any contrast $\underline{\xi}_i\underline{\tau}$, for i=1,2,...,t-1 is called **basic** contrast.

1.2.2 Contrast Matrices for the Dual-Versus-Single Problem:

In this research we are mainly concerned with two factors, namely A and B, at n and m levels respectively. The contrasts of interest are (1.1) and (1.2) and these can be expressed as $C_1\underline{\tau}$ and $C_2\underline{\tau}$ where the contrast matrices are:

$$\begin{aligned} C_1 &= (\ -\mathrm{I}_q \otimes \underline{1}_p \quad 0_{l\times p} \quad E\ ), \\ C_2 &= (\ 0_{l\times q} \quad -\mathrm{I}_p \otimes \underline{1}_q \quad \mathrm{I}_\ell\ ), \\ C &= (\ C_1' \quad C_2'\ )', \end{aligned} \tag{1.12}$$

where I_n is an identity matrix of order n, $O_{u\times v}$ is a zero matrix of u rows and v columns, $\underline{1}_n$ is an $n\times 1$ column vector with all entries 1, $\otimes$ denotes Kronecker product, $\ell = pq$ and

$$E = \begin{bmatrix} E_{11} & E_{12} & E_{13} & \cdots\cdots & E_{1p} \\ E_{21} & E_{22} & E_{23} & \cdots\cdots & E_{2p} \\ E_{31} & E_{32} & E_{33} & \cdots\cdots & E_{3p} \\ \cdots & \cdots & \cdots & \cdots\cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots\cdots & \cdots \\ E_{q1} & E_{q2} & E_{q3} & \cdots\cdots & E_{qp} \end{bmatrix}, \tag{1.13}$$

where E_{ij}'s are $p \times q$ matrices with a 1 in the (j,i)th position and zero elsewhere. Then BLUE of $C_i\underline{\tau}$(i=1,2) will be given by:

$$C_i\underline{\hat{\tau}} = C_i\Omega\underline{Q}(i = 1,2). \tag{1.14}$$

The standard theory for making inferences about the contrasts of interest, by using an analysis of variance under normal assumptions, is described in John(1987 ,p12).

1.3 Design Criteria:

Suppose we have an experiment involving t treatments and b blocks each composed of k units. The notation D(t,b,k) will stand for the set of all designs which are allocations of t treatments to b blocks of size k. In order to determine how the treatments should be allocated to the experimental units we require criteria for design selection.

1.3.1 Optimality Criteria:

In traditional design theory the comparisons of all treatment pairs are often considered to be of equal importance. Let V(d) denote the variance-covariance matrix of the estimators of the contrasts of interest for design d then, in the work of Kiefer and others in the area of optimal designs (see for example Kiefer,1980), the most common criteria for design selection are as follows:

D-Optimality : A design $d^* \in$D(t,b,k) is said to be D-optimal if

$$det(V(d^*)) = \min \det(\mathrm{V(d)}), \forall d \in D(t,b,k)$$

where $det(X)$[1] denotes the determinant of matrix X. Under the normality assumptions for the errors in the model, a D-optimal design minimizes the

[1] Whenever the determinant is defined

volume of the confidence ellipsoid for contrasts and its application is well-known in response surface designs.

MV-Optimality : A design $d^* \in$D(t,b,k) is said to be MV-optimal if

$$\max_i(v_i(d^*)) \leq \min \max_i(v_i(d)),\ \forall d \in D,$$

where $v_i(d)$ is the ith element of the diagonal of the variance-covariance matrix of the estimators of the contrasts of interest. An MV-optimal design minimizes the maximum variance of the BLUE's of the estimators of estimable functions. It should be noted that the E-optimality criterion which minimizes the maximum of the eigenvalues of $V(d)$, is equivalent to MV-optimality if the contrasts of interest are proportional to the basic contrasts.

A-Optimality : A design $d^* \in$D(t,b,k) is said to be A-optimal if

$$tr(V(d^*)) = \min \mathrm{tr(V(d))}\ \forall d \in D;$$

where $tr(X)$ denotes the trace of the matrix X. Assuming the usual normal theory model, A-optimality is equivalent to minimizing the sum of the lengths of the axes of the simultaneous confidence ellipsoid for the given contrasts of interest.

The goal for selecting a design, is to estimate the contrasts $\tau_{ij}-\tau_{i0}$ and $\tau_{ij}-\tau_{0j}$, for i=1,2,...,n-1 and j=1,2,...,m-1 with as much precision as possible in the sense of having small variances for the $\hat{\tau}_{ij} - \hat{\tau}_{i0}$ and $\hat{\tau}_{ij} - \hat{\tau}_{0j}$. Two of the standard criteria used to accomplish this goal are to select designs that minimize $tr(C\Omega C')$(A-optimality) or minimize the maximum variance for the the estimators of $\tau_{ij} - \tau_{i0}$ and $\tau_{ij} - \tau_{0j}$(MV-optimality). These have a meaningful interpretation, namely minimizing the sum of the variances of the estimators of the contrasts of interest over all designs, and minimizing the maximum of the variances of the estimators of the contrast of interest over all designs respectively. However as pointed out by Hedayat, Jacroux and Majumdar(1988) the D-optimality criterion does not seem to be either an intuitively, or statistically suitable criterion, because the designs it selects as being optimal generally do not provide any more information about the contrasts of interest than they do about the other possible contrasts which are not of primary interest. On the other hand, the A- and MV-optimality criteria each have a natural and statistically meaningful interpretation.

It should be noted here that a design which is optimal under any one of the above criteria is not necessarily optimal under the others . However, evidence gained from studies of different types of designs suggests that a design which is optimal or performs well on one criterion tends to perform well on the other criteria(ref: John, 1987,p28).

In our problem A-optimality corresponds to regarding estimation of the two sets of contrasts (1.1) and (1.2) as of equal importance. In some practical problems this may not be appropriate. For example a comparison of the joint effect of A and B with the effect of A alone may be of greater importance than comparing the joint effect with the effect of B alone. In such cases we can consider the average variance within each set of contrasts separately. Alternatively we might minimize a weighted mean of the variances of the estimators of the contrasts of interest(see Chapter 6).

As Hedayat, Jacroux and Majumdar(1988) point out, minimizing the average variance of the estimators of the contrast of interest is usually not easy. As in the other cases of exact design theory, it is highly unlikely that we can obtain one method which is capable of producing A-optimal designs for arbitrary values of t, b and k.

1.3.2 Definitions:

In the this section we bring together some useful definitions concerning our problem.

Definition 1.1 *A block design for two factors A and B at n and m levels respectively which accommodates all the combinations of levels of A and B except 00 is called an* **n×m Factorial Block Design** *with* **00 Censored**, *and is denoted by* $n \times m$ **CFBD(00)**.

In the following we specify some possible forms of balance in a $n \times m$ CFBD(0 0). In the past balance properties were primarily of importance for simplifying the computation of the analysis of the data rather than as a desirable design feature. Since the development of computer software such as GLIM, this feature is no longer so important. The main motivation for balance properties in modern design is to give designs with equal and high precision on the contrasts of interest. In traditional block theory, balance of treatments and blocks has been shown to give designs which are optimal under all the criteria in the previous section and under a wider class of optimality criteria called **Universal Optimality**(see Kiefer,1975, and Cheng and Wu,1980).

Definition 1.2 *An $n \times m$ CFBD(00) is said to be* **Balanced** *for* **Dual versus A** *if:*

$$V(\hat{\tau}_{ij} - \hat{\tau}_{i0}) = \alpha_1(\alpha_1 \neq 0),$$
$$Cov(\hat{\tau}_{ij} - \hat{\tau}_{i0} \ , \ \hat{\tau}_{kl} - \hat{\tau}_{k0}) = \rho_1, \tag{1.15}$$

for $i = 1, 2, \ldots, n-1$, $j = 1, 2, \ldots, m-1$, $k = 1, 2, \ldots, n-1$ and $l = 1, 2, \ldots, m-1$; excluding $ij = kl$; where α_1 and ρ_1 are constant($\alpha_1 \neq \rho_1$), and $\hat{\tau}_{ij} - \hat{\tau}_{i0}$ and $\hat{\tau}_{kl} - \hat{\tau}_{k0}$ are $BLUE's$ of $\tau_{ij} - \tau_{i0}$ and $\tau_{kl} - \tau_{k0}$, respectively and Cov(x,y) stands for the covariance between x and y. This property will be abbreviated to **BDS(A)**.

In other words an n×m CFBD(00) is balanced dual versus A if:

$$V(C_2\underline{\hat{\tau}}) = (\alpha_1 - \rho_1)I_l + \rho_1 J_l(\alpha_1 \neq \rho_1), \tag{1.16}$$

where C_2 was given in(1.12) and $l = (n-1)(m-1)$.

A similar property of balance can be defined as **Balanced Dual versus B**, and denoted by **BDS(B)**. Thus a n× m CFBD(00) is balanced dual versus B if:

$$V(C_1\underline{\hat{\tau}}) = (\alpha_2 - \rho_2)I_l + \rho_2 J_l(\alpha_2 \neq \rho_2), \tag{1.17}$$

where C_1 was given in(1.12), ρ_2 and $\alpha_2(\alpha_2 \neq 0)$ are constants.

Definition 1.3 *An n×2 CFBD(00) is called* **Partly Balanced Dual versus Single(PBDS)** *if it is*

1. *balanced for dual versus A and balanced for dual versus B,*
2. *there are equal correlations between the estimators of every pair of orthogonal dual versus single contrasts,*
   and
3. *there are equal correlations between the estimators of every pair of non-orthogonal dual versus single contrasts, not necessarily equal to the correlations in part 2.*

In other words an $n \times 2$ CFBD(00) is PBDS design if:

$$V(C\hat{\underline{\tau}}) = \begin{bmatrix} (\alpha_1 - \rho_1)I_p + \rho_1 J_p & (\theta - \gamma)I_p + \gamma J_p \\ (\theta - \gamma)I_p + \gamma J_p & (\alpha_2 - \rho_2)I_p + \rho_2 J_p \end{bmatrix}. \tag{1.18}$$

This definition is extended to $n \times m$ experiment in Chapter 5.

If the estimation of the comparisons in (1.1) and (1.2) are of equal importance, then equal variances on all the comparisons is desirable. This motivates the following property.

Definition 1.4 *An $n \times m$ PBDS design is called a* **Balanced Dual versus Single Design(BDSD)** *if all the contrasts of interest are estimated with equal precision and every pair of contrast estimators has equal correlation. In other words the design is a BDSD if:*

$$V(C\hat{\underline{\tau}}) = (\sigma^2 - \rho)I_{2l} + \rho J_{2l}, \tag{1.19}$$

where C is defined in (1.12) and $l = (n-1)(m-1)$.

The following Examples illustrate these definitions.

Example 1.1 *For n=3, m=2, k=2, and b=4 we have t=5 and ,*

$$\underline{\tau} = (\tau_{01}, \tau_{10}, \tau_{20}, \tau_{11}, \tau_{21})',$$

$$C_1 = \begin{bmatrix} -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$C_2 = \begin{bmatrix} 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 1 \end{bmatrix}.$$

Then the design given below is a balanced dual versus single design:

*block*1	01	21
*block*2	01	11
*block*3	10	11
*block*4	20	21

.

The balance property follows since

$$N = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}, NN' = \begin{bmatrix} 2 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 2 & 0 \\ 1 & 0 & 1 & 0 & 2 \end{bmatrix},$$

and hence

$$A = \begin{bmatrix} 1 & 0 & 0 & -0.5 & -0.5 \\ 0 & 0.5 & 0 & -0.5 & 0 \\ 0 & 0 & 0.5 & 0 & -0.5 \\ -0.5 & -0.5 & 0 & 1 & 0 \\ -0.5 & 0 & -0.5 & 0 & 1 \end{bmatrix},$$

$$V(C_1\hat{\underline{\tau}}) = 2I_2,$$

and

$$V(C_2\hat{\underline{\tau}}) = 2I_2.$$

Example 1.2 *For n=4, m=2, k=5 and b=3 we have t=7 and*

$$\underline{\tau} = (\tau_{01}, \tau_{10}, \tau_{20}, \tau_{30}, \tau_{11}, \tau_{21}, \tau_{31})',$$

$$C_1 = \begin{bmatrix} -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$C_2 = \begin{bmatrix} 0 & -1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 \end{bmatrix}.$$

For the design

*block*1	01	10	11	20	21
*block*2	01	20	21	30	31
*block*3	01	30	31	10	11

we have:

$$N' = \begin{bmatrix} 1 & 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 \end{bmatrix}, NN' = \begin{bmatrix} 3 & 2 & 2 & 2 & 2 & 2 & 2 \\ 2 & 2 & 1 & 1 & 2 & 1 & 1 \\ 2 & 1 & 2 & 1 & 1 & 2 & 1 \\ 2 & 1 & 1 & 2 & 1 & 1 & 2 \\ 2 & 2 & 1 & 1 & 2 & 1 & 1 \\ 2 & 1 & 2 & 1 & 1 & 2 & 1 \\ 2 & 1 & 1 & 2 & 1 & 1 & 2 \end{bmatrix}.$$

It follows that:

$$V(C_1\underline{\hat{\tau}}) = \begin{bmatrix} 0.875 & 0.312 & 0.312 \\ 0.312 & 0.875 & 0.312 \\ 0.312 & 0.312 & 0.875 \end{bmatrix},$$

and

$$V(C_2\underline{\hat{\tau}}) = I_3.$$

Hence the design is PBDS but does not have full balance for dual versus single factor comparisons.

Definition 1.5 *A design will be termed efficient for the dual versus single treatment problem if it has very low total variance on the contrasts $C\tau$ where C is given in (1.12).*

1.4 2×2 CFBD(00):

The remainder of this chapter concentrates on the case m=n=2, i.e. where both factors have two levels. The problem then reduces to designing for the comparison of each of the treatments 01 and 10 with the treatment 11. This is a particular case of the general problem of constructing efficient designs for comparing test treatments with a single control treatment which in recent years has received a good deal of attention. The problem is to construct an experiment involving t test treatments and 1 control making a total of t+1 treatments. The treatments are to be arranged in b blocks, each of size k. Let the test treatments be labelled 1,...,t and let 0 denote the control treatment. The term control is used in the sense of a special or standard treatment. An additive linear model without treatment-block interactions is assumed. The objective of the experiment is to estimate the treatment contrasts $\tau_i - \tau_0$ for $1 \leq i \leq t$. Now we give a brief summary of studies which have been done on A- and MV-optimal designs.

1.4.1 Historical Background:

In connection with finding good designs for test treatments versus control treatment, Cox(1958, p238) suggests a design in which the control treatment appears the same number of times(once, twice, or more), within each block and the test treatments form a **Balanced Incomplete Block Design(BIBD)** over the remaining units. He does not give any mathematical analysis to establish the efficiency of such designs. Pesek(cf: Hedayat, Jcroux and Majumdar,1988), compares a BIBD with an augmented BIBD as suggested by Cox(1958) and concludes that the latter is more efficient. Constantine(1983), shows that a BIBD in the test treatments augmented by a replication of the control in each block, is A-optimal in the class of designs with exactly one replication of the control in each block. Jacroux(1984) shows that Constantine's conclusion remains valid even when BIBD's are replaced by certain Group Divisible(GD) design. Stufken(1988) determines the most efficient augmented block design and suggests a lower bound for the efficiency of these designs.

Pearce(1960) proposes the class of supplemented balance designs for investigating the test treatments versus control treatment problem. Gupta(1989) studies the work of Pearce(1960) and derives a lower bound for the average variance of test-control contrast estimators in designs which are binary in terms of all the treatments involved in the block designs. He advocates using this bound for both binary and non-binary designs. However this bound is not the tightest bound available for non-binary designs.

Bechhofer and Tamhane(1981) were the first to propose a class of designs called **Balanced Test Treatment Incomplete Block(BTIB)** designs in order to characterize optimal block designs for the simultaneous test-control confidence region, which includes Cox's(1958) designs. This class will be discussed in Section 1.4.2.

A rigorous treatment for determining optimal designs for comparing test treatments with a control is started by Majumdar and Notz(1983). They initiate the study of A-optimality of BTIB designs and give a method for finding A- and MV-optimal designs. In the course of their work a bound for average variance of the contrast estimators is derived which holds for the cases in which $t + 1 > k$. This bound is extended to the designs with $t + 1 \leq k$ later by Jacroux and Majumdar(1987) and Ting and Notz(1987) separately. The bound of Gupta(1989) equals the bound in which $t + 1 > k$ in the special case when the design is binary in terms of the t+1 treatments involved in the design, t+1 is a perfect square value and an overall BTIB design does exist. For all other cases Gupta's bound is smaller than the two other bounds.

Hedayat and Majumdar(1984, 1985) devise an algorithm for obtaining A-optimal design based on Majumdar and Notz(1983), and provide a catalogue of A-optimal designs and designs which are A-optimal among BTIB designs. They also give a family of optimal designs. Türe(1982,1985) also studies A-optimal designs and highly efficient designs and gives a method of construction. Jacroux(1989) generalizes Hedayat and Majumdar's(1984) algorithm for finding A-optimal designs. Stufken(1986,1987,1988) studies optimal designs and gives families of optimal designs as well as approximate optimal designs.

Cheng, Majumdar, Stufken and Türe(1988) give new families of optimal designs and some approximate optimal designs. Ting and Notz(1987) study optimal block designs. Ting and Notz(1988) give a catalogue of A-optimal designs for the cases where the number of test treatments involved in the design is less than k. The most recent work of Hedayat, Jacroux and Majumdar(1988) outlines existing knowledge on optimal designs for comparing test treatments with a control in incomplete block designs, completely randomized block designs and row-column designs.

In the following we bring together those definitions and theorems underlying the theory of efficient block designs for comparing test treatments with a control treatment which are relevant to the dual-versus-single design problem.

Definition 1.6 *(Keifer, 1975): A block design is said to be a* **Balanced Block Design** *if:*

$$\begin{array}{lll} 1.\ \sum_{j=1}^{b} n_{ij} = r, & for & i = 1,2,\ldots,t, \\ 2.\ \sum_{j=1}^{b} n_{ij}n_{mj} = \lambda & for & i \neq m, i, m = 1,2,\ldots,t, \\ 3.\ \mid n_{ij} - k/t \mid < 1,\ for\ j = 1,2,\ldots,b & and & i = 1,2,\ldots,t. \end{array} \qquad (1.20)$$

A balanced block design for t treatments in b blocks of size k is denoted by **BBD(t,b,k)**. If the balanced block design is *binary*, then it is called a **Balanced Incomplete Block Design** denoted by **BIBD**(t,b,k).

1.4.2 A-optimal Block Designs for Control-Test Treatment Comparisons:

In this section we summarize the definitions and results used in the literature for finding A-optimal block designs for control-test treatment comparisons. We use $\hat{\tau}_i - \hat{\tau}_0$ to denote the BLUE of $\tau_i - \tau_i$(i=0,1,2...,t) and D(t+1,b,k) to denote the set of all possible experimental designs in b blocks of size k each, based on t+1 treatments. The problem is, for given t, b and k, to select a design $d^* \in D(t+1, b, k)$ which minimizes $\sum_{i=1}^{t} V(\hat{\tau}_i - \hat{\tau}_0)$ over all designs belonging to $D(t+1, b, k)$. Thus an A-optimal design criterion is used. Some definitions concerning this problem follow:

Definition 1.7 *(Bechhofer and Tamhane,1981) A design d∈ $D(t+1, b, k)$ is called a* **Balanced Test Treatment Incomplete Block(BTIB)** *design if the following conditions are satisfied:*

1. *d is an incomplete block design, that is $t \geq k$,*
2. *there are constants λ_0 and λ_1 such that:*

$$\begin{array}{ll} \sum_{j=1}^{b} n_{0j} n_{ij} = \lambda_0, & for \quad 1 \leq i \leq t, \\ \sum_{j=1}^{b} n_{ij} n_{i'j} = \lambda_1, & for \quad 1 \leq i, i' \leq t. \end{array} \tag{1.21}$$

Bechhofer and Tamhane(1981,Theorem 3.1) prove that necessary and sufficient conditions for a design to be BTIB is that the variance-covariance matrix for $\hat{\underline{\theta}} = (\hat{\tau}_1 - \hat{\tau}_0\ ,\ \hat{\tau}_2 - \hat{\tau}_0\ ,\ \ldots, \hat{\tau}_t - \hat{\tau}_0)'$ is a completely symmetric matrix. In other words a design is BTIB iff:

$$V(\hat{\underline{\theta}}) = (\eta - \mu) I_t + \mu J_t. \tag{1.22}$$

In the literature designs with this feature are known as totally variance balanced for the test-control contrasts. It should be mentioned here that the same properties can be sought in block designs with $k > t$.

Definition 1.8 *(Ting and Notz,1988,Definition 2) A design $d \in D(t+1, b, k)$ is called a* **Balanced Treatment Block Design(BTBD)** *if condition 2 of Definition.1.6 holds and condition 1 does not hold.*

Definition 1.9 *(Stufken,1987,Definition 2.2) A design d is termed* **BTIB(t+1, b,k;u,s)** *if d∈ $D(t+1, b, k)$ and has the following properties:*

1. *d is a BTIB.*
2. *There are s blocks in d, each with u+1 replications of the control, while each of the remaining b-s blocks contains u replications of the control.*
3. *d is binary in the test treatments, i.e.* $n_{ij} \in \{0,1\}$ *for* $1 \leq i \leq t$ *and* $1 \leq j \leq b$.

Similarly, a design d is termed BTBD(t+1,b,k;u,s) if it has the following properties:

1. d is a BTBD.
2. There are s blocks in d, each with u+1 replications of the control, while each of the remaining b-s blocks contains u replications of the control.

Definition 1.10 *(Hedayat and Majumdar, 1984) A BTIB(t+1,b,k;u,s) is called a* **Rectangular type(R-type)** *design if s=0 or b , and a* **Step type(S-type)** *otherwise.*

Figures 1.1 and 1.2 show the structure of an R-type and an S-type design respectively, where d_0 denotes a BIBD with t treatments in b blocks each of size k-u, d_1 and d_2 denote a BIBD with t treatments in s blocks each of size k-u-1, and b-s blocks of size k-u each respectively. Note that the blocks correspond to the columns of the array.

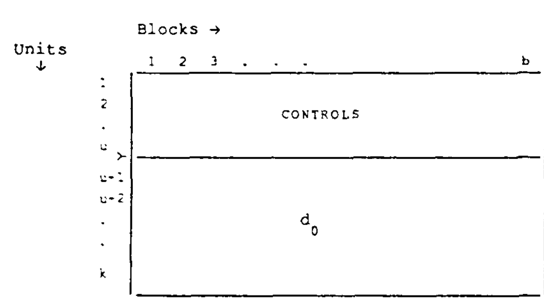

Figure 1.1: An R-type design(s=0).

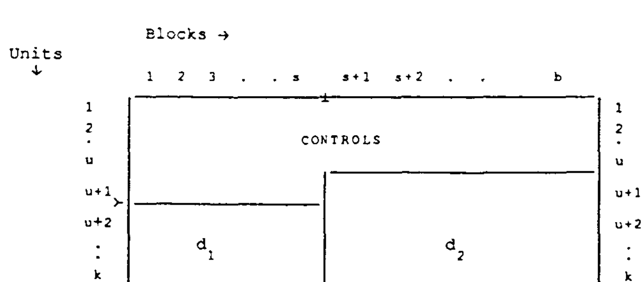

Figure 1.2: An S-type design(s≠0).

The following lemma specifies a necessary relationship amongst the parameters of BTIB(t+1,b,k;u,s).

Lemma 1.1 *(Hedayat and Majumdar,1984,Lemma 2.2): In a BTIB(t+1,b,k; u, s), the following relations must hold:*

$$\begin{aligned} tr &= b(k-u)-s, \\ tc &= s(k-u-1) \\ \lambda(t-1) &= c(k-u-2)+(r-c)(k-u-1), \end{aligned} \tag{1.23}$$

where r denotes the number of replications of each test treatments. For R-type designs c=0; for S-type designs c equals the number of replications of each test treatments in part d_1.

When k=2, the necessary conditions stated in Lemma 1.1 are sufficient, because in an R-type design, d_0 consists of copies of $t\sum 1$ and in an S-type design d_1 and d_2 consist of copies of $t\sum 1$ and $t\sum 2$, respectively, where $b\sum$a: is the set of all $b!/\{a!(b-a)!\}$ distinct blocks of size a each based on b treatments.

1.4.3 Efficient 2×2 CFIBD(00)$(t \geq k)$:

Majumdar and Notz(1983) first showed that the general problem of constructing efficient incomplete block designs, where $t \geq k$ for comparing test treatments with a control can be reduced to finding the number, r_0, of replications of the control in the entire design, and then finding the most efficient design for this value of r_0. They characterize certain A-optimal designs in the incomplete block case, where $t \geq k$ as follows :

Theorem 1.1 *(Majumdar and Notz,1983): For given t, b and k, a BTIB(t+1, b, k; u,s) design is A-optimal when u=x and s=z minimize:*

$$g(x,z) = (t-1)^2\{btk(k-1)-(bx+z)(kt-t+k)+(bx^2+2xz+z)\}^{-1}+ \\ \{k(bx+z)-(bx^2+2xz+z)\}^{-1} \tag{1.24}$$

among the integers x=0,1,....,[k/2] and z=0,1,....,b-1, with the restriction that z is positive when x=0 and z=0 when x=[k/2]. Here [.] *denotes* "the integer part of.".

For the 2×2 dual-versus-single problem the only possible size for $t \geq k$, is k=2. Obviously for the set of parameters t=2, k=2 and b, Theorem.1.1 is not able to provide A-optimal design for every value of b. An A-optimal design exists for any value of b but searching for it through a complete enumeration of all designs is prohibitively costly, even for moderate values of b.

Hedayat and Majumdar(1984) use Theorem 1.1 in an algorithm to produce a catalogue of A-optimal designs, which include 2×2 designs with parameters in the range $2 \leq b \leq 50$.

As an alternative we might use a design which is A-optimal within a class of designs known to have some desirable statistical properties. The class of BTIB designs is a good choice in our case because of the symmetric structure of the variance-covariance matrix for the estimators of the contrasts of interest of such designs. Designs that are A-optimal within the class of BTIB designs are expected to compete well with designs that are A-optimal in the entire class, in most cases.

Hedayat and Majumdar(1984) show that for an S-type design in which u=0, d_1 is w copies of $2\sum 1$ and d_2 is y copies of $2\sum 2$, respectively. For this case the expression:

$$\frac{1}{w+2y}+\frac{1}{w} \tag{1.25}$$

is proportional to the total of the variances of the control test treatments estimators. They characterize designs which minimize the expression in (1.25) over nonnegative integers w and y, satisfying:

$$2w+y=b, \tag{1.26}$$

for $w > 0$.

They used this approach to obtain A-optimal designs by finding A-optimal designs within the BTIB class of designs with S-type structure.

Table 2 of Hedayat and Majumdar(1984) gives a catalogue of A-optimal designs and designs which are A-optimal among BTIB designs with k=2 and $2 \leq b \leq 50$.

1.4.4 Catalogue of A-Optimal 2×2 CFBD(00)($t < k$):

In this section available A-optimal block designs for $t < k$ and both factors at two levels are briefly reviewed and new designs are catalogued. The new designs cover parameter values for which designs are not currently available. The designs are all of the R- and S-type.

Ting and Notz(1987) give the following theorem to characterize a series of A-optimal designs within the BTBD(cf: Definition 1.7) class for the cases when $t < k$.

Theorem 1.2 *(Ting and Notz, 1987, Theorem 3.1)For given t, b, and k suppose* $d \in D(t+1, b, k)$ *is a BTBD such that:*

$$\begin{array}{llllll} 1. & r_i = [(kb - r_0)/t] & or & [(kb - r_0)/t] + 1, & for & 1 \le i \le t \\ 2. & n_{ij} = [r_i/b] & or & [r_i/b] + 1, & for & 1 \le i \le t \quad ,1 \le j \le b \\ 3. & n_{0j} = [r_0/b] & or & [r_0/b] + 1, & for & 1 \le j \le b \quad . \end{array} \tag{1.27}$$

4. r_0 *is the non-negative integer,* $1 \le r_0 \le [bk/2]$ *which minimizes F(r), where F(r) is given below, then d is A-optimal over D(t+1,b,k). Here* [.] *denotes* "the integer part of ." *and*

$$F(r) = \frac{t(t-1)^2}{t\{bk - r - (c/k)\} - \{r - (g/k)\}} + \frac{t}{r - (g/k)};$$

where

$$\begin{gathered} g = r + (2r - b)[r/b] - b[r/b]^2, \\ c = bk - r + (t - bk + r + tp)[p/b](2p - b - b[p/b]) + \\ (bk - r - tp)[(p+1)/b]\{2(p+1) - b - b[(p+1)/b]\}, \end{gathered} \tag{1.28}$$

and

$$p = [(bk - r)/t].$$

Jacroux and Majumdar(1987) obtain the same theorem by permuting the information matrix of the test-control contrasts.

Notice that all the designs satisfying Theorem 1.2 will have the BDS property, because they are BTBD; in particular the contrasts of interest will have equal variances.

Note that $F(r_0)$ is an achievable bound which can be used to assess the efficiency of <u>any</u> connected block design.

Ting and Notz(1988) use Theorem 1.2 in an algorithm to produce a catalogue of A-optimal designs which includes 2×2 designs with parameters in the ranges $2 \le b \le 50$ and $3 \le k \le 30$. However, there are many block sizes for which designs are not given, for example k=3,5,6,8,9,11,12. When k=3, then by Ting and Notz(1988), the randomized block design is A-optimal for each b. It should be noted that this is not true in general for $t > 2$ and k=t+1. The result also follows from Theorem 3.1 of Hedayat and Majumdar(1985). In Table 1.1 at the end of this chapter we give a catalogue of A-optimal designs of the R- and S-type to fill in the gaps for $4 \leq b \leq 50$, and $k \leq 30$.

The BTB designs considered by Ting and Notz(1988) and further investigated here are of three types:

- R-type when $r_0 \equiv 0 mod(b)$ and $(kb - r_0)/(tb)$ is an integer. Then the structure is Figure 1.1, where $u = r_0/b$ and d_0 is a BBD(t,b,k-u) in the test treatments. For this structure, the number of replications of each test treatment within each block is $(kb - r_0)/(tb)$.

- R-type when $r_0 \equiv 0 mod(b)$ and $(kb - r_0)/(tb)$ is not an integer. Then the structure is Figure 1.3, with:

$$\begin{aligned} u &= r_0/b, \\ q &= k - (r_0/b) - t\left[(bk - r_0)/tb\right], \end{aligned} \tag{1.29}$$

  d_{01} and d_{02} are BBD(t,b,k-q-u) and BBD(t,b,q) in the test treatments respectively. For this structure $(kb - r_0)/t$ should be an integer.

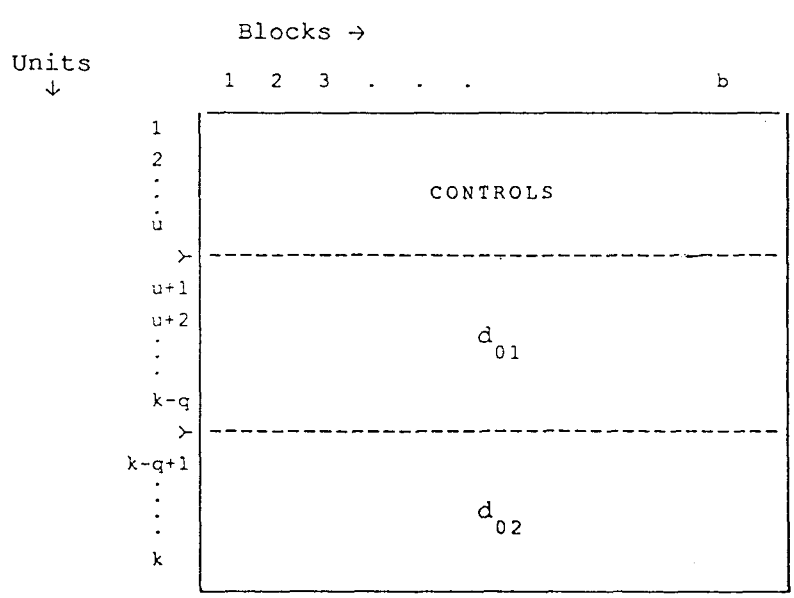

Figure 1.3: An R-type design when $(bk-r_0)/tb$ is not an integer.

- S-type when r_0/b is not an integer. Then the structure is as shown in Figure 1.2, where $u = [r_0/b]$, $s = r_0 - bu$, d_1 and d_2 are BBD(t,s,k-u-1) and

BBD(t,b-s,k-u) in the test treatments respectively. For this structure $(kb - r_0)/t$ should be an integer. Note that t=2 for the case we are considering.

The catalogue in Table 1.1 at the end of this chapter was obtained by using the procedure of Ting and Notz(1988) to fill in the gaps for some practical set of parameters which have not been given previously. The computer algorithm for generating the catalogue in Table 1.1 is outlined in Section 1.4.5.

In the following we give two examples to show how to get designs from the catalogue.

Example 1.3 *For b=2 and k=5, it is clear from Table 1.1 that the design is R-type with* $r_0 = 4$. *Now* $(kb - r_0)/(tb) = 6/4$ *and hence the design has the form shown in Figure 1.3. From (1.29) with t=2 we have q=1. Therefore u=2 units of each block are allocated to the control, labelled 11;* d_{01} *consists of 2 blocks each of size k-q-u=2, where the test treatments(01 and 10) occur once in each block;* d_{02} *consists of two blocks of size 1 with the test treatments 01 and 10 occurring once. The design is:*

*Block*1	11	11	01	10	01
*Block*2	11	11	01	10	10

Example 1.4 *For k=6 and b=6 from Table 1.1 the A-optimal design is S-type with structure as in Figure 1.2, where* d_1 *is a BBD(2,2,3) and* d_2 *a BBD(2,4,4). The design therefore has the control treatment 11 occurring three times in each of blocks 1 and 2 and twice in each of the other blocks. The design is:*

*Block*1	11	11	11	01	10	01
*Block*2	11	11	11	10	10	01
*Block*3	11	11	01	01	10	10
*Block*4	11	11	01	01	10	10
*Block*5	11	11	01	01	10	10
*Block*6	11	11	01	01	10	10

In the following theorem an explicit method of constructing BBD's for t=2 is given. This method is useful for obtaining sections d_1 and d_2 of the above designs and hence for constructing balanced treatment block designs.

Theorem 1.3 *BTBD(3,b,k;u,s) design exists if and only if b(k-u)-s is even.*

Proof: Two cases must be considered:

1. $s = 0$, i.e. the design is R-type. For this case by looking at Figure 1.1 on page 16, we must show d_0 which is BBD(2,b,k-u) does exist. Since b(k-u) is even it follows that either b or k-u must be even. If k-u is even then each of treatments 01 and 10 occurs $(k-u)/2$ times in each block and the resulting design is BBD(2,b,k-u). If k-u is not even then b must be even and we have b/2 pairs of blocks. For each pair of blocks assign $[(k-u)/2]+1$ units of one block to treatment 10 and the remaining units of that block to treatment 01. In the other block of the pair assign $[(k-u)/2]+1$ units to treatment 01 and the remaining units to treatment 10. Then each pair of blocks consists of a BBD and the resulting design is BBD(2,b,k-u).

2. If $s \neq 0$, i.e. design is S-type. For this case we must show that d_1 and d_2 are BBD(2,s,k-u-1) and BBD(2,b-s,k-u), repectively. In this case $bk - r_0 = bk - bu - s$ is even. There are then two possibilities:

   (a) Both s and b(k-u) are even, then by argument in part 1, d_1 and d_2 can be constructed.

   (b) Both s and b(k-u) are odd, then k-u-1 is even and d_1 can be constructed. Also d_2 can be constructed, since b and s are both odd, which implies that b-s is even.

If $b(k-u)-s$ is not even, the design is not equireplicate in terms of test treatments and then a BTBD does not exist. This completes the proof.♣

As an illustration of this result, Examples 1.3 and 1.4 can be constructed as in parts 1 and 2 of the proof of Theorem 1.3 respectively.

1.4.5 Computer Algorithm:

The computer algorithm(Appendix B) for generating the catalogue of A-optimal designs in Table 1.1 consists of the following steps:

STEP 1 : Find r_0, the value for r which minimize F(r), for all r∈L.

STEP 2 : Check whether bk-r_0 is even or odd. If it is odd, then by Theorem 1.3, an overall A-optimal BTBD does not exist.

STEP 3 : Specify the layout of the A-optimal design based on Figures 1.1 to 1.3.

STEP 4 : Determine the detailed structure of the design specified in STEP 3.

1.4.6 Near Optimal and New Optimal Balanced Treatment Block Designs:

It is clear that for parameters $4 \leq k \leq 30$, and $b \leq 50$, *there still remain gaps* where the A-optimal BTBD does not satisfy Theorem 1.2. This is because the A-optimal designs are not balanced and this is the case whenever $(bk - r_0)/t$ is not an integer, where r_0 is the value which minimizes F(r) in Theorem 1.2. For these cases, as we have already pointed out, to search for A-optimal designs through a complete enumeration of all designs is costly. Examination of the class of BTBD is a natural choice in our context since this class guarantees equal precision for the estimators of the contrasts of interest. Designs that are A-optimal within this class are expected to compete with designs that are A-optimal in the entire class, in most cases(ref: Hedayat and Majumdar,1984).

In this section we find A-optimal designs within the BTBD class. The A-optimal BTBD could be obtained by using the Ting and Notz(1988) algorithm. Let L={r;r=1,2,...,bk/2} and let r_0 ∈L be the value which minimizes F(r) in Theorem 1.2. Then if $bk - r_0$ is even, the A-optimal design belongs to the BTBD class which is given in Table 1.1. If $bk - r_0$ is not even then the design which is A-optimal among BTBD's could be obtained by finding $r_1 \in L$ which (i) minimizes F(r) in Theorem 1.2 among all the possible values of $r \in L$ excluding $r = r_0$ and (ii) makes $bk - r_1$ equal to an even number.

Cheng, Majumdar, Stufken and Türe(1988), proved that if $F(r_0)$=min F(r) $\forall r \in L$, then F(r) is decreasing on $\{r_1 \in L; r_1 \leq r_0\}$ and increasing over $\{r_1 \in L; r_1 \geq r_0\}$. Based on this theorem, if bk-r_0 is not even, then the most efficient BTBD will be obtained by taking either $r_0 - 1$ or $r_0 + 1$ as the number of replications of the control treatment in the optimal design according to one which gives the smaller value for F(r).

Consequently when an A-optimal BTBD does not exist, then a near optimal BTBD is obtained by requiring that the number of replications of the control should be exactly 1 less than or greater than the value which minimizes F(r) in Theorem 1.2 i.e. we take $r_0 - 1$ or $r_0 + 1$ as the number of replications of the control treatment in the A-optimal BTBD. A design, d, is called **near optimal** or **efficient** if the trace of the variance-covariance matrix of contrasts of interest is very close to the minimum value of F(r) i.e. $F(r_0)$, the lower bound for the contrasts of interest. In other words if $E_d = F(r_0)/tr(V_d)$, where V is the variance-covariance matrix of design d, then d is efficient if E_d is very close to 1.

When $bk - r_0$ is not even, a computer algorithm(Appendix B) similar to the algorithm given earlier has been used to determine the A-optimal designs within the class of BTBD. Table 1.2 at the end of this chapter gives a catalogue of these designs. Note that all the designs in this table have E_d greater than 0.96.

In the following examples we will show how these A-optimal designs within the BTBD class are efficient relative to the minimum value of F(r) and relative to the most efficient design which can be generated by using the algorithm of Jones and Eccleston(1980). Henceforth we denote this algorithm by JE.

Example 1.5 *For given parameter values b=5 and k=5, minimizing F(r) in Theorem 1.2 by the computer algorithm gives* $r_0 = 10$. *The efficient design for* $r_0 = 10$, *found by JE, is shown below:*

*Block*1	11	11	01	01	10
*Block*2	11	11	01	10	10
*Block*3	11	11	01	01	10
*Block*4	11	11	01	10	10
*Block*5	11	11	01	01	10

The individual variances for $\hat{\tau}_{01} - \hat{\tau}_{11}$ *and* $\hat{\tau}_{10} - \hat{\tau}_{11}$ *are 0.1145 and 0.1240 respectively with E=0.998 which shows that the design is not a BTBD. It has* $tr(V) = 0.238550$. *To find a competing efficient BTBD for these parameters we use the control replication* $r_1 = r_0 + 1 = 11$, *and construct the following BTBD using the computer algorithm of Section 1.4.5:*

*Block*1	11	11	01	01	10
*Block*2	11	11	01	10	10
*Block*3	11	11	01	01	10
*Block*4	11	11	01	10	10
*Block*5	11	11	11	01	10

The individual variances for $\hat{\tau}_{01} - \hat{\tau}_{11}$ *and* $\hat{\tau}_{10} - \hat{\tau}_{11}$ *are both 0.1212 and the design is a BTBD with* $E_d = 0.982$. *This is not an overall A-optimal design but is A-optimal within the BTBD class and is, therefore, included in Table 1.2.*

Example 1.6 *For given parameter values b=4 and k=6, minimizing F(r) gives* $r_0 = 9$ *and the efficient design for* $r_0 = 9$ *obtained by JE, is shown below:*

*Block*1	11	11	11	01	01	10
*Block*2	11	11	01	01	10	10
*Block*3	11	11	01	01	10	10
*Block*4	11	11	01	01	10	10

The individual variances for $\hat{\tau}_{01} - \hat{\tau}_{11}$ *and* $\hat{\tau}_{10} - \hat{\tau}_{11}$ *are 0.1189 and 0.1311 respectively with* $tr(V) = 0.2500$. *The design is neither BTBD nor A-optimal with E=0.997. To find a competing and more efficient BTBD for these parameters we use* $r_0 = 9$. *Then putting* $r_0 + 1$ *as the number of replications,* r_1, *of the control treatment, we obtain from Table 1.2 the following S-type BTBD:*

*Block*1	11	11	11	01	01	10
*Block*2	11	11	11	01	10	10
*Block*3	11	11	01	01	10	10
*Block*4	11	11	01	01	10	10

with $tr(V) = 0.249641$ $V(\hat{\tau}_{01} - \hat{\tau}_{11}) = V(\hat{\tau}_{10} - \hat{\tau}_{11}) = 0.1248$ *and* $E_d = 0.998$.

Table 1.1: Catalogue[2] of overall A-optimal designs of the R- and S-type for t=2, $2 \leq b \leq 50$, $4 \leq k \leq 30$, which were not listed in Ting and Notz(1988).

k	b	r_0	type	section of the design			
5	2m	2b	R	d_{01} :	1 rep;	d_{02} :	m copies of $2\sum 1$
6	6	14	S	d_1 :	BBD(2, 2,3);	d_2 :	BBD(2, 4,4)
	7	16	S	d_1 :	"	d_2 :	BBD(2, 5,4)
	8	18	S	d_1 :	"	d_2 :	BBD(2, 6,4)
	12	28	S	d_1 :	BBD(2, 4,3);	d_2 :	BBD(2, 8,4)
	13	30	S	d_1 :	"	d_2 :	BBD(2, 9,4)
	14	32	S	d_1 :	"	d_2 :	BBD(2,10,4)
	15	34	S	d_1 :	"	d_2 :	BBD(2,11,4)
	19	44	S	d_1 :	BBD(2, 6,3);	d_2 :	BBD(2,13,4)
	20	46	S	d_1 :	"	d_2 :	BBD(2,14,4)
	21	48	S	d_1 :	"	d_2 :	BBD(2,15,4)
	22	50	S	d_1 :	"	d_2 :	BBD(2,16,4)
	26	60	S	d_1 :	BBD(2, 8,3)	d_2 :	BBD(2,18,4)
	27	62	S	d_1 :	"	d_2 :	BBD(2,19,4)
	28	64	S	d_1 :	"	d_2 :	BBD(2,20,4)
	33	76	S	d_1 :	BBD(2,10,3)	d_2 :	BBD(2,23,4)
	34	78	S	d_1 :	"	d_2 :	BBD(2,24,4)
	35	80	S	d_1 :	"	d_2 :	BBD(2,25,4)
	40	92	S	d_1 :	BBD(2,12,3)	d_2 :	BBD(2,28,4)
	41	94	S	d_1 :	"	d_2 :	BBD(2,29,4)
	42	96	S	d_1 :	"	d_2 :	BBD(2,30,4)
	46	106	S	d_1 :	BBD(2,14,3)	d_2 :	BBD(2,32,4)
	47	108	S	d_1 :	"	d_2 :	BBD(2,33,4)
	48	110	S	d_1 :	"	d_2 :	BBD(2,34,4)
	49	112	S	d_1 :	"	d_2 :	BBD(2,35,4)

[2]Note

1. Selections d_0, d_1, d_2, d_{01} and d_{02} are amalgamated as shown in Figures 1.1 to 1.3 on pages 16 and 20.
2. m is any positive integer.
3. z rep means z replications for each test treatment in each block.
4. $x \sum y$ is the set of all $x!/\{y!(x-y)!\}$ blocks obtained from all the distinct selections of y treatments from x.

Table 1.1: continued...

k	b	r_0	type		section of the design		
8	2m	3b	R	d_{01} :	2 rep;	d_{02} :	m copies of $2\sum 1$
9	2m	4b	R	d_{01} :	2rep;	d_{02} :	m copies of $2\sum 1$
	$m < 6$						
	2m+1	4b-1	S	d_1 :	BBD(2,2m,5);	d_2 :	BBD(2, 1,6)
	$4 < m < 15$						
	2m	4b-2	S	d_1 :	BBD(2,b-2,5);	d_2 :	BBD(2,2,6)
	$15 < m < 26$						
11	b	5b	R	d_0 :	3 rep		
	$b < 7$						
	b	5b-2	S	d_1 :	BBD(2,b-2,6);	d_2 :	BBD(2,2,7)
	$20 < b < 34$						
	b	5b-4	S	d_1 :	BBD(2,b-4,6);	d_2 :	BBD(2,4,7)
	$46 < b < 51$						
12	2m	5b	R	d_{01} :	3 rep;	d_{02} :	m copies of $2\sum 1$
15	2m	6b	R	d_{01} :	4 rep;	d_{02} :	m copies of $2\sum 1$
16	3	20	S	d_1 :	BBD(2, 2,9);	d_2 :	BBD(2,1,10)
	5	34	S	d_1 :	BBD(2, 4,9);	d_2 :	"
	6	40	S	d_1 :	"	d_2 :	BBD(2,2,10)
	8	54	S	d_1 :	BBD(2, 6,9);	d_2 :	"
	9	60	S	d_1 :	"	d_2 :	BBD(2,3,10)
	11	74	S	d_1 :	BBD(2, 8,9);	d_2 :	"
	14	94	S	d_1 :	BBD(2,10,9);	d_2 :	BBD(2,4,10)
	17	114	S	d_1 :	BBD(2,12,9);	d_2 :	BBD(2,5,10)
	19	128	S	d_1 :	BBD(2,14,9);	d_2 :	"
	20	134	S	d_1 :	"	d_2 :	BBD(2,6,10)
	22	148	S	d_1 :	BBD(2,16,9);	d_2 :	"
	23	154	S	d_1 :	"	d_2 :	BBD(2,7,10)
	25	168	S	d_1 :	BBD(2,18,9);	d_2 :	"
	26	174	S	d_1 :	"	d_2 :	BBD(2,8,10)
	28	188	S	d_1 :	BBD(2,20,9);	d_2 :	"

Table 1.1: continued...

k	b	r_0	type		section of the design		
16	31	208	S	d_1 :	BBD(2,22,9);	d_2 :	BBD(2,9,10)
	34	228	S	d_1 :	BBD(2,24,9);	d_2 :	BBD(2,10,10)
	36	242	S	d_1 :	BBD(2,26,9);	d_2 :	"
	37	248	S	d_1 :	"	d_2 :	BBD(2,11,10)
	39	262	S	d_1 :	BBD(2,28,9);	d_2 :	"
	40	268	S	d_1 :	BBD(2,28,9);	d_2 :	BBD(2,12,10)
	42	282	S	d_1 :	BBD(2,30,9);	d_2 :	"
	45	302	S	d_1 :	BBD(2,32,9);	d_2 :	BBD(2,13,10)
	48	322	S	d_1 :	BBD(2,34,9);	d_2 :	BBD(2,14,10)
	50	336	S	d_1 :	BBD(2,36,9);	d_2 :	"
18	4	30	S	d_1 :	BBD(2,2,10);	d_2 :	BBD(2,2,11)
	5	38	S	d_1 :	BBD(2,3,10);	d_2 :	"
	9	68	S	d_1 :	BBD(2,5,10);	d_2 :	BBD(2,4,11)
	10	76	S	d_1 :	BBD(2,6,10);	d_2 :	"
	13	98	S	d_1 :	BBD(2,7,10);	d_2 :	BBD(2,6,11)
	14	106	S	d_1 :	BBD(2,8,10);	d_2 :	"
	15	114	S	d_1 :	BBD(2,9,10);	d_2 :	"
	18	136	S	d_1 :	BBD(2,10,10);	d_2 :	BBD(2,8,11)
	19	144	S	d_1 :	BBD(2,11,10);	d_2 :	"
	22	166	S	d_1 :	BBD(2,12,10);	d_2 :	BBD(2,10,11)
	23	174	S	d_1 :	BBD(2,13,10);	d_2 :	"
	24	182	S	d_1 :	BBD(2,14,10);	d_2 :	"
	27	204	S	d_1 :	BBD(2,15,10);	d_2 :	BBD(2,12,11)
	28	212	S	d_1 :	BBD(2,16,10);	d_2 :	"
	32	242	S	d_1 :	BBD(2,18,10);	d_2 :	BBD(2,14,11)
	33	250	S	d_1 :	BBD(2,19,10);	d_2 :	"
	36	272	S	d_1 :	BBD(2,20,10);	d_2 :	BBD(2,16,11)
	37	280	S	d_1 :	BBD(2,21,10);	d_2 :	"
	38	288	S	d_1 :	BBD(2,22,10);	d_2 :	"
	41	310	S	d_1 :	BBD(2,23,10);	d_2 :	BBD(2,18,11)
	42	318	S	d_1 :	BBD(2,24,10);	d_2 :	"
	46	348	S	d_1 :	BBD(2,26,10);	d_2 :	BBD(2,20,11)
	47	356	S	d_1 :	BBD(2,27,10);	d_2 :	"
	50	378	S	d_1 :	BBD(2,28,10);	d_2 :	BBD(2,22,11)

Table 1.1: continued...

k	b	r_0	type	section of the design			
19	2m	8b	R	d_{01} :	5 rep;	d_{02} :	m copies of $2\sum 1$
23	4	38	S	d_1 :	BBD(2,2,13);	d_2 :	BBD(2,2,14)
	5	47	S	d_1 :	"	d_2 :	BBD(2,3,14)
	6	56	S	d_1 :	"	d_2 :	BBD(2,4,14)
	9	85	S	d_1 :	BBD(2,4,13);	d_2 :	BBD(2,5,14)
	10	94	S	d_1 :	"	d_2 :	BBD(2,6,14)
	11	103	S	d_1 :	"	d_2 :	BBD(2,7,14)
	14	132	S	d_1 :	BBD(2,6,13);	d_2 :	BBD(2,8,14)
	15	141	S	d_1 :	"	d_2 :	BBD(2,9,14)
	16	150	S	d_1 :	"	d_2 :	BBD(2,10,14)
	19	179	S	d_1 :	BBD(2,8,13);	d_2 :	BBD(2,11,14)
	20	188	S	d_1 :	"	d_2 :	BBD(2,12,14)
	21	197	S	d_1 :	"	d_2 :	BBD(2,13,14)
	25	235	S	d_1 :	BBD(2,10,13);	d_2 :	BBD(2,15,14)
	26	244	S	d_1 :	"	d_2 :	BBD(2,16,14)
	30	282	S	d_1 :	BBD(2,12,13);	d_2 :	BBD(2,18,14)
	31	291	S	d_1 :	"	d_2 :	BBD(2,19,14)
	35	329	S	d_1 :	BBD(2,14,13);	d_2 :	BBD(2,21,14)
	36	338	S	d_1 :	"	d_2 :	BBD(2,22,14)
	40	376	S	d_1 :	BBD(2,16,13);	d_2 :	BBD(2,24,14)
	41	385	S	d_1 :	"	d_2 :	BBD(2,25,14)
	45	423	S	d_1 :	BBD(2,18,13);	d_2 :	BBD(2,27,14)
	46	432	S	d_1 :	"	d_2 :	BBD(2,28,14)
	50	470	S	d_1 :	BBD(2,20,13);	d_2 :	BBD(2,30,14)
25	2	20	R	d_{01} :	7 rep;	d_{02} :	1 copy of $2\sum 1$
	3	31	S	d_1 :	BBD(2,1,14);	d_2 :	BBD(2,2,15)
	5	51	S	d_1 :	"	d_2 :	BBD(2,4,15)
	7	71	S	d_1 :	"	d_1 :	BBD(2,6,15)
	8	82	S	d_1 :	BBD(2,2,14);	d_2 :	"
	10	102	S	d_1 :	"	d_2 :	BBD(2,8,15)
	12	122	S	d_1 :	"	d_2 :	BBD(2,10,15)
	13	133	S	d_1 :	BBD(2,3,14);	d_2 :	"
	15	153	S	d_1 :	"	d_2 :	BBD(2,12,15)
	17	173	S	d_1 :	"	d_2 :	BBD(2,14,15)

Table 1.1: continued...

k	b	r_0	type	section of the design			
25	18	184	S	d_1 :	BBD(2,4,14);	d_2 :	BBD(2,14,15)
	20	204	S	d_1 :	"	d_2 :	BBD(2,16,15)
	22	224	S	d_1 :	"	d_2 :	BBD(2,18,15)
	25	255	S	d_1 :	BBD(2,5,14);	d_2 :	BBD(2,20,15)
	27	275	S	d_1 :	"	d_2 :	BBD(2,22,15)
	30	306	S	d_1 :	BBD(2,6,14);	d_2 :	BBD(2,24,15)
	32	326	S	d_1 :	"	d_2 :	BBD(2,26,15)
	35	357	S	d_1 :	BBD(2,7,14);	d_2 :	BBD(2,28,15)
	37	377	S	d_1 :	"	d_2 :	BBD(2,30,15)
	40	408	S	d_1 :	BBD(2,8,14);	d_2 :	BBD(2,32,15)
	42	428	S	d_1 :	"	d_2 :	BBD(2,34,15)
	45	459	S	d_1 :	BBD(2,9,14);	d_2 :	BBD(2,36,15)
	47	479	S	d_1 :	"	d_2 :	BBD(2,38,15)
	50	510	S	d_1 :	BBD(2,10,14);	d_2 :	BBD(2,40,15)
30	b $b < 11$	12b	R	d_0 :	9 rep		
	b $30 \leq b \leq 50$	12b+2	S	d_1 :	BBD(2,2,17);	d_2 :	BBD(2,b-2,18)

Table 1.2: Catalogue[3] of R- and S-type A-optimal designs within the BTBD class for t=2, $2 \leq b \leq 50$, $4 \leq k \leq 30$.

k	b	r_1	type	section of the design			
5	2m+1	2b+1	S	d_1 :	BBD(2,1,2);	d_2 :	BBD(2,b-1,3)
6	b(=2,3)	2b	R	d_0 :	2 rep		
	4	10	S	d_1 :	BBD(2,2,3);	d_2 :	BBD(2,2,4)
	5	12	S	d_1 :	BBD(2,2,3);	d_2 :	BBD(2,3,4)
	9	20	S	d_1 :	BBD(2,2,3);	d_2 :	BBD(2,7,4)
	10	22	S	d_1 :	BBD(2,2,3);	d_2 :	BBD(2,8,4)
	11	26	S	d_1 :	BBD(2,4,3):	d_2 :	BBD(2,7,4)
	16	36	S	d_1 :	BBD(2,4,3);	d_2 :	BBD(2,12,4)
	17	38	S	d_1 :	BBD(2,4,3);	d_2 :	BBD(2,13,4)
	18	42	S	d_1 :	BBD(2,6,3);	d_2 :	BBD(2,12,4)
	23	52	S	d_1 :	BBD(2,6,3);	d_2 :	BBD(2,17,4)
	24	56	S	d_1 :	BBD(2,8,3);	d_2 :	BBD(2,16,4)
	25	58	S	d_1 :	BBD(2,8,3);	d_2 :	BBD(2,17,4)
	29	66	S	d_1 :	BBD(2,8,3);	d_2 :	BBD(2,21,4)
	30	68	S	d_1 :	BBD(2,8,3);	d_2 :	BBD(2,22,4)
	31	72	S	d_1 :	BBD(2,10,3);	d_2 :	BBD(2,21,4)
	32	74	S	d_1 :	BBD(2,10,3);	d_2 :	BBD(2,22,4)
	36	82	S	d_1 :	BBD(2,10,3);	d_2 :	BBD(2,26,4)
	37	84	S	d_1 :	BBD(2,10,3);	d_2 :	BBD(2,27,4)
	38	88	S	d_1 :	BBD(2,12,3);	d_2 :	BBD(2,26,4)
	39	90	S	d_1 :	BBD(2,12,3);	d_2 :	BBD(2,27,4)
	43	98	S	d_1 :	BBD(2,12,3);	d_2 :	BBD(2,31,4)
	45	104	S	d_1 :	BBD(2,14,3);	d_2 :	BBD(2,31,4)
	50	114	S	d_1 :	BBD(2,14,3);	d_2 :	BBD(2,36,4)
8	2m+1	3b+1	S	d_1 :	BBD(2,1,4);	d_2 :	BBD(2,b-1,5)
9	2m+1	4b-1	S	d_1 :	BBD(2,b-1,5);	d_2 :	BBD(2,1,6)
	$1 \leq m \leq 4$						
	2m	4b	R	d_{01} :	2 rep	d_{02} :	m copies of $2\sum 1$
	$6 \leq m \leq 10$						
	2m	4b-2	S	d_1 :	BBD(2,b-2,5);	d_2 :	BBD(2,2,6)
	$11 \leq m \leq 15$						

[3] r_1 is the replication of the control treatment.

Table 1.2: continued...

k	b	r_1	type	section of the design			
9	2m+1	4b-1	S	d_1 :	BBD(2,b-1,5);	d_2 :	BBD(2,1,6)
	$16 \leq m \leq 19$						
	2m+1	4b-3	S	d_1 :	BBD(2,b-3,5);	d_2 :	BBD(2,3,6)
	$20 \leq m \leq 24$						
11	b	5b	R	d_0 :	3 rep		
	$7 \leq m \leq 13$						
	b	5b-2	S	d_1 :	BBD(2,b-2,6);	d_2 :	BBD(2,2,7)
	$14 \leq b \leq 40$						
	b	5b-4	S	d_1 :	BBD(2,b-4,6);	d_2 :	BBD(2,4,7)
	$41 \leq b \leq 46$						
12	2m+1	5b-1	S	d_1 :	BBD(2,b-1,7);	d_2 :	BBD(2,1,8)
15	2m+1	6b+1	S	d_1 :	BBD(2,1,8);	d_2 :	BBD(2,b-1,9)
16	2	14	R	d_{01} :	4 rep;	d_{02} :	1 copy of $2\sum 1$
	4	26	S	d_1 :	BBD(2,2,9);	d_2 :	BBD(2,2,10)
	7	46	S	d_1 :	BBD(2,4,9);	d_2 :	BBD(2,3,10)
	10	68	S	d_1 :	BBD(2,8,9);	d_2 :	BBD(2,2,10)
	12	80	S	d_1 :	BBD(2,8,9);	d_2 :	BBD(2,4,10)
	13	88	S	d_1 :	BBD(2,10,9);	d_2 :	BBD(2,3,10)
	15	100	S	d_1 :	BBD(2,10,9);	d_2 :	BBD(2,5,10)
	16	108	S	d_1 :	BBD(2,12,9);	d_2 :	BBD(2,4,10)
	18	120	S	d_1 :	BBD(2,12,9);	d_2 :	BBD(2,6,10)
	21	140	S	d_1 :	BBD(2,14,9);	d_2 :	BBD(2,7,10)
	24	162	S	d_1 :	BBD(2,18,9);	d_2 :	BBD(2,6,10)
	27	180	S	d_1 :	BBD(2,20,9);	d_2 :	BBD(2,7,10)
	29	194	S	d_1 :	BBD(2,20,9);	d_2 :	BBD(2,9,10)
	30	202	S	d_1 :	BBD(2,22,9);	d_2 :	BBD(2,8,10)
	32	214	S	d_1 :	BBD(2,22,9);	d_2 :	BBD(2,10,10)
	33	222	S	d_1 :	BBD(2,24,9);	d_2 :	BBD(2,9,10)
	35	234	S	d_1 :	BBD(2,24,9);	d_2 :	BBD(2,11,10)
	38	256	S	d_1 :	BBD(2,28,9);	d_2 :	BBD(2,10,10)
	41	276	S	d_1 :	BBD(2,30,9);	d_2 :	BBD(2,11,10)
	43	288	S	d_1 :	BBD(2,30,9);	d_2 :	BBD(2,13,10)
	44	296	S	d_1 :	BBD(2,32,9);	d_2 :	BBD(2,12,10)

Table 1.2: continued...

k	b	r_1	type	section of the design			
16	46	308	S	d_1 :	BBD(2,32,9);	d_2 :	BBD(2,14,10)
	47	316	S	d_1 :	BBD(2,34,9);	d_2 :	BBD(2,13,10)
	49	328	S	d_1 :	BBD(2,34,9);	d_2 :	BBD(2,15,10)
18	2	16	R	d_0 :	5 rep		
	3	22	S	d_1 :	BBD(2,1,10);	d_2 :	BBD(2,2,11)
	6	46	S	d_1 :	BBD(2,4,10);	d_2 :	BBD(2,2,11)
	7	52	S	d_1 :	BBD(2,3,10);	d_2 :	BBD(2,4,11)
	8	60	S	d_1 :	BBD(2,4,10);	d_2 :	BBD(2,4,11)
	11	84	S	d_1 :	BBD(2,7,10);	d_2 :	BBD(2,4,11)
	12	90	S	d_1 :	BBD(2,6,10);	d_2 :	BBD(2,6,11)
	16	122	S	d_1 :	BBD(2,10,10);	d_2 :	BBD(2,6,11)
	17	128	S	d_1 :	BBD(2,9,10);	d_2 :	BBD(2,8,11)
	18	152	S	d_1 :	BBD(2,12,10);	d_2 :	BBD(2,8,11)
	21	158	S	d_1 :	BBD(2,11,10);	d_2 :	BBD(2,10,11)
	25	190	S	d_1 :	BBD(2,15,10);	d_2 :	BBD(2,10,11)
	26	196	S	d_1 :	BBD(2,14,10);	d_2 :	BBD(2,12,11)
	29	220	S	d_1 :	BBD(2,17,10);	d_2 :	BBD(2,12,11)
	30	228	S	d_1 :	BBD(2,18,10);	d_2 :	BBD(2,12,11)
	31	234	S	d_1 :	BBD(2,17,10);	d_2 :	BBD(2,14,11)
	34	258	S	d_1 :	BBD(2,20,10);	d_2 :	BBD(2,14,11)
	35	264	S	d_1 :	BBD(2,19,10);	d_2 :	BBD(2,16,11)
	39	296	S	d_1 :	BBD(2,23,10);	d_2 :	BBD(2,16,11)
	40	302	S	d_1 :	BBD(2,22,10);	d_2 :	BBD(2,18,11)
	43	326	S	d_1 :	BBD(2,25,10);	d_2 :	BBD(2,18,11)
	44	332	S	d_1 :	BBD(2,24,10);	d_2 :	BBD(2,20,11)
	45	340	S	d_1 :	BBD(2,25,10);	d_2 :	BBD(2,20,11)
	48	364	S	d_1 :	BBD(2,28,10);	d_2 :	BBD(2,20,11)
	49	370	S	d_1 :	BBD(2,27,10);	d_2 :	BBD(2,22,11)
19	2m+1	8b-1	S	d_1 :	BBD(2,b-1,11);	d_2 :	BBD(2,1,12)
22	2m+1	9b+1	S	d_1 :	BBD(2,1,12);	d_2 :	BBD(2,b-1,13)

Table 1.2: continued...

k	b	r_1	type	section of the design			
23	2	18	R	d_0 :	7 rep		
	3	29	S	d_1 :	BBD(2,2,13);	d_2 :	BBD(2,1,14)
	7	65	S	d_1 :	BBD(2,2,13);	d_2 :	BBD(2,5,14)
	8	76	S	d_1 :	BBD(2,4,13);	d_2 :	BBD(2,4,14)
	12	112	S	d_1 :	BBD(2,4,13);	d_2 :	BBD(2,8,14)
	13	123	S	d_1 :	BBD(2,6,13);	d_2 :	BBD(2,7,14)
	17	159	S	d_1 :	BBD(2,6,13);	d_2 :	BBD(2,11,14)
	18	170	S	d_1 :	BBD(2,8,13);	d_2 :	BBD(2,10,14)
	22	206	S	d_1 :	BBD(2,8,13);	d_2 :	BBD(2,14,14)
	23	217	S	d_1 :	BBD(2,10,13);	d_2 :	BBD(2,13,14)
	24	226	S	d_1 :	BBD(2,10,13);	d_2 :	BBD(2,14,14)
	27	253	S	d_1 :	BBD(2,10,13);	d_2 :	BBD(2,17,14)
	28	264	S	d_1 :	BBD(2,12,13);	d_2 :	BBD(2,16,14)
	29	273	S	d_1 :	BBD(2,12,13);	d_2 :	BBD(2,17,14)
	32	300	S	d_1 :	BBD(2,12,13);	d_2 :	BBD(2,20,14)
	33	311	S	d_1 :	BBD(2,14,13);	d_2 :	BBD(2,19,14)
	34	320	S	d_1 :	BBD(2,14,13);	d_2 :	BBD(2,20,14)
	37	347	S	d_1 :	BBD(2,14,13);	d_2 :	BBD(2,23,14)
	38	358	S	d_1 :	BBD(2,16,13);	d_2 :	BBD(2,22,14)
	39	367	S	d_1 :	BBD(2,16,13);	d_2 :	BBD(2,23,14)
	42	394	S	d_1 :	BBD(2,16,13);	d_2 :	BBD(2,26,14)
	43	405	S	d_1 :	BBD(2,18,13);	d_2 :	BBD(2,25,14)
	44	414	S	d_1 :	BBD(2,18,13);	d_2 :	BBD(2,26,14)
	47	441	S	d_1 :	BBD(2,18,13);	d_2 :	BBD(2,29,14)
	48	450	S	d_1 :	BBD(2,18,13);	d_2 :	BBD(2,30,14)
	49	461	S	d_1 :	BBD(2,20,13);	d_2 :	BBD(2,29,14)
25	4	40	R	d_{01} :	7 rep;	d_{02} :	2 copies of $2\sum 1$
	6	62	S	d_1 :	BBD(2,2,14);	d_2 :	BBD(2,4,15)
	9	91	S	d_1 :	BBD(2,1,14);	d_2 :	BBD(2,8,15)
	11	113	S	d_1 :	BBD(2,3,14);	d_2 :	BBD(2,8,15)
	14	142	S	d_1 :	BBD(2,2,14);	d_2 :	BBD(2,12,15)

Table 1.2: continued...

k	b	r_1	type	section of the design			
25	16	164	S	d_1 :	BBD(2,4,14);	d_2 :	BBD(2,12,15)
	19	193	S	d_1 :	BBD(2,3,14);	d_2 :	BBD(2,16,15)
	21	215	S	d_1 :	BBD(2,5,14);	d_2 :	BBD(2,16,15)
	23	235	S	d_1 :	BBD(2,5,14);	d_2 :	BBD(2,18,15)
	24	244	S	d_1 :	BBD(2,4,14);	d_2 :	BBD(2,20,15)
	26	266	S	d_1 :	BBD(2,6,14);	d_2 :	BBD(2,20,15)
	28	286	S	d_1 :	BBD(2,6,14);	d_2 :	BBD(2,22,15)
	29	295	S	d_1 :	BBD(2,5,14);	d_2 :	BBD(2,24,15)
	31	317	S	d_1 :	BBD(2,7,14);	d_2 :	BBD(2,24,15)
	33	337	S	d_1 :	BBD(2,7,14);	d_2 :	BBD(2,26,15)
	34	346	S	d_1 :	BBD(2,6,14);	d_2 :	BBD(2,28,15)
	36	368	S	d_1 :	BBD(2,8,14);	d_2 :	BBD(2,28,15)
	38	388	S	d_1 :	BBD(2,8,14);	d_2 :	BBD(2,30,15)
	39	397	S	d_1 :	BBD(2,7,14);	d_2 :	BBD(2,32,15)
	41	417	S	d_1 :	BBD(2,7,14);	d_2 :	BBD(2,34,15)
	43	439	S	d_1 :	BBD(2,9,14);	d_2 :	BBD(2,34,15)
	44	448	S	d_1 :	BBD(2,8,14);	d_2 :	BBD(2,36,15)
	46	468	S	d_1 :	BBD(2,8,14);	d_2 :	BBD(2,38,15)
	48	490	S	d_1 :	BBD(2,10,14);	d_2 :	BBD(2,38,15)
	49	499	S	d_1 :	BBD(2,9,14);	d_2 :	BBD(2,40,15)
26	2m+1	11b-1	S	d_1 :	BBD(2,b-1,15);	d_2 :	BBD(2,1,16)
29	2m+1	12b-1	S	d_1 :	BBD(2,1,16);	d_2 :	BBD(2,b-1,17)
30	b $11 \leq b \leq 20$	12b	R	d_0 :	9 rep		
	b $21 \leq b \leq 30$	12b+2	S	d_1 :	BBD(2,2,17);	d_2 :	BBD(2,b-2,18)

Chapter 2

Dual Versus Single Treatment Block Designs for $n \times 2$ Experiments with $n > 2$.

2.1 Introduction:

In Chapter 1 we found that the class of **Balanced Dual versus Single Designs(BDSD)** is a rich source of optimal and near optimal designs for the dual versus single treatment design problem when both factors have two levels. When one or both factors have more than 2 levels it is therefore natural to ask if the subclass of designs having the property of balance again includes A-optimal designs. In this chapter we extend our consideration of designs to those which are partly balanced as in Definition 1.3. These include totally balanced designs as a special case. We establish the necessary and sufficient condition on the A-matrix of a design to be PBDS. A method of constructing a series of PBDS designs based on reinforcing group divisible designs is suggested and some of the properties of this series of designs are investigated. The class of BDSD's which is a special case of the class of PBDS designs is considered in detail. It is shown that restricting to designs with the balance property incurs unnecessarily large treatment replications and other disadvantages. It is proved that BDSD's exist only for m=2 or n=2. Further, the feasibility of certain desirable structures of the variance-covariance matrix of the contrast estimators is considered. Also combinatorial problems of the designs are investigated.

2.2 Contrasts:

For the $n \times 2$ case the ordering of the treatments shown in (1.4) is used in the treatment vector:

$$\underline{\tau} = (\tau_{01}, \tau_{10}, \tau_{20}, \ldots, \tau_{p0}, \tau_{11}, \tau_{21}, \ldots, \tau_{p1})', \tag{2.1}$$

where p=n-1, $\underline{\tau}$ is a $t \times 1$ column vector and t=2n-1. The contrasts of interest are the dual versus single treatment comparisons:

$$(i) \quad \tau_{i1} - \tau_{01}, \tag{2.2}$$

and

$$(ii) \quad \tau_{i1} - \tau_{i0}, \tag{2.3}$$

for i=1,2,...,p; where (2.2) and (2.3) consist of the contrasts for dual versus B and dual versus A respectively. In matrix form, the contrasts of interest are given as $C\underline{\tau}$, where

$$C = \begin{bmatrix} -\underline{1}_p & 0_p & I_p \\ \underline{0}_p & -I_p & I_p \end{bmatrix}. \tag{2.4}$$

We can view the problem as comparing each dual treatment **i1** with the two single treatments **i0** and **01** (i=1,2,...,p). Majumdar(1986) found A-optimal designs for comparing a set of test treatments with a set of control treatments. In his context all the elementary treatment contrasts for comparing any test treatment with any control treatment are of equal interest. The dual versus single design problem can be viewed as comparing a set of test treatments(the dual treatments 11,21,...,p1) with a set of control treatments(the single treatments 01,10,20,...,p0). However, the problem differs from that considered by Majumdar(1986) in that any particular test treatment is to be compared with only **two specific** control treatments. We have found nothing in the literature relevant to this problem for $n > 2$.

2.3 Information Matrix of the Contrast Estimators:

Before going further we give a definition which will be used to specify the structure of the A-matrix of designs belonging to a specific class.

Definition 2.1 *Let $C\underline{\hat{\tau}}$ be a set of independent contrast estimators of $C\underline{\tau}$ in a connected design with Ω as a g-inverse of the A-matrix of the design, then*

$$M = (C\Omega C')^{-1}, \tag{2.5}$$

will be called the **Information matrix of the contrast estimators.** *The information matrix M depends on the design as well as the contrasts of interest, but throughout this thesis we use M rather than M(C,d).*

We now specify the information matrix for the estimators of the contrast of interest. From Definition 2.1 it is clear that the variance-covariance matrix of the contrast estimators is $V = M^{-1}$. The determination of M is an important, but not always an easy, job. Fortunately for $n \times 2$ experiments it is not difficult to specify it. The following lemmas and theorem leads us to give M in terms of the elements of the A-matrix of the design.

Lemma 2.1 *The A-matrix of any connected(block or row-column) design can always be partitioned as follows :*

$$A = \begin{bmatrix} a_{11} & \underline{a}'_{12} \\ \underline{a}_{12} & U \end{bmatrix}, \tag{2.6}$$

where a_{11} is a scalar, $\underline{a}_{12}$ is a column vector, U is a $(t-1)\times(t-1)$ nonsingular symmetric matrix and t is the number of treatments.

<u>Proof</u>: We know $A\underline{1}_t = \underline{0}_t$, where $\underline{1}_t$ is a vector with every entry unity. Hence in order for a partition (2.6) to hold we must have:

$$\begin{bmatrix} a_{11} \\ \underline{a}_{12} \end{bmatrix} = -\begin{bmatrix} \underline{a}'_{12} \\ U \end{bmatrix} \times \underline{1}_{t-1}. \tag{2.7}$$

This gives us:

$$R(A) = R\left(\begin{bmatrix} \underline{a}'_{12} \\ U \end{bmatrix}\right). \tag{2.8}$$

Also we know that $\underline{1}'_{t-1}U + \underline{a}'_{12} = \underline{0}$, since $(A\underline{1}_t)' = \underline{1}'_t A = \underline{0}$. This implies that $R(A) = R(U)$. U must be nonsingular, since connectivity implies R(A)=t-1.♣

The following lemma gives a specific g-inverse for the A-matrix of any connected(block or row-column) design.

Lemma 2.2 *Let the A-matrix of a connected design be partitioned as in Lemma 2.1, then it has the following matrix as a g-inverse:*

$$\Omega = \begin{bmatrix} 0 & \underline{0}' \\ \underline{0} & U^{-1} \end{bmatrix}. \tag{2.9}$$

Proof: It is sufficient to show that $A\Omega A = A$. From Lemma 2.1. we have:

$$A = \begin{bmatrix} a_{11} & \underline{a}'_{12} \\ \underline{a}_{12} & U \end{bmatrix},$$

therefore:

$$A\Omega A = \begin{bmatrix} a_{11} & \underline{a}'_{12} \\ \underline{a}_{12} & U \end{bmatrix} \times \begin{bmatrix} 0 & \underline{0}' \\ \underline{0} & U^{-1} \end{bmatrix} \times \begin{bmatrix} a_{11} & \underline{a}'_{12} \\ \underline{a}_{12} & U \end{bmatrix}$$

$$= \begin{bmatrix} \underline{a}'_{12}U^{-1}\underline{a}_{12} & \underline{a}'_{12} \\ \underline{a}_{12} & U \end{bmatrix}. \tag{2.10}$$

But from Lemma 2.1 we have $\underline{a}'_{12} = -\underline{1}'U$ and this implies that $\underline{a}'_{12}U^{-1} = -\underline{1}'$. Hence $\underline{a}'_{12}U^{-1}\underline{a}_{12} = -\underline{1}'\underline{a}_{12}$. Also from Lemma 2.1 we have $\underline{1}'\underline{a}_{12} = a_{11}$. Therefore $A\Omega A = A$ and Ω is a g-inverse of the A-matrix of the design.♣

Note: Lemmas 2.1 and 2.2 apply to both block and row-column designs under the model in which there are no interactions involving blocking or row and column factors.

Two things should be noted here. Firstly for the estimable parametric functions such as contrasts, both the estimators and variance-covariance matrix of the estimators are invariant under any choice of g-inverse of the A-matrix(Ref: John,1987;p11). Secondly the Lemmas 2.1 and 2.2 are valid for any ordering of treatments in $\underline{\tau}$.

In the following theorem we will determine the information matrix, M, for the dual versus single treatment contrast estimators.

Theorem 2.1 *For any connected $n \times 2$ CFBD(00), let the A-matrix of the design be represented by:*

$$A = \begin{bmatrix} a_{11} & \underline{a}_{12}' & \underline{a}_{13}' \\ \underline{a}_{12} & A_{22} & A_{23} \\ \underline{a}_{13} & A_{23}' & A_{33} \end{bmatrix}, \tag{2.11}$$

where a_{11} is a scalar, $\underline{a}_{12}$ and $\underline{a}_{13}$ are column vectors both of order $(n-1) \times 1$, A_{22} , A_{23} and A_{33} are matrices of order $(n-1) \times (n-1)$. Then the information matrix of the contrast estimators for the dual versus single treatment problem has the form:

$$M = \begin{bmatrix} A_{22} + A_{33} + A_{23} + A_{23}' & -A_{22} - A_{23}' \\ -A_{22} - A_{23} & A_{22} \end{bmatrix}. \tag{2.12}$$

Proof: The variance-covariance matrix for the dual versus single estimators is $C\Omega C'$. By Definition 2.1 we have $M = (C\Omega C')^{-1}$. From Lemma 2.2 the following matrix can be used as Ω:

$$\Omega = \begin{bmatrix} 0 & \underline{0}' \\ \underline{0} & U^{-1} \end{bmatrix}, \tag{2.13}$$

where,

$$U = \begin{bmatrix} A_{22} & A_{23} \\ A_{23}' & A_{33} \end{bmatrix}. \tag{2.14}$$

From (2.4) we can partition C as follows:

$$C = \begin{bmatrix} V_1 & , & V_2 \end{bmatrix}, \tag{2.15}$$

where

$$V_1 = \begin{bmatrix} -\underline{1}_p \\ \underline{0}_p \end{bmatrix} \quad and \quad V_2 = \begin{bmatrix} 0_p & I_p \\ -I_p & I_p \end{bmatrix}. \tag{2.16}$$

Then after some manipulation we get: $C\Omega C' = V_2 U^{-1} V_2'$. But V_2 is a nonsingular matrix, therefore we have:

$$M = (C\Omega C')^{-1} = (V_2 U^{-1} V_2')^{-1} = V'UV, \tag{2.17}$$

where,

$$V = V_2^{-1} = \begin{bmatrix} I_p & -I_p \\ I_p & 0_p \end{bmatrix}. \tag{2.18}$$

Substituting from (2.14) and (2.18) into (2.17) we will get (2.12). Hence the theorem is proved.♣

2.4 Class of PBDS Designs:

One major problem in establishing A-optimal designs is to specify a class of designs which includes highly efficient or A-optimal designs. The class of PBDS designs not only gives equal precision for estimated contrasts within the dual versus A set and equal precision within the dual versus B set, but also satisfies this requirement. In fact the A-optimal design in this class is a highly efficient design in most cases and is sometimes A-optimal in the entire class of designs(see Chapter 4).

Based on Definition 1.3, a design is PBDS if the variance-covariance matrix of the contrast estimators corresponding to dual versus A and dual versus B is of the form:

$$C\Omega C' = \begin{bmatrix} (\alpha_1 - \rho_1)I_p + \rho_1 J_p & (\delta - \phi)I_p + \phi J_p \\ (\delta - \phi)I_p + \phi J_p & (\alpha_2 - \rho_2)I_p + \rho_2 J_p \end{bmatrix}, \tag{2.19}$$

for $\alpha_i \neq \rho_i (i = 1, 2)$, where C is given in (2.4).

This structure for the variance-covariance matrix allows equal precision and correlation for the contrast estimators corresponding to dual versus A, as well as for those corresponding to dual versus B. It has two values(not necessarily equal) for the correlations among the contrast estimators; one value for orthogonal contrasts and another value for non-orthogonal contrasts.

Example 2.1 *For n=4, b=3 and k=5, the following design is PBDS design:*

*Block*1	01	10	11	20	21
*Block*2	01	10	11	30	31
*Block*3	01	20	21	30	31

with the variance-covariance matrix for the dual versus single contrast estimators:

$$C\Omega C' = \begin{bmatrix} 0.56I_3 + 0.31J_3 & 0.50I_3 \\ 0.50I_3 & I_3 \end{bmatrix}.$$

In Chapter 4 it will be shown that this is a very highly efficient design in the entire class of designs(see Table 4.2).

2.4.1 A-matrix of the Class of PBDS Designs:

So far we have specified the class of PBDS designs in terms of its variance-covariance matrix structure. Now in what follows in this section we characterize this class of designs in terms of the structure of their A-matrices. This simplifies the characterization of this class of designs. But first, we need the following definition.

Definition 2.2 *A matrix has* **structure** *W if it has the form:*

$$W = \begin{bmatrix} a & b\underline{1}'_p & c\underline{1}'_p \\ b\underline{1}_p & dI_p + fJ_p & gI_p + hJ_p \\ c\underline{1}_p & gI_p + hJ_p & qI_p + sJ_p \end{bmatrix}. \tag{2.20}$$

The following theorem specifies the A-matrix of the PBDS designs.

Theorem 2.2 *A necessary and sufficient condition for a connected design d to be a PBDS design is that its A-matrix has structure W.*

Proof: (i)- If the A-matrix of d has structure W then, applying Theorem 2.1, we will show that the variance-covariance matrix of the estimators of the contrast of interest of d has the same structure as a PBDS.

By Lemma 2.2 a g-inverse of the A-matrix is:

$$\Omega = \begin{bmatrix} 0 & \underline{0}'_{2p} \\ \underline{0}_{2p} & U^{-1} \end{bmatrix}, \tag{2.21}$$

where

$$U = \begin{bmatrix} dI_p + fJ_p & gI_p + hJ_p \\ gI_p + hJ_p & qI_p + sJ_p \end{bmatrix}.$$

By matrix algebra theory we have(see Graybill,1983,p195)

$$U^{-1} = \begin{bmatrix} \delta I_p + \phi J_p & \gamma I_p + \eta J_p \\ \gamma I_p + \eta J_p & \theta I_p + \sigma J_p \end{bmatrix}, \quad (2.22)$$

where θ, σ, γ, δ, η and ϕ are functions in terms of d, f, g, h, q and s. Substituting from (2.22) into (2.21), using the definition of C from (2.4) and applying (2.17) we obtain $C\Omega C' = V^{-1}U^{-1}(V')^{-1}$. Then after some algebra we have:

$$C\Omega C' = \begin{bmatrix} \theta I_p + \sigma J_p & (\theta-\gamma)I_p + (\sigma-\eta)J_p \\ (\theta-\gamma)I_p + (\sigma-\eta)J_p & (\theta+\delta-2\gamma)I_p + (\sigma+\phi-2\eta)J_p \end{bmatrix}. \quad (2.23)$$

This gives $\theta I_p + \sigma J_p$ and $(\theta+\delta-2\gamma)I_p + (\sigma+\phi-2\eta)J_p$ as the variance-covariance matrix for the dual versus B and dual versus A contrasts estimators respectively. Therefore, by definition, d is a PBDS design.

(ii)- If we have a design d_1 with A_1 and Ω_1 as its A-matrix and a g-inverse respectively, with:

$$C\Omega_1 C' = \begin{bmatrix} \theta I_p + \sigma J_p & \gamma I_p + \eta J_p \\ \gamma I_p + \eta J_p & \delta I_p + \phi J_p \end{bmatrix}, \quad (2.24)$$

then by Definition 2.1 we have:

$$M_1 = (C\Omega_1 C')^{-1} = \begin{bmatrix} \theta I_p + \sigma J_p & \gamma I_p + \eta J_p \\ \gamma I_p + \eta J_p & \delta I_p + \phi J_p \end{bmatrix}^{-1}. \quad (2.25)$$

But by Theorem 2.1 we have:

$$M_1 = \begin{bmatrix} A_{22} + A_{33} + A_{23} + A'_{23} & -A_{22} - A'_{23} \\ -A_{22} - A_{23} & A_{22} \end{bmatrix}. \quad (2.26)$$

Equating (2.25) and (2.26) we get: $A_{22} = x_1 I_p + y_1 J_p$, $A_{23} = x_2 I_p + y_2 J_p$ and $A_{33} = x_3 I_p + y_3 J_p$, where x_i and y_i(i=1,2,3) are functions of θ , σ , γ , η , δ and ϕ . By a property of the A-matrix of any design(namely, that the sum of the rows and the sum of the columns equal zero) we can easily show that $\underline{a}_{1i} = \psi_i \underline{1} (i = 1, 2)$ where ψ_i's are functions in terms of x_i and y_i(i=1,2,3). Substituting these into the A-matrix given in (2.11) we have:

$$A_1 = \begin{bmatrix} a_{11} & \psi_1 \underline{1}' & \psi_2 \underline{1}' \\ \psi_1 \underline{1} & x_1 I_p + y_1 J_p & x_2 I_p + y_2 J_p \\ \psi_2 \underline{1} & x_2 I_p + y_2 J_p & x_3 I_p + y_3 J_p \end{bmatrix}.$$

Hence the theorem is proved.♣

2.4.2 Information Matrix of the Class of PBDS Designs:

The following Corollary gives the information matrix, M, for the estimators of the contrasts of interest:

Corollary 2.1 *The information matrix for the estimators of the dual versus single treatment contrasts in the class of PBDS designs has the following structure:*

$$M = \begin{bmatrix} (d+q+2g)I_p + (f+s+2h)J_p & -(d+g)I_p - (f+h)J_p \\ -(d+g)I_p - (f+h)J_p & dI_p + fJ_p \end{bmatrix}. \qquad (2.27)$$

Proof: Using structure W, for the A-matrix of the design and applying Theorem 2.2 gives M.♣

Example 2.2 *For n=3, b=3 and k=6, the design:*

*Block*1	01	01	11	21	10	20
*Block*2	01	11	11	21	10	20 ,
*Block*3	01	11	21	21	10	20

has the A-matrix:

$$A = \begin{bmatrix} 3.00 & -0.67\underline{1}_2' & -0.83\underline{1}_2' \\ -0.67\underline{1}_2 & 3I_2 - 0.50J_2 & -0.67J_2 \\ -0.83\underline{1}_2 & -0.67J_2 & 3.83I_2 - 0.83J_2 \end{bmatrix}.$$

The A-matrix of this design has structure W. The information matrix for the dual versus single treatment contrast estimators for this is:

$$M = \begin{bmatrix} 6.83I_2 - 2.67J_2 & -3I_2 + 1.17J_2 \\ -3I_2 + 1.17J_2 & 3I_2 - 0.5J_2 \end{bmatrix}.$$

2.4.3 Combinatorial Properties of PBDS Designs:

We consider the number of occurrences of each treatment in each block and group the treatments according to whether they are B alone, A alone or a dual treatment. In an $n \times 2$ CFBD(00) let n_{Aij}, n_{Bj} and n_{Dij} denote the replications within the jth block(j=1,2,...,b) of the treatment combinations i0, 01 and i1 belonging to sets $A = \{i0; i = 1, 2, ..., p\}$, $B = \{01\}$ and $D = \{i1; i = 1, 2, ..., p\}$ respectively. Let $r_{Ai} = \sum_{j=1}^{b} n_{Aij}$, $r_B = \sum_{j=1}^{b} n_{Bj}$ and $r_{Di} = \sum_{j=1}^{b} n_{Dij}$ denote the respective replications of i0, 01 and i1 in the entire design for i=1,2,...,p. Then from Theorem 2.2, it can be shown that for any PBDS design the following conditions must be satisfied:

1. $\sum_{j=1}^{b} n_{Xij}n_{Xi'j} = \lambda_X$, for $i \neq i'$, i, i'=1,2,...,n-1, X=A and D.
2. $\sum_{j=1}^{b} n_{Aij}n_{Dij} = \lambda_1$, for i=1,2,...,n-1.
3. $\sum_{j=1}^{b} n_{Aij}n_{Di'j} = \lambda_2$, for $i \neq i'$, i, i'=1,2,...,n-1.
4. $\sum_{j=1}^{b} n_{Xij}n_{Bj} = \lambda_{BX}$, for i=1,2,...,n-1, X=A and D.
5. $\sum_{j=1}^{b} n_{Bj}^2 + (n-1)(\lambda_{BA} + \lambda_{BD}) = kr_B$.
6. $\sum_{j=1}^{b} n_{Aij}^2 + (n-2)(\lambda_A + \lambda_2) + \lambda_{BA} + \lambda_1 = kr_{Ai}$.
7. $\sum_{j=1}^{b} n_{Dij}^2 + (n-2)(\lambda_D + \lambda_2) + \lambda_{BD} + \lambda_1 = kr_{Di}$.

2.5 Series of RGDD:

In this section firstly we will introduce a series of block designs for $k < t = 2n-1$, which is useful in our context, and then we will consider its properties. This series of designs is constructed by using a group divisible design for all the treatment combinations involved in the design except the treatment combination 01, and then reinforcing each of the blocks once by 01. Before introducing the class of RGDD we give the definition and a brief summary of some properties of group divisible designs. Further details are given in Clatworthy(1973).

2.5.1 Group Divisible Designs:

A Group Divisible(GD) design is a block design with $t \geq k$ for $t = m_1 \times m_2$ treatments each with replication r. The treatments are divided into m_1 groups of m_2 treatments each. The designs are such that all pairs of treatments belonging to the same group occur together in say, λ_1 blocks, while pairs of treatments from different groups occur together in λ_2 blocks. Two treatments in the same group are said to be **first associates** and those from different groups are said to be **second associates**. Hereafter we will denote a group divisible design by $\mathbf{GD(t, b, k, m_1, m_2, r, \lambda_1, \lambda_2)}$ or simply by **GD** design.

1.5.1.1 Combinatorial Properties of GD Designs:

The parameters of a GD design must satisfy the following conditions:

$$\begin{array}{ll} (i) & t = m_1 m_2 \\ (ii) & r(k-1) = (m_2 - 1)\lambda_1 + m_2(m_1 - 1)\lambda_2. \end{array} \tag{2.28}$$

GD designs have been classified into three subtypes:

$$\begin{array}{llllll} (i) & \textbf{Singular(S)}, & with & \lambda_1 = r & & \\ (ii) & \textbf{Semi}-\textbf{Regular(SR)}, & with & \lambda_1 < r & and & t\lambda_2 = kr \\ (iii) & \textbf{Regular(R)}, & with & \lambda_1 < r & and & t\lambda_2 < kr. \end{array} \tag{2.29}$$

2.5.1.2 Variances and Efficiencies in GD Designs:

The variances of the elementary contrasts can be expressed as functions of the parameters of the GD design as follows:

Let u_1 and u_2 denote the variances of the estimated comparisons of the effects of two treatments which are first and second associates respectively, then

$$u_1 = \frac{2k}{r(k-1) + \lambda_1} \tag{2.30}$$

and

$$u_2 = u_1\{1 - \frac{\lambda_2 - \lambda_1}{t\lambda_2}\}.$$

Comparing these with a **randomized block design** having the same r and the same σ^2(that is having common variances for the error terms in model 1.3 on page 3), gives the following efficiency factors for comparing two first associates and two second associates respectively:

$$E_1^{-1} = \frac{rk}{r(k-1) + \lambda_1} \tag{2.31}$$

and

$$E_2 = E_1\{1 - \frac{\lambda_2 - \lambda_1}{t\lambda_2}\}^{-1}.$$

2.5.2 Reinforced Group Divisible Designs:

Before introducing this class of designs, we give brief definitions and discuss **supplementation balance** and **reinforcement balance** from the literature. These concepts have been introduced when the contrasts among the treatments involved in the design are of unequal importance, such as in the test treatments versus the control treatment problem. To cope with this, traditionally two suggestions have been made. One is supplementation balance(Hoblyn,Pearce and Freeman,1954, Pearce 1960), the other is reinforcement(Das, 1958). The definitions given are: a design is said to have supplemented balance if all the test treatments are replicated r times except for the control(supplementing) treatment which has r_0 replicates. In addition all pairs of test treatments concur λ times in blocks, unless one of the pair is the control treatment, in which case there are λ_0 concurrences. According to Das(1958), if we have a proper block design d, and if a further treatment is added equally often to each block, the resulting design, d^*, is said to be a reinforced design. If design d is a BIBD or a Partially Balanced Incomplete Block Design(PBIBD), then design d^* is called a reinforced balanced or a partially balanced block design respectively(For definitions of these classes of designs refer to Raghavarao,1971, Chapter 8 and Giri,1958). The important feature of supplemented balance is that the non-supplemented treatment is in total balance; in reinforced designs the special treatment is orthogonal to blocks.

For the test treatments versus control treatment problem which is the special case of our problem with n=2, the balance defined in Definitions 1.6 and 1.7 in Chapter 1, is exactly the same as supplemented or reinforcement balance. However for $n > 2$, the partly balanced dual versus single contrasts do not meet the definitions, because this case is concerned with comparisons involving three groups of treatments. Pearce(1983,p 135) extends supplemented balance to m groups of treatments and defines **multipartite** designs, which are mainly used when the treatments fall into groups such that the main comparisons are within groups and only subsidiarily between them. This appears similar to our requirement on designs. However it differs in that it is looking at all contrasts(first group against second group and first group against third group and so on) whereas we are concerned with estimating only proper subsets of these contrasts.

Definition 2.3 *If we reinforce each block of the GD(t-1, b, k-1,* $m_1, m_2, r, \lambda_1, \lambda_2$*) design once by a new treatment then such a design will be called a* **Reinforced Group Divisible Design** *and will be denoted by* **RGDD(t-1, b, k,** m_1, m_2**, r,** λ_1, λ_2**)**.

2.5.2.1 Combinatorial Properties of RGDD

The parameters of a RGDD design must satisfy the following conditions:

$$\begin{array}{ll} (i) & t-1 = m_1 m_2 \\ (ii) & r(k-2) = (m_2-1)\lambda_1 + m_2(m_1-1)\lambda_2. \end{array} \tag{2.32}$$

Later in Chapter 3, we assess the efficiency and usefulness of these designs under the A-optimality criterion by comparing the total variances of the estimators of the contrasts with lower bounds derived in Chapter 3.

We further consider the appropriateness of the designs for experiments in which we require equal variances for dual versus A and dual versus B contrast estimators, but one of the sets of contrasts is to be estimated with greater precision than the other. An A-optimal design is then not necessarily appropriate to the experimenter. We would seek a design which gives us variance balance for the contrasts corresponding to the dual versus A comparisons provided low variance can be achieved. We will show in Chapter 4 that the best design having this balance feature is a highly efficient or is sometimes A-optimal in the entire class of designs. This leads us to consider a group divisible design for the 2(n-1) treatments i0, i1(i=1,2,...,n-1) in which the dual treatments i1 and single treatments i0 are first associates(for i=1,2,...,n-1) whilst the other treatments, excluding 01, are second associates of each other. Also we want all the dual versus B contrasts to have the same variance. This suggests a design in which each of the dual treatments i1(i=1,2,...,n-1) and single treatment 01 occur the same number of times in each block. Therefore this leads us to a $RGDD(2n-2, b, k, n-1, 2, r, \lambda_1, \lambda_2)$, which was defined in Section 2.5.2.

In the next section we consider some further properties of this new class of designs.

2.5.2.2 A-matrix of RGDD:

The A-matrix of RGDD(2p,b,k,p,2,λ_1, λ_2) is as follows:

$$A = \frac{1}{k}\begin{bmatrix} b(k-1) & -r\underline{1}'_p & -r\underline{1}'_p \\ -r\underline{1}_p & F_{11} & F_{12} \\ -r\underline{1}_p & F'_{12} & F_{11} \end{bmatrix}, \tag{2.33}$$

where p=n-1, $F_{11} = \{r(k-1)+\lambda_2\}I_p - \lambda_2 J_p$ and $F_{12} = F'_{12} = (\lambda_2-\lambda_1)I_p - \lambda_2 J_p$. Also $RGDD$'s are binary designs with tr(A)=b(k-1).

2.5.2.3 Variance-Covariance Matrix:

We now consider the structure of the variance-covariance matrix of an RGDD and establish the relationship between the variance of the dual versus A and the dual versus B contrast estimators. We need the following lemma.

Lemma 2.3 *Let I be an identity matrix and J be a matrix in which all entries are 1, where both matrices have order $p \times p$. Let X and Y be two square matrices of size $q \times q$, then if X^{-1} and $(X + pY)^{-1}$ exist we have:*

$$(X \otimes I + Y \otimes J)^{-1} = X^{-1} \otimes I - (X + pY)^{-1} Y X^{-1} \otimes J; \tag{2.34}$$

where $\otimes$ is Kronecker product.

Proof: Let the inverse of $X \otimes I + Y \otimes J$ be of the form $Z \otimes I + S \otimes J$, then, on equating the product of the two matrices to an identity matrix, the result is obtained.♣

Theorem 2.3 *Let d be an RGDD($2p,b,k,p,2,\lambda_1,\lambda_2$), then the variance-covariance matrix of the BLUE's of the dual versus single treatment contrasts is:*

$$C\Omega C' = \begin{bmatrix} x_1 I_p + y J_p & (x_1 - x_2) I_p \\ (x_1 - x_2) I_p & 2(x_1 - x_2) I_p \end{bmatrix}; \tag{2.35}$$

where

$$x_1 = \frac{k\{r(k-1) + \lambda_2\}}{(r + 2p\lambda_2)\{r(k-1) + \lambda_1\}},$$

$$x_2 = \frac{k(\lambda_1 - \lambda_2)}{(r + 2p\lambda_2)\{r(k-1) + \lambda_1\}},$$

$$y = \frac{k\lambda_2}{r(r + 2p\lambda_2)}.$$

Proof: Deletion of the first row and first column from the A-matrix of any $RGDD(2p, b, k, p, 2, r, \lambda_1, \lambda_2)$, in which the rows and columns correspond to the treatments as ordered in (2.1), gives:

$$U = \frac{1}{k} \begin{bmatrix} F_{11} & F_{12} \\ F'_{12} & F_{11} \end{bmatrix}, \tag{2.36}$$

where F_{11} and F_{12} are given in (2.33). From (2.33) we have:

$$U = \frac{1}{k}\begin{bmatrix} r(k-1)+\lambda_2 & \lambda_2-\lambda_1 \\ \lambda_2-\lambda_1 & r(k-1)+\lambda_2 \end{bmatrix} \otimes I_p - \frac{\lambda_2}{k} J_2 \otimes J_p. \tag{2.37}$$

Applying Lemma 2.3 gives:

$$U^{-1} = \begin{bmatrix} x_1 I_p + yJ_p & x_2 I_p + yJ_p \\ x_2 I_p + yJ_p & x_1 I_p + yJ_p \end{bmatrix}; \tag{2.38}$$

where x_1, x_2 and y are given in (2.35). It follows from Lemma 2.2 that:

$$C\Omega C' = \begin{bmatrix} x_1 I_p + yJ_p & (x_1-x_2)I_p \\ (x_1-x_2)I_p & 2(x_1-x_2)I_p \end{bmatrix}. \tag{2.39}$$

Hence the theorem is proved.♣

Corollary 2.2 *All RGDD(2p,b,k,p,2,λ_1, λ_2)'s are PBDS design.*

Proof: The proof simply follows from (2.35) and (1.18) in Chapter 1.♣

From the variance-covariance matrix of a RGDD(2p,b,k,p,2,λ_1, λ_2), it follows that:

1. $V(\hat{\tau}_{i1} - \hat{\tau}_{01}) = x_1 + y = v_1$, say, and
2. $V(\hat{\tau}_{i1} - \hat{\tau}_{i0}) = 2(x_1 - x_2) = v_2$, say, for i=1,2,...,n-1.

It is easy to show that v_1 and v_2 can be written in terms of the parameters of an RGDD(2p,b,k,p,2,λ_1, λ_2):

$$v_1 = \frac{k}{r+2p\lambda_2}\left\{\frac{r(k-1)+\lambda_2}{r(k-1)+\lambda_1} + \frac{\lambda_2}{r}\right\},$$

$$v_2 = \frac{2k}{r(k-1)+\lambda_1}. \tag{2.40}$$

Example 2.3 *For n=4, b=3, k=5, $r = \lambda_1 = 2$ and $\lambda_2 = 1$, the following design is RGDD(6,3,5,3,2,2,2,1):*

*Block*1	01	10	11	20	21
*Block*2	01	20	21	30	31
*Block*3	01	30	31	10	11

with variance-covariance matrix for the dual versus single contrast estimators.

$$C\Omega C' = \begin{bmatrix} 0.5625 I_3 + 0.3125 J_3 & 0.5 I_3 \\ 0.5 I_3 & I_3 \end{bmatrix}.$$

For this example the average variances of the estimators of the contrast of interest given from $C\Omega C'$ in above is 0.9375. JE gives the same efficient design as the above design. Also we will show in later chapters, this design is A-optimal within the class of PBDS designs.

We now prove a further property of RGDD's, namely that they are more efficient for estimating the dual versus B contrasts than for estimating the dual versus A contrasts.

Theorem 2.4 *For any RGDD(2p,b,k,p,2,λ_1, λ_2), let v_1 and v_2 be the common variances for the dual versus B and dual versus A contrasts estimators respectively as given in (2.40), then $v_1 \leq v_2$.*

Proof: It is sufficient to show that $v_1 - v_2 \leq 0$. We know that for any RGDD(2p,b,k,p,2,λ_1, λ_2), $d = v_1 - v_2$, where v_1 and v_2 were given in (2.40). Substituting into d, we obtain:

$$d = \frac{k}{r + 2p\lambda_2}\left\{\frac{3(\lambda_1 - \lambda_2)}{r(k-1) + \lambda_1} + \frac{\lambda_2}{r} - 1\right\}. \qquad (2.41)$$

Since k and $r + 2p\lambda_2$ are positive, we consider the sign of

$$Q = \frac{3(\lambda_1 - \lambda_2)}{r(k-1) + \lambda_1} + \frac{\lambda_2}{r} - 1. \qquad (2.42)$$

If Q=0 then $v_1 = v_2$, and if $Q > 0$ then $v_1 > v_2$; otherwise $v_1 < v_2$.
On rearranging (2.42) we obtain:

$$Q = \frac{(\lambda_2 - r)\{r(k-1) + \lambda_1\} + 3r(\lambda_1 - \lambda_2)}{r\{r(k-1) + \lambda_1\}}. \qquad (2.43)$$

Since $r\{r(k-1) + \lambda_1\}$ is positive, the problem reduces to considering the sign of the numerator:

$$(\lambda_2 - r)\{r(k-1) + \lambda_1\} + 3r(\lambda_1 - \lambda_2). \qquad (2.44)$$

But the RGDD parameters, λ_1 and λ_2, are related through the equation (2.32), i.e. $r(k-2) = \lambda_1 + 2(n-2)\lambda_2$. On substituting for λ_2 from this expression into (2.44) and multiplying throughout by 2(n-2) we obtain:

$$P = -\lambda_1^2 + 2(2n-3)r\lambda_1 + r^2\{(k-1)^2 - 2n(k-1) + 3\}. \qquad (2.45)$$

Since $n > 2$ so that $2(n-2) > 0$, the sign of P is the same as that of Q.

We now find the sign of P across the range of λ_1 values, by solving the quadratic equation $P = 0$ and hence locating the values of λ_1 at which the sign of P changes. Solving $P = 0$ gives two roots: $r(2n-3-s)$ and $r(2n-3+s)$, where

$$s^2 = (2n-1-k)^2 + 2(k-3)(n-2). \tag{2.46}$$

We denote the smaller root by c=r(2n-3-s). Since in a GD design we have $\lambda_1 \leq r$, it will be sufficient to prove that $c \geq r$ for $k \geq 3$, $n > 2$ and any b. However for a GD design the values of λ_1 are restricted to $\lambda_1 \leq r$. Hence we can establish that P is always negative for a GD design by proving that $\lambda_1 \leq c$. We achieve this by proving that $c \geq r$.

We consider two cases: k=3 and $k > 3$. We do not consider $k < 3$ because there is no GD design with block size less than 2.

For k=3, we have s=2n-4 and hence c=r$\geq \lambda_1$. For $k > 3$, we can assume k=3+ℓ for $\ell > 0$. Substituting for k into s^2 we obtain $s^2 = (2n-4)^2 + \ell(\ell - 2n + 4)$. In a RGDD(2p,b,k,p,2,$\lambda_1, \lambda_2$) we have $k - 1 \leq 2p$ which implies that $\ell \leq 2n - 4$ and thus $s^2 \leq (2n-4)^2$ for $n > 2$. This implies that $s \leq 2n - 4$ and consequently $c \geq r(2n - 3 - 2n + 4) = r$. Therefore c is always not smaller than r. Hence the theorem is proved.♣

We now prove a theorem to determine which subtype of GD designs gives a more A-efficient RGDD.

Theorem 2.5 *For any RGDD(2p,b,k,p,2,λ_1, λ_2), if $k \geq 4$, then the average variance of the dual versus single contrast estimators is an increasing function of λ_2(or a decreasing function of λ_1).*

Proof: In an RGDD(2p,b,k,p,2,λ_1, λ_2), since there are n-1 dual versus A contrasts and n-1 dual versus B contrasts the average variances of these contrasts is $v = \frac{1}{2}(v_1 + v_2)$, where v_1 and v_2 are given in (2.40). Hence:

$$Q = \frac{2v}{k} = \frac{2}{r(k-1)+\lambda_1} + \frac{1}{r+2p\lambda_2}\{\frac{r(k-1)+\lambda_2}{r(k-1)+\lambda_1} + \frac{\lambda_2}{r}\}. \tag{2.47}$$

We know that $r(k-2) = \lambda_1 + 2(n-2)\lambda_2$, by property (2.32) of a RGDD. Therefore for fixed values of n, b, k, and r, Q can be regarded as a function of λ_2(or of λ_1) only. Let $Q = Q(\lambda_2)$. Suppose λ_2 is a continuous variable, then the derivative of $Q(\lambda_2)$ with respect to λ_2 is after some calculus:

$$\partial Q(\lambda_2)/\partial\lambda_2 = \frac{4(n-2)}{\{r(k-1)+\lambda_1\}^2} - \frac{2px}{(r+2p\lambda_2)^2} + \frac{y}{r+2p\lambda_2}, \tag{2.48}$$

where

$$x = \frac{r(k-1)+\lambda_2}{r(k-1)+\lambda_1} + \frac{\lambda_2}{r},$$

and

$$y = \frac{\{r(k-1)+\lambda_1\} + 2(n-2)\{r(k-1)+\lambda_2\}}{\{r(k-1)+\lambda_1\}^2} + \frac{1}{r}.$$

Then we need to find the sign of this derivative. After some algebra we can show that:

$$x = \frac{r(k-1)(r+\lambda_2)+\lambda_2(r+\lambda_1)}{r\{r(k-1)+\lambda_1\}},$$

and

$$y = \frac{\{r(k-1)+\lambda_1\}(kr+\lambda_1) + 2(n-2)r\{r(k-1)+\lambda_2\}}{r\{r(k-1)+\lambda_1\}^2}.$$

Then

$$\partial Q(\lambda_2)/\partial\lambda_2 = \frac{a+b+c}{d},$$

where

$$a = \{r(k-1)+\lambda_1\}\{kr+\lambda_1-2p(k-1)r\},$$

$$b = 2(n-2)\{r(k-1)+\lambda_2\}(r+2p\lambda_2),$$

$$c = 4(n-2)(r+2p\lambda_2)^2,$$

and

$$d = \{r(k-1)+\lambda_1\}^2(r+2p\lambda_2)^2.$$

Since d is always positive, the sign of this derivative is the same as the sign of Z=a+b+c. Since

$$r+2p\lambda_2 = r(k-1)+\lambda_1+2(\lambda_2-\lambda_1), \tag{2.49}$$

we have

$$c = 4(n-2)(r+2p\lambda_2)\{r(k-1)+\lambda_1+2(\lambda_2-\lambda_1)\}.$$

After further algebra we get:

$$c = 4(n-2)\{r(k-1)+\lambda_1\}(r+2p\lambda_2) + 8(n-2)(\lambda_2-\lambda_1)(r+2p\lambda_2). \quad (2.50)$$

Substituting from (2.49) into b, after some algebra we get

$$b + c = 4(n-2)(r+2p\lambda_2)\{r(k-1)+\lambda_1\} + 8(n-2)(\lambda_2-\lambda_1)(r+2p\lambda_2)+$$
$$2(n-2)(r+2p\lambda_2)\{r(k-1)+\lambda_2\} \quad (2.51)$$
$$= 6(n-2)(r+2p\lambda_2)\{r(k-1)+\lambda_1\} + 10(n-2)(\lambda_2-\lambda_1)(r+2p\lambda_2)$$
$$= 20(n-2)(\lambda_2-\lambda_1)^2 + \{r(k-1)+\lambda_1\}\{r(-6n+6kn-k-10)-(16n-21)\lambda_1\}.$$

Also

$$Z = 20(n-2)(\lambda_2-\lambda_1)^2 + \{r(k-1)+\lambda_1\}\{r(4kn+2k-4n-12)-(16n-22)\lambda_1\}. \quad (2.52)$$

But in a GD we have $r \geq \lambda_i (i=1,2)$, so that $-r \leq -\lambda_i (i=1,2)$. Therefore $-\lambda_1(16n-22) \geq -r(16n-22)$, which implies that:

$$Z \geq 20(n-2)(\lambda_2-\lambda_1)^2 + r(4kn-20n+2k+10)\{r(k-1)+\lambda_1\}. \quad (2.53)$$

The first term in the RHS of the above inequality is always positive. Also r and $r(k-1)+\lambda_1$ are both positive, therefore if 4kn-20n+2k+10 is positive then $\partial Q(\lambda_2)/\partial\lambda_2$ will be positive. For $k > 4$, this last expression is always positive, i.e. the average variance of the contrast estimators is an increasing function in terms of λ_2. This establishes the proof for $k > 4$. If k=4, then we have $2(n-2)\lambda_2 = 2r - \lambda_1$ and

$$Z = 20(n-2)(\lambda_2-\lambda_1)^2 + (3r+\lambda_1)\{r(12n-4)-(16n-22)\lambda_1\}.$$

Multiplying Z by n-2 and substituting for λ_2, from here we will get

$$z = 5\{2r-(2n-3)\lambda_1\}^2 + (n-2)(3r+\lambda_1)\{r(12n-4)-(16n-22)\lambda_1\}, \quad (2.54)$$

where z=(n-2)Z. After some manipolation we get

$$z = u\lambda_1^2 - vr\lambda_1 + wr^2, \quad (2.55)$$

where

$$u = 4n^2 - 6n + 1,$$

$$v = 36n^2 - 94n + 64,$$

and

$$w = 36n^2 - 84n + 44.$$

But we know that $\lambda_1 \leq r$, and also for $n \geq 2$, v is nonnegative, this implies that $vr\lambda_1 \leq vr^2$. Therefore $-vr\lambda_1 \geq -vr^2$, i.e. $z \geq u\lambda_1^2 - vr^2 + wr^2 = u\lambda_1^2 + (w-v)r^2$. For $n \geq 2$, u and $w - u = 10(n-2)$ are both nonnegative. Hence $z \geq 0$ and consequently $\partial Q(\lambda_2)/\lambda_2 \geq 0$. This establishes the proof of the theorem.♣

Consequnces of Theorem 2.5 are Corollaries 2.3 and 2.4. It should be noted here that for k=3 the problem remains unsolved. Obviously k can never be less than 3 in the RGDD.

Corollary 2.3 *Singular Group Divisible designs, when they exist, are the most efficient RGDD under the A-criterion for the dual versus single treatment problem.*

Proof: For singular group divisible designs $\lambda_1 = r$, whereas $\lambda_1 < r$ for other two types. The result follows from Theorem 2.5.♣

Note : Singular GD designs have full efficiency for comparing dual versus A, as is clear from (2.40) since for these type of designs $v_2 = 2/r$ which is the same as the variance obtained from a randomized block design($\sigma^2 = 1$).

Corollary 2.4 *Regular GD designs are more A-efficient than semi-regular GD designs.*

Proof: For fixed values of n, b and k if there exists a semi-regular and a regular GD, then by (2.29), λ_2 for a regular GD is less than λ_2 for a semi-regular GD. In other words λ_1 for a regular GD is greater than λ_1 for a semi-regular GD. Then by Theorem 2.5 the corollary is proved.♣

Discussion 2.1 *For particular values of n, b and k we sometimes have a choice of GD designs with different parameter values λ_1, λ_2 to use in the RGDD construction. For such cases we recommend that the experimenter selects the GD design with the biggest λ_1 value. For example, for n=5, k=5 and b=12 the experimenter has two choices for selecting a GD for 8 treatments in 12 blocks each of size 4. The first choice is a singular GD (Clatworthy,1973,S7,p 103) which leads to a RGDD with average variance for the contrast estimators of 0.60. As a second* *choice consider a semi-regular GD (Clatworthy, 1973, SR37, p 138) which gives the average variance for the same set of the contrast estimators as 0.66. However, there are sizes of experiment for which there is only one sensible choice of GD design to use in the construction. An example is parameter values n=5, b=8 and k=5 for which only one design, SR36 is listed in the Clatworthy's catalogue.*

2.5.2.4 Relationship Between GD Designs and RGDD:

We now show how the variances for the RGDD can be obtained simply from the variances of the GD designs. This enables the variances to be derived directly from the tabulated information in Clatworthy(1973).

Theorem 2.6 *Let* u_1 *and* E_1 *be the variance and efficiency of the first associate of a* $GD(2n-2, b, k-1, n-1, 2, r, \lambda_1, \lambda_1)$ *respectively. Let* v_1 *and* v_2 *be the variances of the dual versus B and dual versus A contrasts estimators respectively, then*

$$v_1 = \frac{k}{r(r+2p\lambda_2)}\left\{\frac{r(k-1)E_1 - \lambda_1 + \lambda_2 + r}{1+(k-1)E_1} + \lambda_2\right\}. \tag{2.56}$$

and

$$v_2 = \frac{2k}{r + r(k-1)E_1}.$$

Proof: For a $GD(2n-2, b, k-1, n-1, 2, r, \lambda_1, \lambda_2)$, from (2.30) and (2.31):

$$u_1 = \frac{2(k-1)}{r(k-2)+\lambda_1}, \tag{2.57}$$

and

$$E_1^{-1} = \frac{r(k-1)}{r(k-2)+\lambda_1}.$$

We can show, by algebraic manipulation, that the expressions in (2.40) can be written in terms of E_1 as

$$v_1 = \frac{k}{r(r+2p\lambda_2)}\left\{\frac{r(k-1)E_1 - \lambda_1 + \lambda_2 + r}{1+(k-1)E_1} + \lambda_2\right\}, \tag{2.58}$$

and

$$v_2 = \frac{2k}{r + r(k-1)E_1}.$$

Hence the theorem is proved.♣

Note: Since dual treatments i1 and single treatments i0 for i=1,2,...,n-1, are replicated the same number of times, we can define $E_2^* = 2/(rv_2)$, as the efficiency factor of the RGDD for estimating the dual versus A contrasts. In terms of E_1,

$$E_2^* = \frac{1 + (k-1)E_1}{k}.$$

For $\lambda_1 = r$, we can easily show that $E_2^* = E_1 = 1$.

Example 2.4 *From Example 2.3 on page 50, on substituting the parameter values into (2.56) we obtain* $v_1 = 0.875$, $v_2 = 1.0$, *and hence* $E_2^* = 1$. *Thus the design has full efficiency for dual versus A comparisons and lower precision on the dual versus B contrasts.*

Discussion 2.2 *As we will show in Chapter 3, all the reinforced singular group divisible designs are highly efficient relative to derived bounds. But for reinforced regular and semi-regular group divisible designs this may not be true. But one benefit of considering optimal designs within the RGDD class is that their construction is very simple since one may appeal to the vast literature on GD designs. This is an appreciable advantage over other PBDS designs, which have a less straightforward construction but, in some case, are more efficient than RGDD designs. These will be studied in Chapter 4.*

2.5.2.5 Availability of Designs in the RGDD Class:

GD designs are widely available in the literature. The largest source of designs is the catalogue of Clatworthy(1973). Further designs have been given, for example in Freeman(1976a) and John and Turner(1977). One advantage of RGDD's is that they are easily constructed from available GD designs.

1. For $k > 3$ the best design available is chosen from Clatworthy by taking a singular GD design if available and otherwise taking the best of the remaining categories of GD designs(guided by Theorem 2.5).

2. For k=3 many of the designs listed in Clatworthy give RGDD designs which will have high variances for comparing i0 with i1(by the construction method given in Section 2.5.2). However, for the parameter ranges in Clatworthy it was found that we can obtain a more suitable GD design by forcing $\lambda_2 = 0$ and obtaining the value of λ_1 from the expression

$r(k-2) = \lambda_1 + 2(n-2)\lambda_2$. It was straightforward to write down the designs in these cases by taking treatment combinations i0 and i1 in the same block and accommodating treatment combination 01 in each block of the design. The resulting RGDD designs had much smaller average variances than those derived directly from the catalogue.

Example 2.5 *For n=3, b=4 and k=3, the only available design which can be constructed from the catalogue of Clatworthy(1973,p141) is reinforced SR1 with* $\lambda_1 = 0$*, which is the RGDD(5,4,2,2,0,1) given below:*

*Block*1	01	10	21
*Block*2	01	10	20
*Block*3	01	11	21
*Block*4	01	11	20

with the discrepancy 34.58%*(see Definition 3.2 on page 73). However the design*

*Block*1	01	10	11
*Block*2	01	10	11
*Block*3	01	20	21
*Block*4	01	20	21

gives discrepancy 13.331%*. Note that although the GD design employed here, namely*

*Block*1	10	11
*Block*2	10	11
*Block*3	20	21
*Block*4	20	21

with $\lambda_1 = 2$ *and* $\lambda_2 = 0$ *is a disconnected design, the RGDD obtained is connected. This is a substantial improvement on the best RGDD based on the appropriate GD design from Clatworthy's catalogue.*

An assessment of the performance of the RGDD's obtained as in 1 and 2, is made in Chapter 3 by comparing their average variance for the contrast of interest with a lower bound.

2.6 Class of BDSD:

In the remainder of this chapter we look at tighter requirements on the variance-covariance matrix in an attempt to eliminate correlations between some or all of the contrast estimators. We investigate if it is possible to find efficient designs satisfying these requirements.

From Definition 1.4 in Chapter 1, a design is said to be a Balanced Dual versus Single treatment Design(BDSD), if $V(C\hat{\underline{\tau}}) = (\alpha - \rho)I_{2\ell} + \rho J_{2\ell}(\alpha \neq \rho)$, where $\ell = (m-1)(n-1)$. This design gives equal precision for all the estimators of the dual versus single treatment contrasts. Also it gives equal correlations between any two individual contrast estimators. Now we prove that for a general $n \times m$ factorial experiment, a connected BDSD exists if and only if n=2 or m=2.

Theorem 2.7 *An $n \times m$ BDSD connected(block or row-column) design exists if and only if m=2 or n=2.*

Proof: Let $C\hat{\underline{\tau}}$ denote the BLUE of $C\underline{\tau}$, where $\underline{\tau}$ is given in (1.4). Then we have $V(C\hat{\underline{\tau}}) = C\Omega C'$; where C was defined in (1.12) and Ω is a g-inverse of the A-matrix defined in Chapter 1. We know from matrix algebra theory that $R(XY) \leq \min\{R(X), R(Y)\}$, where R(X) stands for the rank of matrix X, and min(a,b) stands for the minimum of a and b. Since $A\Omega A = A$ and the design is connected, $R(\Omega) \geq mn - 2$(ref Rao,1973;p 25). Also

$$R(C) = R(C'C) = \min\{2\ell, mn - 2\}, \tag{2.59}$$

where ℓ=(m-1)(n-1), and $R(C\Omega C') \leq \min\{R(\Omega), R(C)\}$. Therefore

$$R(C\Omega C') \leq \min\{2\ell, mn - 2\}. \tag{2.60}$$

If the design is a BDSD then from Definition 1.4, $V(C\hat{\underline{\tau}}) = (\alpha-\rho)I_{2\ell}+\rho J_{2\ell}(\rho \neq 0)$, and this variance-covariance matrix is of rank 2ℓ if $\rho \neq \alpha$. Hence we must have $2\ell = \min\{2\ell, mn-2\}$, i.e. $2\ell \leq mn - 2$. It follows that $(m-2)(n-2) \leq 0$. But neither n nor m can be less than 2. Therefore $(n-2)(m-2) = 0$, which is valid if and only if m=2 or n=2. Hence the theorem is proved.♣

2.6.1 A-matrix of a BDSD:

The following theorem specifies the A-matrix of a BDSD:

Theorem 2.8 *Any $n \times 2$ CFBD(00) is a BDSD if and only if its A-matrix has the following structure:*

$$A = \frac{1}{\alpha}\begin{bmatrix} p & \underline{0}'_p & -\underline{1}'_p \\ \underline{0}_p & I_p & -I_p \\ -\underline{1}_p & -I_p & 2I_p \end{bmatrix}, \tag{2.61}$$

where p=n-1 and α is a design dependent constant.

Proof:

(i) To prove necessity of the A-matrix structure: Assume the design is a BDSD, then $C\Omega C' = (\alpha - \rho)I_{2p} + \rho J_{2p}$. From Theorem 2.1 we have $U = (V')^{-1}(C\Omega C')^{-1}V^{-1} = (VC\Omega C'V')^{-1}$, where U and V are defined in (2.14) and (2.18) respectively. Substituting for U in terms of the elements of the A-matrix from (2.14) and for $C\Omega C'$ from above, we obtain:

$$U = \frac{1}{\alpha - \rho}\begin{bmatrix} I_p - (\rho/d)J_p & -I_p + 2(\rho/d)J_p \\ -I_p + 2(\rho/d)J_p & 2I_p - 4(\rho/d)J_p \end{bmatrix}, \tag{2.62}$$

where $d = \alpha + (2n-3)\rho$.

Since none of the off-diagonal elements of the A-matrix or of matrix U can be positive, the only valid form for U is when $\rho = 0$. In this case:

$$U = \frac{1}{\alpha}\begin{bmatrix} I_p & -I_p \\ -I_p & 2I_p \end{bmatrix}. \tag{2.63}$$

By Lemma.2.1, $\underline{a}_{12} = -U\underline{1}_{t-1}$, $\underline{a}'_{12}$ is the transpose of $\underline{a}_{12}$ and $a_{11} = -\underline{a}'_{12}\underline{1}$. Therefore we have:

$$A = \frac{1}{\alpha}\begin{bmatrix} p & \underline{0}'_p & -\underline{1}'_p \\ \underline{0}_p & I_p & -I_p \\ -\underline{1}_p & -I_p & 2I_p \end{bmatrix}. \tag{2.64}$$

(ii) To prove sufficiency of the structure:

If the A-matrix of a design is of the form (2.61), then by Lemma 2.2 a g-inverse of the A-matrix is:

$$\Omega = \alpha\begin{bmatrix} 0 & \underline{0}'_p & \underline{0}'_p \\ \underline{0}_p & 2I_p & I_p \\ \underline{0}_p & I_p & I_p \end{bmatrix}. \tag{2.65}$$

Hence

$$C\Omega C' = \alpha \begin{bmatrix} I_p & 0_p \\ 0_p & I_p \end{bmatrix}, \tag{2.66}$$

and the design is BDSD.♣

In the following section we specify some conditions for a block design to be a BDSD.

2.6.2 Combinatorial Properties of a BDSD:

By using the notation on page 44, the following theorem gives combinatorial restrictions on a design which is a BDSD.

Theorem 2.9 *For a block design to be a BDSD, the following conditions must be satisfied:*

1.

$$\sum_{j=1}^{b} n_{Aij}(k - n_{Aij}) = \frac{1}{2}\sum_{j=1}^{b} n_{Dij}(k - n_{Dij}) = \sum_{j=1}^{b} n_{Aij}n_{Dij} = \sum_{j=1}^{b} n_{Bj}n_{Dij} =$$

$$\frac{1}{p}\sum_{j=1}^{b} n_{Bj}(k - n_{Bj}) = \frac{k}{\alpha}, \tag{2.67}$$

2.

$$\sum_{j=1}^{b} n_{Bj}n_{Aij} = \sum_{j=1}^{b} n_{Aij}n_{Alj} = \sum_{j=1}^{b} n_{Aij}n_{Dlj} = \sum_{j=1}^{b} n_{Dij}n_{Dlj} = 0,$$

for i=1,2,...,p and $i \neq l$.

Proof: By Theorem 2.8 the structure of the A-matrix necessary for a block design to be a BDSD is as shown in (2.61). Therefore:

$$r_{Ai} - \frac{1}{k}\sum_{j=1}^{b} n_{Aij}^2 = \frac{1}{2}(r_{Di} - \frac{1}{k}\sum_{j=1}^{b} n_{Dij}^2) =$$

$$\frac{1}{p}(r_B - \frac{1}{k}\sum_{j=1}^{b} n_{Bj}^2) = \frac{1}{k}\sum_{j=1}^{b} n_{Aij}n_{Dij} = \frac{1}{k}\sum_{j=1}^{b} n_{Bj}n_{Dij}.$$

Also from the A-matrix of the design given in (2.61) we have:

$$p\sum_{j=1}^{b} n_{Aij}(k - n_{Aij}) = \frac{p}{2}\sum_{j=1}^{b} n_{Dij}(k - n_{Dij}) = \sum_{j=1}^{b} n_{Bj}(k - n_{Bj}) = \frac{pk}{\alpha},$$

which establishes the necessity of the first condition. Establishing the second condition as necessary is straightforward from the structure of the A-matrix of the BDSD.♣

Corollary 2.5 *Suppose design d is a BDSD, then in each block of d we have present either the pair of treatment combinations (01,i1) or (i0,i1); for some i=1,2,...,p.*

Proof: The proof follows from condition 2 of Theorem 2.9.♣

Now we are in a position to characterize A-optimal designs within the BDSD class in the following section.

2.6.3 A-optimal Designs within the BDSD Class:

Before giving the theorem which specifies the A-optimal designs within the BDSD class for parameter values n, b and k, a lemma is needed.

Lemma 2.4 *Let x and y be positive real numbers, such that $x \leq y$, then for fixed values for y, f(x)=x(y-x) has a unique maximum value at the point x=y/2. If x and y are assumed to be integers*

1. *if $y = 2y'$ is even, then $x = y'$ maximizes f(x);*
2. *if y is odd, then $x = y'$ and $y'+1$ will maximize f(x) with the same maximum value $y'(y'+1)$.*

Proof: If x is assumed to be a real number, then $\partial f(x)/\partial x = y - 2x$, and $y - 2x = 0$ gives $x_0 = y/2$ as the only critical point of f(x) which maximizes it. Assume y is an even number, i.e. y=2y′, then $x_0 = y'$ is an integer value. f(x) is an increasing function on the interval $x \in [0, y/2]$ and a decreasing function over $x \in [y/2, y]$. In other words f(x) is a concave function(see Roberts and Varberg,1973,page2). Therefore if y is not even, i.e. $y = 2y' + 1$, where y' is an integer, then it can be shown that $f(y'+1) = f(y')$. Hence the lemma is proved.♣

Now we are in a position to establish conditions under which a BDSD is A-optimal within the class of BDSD for the parameters n, b and k.

Theorem 2.10 *A BDSD is A-optimal among all the BDSD's if the following conditions are satisfied:*

1. *for each block j which contains i0,* $\mid n_{Aij} - k/2 \mid \leq 1$,
2. *for each block j which contains i1,* $\mid n_{Dij} - k/2 \mid \leq 1$,
3. *for each block j which contains 01,* $\mid n_{Bj} - k/2 \mid \leq 1$,

4. *for each block j which contains i0 and i1,* $| n_{Aij} - n_{Dij} | \leq 1$,

5. *for each block j which contains i1 and 01,* $| n_{Dij} - n_{Bj} | \leq 1$.

Proof: If the design is a BDSD, then we have $tr(C\Omega C') = 2p\alpha$, and the design is A-optimal if it minimizes α, since p(=n-1) is fixed. Minimizing α subject to the conditions in (2.67) and applying Lemma 2.4 and Corollary 2.5, gives conditions 1 to 5.♣

The following example illustrates the structure established as sufficient for a design to be a BDSD. It also shows that a BDSD is not necessarily efficient.

Example 2.6 *For n=3, b=4 and k=3 we have:*

*Block*1	01	11	11
*Block*2	01	21	21
*Block*3	10	11	11
*Block*4	20	21	21

which gives:

$$A = \begin{bmatrix} 1.33 & \underline{0}_2' & -0.67\underline{1}_2' \\ \underline{0}_2 & 0.67I_2 & -0.67I_2 \\ -0.67\underline{1}_2 & -0.67I_2 & 1.33I_2 \end{bmatrix}.$$

Hence by Theorem 2.8 the design is a BDSD. Also $V(C\hat{\underline{\tau}}) = C\Omega C' = 1.5I_4$, $\alpha = 1.5$, *and* $tr(C\Omega C') = 6$. *However the design is not highly efficient since the following design which is not a BDSD has* $tr(C\Omega C') = 3.84$.

*Block*1	01	20	21
*Block*2	01	10	11
*Block*3	01	11	21
*Block*4	10	20	11

Now we can specify the layout of a BDSD to be A-optimal among all possible designs within the class of BDSD.

2.6.4 Layout of A-optimal Designs within the BDSD Class:

The general layout of an A-optimal BDSD depends on the block size k and can be deduced from Corollary 2.5 and Theorem 2.10. The layout of designs with odd block size differs from those with even block size as follows:

1. When k is even, Figure 2.1 shows the layout of a BDSD which is A-optimal.

Units →

Blocks ↓	1	2	3	...	$\frac{k}{2}$	$\frac{k}{2}+1$	$\frac{k}{2}+2$	...	k
1	10	10	10	...	10	11	11	...	11
2	20	20	20	...	20	21	21	...	21
3	30	30	30	...	30	31	31	...	31
.	..	..	..	...	..	..	..	...	..
.	..	..	..	...	..	..	..	...	..
p	p0	p0	p0	...	p0	p1	p1	...	p1
p+1	01	01	01	...	01	11	11	...	11
p+2	01	01	01	...	01	21	21	...	21
.	..	..	..	...	..	..	..	...	..
.	..	..	..	...	..	..	..	...	..
2p	01	01	01	...	01	p1	p1	...	p1

Figure 2.1: Layout of A-optimal BDSD when k is even.

Example 2.7 *When n=3, k=2 and b=4:*

*Block*1	10	11
*Block*2	20	21
*Block*3	01	11
*Block*4	01	21

For this case:

$$A = \begin{bmatrix} 1 & \underline{0}_2' & -0.5\underline{1}_2' \\ \underline{0}_2 & 0.5I_2 & -0.5I_2 \\ -0.5\underline{1}_2 & -0.5I_2 & I_2 \end{bmatrix}$$

and $V(C\hat{\underline{\tau}}) = (C\Omega C') = 2I_4$, *which gives* $\alpha = 2$ *and design is BDSD.*

2. When <u>k is odd</u>, then the layout of the A-optimal design is given in Figure 2.2, where $f = [k/2]$ and [.] denotes the *"integer part of."*.

Units →

		1	2	3	...	f	f+1	f+2	...	k
	1	10	10	10	...	10	11	11	...	11
	2	20	20	20	...	20	21	21	...	21
	3	30	30	30	...	30	31	31	...	31
	.	..	..	..	...	..	..	..	...	..
Blocks ↓	.	..	..	..	...	..	..	..	...	..
	p	p0	p0	p0	...	p0	p1	p1	...	p1
	p+1	01	01	01	...	01	11	11	...	11
	p+2	01	01	01	...	01	21	21	...	21
	.	..	..	..	...	..	..	..	...	..
	.	..	..	..	...	..	..	..	...	..
	2p	01	01	01	...	01	p1	p1	...	p1

Figure 2.2: Layout of A-optimal BDSD when k is odd.

2.6.5 Advantages and Disadvantages of A-optimal BDSD:

In this section we note some advantages and disadvantages of an A-optimal BDSD.

The main advantages of the designs are that they are:

1. Easy to construct.

2. Optimal in the class of BDSD.

3. Useful when k=2, since then the number of replications of the treatments in each block is not impractically large.

However, there are disadvantages of these designs:

1. They exist only for $b \equiv 0 mod(2n-2)$.

2. For $k > 3$, the number of replications of each of the treatments 01, 11, 21, ..., p1 is large, being more than one in every block.

3. An A-optimal BDSD is not A-optimal in the entire class of designs except for a few parameter values, mainly when k=2.

2.7 Other Forms of Designs:

As we have shown in the previous section, that although BDSD's have the feature of giving equal precision for both dual versus A and dual versus B contrast estimators, their efficiencies are not necessarily high. We now consider two further types of designs with variance-covariance matrix having particular features which are desirable, provided efficient designs can be found with the features.

1. $C\Omega C'$=F, where F is a diagonal matix so that the estimators of the contrasts of interest are uncorrelated. For this type of designs, based on Definition 2.1, we have:

$$M = (C\Omega C')^{-1} = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix}, \tag{2.68}$$

where the E_i's(i=1,2) are $p \times p$ diagonal matrices with positive diagonal elements and M is the information matrix of the estimators of the contrasts of interest. Let the A-matrix of the design be partitioned as in (2.11), on page 40, then by applying Theorem 2.1, we obtain

$$\begin{bmatrix} A_{22} + A_{23} + A'_{23} + A_{33} & -A_{22} - A'_{23} \\ -A_{22} - A_{23} & A_{22} \end{bmatrix} = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix}. \tag{2.69}$$

From this we obtain $A_{22} = E_2$, $A_{23} = A'_{23} = -E_2$ and $A_{33} = E_1 + E_2$. Other parts of the A-matrix can be obtained by applying the facts that the A-matrix is symmetrical and has the sum of its rows equal to zero. Therefore for a design with property 1, we have:

$$A = \begin{bmatrix} a_{11} & \underline{0}' & -\underline{1}'E_1 \\ \underline{0} & E_2 & -E_2 \\ -E_1\underline{1} & -E_2 & E_1 + E_2 \end{bmatrix}. \tag{2.70}$$

By using the notation on page 44, the following combinatorial restrictions apply to this type of design:

(a)

$$\sum_{j=1}^{b} n_{Bj}n_{Aij} = \sum_{j=1}^{b} n_{Aij}n_{Alj} = \sum_{j=1}^{b} n_{Aij}n_{Dlj} = \sum_{j=1}^{b} n_{Dij}n_{Dlj} = 0$$

for $i \neq l$=1,2,...,n-1.

(b)

$$\sum_{j=1}^{b} n_{Aij}(k - n_{Aij}) = \sum_{j=1}^{b} n_{Aij}n_{Dij}. \quad (2.71)$$

From these properties we deduce that in each block we have present either the pair of treatment combinations (01,i1) or (i0,i1); for some i=1,2,...,n-1. Major disadvantages of this type of designs are:

(a) Number of blocks increases as n is increased, since the minimum number of required blocks is b=2(n-1) in order to accommodate all the treatment combinations involved in the design.

(b) For $k > 2$, some of the treatment combinations occur more than once in a block whilst other treatment combinations in the same group do not occur at all in the block. In other words the design is non-binary even for k=3.

(c) The efficiencies of designs in this class as, follows from the work of Chapter 4, are low.

Example 2.8 *For n=3, b=4 and k=4, the most efficient design of this type generated by applying JE is:*

*Block*1	01	01	01	11
*Block*2	10	10	11	11
*Block*3	01	01	21	21
*Block*4	20	21	21	21

This design is not binary, for example in block 1 treatment combination 11 occurs twice but combinatorial restrictions dictate that treatment combination 21 cannot be present in this block.

For this design we have:

$$C\Omega C' = \begin{bmatrix} 1.33 & 0.00 & 0.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 \\ 0.00 & 0.00 & 1.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 1.33 \end{bmatrix}$$

in which $tr(C\Omega C') = 4.67$. *For this example the most efficient design which could be generated by the algorithm without restricting to the designs with* *property 1 has* $tr(C\Omega C') = 2.639$ *and the deficiency of the first design is clear from here.*

2. In view of the poor performance of the designs with property 1, we consider relaxing the requirement to allow correlations between any two contrast estimators for comparing 01 with any treatment combination belonging to group D and between any two contrast estimators corresponding to dual versus A comparisons. In other words we consider designs with the property:

$$C\Omega C' = \begin{bmatrix} aI_p + bJ_p & 0 \\ 0 & cI_p + dJ_p \end{bmatrix}, \tag{2.72}$$

where p=n-1.

This type of design is a special case of the wider class of PBDS designs. However we will show in Chapter 4 that the designs which have such a restricted structure for the variance-covariance matrix again are not the most efficient in the sense of not having the smallest average variance of the estimators of the contrast of interest.

Conclusions: Various types of designs based on features of the variance-covariance matrix for the estimators of the contrast of interest have been considered in this chapter. We conclude that restricting to each type of design reduces efficiency except for the general class of PBDS designs. Therefore for $n \times 2$ experiments we confine ourselves within the PBDS class of designs. As was pointed out in Chapter 1, we have no guarantee that all the A-optimal designs belong to this class for all parameter values. However, as we shall establish in Chapter 4, it contains a wide range of highly efficient designs and some overall A-optimal designs.

In the next chapter we give bounds to assess the performance of the designs.

Chapter 3

Bounds for $n \times m$ Experiments

3.1 Introduction:

In Chapter 2 we introduced the class of RGDD, which is a subclass of PBDS designs, and considered properties of this subclass including the characterization of efficient designs. The question now considered is how the performance of the best designs within this class compares with the best in the entire class of designs for particular parameter values, n, b and k. In the present chapter, we give two different lower bounds on the total of the variances of the contrast estimators for the dual treatments versus single treatment comparisons in a general $n \times m$ censored factorial experiments. We establish which bound is the tighter for different parameter ranges, and use the bounds to assess the performance of designs such as RGDD designs.

3.2 Bound $1(b_1)$:

In the following we give theorems and lemmas which lead us to the first bound. The main idea is developed from the result of Wu(1980). Majumdar(1986) has used a similar approach to establish A-optimal designs for comparing a set of test treatments with a set of control treatments. Following these ideas we were able to establish only a few A-optimal designs for our problem, due to the nature of the contrasts of interest. Nevertheless it leads us to find a tight bound b_1 for a specific range of parameter values.

Lemma 3.1 *For any connected(block or row-column) design with replication matrix r^{δ} and any contrast matrix C,*

$$tr(C\Omega C') \geq tr(Cr^{-\delta}C'), \tag{3.1}$$

where Ω is a g-inverse of the A-matrix of the design and

$$r^{\delta} = diag(r_1, r_2, \ldots, r_t),$$

where r_i gives the replication of the ith *treatment in the entire design and $r^{-\delta}$ is the inverse of r^{δ}.*

Proof: Applying Wu(1980,Theorem 3), there exists a g-inverse Ω, such that $\Omega - r^{-\delta}$ is non-negative definite(n.n.d.). Hence

$$0 \leq tr\left\{C(\Omega - r^{-\delta})C'\right\} = tr(C\Omega C') - tr(Cr^{-\delta}C'), \tag{3.2}$$

and the lemma follows.♣

The following notation is needed to establish corollaries which lead to bound b_1.

Notation: In an $n \times m$ CFBD(00), let $A = \{i0;\ i = 1, 2, \ldots, n-1\}$, $B = \{0j;\ j = 1, 2, \ldots, m-1\}$ and $D = \{ij;\ i = 1, 2, \ldots, n-1,\ j = 1, 2, \ldots, m-1\}$. Let n_{Ail}, n_{Bjl} and n_{Dijl} denote the respective number of times that the treatment combinations i0, 0j and ij(belonging to sets A, B and D respectively) occur in block l, for $l = 1, 2, \ldots, b$, $i = 1, 2, \ldots, n-1$ and $j = 1, 2, \ldots, m-1$. Then $r_{Ai} = \sum_{l=1}^{b} n_{Ail}$, $r_{Bj} = \sum_{l=1}^{b} n_{Bjl}$ and $r_{Dij} = \sum_{l=1}^{b} n_{Dijl}$ denote the respective replications of treatment combinations i0, 0j and ij belonging to sets A, B and D in the entire design. Also let $r^A = diag(r_{Ai})$, $r^B = diag(r_{Bj})$ and $r^D = diag(r_{Dij})$ denote the diagonal matrix of the replications for treatment combinations belonging to sets A, B and D respectively. Then

$$r^{\delta} = \begin{bmatrix} r^B & 0 & 0 \\ 0 & r^A & 0 \\ 0 & 0 & r^D \end{bmatrix}, \tag{3.3}$$

denotes the replication matrix of an $n \times m$ CFBD(00).

Immediate consequences of using Lemma 3.1 in an $n \times m$ CFBD(00) experiment are the following corollaries.

Corollary 3.1 *For any $n \times m$ CFBD(00) design d*

$$tr(C\Omega C') \geq tr(Cr^{-\delta}C') = p\sum_{j=1}^{q}\frac{1}{r_{Bj}} + q\sum_{i=1}^{p}\frac{1}{r_{Ai}} + 2\sum_{i=1}^{p}\sum_{j=1}^{q}\frac{1}{r_{Dij}}, \tag{3.4}$$

where C is given in (1.12) on page 5.

Proof: By applying Lemma 3.1 we have: $tr(C\Omega C') \geq tr(Cr^{-\delta}C')$. But $tr(Cr^{-\delta}C') = tr(C'Cr^{-\delta})$. It can be shown that:

$$C'C = \begin{bmatrix} pI_q & o_{q\times p} & -\underline{1}'_p \otimes I_q \\ o_{p\times q} & qI_p & -I_p \otimes \underline{1}'_q \\ -\underline{1}_p \otimes I_q & -I_p \otimes \underline{1}_q & 2I_l \end{bmatrix}, \tag{3.5}$$

where p=n-1, q=m-1 and l=pq.

Therefore

$$tr(Cr^{-\delta}C') = ptr(r^{-B}) + qtr(r^{-A}) + 2tr(r^{-D}).$$

The proof follows from here.♣

The following corollary characterizes the designs which achieve the bound in Corollary 3.1(cf Majumdar,1986).

Corollary 3.2 *If d is an $n \times m$ CFBD(00) design, such that $N'r^{-\delta}C' = 0$, then*

$$tr(C\Omega C') = tr(Cr^{-\delta}C') = p\sum_{j=1}^{q}\frac{1}{r_{Bj}} + q\sum_{i=1}^{p}\frac{1}{r_{Ai}} + 2\sum_{i=1}^{p}\sum_{j=1}^{q}\frac{1}{r_{Dij}}, \tag{3.6}$$

where C is the dual versus single contrast matrix given in (1.12) on page 5 and N is the incidence matrix of the design.

Proof: Since $N'r^{-\delta}C' = 0$, it follows that

$$Ar^{-\delta}C' = (r^{\delta} - 1/kNN')r^{-\delta}C' = C' - 1/kNN'r^{-\delta}C' = C'. \tag{3.7}$$

On premultiplying by $C\Omega$ and using the estimability condition $C\Omega A = C$, we obtain:

$$C\Omega C' = C\Omega Ar^{-\delta}C' = Cr^{-\delta}C'. \tag{3.8}$$

Thus $tr(C\Omega C') = tr(Cr^{-\delta}C')$, and the result follows from Corollary 3.1.♣

Note: Corollary 3.2 gives a sufficient condition for an A-optimal design. It is straightforward to apply the same argument to the convex function Ψ of Kiefer(1975) to establish that the condition in Corollary 3.2 is sufficient for a design to be universally optimal(see Majumdar,1986,Theorem 3.1). However, it is an unfruitful means of obtaining designs for our problem, because the condition is only satisfied for sparse and large values of k(for m=n=3, k=8,16,24,... and for n=3 and m=9, k=28,56,...). This point will be considered further in Chapter 5. However Corollary 3.2 is useful for establishing a bound in conjunction with the following lemma.

Lemma 3.2 *Let r_i(i=1,2,...,L) be L integer values and* $\sum_{i=1}^{L} r_i = r$ *be regarded as fixed and such that* $r \geq L$. *Also let* $\bar{r} = [r/L]$, *where* [.] *means* "integer part of .", *then*

$$\sum_{i=1}^{L} \frac{1}{r_i} \geq \frac{2L\bar{r} + L - r}{\bar{r}(\bar{r}+1)}. \tag{3.9}$$

Proof: Since $f(x) = 1/x$ is a convex function, then by Marshall and Olkin(1979 ,p3), the values of r_i which minimize $\sum 1/r_i$ subject to the condition $\sum r_i = fixed$, are the values which minimize $\sum r_i^2$ subject to the same constraint. By Cheng and Wu(1980, Lemma 2.3) the minimum is obtained when r_i's are as close as possible, i.e. if:

$$r_i = \begin{cases} \bar{r}+1 & \text{if } i = 1, 2, \ldots, r - L\bar{r} \\ \bar{r} & \text{if } i = r - L\bar{r} + 1, \ldots, L \end{cases} \tag{3.10}$$

Substituting these values for $r_i(i = 1, 2, \ldots, L)$ into $\sum_{i=1}^{L} r_i^{-1}$ the required expression is obtained.♣

Theorem 3.1 *In an* $n \times m$ *CFBD(00) design, let* $T_B = \sum_{i=1}^{q} r_{Bi}$, $T_A = \sum_{i=1}^{p} r_{Ai}$ *and* $T_D = \sum_{i=1}^{p}\sum_{j=1}^{q} r_{Dij}$ *be regarded as fixed, such that* $T_B \geq q$, $T_A \geq p$, $T_D \geq pq$ *and* $T_A + T_D \leq bk - q$. *Also let* $\bar{r}_A = [T_A/p]$, $\bar{r}_B = [T_B/q]$ *and* $\bar{r}_D = [T_D/pq]$, *then*

$$tr(Cr^{-\delta}C') \geq p\left\{\frac{2q\bar{r}_B + q - T_B}{\bar{r}_B(\bar{r}_B+1)}\right\} + q\left\{\frac{2p\bar{r}_A + p - T_A}{\bar{r}_A(\bar{r}_A+1)}\right\} + 2\left\{\frac{2pq\bar{r}_D + pq - T_D}{\bar{r}_D(\bar{r}_D+1)}\right\}. \tag{3.11}$$

Proof: Follows from the fact that if T_A and T_D are regarded as fixed, then $T_B = bk - T_A - T_D$ is fixed, and the minimization of $tr(Cr^{-\delta}C')$ follows from Lemma 3.2.♣

The minimum value for $tr(Cr^{-\delta}C')$ in Theorem 3.1 is a function in terms of T_A and T_D only since p and q are fixed and $\bar{r}_A$, $\bar{r}_B$ and $\bar{r}_D$ are functions in terms of T_A, T_B and T_D respectively. Therefore let

$$F(T_A,T_D) = p\left\{\frac{2q\bar{r}_B + q - T_B}{\bar{r}_B(\bar{r}_B+1)}\right\} + q\left\{\frac{2p\bar{r}_A + p - T_A}{\bar{r}_A(\bar{r}_A+1)}\right\} + 2\left\{\frac{2pq\bar{r}_D + pq - T_D}{\bar{r}_D(\bar{r}_D+1)}\right\}. \tag{3.12}$$

Let $T_B = q\bar{r}_B + a_B$, where $0 \leq a_B < q$, $T_D = pq\bar{r}_D + a_D$; $0 \leq a_D < pq$ and $T_A = p\bar{r}_A + a_A$; $0 \leq a_A < p$. Then if we substitute T_A, T_B and T_D from here into $F(T_A, T_D)$, we will obtain the function in terms of a_A, $\bar{r}_A$, a_B, $\bar{r}_B$ and a_D, $\bar{r}_D$, viz

$$F(T_A,T_D) = \tag{3.13}$$

$$= pq\left(\frac{1}{\bar{r}_B} + \frac{1}{\bar{r}_A} + \frac{2}{\bar{r}_D}\right) - \left\{\frac{pa_B}{\bar{r}_B(\bar{r}_B+1)} + \frac{qa_A}{\bar{r}_A(\bar{r}_A+1)} + \frac{2a_D}{\bar{r}_D(\bar{r}_D+1)}\right\}.$$

Definition 3.1 *Let*

$$b_1 = \min\{F(t_A,t_D);\ (t_A,t_D) \in \Xi\}, \tag{3.14}$$

where

$$\Xi = \{(t_A,t_D);\ t_A \geq p,\ t_D \geq pq; t_A + t_D \leq bk - q;\ t_A, t_D \in N^+\},$$

and N^+ *denotes the set of integers, positive numbers, then* b_1 *is called the* **first bound** *on the sum of the variances for the dual versus single estimators.*

Now we are in a position to establish the following corollary.

Corollary 3.3 *For any* $n \times m$ *CFBD(00) design, d, with a g-inverse* Ω*, then*

$$tr(C\Omega C') \geq F(T_A,T_D) \geq b_1. \tag{3.15}$$

Proof: It follows from Theorem 3.1 and the fact that b_1 is the overall minimum value for $tr(Cr^{-\delta}C')$.♣

Definition 3.2 *Let* b_l *denote a lower bound for the total of the variances of the estimators of the contrasts of interest. Then*

$$D(d,C) = \frac{tr(C\Omega C') - b_l}{b_l} \times 100 \tag{3.16}$$

is called the **discrepancy** *of design d for the contrast estimators* $C\hat{\underline{\tau}}$ *relative to the bound* b_l.

The following three examples show the capability of b_1 in assessing design performance.

Example 3.1 *For m=n=3, b=3 and k=8, the following design has* $tr(C\Omega C') =$ 5.333, *which is equal to* b_1, *is overall A-optimal.*

*Block*1	01	01	10	20	11	12	21	22
*Block*2	01	01	10	20	11	12	21	22
*Block*3	01	01	10	20	11	12	21	22

Example 3.2 *For m=n=3, b=3 and k=9,* $b_1 = 4.833$ *and for these parameter values the most efficient design which is generated by JE,* $tr(C\Omega C') = 4.862$. *The discrepancy for this design is 0.6% which is very small, indicating that bound is a good bound for these parameter values.*

Example 3.3 *For m=n=3, b=18 and k=2, we have* b_1*=3.6, and the most efficient design generated by JE gives tr(*$C\Omega C'$*)= 5.996, with 66% discrepancy with* b_1. *For these parameter values* b_1 *is a poor bound.*

Discussion 3.1 *Examples 3.1 and 3.2 indicate that* b_1 *is a tight lower bound for* $tr(C\Omega C')$, *for big values of k relative to t=mn-1. However, Example 3.3 suggests that for small values of k relative to t=mn-1,* b_1 *cannot be used to judge the performance of the design.*

3.3 Bound 2(b_2):

We need to establish a bound which is tighter than b_1 for small values of k. The new bound, b_2, which will be given in this section is based on the eigenvalues of the A-matrix of the design and $C'C$, where C is the contrast matrix for the dual treatments versus single treatment problem. Before going further we need to investigate the $C'C$ matrix.

3.3.1 Structure and Eigenvalues of $C'C$:

For a general $n \times m$ CFBD(00), from the coefficient matrix C, given in (1.12), from (3.5) we have:

$$C'C = \begin{bmatrix} pI_q & o_{q\times p} & -\underline{1}'_p \otimes I_q \\ o_{p\times q} & qI_p & -I_p \otimes \underline{1}'_q \\ -\underline{1}_p \otimes I_q & -I_p \otimes \underline{1}_q & 2I_l \end{bmatrix}, \tag{3.17}$$

Table 3.1: Eigenvalues of $C'C$ matrix(p=n-1, q=m-1).

Eigenvalues(θ_i)	multiplicities
$\frac{p+q+2+\sqrt{(p+q+2)^2-4(pq+p+q)}}{2}$	1
$\frac{p+q+2-\sqrt{(p+q+2)^2-4(pq+p+q)}}{2}$	1
$\frac{p+2+\sqrt{(p+2)^2-4p}}{2}$	q-1
$\frac{p+2-\sqrt{(p+2)^2-4p}}{2}$	q-1
$\frac{q+2+\sqrt{(q+2)^2-4q}}{2}$	p-1
$\frac{q+2-\sqrt{(q+2)^2-4q}}{2}$	p-1
2	$(p-1)\times(q-1)$
0	1

where p=n-1, q=m-1 and l=pq.

The eigenvalues of $C'C$ are given in Table 3.1.

3.3.2 Properties of $C'C$:

1. $C'C$ is a symmetric and non-negative definite(n.n.d.) matrix with eigenvalues $\theta_1 \geq \theta_2 \geq \ldots \geq \theta_{t-1} > \theta_t = 0$ given in Table 3.1. Let the corresponding eigenvectors be denoted by $\underline{\mu}_1, \underline{\mu}_2, \ldots, \underline{\mu}_{t-1}$ and $\underline{\mu}_t = t^{-1/2}\underline{1}_t$ respectively.

2. $C'C\underline{1} = \underline{0}$. Therefore $\underline{\mu}_t = t^{-1/2}\underline{1}_t$ is an eigenvector of $C'C$ corresponding to the eigenvalue $\theta_t = 0$, where t=mn-1.

3. R($C'C$)=t-1=mn-2, since $C'C\underline{1}_t = \underline{0}$, which simply means that one of the rows or columns of $C'C$ is a linear functions of the other rows or columns respectively.

In the following we give a theorem and some corollaries which lead us to the new bound, b_2.

Theorem 3.2 *Let* $C\underline{\tau}$ *be a set of* L *contrasts of interest in a design(block or row-column), involving* t *treatments such that* $L \geq t-1$ *and* $R(C) = t-1$. *Then if* $\theta_1 \geq \theta_2 \geq \ldots \geq \theta_{t-1} > \theta_t = 0$ *are the eigenvalues of* $C'C$ *and* $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{t-1} > \lambda_t = 0$, *are the eigenvalues of the A-matrix of the design, Then:*

$$tr\{V(C\hat{\underline{\tau}})\} = tr(C\Omega C') \geq \sum_{i=1}^{t-1} \frac{\theta_i}{\lambda_i}. \tag{3.18}$$

Proof: We prove the theorem by considering two cases:

(i)- $L \geq t$. Let Ω be the Moore-Penrose g-inverse of the A-matrix of the design, then we have: $V(C\hat{\tau}) = C\Omega C'$. Therefore

$$tr(C\Omega C') = tr\left\{C(\sum_{i=1}^{t-1} \lambda_i^{-1} \underline{\xi}_i \underline{\xi}_i')C'\right\}, \tag{3.19}$$

where the ξ_i's are normalized eigenvectors of the A-matrix of the design corresponding to the eigenvalues λ_i's with the property (1.9) as given in Chapter 1. This implies that

$$tr(C\Omega C') = tr\left(\sum_{i=1}^{t-1} \lambda_i^{-1} C\underline{\xi}_i \underline{\xi}_i' C'\right) = \sum_{i=1}^{t-1} \lambda_i^{-1} \underline{\xi}_i' C'C\underline{\xi}_i. \tag{3.20}$$

Let $\underline{\gamma}_i = \lambda_i^{-1/2}\underline{\xi}_i$, for $i = 1, 2, \ldots, t-1$, then we have:

$$tr(C\Omega C') = \sum_{i=1}^{t-1} \underline{\gamma}_i' C'C\underline{\gamma}_i. \tag{3.21}$$

Also let $\Gamma = (\underline{\gamma}_1, \underline{\gamma}_2, \cdots, \underline{\gamma}_{t-1}, d^{-1}t^{-1}\underline{1}_t)$, where d is a positive real, such that $td^2 \leq \lambda_{t-1}$. Since $\underline{1}'C'C\underline{1} = 0$, we have:

$$tr(C\Omega C') = tr(\Gamma' C'C\Gamma). \tag{3.22}$$

By applying Theorem A.4 of Marshall and Olkin(1979,p513), we obtain:

$$tr(\Gamma' C'C\Gamma) \geq \sum_{i=1}^{t} \theta_{t-i+1}\eta_i, \tag{3.23}$$

where η_i's are eigenvalues of $\Gamma'\Gamma$. To obtain η_i's notice that

$$\Gamma'\Gamma = diag(\lambda_1^{-1}, \lambda_2^{-1}, \ldots, \lambda_{t-1}^{-1}, t^{-1}d^{-2}),$$

then if we let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_t$, we have $\eta_1 = d^{-2}t^{-1}$ and

$$\eta_i = \lambda_{t-i+1}^{-1}, \text{ for } i = 2, 3, \ldots, t.$$

It follows that

$$tr(C\Omega C') \geq \sum_{i=1}^{t} \theta_{t-i+1}\eta_i = \theta_t\eta_1 + \sum_{i=2}^{t} \frac{\theta_{t-i+1}}{\lambda_{t-i+1}}. \tag{3.24}$$

But the first term in the RHS of the above inequality is zero since $\theta_t = 0$, and it is easy to show that the second term is $\sum_{i=1}^{t-1} \theta_i/\lambda_i$. This completes the proof of the first case.

(ii)- L=t-1, let $(C^*)' = (d\underline{1}_t\ , C')$, where C^* is an $t \times t$ full rank matrix and $C^*(C^*)'$ has eigenvalues $\chi_1 \geq \chi_2 \geq \ldots \geq \chi_t > 0$, where d is an arbitrary positive constant, such that $\chi_1 = d^2 t$, and $\chi_i = \theta_{i-1}$, for $i = 2, 3, \ldots, t$. Since

$$C^*(C^*)' = \begin{bmatrix} d^2 t & \underline{0}' \\ \underline{0} & CC' \end{bmatrix},$$

it follows that: $|C^*(C^*)' - \chi_i I| = (td^2 - \chi_i)|CC' - \theta_i I| = 0$, for i=1,2,...,t. It is clear from this that t-1 eigenvalues of $C^*(C^*)'$ are those of CC'. If we let Ω be the Moore-Penrose g-inverse of the A-matrix of the design with $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_{t-1} > \eta_t = 0$, as its eigenvalues then we have $\eta_i = \lambda_{t-i}^{-1}$, for $i = 1, 2, \ldots, t-1$. It can be easily shown that $tr(C\Omega C') = tr(C^*\Omega(C^*)')$, since $tr(C^*\Omega(C^*)') = tr(C\Omega C') + d^2\underline{1}'\Omega\underline{1}$, but $\underline{1}'\Omega\underline{1} = 0$. By applying Marshall and Olkin(1979, p513) we have:

$$tr\{C^*\Omega(C^*)'\} \geq \sum_{i=1}^{t} \chi_i\eta_{t-i+1} = \chi_1\eta_t + \sum_{i=2}^{t} \chi_i\eta_{t-i+1} = \sum_{i=2}^{t} \chi_i\eta_{t-i+1}$$

since $\eta_t = 0$. But $\chi_i = \theta_{i-1}$ for $i \geq 2$ and $\eta_{t-i+1} = \lambda_{i-1}^{-1}$. This implies that $tr(C\Omega C') \geq \sum_{i=2}^{t} \theta_{i-1}\lambda_{i-1}^{-1} = \sum_{i=1}^{t-1} \theta_i\lambda_i^{-1}$. Hence the theorem is proved.♣

Corollary 3.4 *If the C matrix in the statement of Theorem 3.2 is the contrast matrix for the dual treatments versus single treatment comparisons in an $n \times m$ CFBD(00), then*

$$tr(C\Omega C') \geq \sum_{i=1}^{t-1} \frac{\theta_i}{\lambda_i}, \tag{3.25}$$

where θ_i's are given in Table 3.1.

Proof: The result follows immediately from Theorem 3.2 and values for θ_i's given in Table 3.1.♣

Corollary 3.5 *If we have a class of designs with fixed trace for the A-matrix, i.e. $tr(A) = c$, where c is a constant, then for any design belonging to this class we have*

$$tr(C\Omega C') \geq \frac{(\sum_{i=1}^{t-1}\sqrt{\theta_i})^2}{c}, \tag{3.26}$$

where C is the contrast matrix of interest and the θ_i's are the eigenvalues of $C'C$ given in Table 3.1.

Proof: From Theorem 3.2 we have $tr(C\Omega C') \geq \sum_{i=1}^{t-1}\theta_i/\lambda_i$. Then if we let $\sum_{i=1}^{t}\lambda_i = c$ be regarded as fixed, by applying Lagrangian Multiplier, γ, we can minimize $\sum_{i=1}^{t-1}\theta_i/\lambda_i$, subject to the condition $\sum_{i=1}^{t}\lambda_i = c$. This minimum value will be

$$tr(C\Omega C') \geq \sum_{i=1}^{t-1}\frac{\theta_i}{\lambda_i} \geq \frac{(\sum_{i=1}^{t-1}\sqrt{\theta_i})^2}{c}, \tag{3.27}$$

which is only a function of the eigenvalues of $C'C$, given in Table 3.1, where

$$\sum_{i=1}^{t}\sqrt{\theta_i} = \sqrt{p+q+2+2\sqrt{pq+p+q}} + (p-1)(q-1)\sqrt{2} + \tag{3.28}$$

$$(q-1)\sqrt{p+2+2\sqrt{p}} + (p-1)\sqrt{q+2+2\sqrt{q}}.$$

Hence the corollary is proved.♣

Note: We know that only for the binary block designs and balanced block designs the value c is fixed and for the other cases it depends on the design. Therefore this bound is only applicable to these two kinds of designs unless we restrict consideration to all block designs with a specific value of c.

The RHS of the inequality in (3.26) is a decreasing function in terms of c, i.e. it will be minimized if c is maximized. But for any design we have

$$c = tr(A) = bk - \frac{1}{k}\sum_{i=1}^{t}\sum_{j=1}^{b}n_{ij}^2. \tag{3.29}$$

This is maximized if $\sum_{i=1}^{t}\sum_{j=1}^{b}n_{ij}^2$ is minimized. That is if the n_{ij}'s are as equal as possible. For $t \geq k$ the minimum value is obtained when the design is binary, that is $n_{ij} \in \{0,1\}$. In this case c=b(k-1) which is fixed.

Definition 3.3 *Let*

$$b_2 = \frac{(\sum_{i=1}^{t} \sqrt{\theta_i})^2}{c'}, \tag{3.30}$$

where θ_i's are eigenvalues of $C'C$ given in Table 3.1 and c' is the maximum value for c, where c is the trace of the A-matrix of the design. Then b_2 is a lower bound on the total variances for the estimators of the contrasts of interest and will be called the **second bound**.

Now we reconsider Examples 3.1 to 3.3 and give a new example to illustrate the use of bound b_2 to assess the performance of designs and to show that it is not always a tighter bound than b_1.

Example 3.4 *For $m=n=3$, $b=18$ and $k=2$, we have $b_2=5.616$. For the most efficient design generated by JE, $tr(C\Omega C')$ =5.996. For this example the discrepancy between this figure b_2 and this design i.e. $D(b_2, d)$ is 6.7% which is a substantial improvement on b_1 (see Example 3.3).*

Example 3.5 *For $m=n=3$, $b=3$ and $k=8$, $b_2=4.814$. For this set of parameters values the A-optimal design, given in Example 3.1, has 5.333 as the total of the variances of the estimators of the contrasts of interest. The discrepancy between this figure and the bound b_2 is 10.8%. Comparing the value of b_2 with b_1=5.333 shows that b_2 is a poor bound*

Example 3.6 *For $m=n=3$, $b=8$ and $k=3$, we obtain $b_2=6.319$. The discrepancy between this value and $tr(C\Omega C')$ for the most efficient design generated by JE is* 1.7% *which is very small. The discrepancy between b_1 and $tr(C\Omega C')$ for the same design is* 20.5%, *showing that b_2 is a much tighter bound than b_1 for the particular parameter values.*

Example 3.7 *For $m=n=3$, $b=3$ and $k=9$, $b_2=4.212$. The discrepancy between b_2 and $tr(C\Omega C')$ for the highly efficient design cited in Example 3.2 is* 15.4%. *Comparison with the discrepancy for b_1 namely* 0.6%, *shows that b_2 is a poorer bound for the parameter values.*

In the following section we will compare bounds b_1 and b_2, in order to specify those ranges of parameters for which b_1 is a tighter bound than b_2, and vice versa. On the basis of this study we shall recommend which of b_1 or b_2 should be used to assess a particular design.

3.4 Comparison Between b_1 and b_2:

A numerical computation has been carried out to compare bounds b_1 and b_2 for the parameter values $2 \leq n, m \leq 10$, $b \leq 30$ and $2 \leq k \leq 15$, excluding (m,n)=(2,2). The results are given in Table 3.2 at the end of this chapter.

Analytical comparison between the bounds is very difficult, because the ratio of the bounds is a messy function.

As we can see from the Table 3.2, for $k \geq t = mn-1$, b_1 is a tighter bound than b_2. Therefore for such cases we recommend the use of b_1 to assess the performance of the designs. In fact, for $k > t$ there are many designs which achieve or almost achieve bound b_1, as will be shown in Section 4.3(Theorem 4.8) and Table 4.2 for n=3. For $k < t$ one bound is not uniformly tighter than the other.

3.5 Assessment of RGDD Using the Bounds:

As we mentioned in Section 3.4, for $k < t$ one bound is not uniformly tighter than the other. Therefore in order to assess the performance of the designs for this case we use the bound:

$$b_m = \max(b_1, b_2). \tag{3.31}$$

A study of all possible RGDD which can be built up from the Clatworthy(1973) catalogue was made. For each design the total of the variances of the dual versus single contrast estimators was compared with b_m. Notice that for this class of designs the trace of the A-matrix has value c=b(k-1), which is fixed.

An extensive numerical investigation has been carried out over all the RGDD designs described in Section 2.5.2.5. The following conclusion have been drawn from this investigation:

1. There are in total 57 designs which are reinforced singular GD designs. These are the best in this class, if they exist, and $tr(C\Omega C')$ has a discrepancy of not more than 12.3% compared with b_m. We found that 72% of the designs in this subtype of designs have discrepancy of not more than 7%.

2. There are in total 28 designs which are reinforced semi-regular GD designs. The maximum discrepancy is 27.2%, while 64% of the designs within the subtype have a discrepancy of not more than 13.3%.

3. The total number of designs which are reinforced regular GD designs is 75. The maximum discrepancy is not more than 27.7%. We found that 49% of these designs have a discrepancy less than 13.4%.

In conclusion, we have established that best subclass of GD designs for forming RGDD is the class of singular GD designs.

Table 3.2: Values of n, m and k, where $b_2 > b_1$.

(m,n)	k
(2,3)	k≤ 3
(2,4)	k≤ 3 and k=4(b≠ 6)
(2,5)	k≤ 4
(2,6)	k≤ 4
(2,7)	k≤ 4 and k=5(b≠6,8,9)
(2,8)	k≤ 4 and k=5(b≠7,9,10)
(2,9)	k≤ 4 and k=5(b≠8,11)
(2,10)	k≤ 4 and k=5(b≠8)
(3,3)	k≤ 4
(3,4)	k≤ 4 and k=5(b≠6)
(3,5)	k≤ 5 and k=6(b≠6–9, 11–14, 16)
(3,6)	k≤ 5 and k=6(b≠7,8)
(3,7)	k≤ 5 and k=6(b≠9)
(3,8)	k≤ 5, k=6(b≠10) and k=7(b≠8–13, 15–17, 19,20)
(3,9)	k≤ 6 and k=7(b≠9–11, 13–15)
(3,10)	k≤ 6 and k=7(b≠10–12, 15,16)
(4,4)	k≤ 5 and k=6(b≠7)
(4,5)	k≤ 6 and k=7(b≠10,11,13,14)
(4,6)	k≤ 6 and k=7(b≠9)
(4,7)	k≤ 7 and k=8(b≠13,14, 16–18, 21)
(4,8)	k≤ 7 and k=8(b≠10–12, 15,16)
(4,9)	k≤ 7 and k=8(b≠12,13)
(4,10)	k≤ 7 and k=8(b≠13,14)

Table 3.2: continued...

(m,n)	k
(5,5)	k≤ 6 and k=7(b≠9,10)
(5,6)	k≤ 7 and k=8(b≠10,11,14,15)
(5,7)	k≤ 7, k=8(b≠12,13) and k=9(b≠10–12, 14–16, 19,20,24)
(5,8)	k≤ 7, k=8(b≠14,15) and k=9(b≠10–14, 17,18)
(5,9)	k≤ 8, k=9(b≠13–15) and k=10(b=21,26,30)
(5,10)	k≤ 8, k=9(b≠15–17) and k=10(b≠13–16, 19–21, 25–27)
(6,6)	k≤ 7, k=8(b≠12,13) and k=9(b≠10–12, 15–17, 20)
(6,7)	k≤ 8, k=9(b≠12–14) and k=10(b=19,24,29)
(6,8)	k≤ 8, k=9(b≠15,16) and k=10(b≠12–15, 18–21)
(6,9)	k≤ 9, k=10(b≠14–17, 21,22) and k=11(b=23,28,29)
(6,10)	k≤ 9, k=10(b≠16–19) and k=11(b=13,19,20,25,26,27,30)
(7,7)	k≤ 8, k=9(b≠15,16) and k=10(b≠13–16, 19,20)
(7,8)	k≤ 8, k=9(b≠18) and k=10(b≠15–18)
(7,9)	k≤ 9, k=10(b≠17–19) and k=11(b≠15–19, 23,24)
(7,10)	k≤ 9, k=10(b≠20,21), k=11(b≠17–20) and k=12(b≠14,20,21,27,28)
(8,8)	k≤ 9, k=10(b≠17–20), k=11(b≠15–19, 23–25) and k=12(b=19,25)
(8,9)	k≤ 9, k=10(b≠20–22), k=11(b≠17–21) and k=12(b=14,21,22, 27–30)
(8,10)	k≤ 9, k=10(b≠23,24) and k=11(b≠20–23), k=12(b≠17–22, 26–29) and k=13(b=22,29,30)
(9,9)	k≤ 10, k=11(b≠20–23), k=12(b=16,17, 23–26, 30) and k=13(b=22,29,30)
(9,10)	k≤ 10, k=11(b≠23–25), k=12(b≠20–24), k=13(b=16,17, 24–26) and k=14(b=23)
(10,10)	k≤ 10, k=11(b≠26–28), k=12(b=19–22, 28–30), k=13(b=18,19, 26–29) and k=14(b=17,25,26)

Chapter 4

Highly Efficient PBDS Designs

4.1 Introduction:

In Chapter 2 we derived some properties of the class of PBDS designs, such as the form of the A-matrix and the structure of the information matrix for the estimators of the contrasts of interest. A method of constructing such designs for $k < t = 2n - 1$, namely RGDD's, was introduced and some of its properties were considered. The performance of RGDD's was assessed against given bounds in Chapter 3. Also the class of BDSD, viewed as a special case of PBDS designs, was considered in detail.

The class of PBDS designs is a source of designs which have a symmetric structure for the variance-covariance matrix for the contrast estimators corresponding to the dual versus single treatment comparisons. In the previous chapters it has been shown by example that highly efficient and, in some cases, overall A-optimal designs can be found in the PBDS class.

In the present chapter we will give theorems which lead us to characterize a wide range of highly efficient PBDS designs. It will be shown that, provided three conjectures are true, we can characterize those designs which are overall A-optimal or A-optimal within the PBDS class.

The approach used is to reconsider the structure of the information matrix for the contrasts of interest(given in 2.12). We shall then apply the permutation method(see Kiefer,1975) to obtain a design-dependent lower bound on the total variance of the estimators of the contrasts. This is described in Section 4.3.

The aim of Section 4.2 is to move towards a lower bound which is not design-dependent on the total variance of the estimators of the contrasts of interest and which is achievable or nearly achievable in the sense of having small discrepancy with the minimum value of $tr(C\Omega C')$ for a wide range of design parameters. Such a bound would be a great improvement on bound b_m(of Chapter 3, Section 3.5) as a tool for locating optimal designs since b_m is not achievable except for large block sizes(see Chapter 3, Section 3.4). To this end an investigation is made in Section 4.3 on the conditions under which the design-dependent bound is minimized. In the final stages of the analytical argument it is found that the conjectures are needed to formulate a conjectured bound. This is due to the need to minimize a very complicated function.

This conjectured bound is the same as b_m given in Chapter 3 whenever $N'r^{-\delta}C' = 0$, $T_A = b(n-1)r_A$ $T_D = b(n-1)r_D$ satisfy condition (3.14) on page 73. For $b > 3$ the conjectured bound is tighter than b_m and more widely achievable by designs(see Table 4.2). Analytical results are presented which tell us how the replications of the treatments should be spread across the blocks(see Theorems 4.4 and 4.8).

The layouts of the best designs are specified and a catalogue of designs which achieve this conjectured bound is given. The high efficiency of designs with block size greater than the number of treatments involved in the design, i.e. $k \geq t$, is demonstrated by comparison with b_m. The designs having small block size($k < t$) are shown to be highly efficient by comparison with the best obtained by JE.

4.2 A Bound Based on the Permutation Method:

In this section we briefly review the permutation method and then apply it to our particular problem to get a bound under certain conditions.

4.2.1 Review of the Permutation Method:

In order to outline the permutation method we need to give a definition of a convex function.

Let U be a subset of $n \times n$ real matrices and R be the set of real numbers, then a real valued function $\Phi : U \rightarrow R$, is said to be a **convex function** if for $X_1, X_2, ..., X_m \in U$ and $\alpha_1, \alpha_2, ..., \alpha_m \in [0,1]$, such that $\sum_{i=1}^{m} \alpha_i = 1$, then

$$\Phi(\sum_{i=1}^{m} \alpha_i X_i) \leq \sum_{i=1}^{m} \alpha_i \Phi(X_i), \tag{4.1}$$

for $m \geq 2$(see Roberts and Varberg, 1973,p89).

A square matrix p is said to be a **permutation matrix** if each row and column has a single unit, and all other entries are zero. Let P be a set of permutation matrices, then Φ is said to be invariant under the set of permutations P applied to rows and columns if

$$\Phi(p_i X p_i') = \Phi(X), \forall p_i \in P.$$

Kiefer(1975) was the first person to employ this concept to provide a sufficient condition for a block design or row-column design to be universally optimal.

Majumdar and Notz(1983) used a similar approach to characterize A- and MV-optimal designs for the test treatments versus control treatment problem.

Yeh(1986), by utilizing this approach, generalized the work of Kiefer(1975) when the required conditions for the universal optimality cannot be achieved and found justification of universal optimality over the class of binary block designs.

Majumdar(1986) used this method to characterize A-optimal designs for comparing a set of test treatments with a set of control treatments, but found that it led to the identification of only a small number of designs.

A key feature of Kiefer's approach is that it uses a set of permutation matrices which leave Φ invariant.

4.2.2 Application to Our Specific Problem:

We now apply the permutation method to establish a design-dependent bound on the total variance of the estimators of the dual versus single treatment contrasts. In other words we want a design-dependent bound on $tr(M^{-1})$, where M is the information matrix for the contrasts of interest, defined in Chapter 2(2.12).

Let the information matrix, M, for the contrasts of interest given in (2.12) be partitioned as follows

$$M = \begin{bmatrix} M_{11} & M_{12} \\ \\ M_{12}' & M_{22} \end{bmatrix}, \tag{4.2}$$

where the M_{ij}'s are $(n-1) \times (n-1)$ matrices for i,j=1,2.

Suppose $\{p_i; i = 1, 2, \ldots, (n-1)!\}$ is the full set of permutation matrices each having order (n-1). The set of permutations we shall employ is $\prod = \{\pi_i; \pi_i = I_2 \otimes p_i\}$.

Now define $\bar{M}$ as the average of M over all permutations in $\prod$, i.e.

$$\bar{M} = \frac{1}{(n-1)!} \sum_{i=1}^{(n-1)!} \pi_i M \pi_i' = \begin{bmatrix} \bar{M}_{11} & \bar{M}_{12} \\ \\ \bar{M}_{12}' & \bar{M}_{22} \end{bmatrix}, \tag{4.3}$$

where

$$\bar{M}_{\ell\ell'} = \frac{1}{(n-1)!} \sum_{i=1}^{(n-1)!} p_i M_{\ell\ell'} p_i', \tag{4.4}$$

for $\ell, \ell' = 1, 2$.

We now utilize the approach of permuting the rows and columns of M, to obtain a bound.

Theorem 4.1 *For any connected design d∈ $n \times 2$ CFBD(00), we have:*

$$tr(C\Omega C') = tr(M^{-1}) \geq tr(\bar{M}^{-1}), \tag{4.5}$$

where $\bar{M}$ is given in (4.3).

Proof: For any connected $n \times 2$ CFBD(00) design, the information matrix, M, is a positive definite matrix with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_{2p}$, where p=n-1. Let $\prod$ be the set of permutation matrices defined above. Then, define $X_i = \pi_i M \pi_i'$ for i=1,2,...,(n-1)!. It is obvious that X_i's are all positive definite matrices and $tr(X_i) = tr(\pi_i M \pi_i') = tr(M)$.

Now if we define

$$\Phi(M) = tr(M^{-1}) = \sum_{i=1}^{2p} \frac{1}{\lambda_i},$$

where λ_i's are the eigenvalues of matrix M, then Φ is a convex function(see Majumdar and Notz,1983,Theorem 2.1). It follows from (4.1) with $\alpha_i = [(n-1)!]^{-1}$(i=1,2,...,(n-1)!) that

$$\Phi(\bar{M}) \leq \sum_{i=1}^{(n-1)!} \frac{1}{(n-1)!} \Phi(\pi_i M \pi_i'). \tag{4.6}$$

But $\Phi(\pi_i M \pi_i') = tr\{(\pi_i M \pi_i')^{-1}\} = tr(M^{-1})$. Therefore the RHS of the inequality in (4.6) is $tr(M^{-1})$. Hence the theorem is proved.♣

The purpose of the following lemmas is to formulate a bound as a function of the elements of the incidence matrix of the design, i.e. as function of the number of occurrences of each treatment combination in each block. This will then facilitate the calculation of a bound and, more importantly, the identification of designs whose total variance achieves the bound. Since the bound is in terms of elements of $\bar{M}$ we need to express the elements of $\bar{M}$ as functions of the entries of the incidence matrix of the design. In doing this we shall use the following notation.

Notation: In addition to the notation used on page 44, we define the following notation. We define

$$T_{Aj} = \sum_{i=1}^{n-1} n_{Aij},\ T_{Dj} = \sum_{i=1}^{n-1} n_{Dij} \text{ and } T_{Bj} = n_{Bj},$$

which denote the total number of units assigned to treatment combinations belonging to sets A, D and B respectively in block j and

$$T_A = \sum_{j=1}^{b} T_{Aj},\ T_D = \sum_{j=1}^{b} T_{Dj} \text{ and } T_B = \sum_{j=1}^{b} T_{Bj}$$

denote the total number of units assigned to treatment combinations in sets A, D and B respectively in the entire design.

The following lemma gives the entries of M in terms of the entries of the incidence matrix of the design. In order to achieve this we note that the submatrices in the partition of M are given from (2.12) in Chapter 2 as

$$\begin{aligned} M_{11} &= A_{22} + A_{23} + A'_{23} + A_{33}, \\ M_{12} &= -A_{22} - A'_{23}, \qquad (4.7) \\ M_{22} &= A_{22}, \end{aligned}$$

where A_{22}, A_{23} and A_{33} are submatrices of the A-matrix of the design such that

$$A = \begin{pmatrix} a_{11} & \underline{a}'_{12} & \underline{a}'_{13} \\ \underline{a}_{12} & A_{22} & A_{23} \\ \underline{a}_{13} & A'_{23} & A_{33} \end{pmatrix}.$$

Lemma 4.1 *For the matrix M given in (4.2), let $m_{j\ell(ii')}$ denote the (i,i')th entry of $M_{j\ell}$, then*

$$m_{11(ii')} = \begin{cases} r_{Di} + r_{Ai} - (1/k)\sum_{j=1}^{b}(n_{Aij} + n_{Dij})^2 & \textit{if } i = i', \\ -(1/k)\sum_{j=1}^{b}(n_{Aij} + n_{Dij})(n_{Ai'j} + n_{Di'j}) & \textit{if } i \neq i', \end{cases}$$

$$m_{12(ii')} = \begin{cases} -r_{Ai} + (1/k)\sum_{j=1}^{b} n_{Aij}(n_{Aij} + n_{Dij}) & \textit{if } i = i', \\ (1/k)\sum_{j=1}^{b} n_{Aij}(n_{Ai'j} + n_{Di'j}) & \textit{if } i \neq i', \end{cases} \tag{4.8}$$

$$m_{22(ii')} = \begin{cases} r_{Ai} - (1/k)\sum_{j=1}^{b} n_{Aij}^2 & \textit{if } i = i', \\ -(1/k)\sum_{j=1}^{b} n_{Aij}n_{Ai'j} & \textit{if } i \neq i'. \end{cases}$$

Proof: Since A_{22}, A_{23} and A_{33} are parts of the A-matrix of the design, if we let $a_{j\ell(ii')}$ denote the $(i,i')th$ entry of $A_{j\ell}$ for j,ℓ=2,3 and i,i'=1,2,...,n-1, then by (1.6) in Chapter 1 we have

$$a_{22(ii')} = \begin{cases} r_{Ai} - (1/k)\sum_{j=1}^{b} n_{Aij}^2 & \text{if } i = i', \\ -(1/k)\sum_{j=1}^{b} n_{Aij}n_{Ai'j} & \text{if } i \neq i', \end{cases}$$

$$a_{23(ii')} = -(1/k)\sum_{j=1}^{b} n_{Aij}n_{Di'j} \tag{4.9}$$

$$a_{33(ii')} = \begin{cases} r_{Di} - (1/k)\sum_{j=1}^{b} n_{Dij}^2 & \text{if } i = i', \\ -(1/k)\sum_{j=1}^{b} n_{Dij}n_{Di'j} & \text{if } i \neq i'. \end{cases}$$

From these and (4.7), after some algebra, the result follows.♣

Now we are in position to express the entries of $\bar{M}$ in terms of the elements of the incidence matrix.

Lemma 4.2 *Let $\bar{m}_{\ell\ell'(ii')}$ denote the $(i,i')th$ entry of $\bar{M}_{\ell\ell'}$ as defined in (4.4), then*

$$\bar{m}_{11(ii')} = \begin{cases} \frac{T_A+T_D}{n-1} - \frac{1}{k(n-1)} \sum_{i=1}^{n-1} \sum_{j=1}^{b} (n_{Aij} + n_{Dij})^2 & \text{if } i = i', \\ \\ -\frac{\sum_{j=1}^{b} \{(T_{Aj}+T_{Dj})^2 - \sum_{i=1}^{n-1} (n_{Aij}+n_{Dij})^2\}}{k(n-1)(n-2)} & \text{if } i \neq i', \end{cases}$$

$$\bar{m}_{12(ii')} = \begin{cases} -\frac{T_A}{n-1} + \frac{1}{k(n-1)} \sum_{i=1}^{n-1} \sum_{j=1}^{b} n_{Aij}(n_{Aij} + n_{Dij}) & \text{if } i = i', \\ \\ \frac{\sum_{j=1}^{b} \{T_{Aj}(T_{Aj}+T_{Dj}) - \sum_{i=1}^{n-1} n_{Aij}(n_{Aij}+n_{Dij})\}}{k(n-1)(n-2)} & \text{if } i \neq i', \end{cases} \quad (4.10)$$

$$\bar{m}_{22(ii')} = \begin{cases} \frac{T_A}{n-1} - \frac{1}{k(n-1)} \sum_{i=1}^{n-1} \sum_{j=1}^{b} n_{Aij}^2 & \text{if } i = i', \\ \\ -\frac{1}{k(n-1)(n-2)} \sum_{j=1}^{b} \{T_{Aj}^2 - \sum_{i=1}^{n-1} n_{Aij}^2\} & \text{if } i \neq i', \end{cases}$$

Proof: From (4.4) we obtain

$$\bar{m}_{11(ii')} = \begin{cases} \frac{1}{n-1} \sum_{i=1}^{n-1} m_{11(ii)} & \text{if } i = i', \\ \\ \frac{1}{(n-1)(n-2)} \sum_{i=1}^{n-1} \sum_{i' \neq i} m_{11(ii')} & \text{if } i \neq i', \end{cases}$$

$$\bar{m}_{12(ii')} = \begin{cases} \frac{1}{n-1} \sum_{i=1}^{n-1} m_{12(ii)} & \text{if } i = i', \\ \\ \frac{1}{(n-1)(n-2)} \sum_{i=1}^{n-1} \sum_{i' \neq i} m_{12(ii')} & \text{if } i \neq i', \end{cases} \quad (4.11)$$

$$\bar{m}_{22(ii')} = \begin{cases} \frac{1}{n-1} \sum_{i=1}^{n-1} m_{22(ii)} & \text{if } i = i', \\ \\ \frac{1}{(n-1)(n-2)} \sum_{i=1}^{n-1} \sum_{i' \neq i} m_{22(ii')} & \text{if } i \neq i', \end{cases}$$

Substituting from Lemma 4.1 gives the required expressions.♣

Corollary 4.1 *The matrix $\bar{M}$ defined in Lemma 4.2 has the following structure*

$$\bar{M} = \begin{bmatrix} (x_1 - y_1)I_p + y_1 J_p & (x_2 - y_2)I_p + y_2 J_p \\ \\ (x_2 - y_2)I_p + y_2 J_p & (x_3 - y_3)I_p + y_3 J_p \end{bmatrix}, \quad (4.12)$$

where $x_1 = \bar{m}_{11(ii)}$, $y_1 = \bar{m}_{11(ii')}(i \neq i')$, $x_2 = \bar{m}_{12(ii)}$, $y_2 = \bar{m}_{12(ii')}(i \neq i')$, $x_3 = \bar{m}_{22(ii)}$, $y_3 = \bar{m}_{22(ii')}(i \neq i')$ and $\bar{m}_{\ell\ell'(ii')}$'s are given in Lemma 4.2.

Proof: Follows from Lemma 4.2.♣

The next step is to evaluate $tr(\bar{M}^{-1})$ in terms of the elements of the incidence matrix of the design. To achieve this the following lemma is needed.

Lemma 4.3 *For any nonsingular symmetric matrix L of the form:*

$$L = \begin{bmatrix} (x_1 - y_1)I_m + y_1 J_m & (x_2 - y_2)I_m + y_2 J_m \\ (x_2 - y_2)I_m + y_2 J_m & (x_3 - y_3)I_m + y_3 J_m \end{bmatrix}, \quad (4.13)$$

we have:

$$tr(L^{-1}) = \frac{(m-1)(x_1 + x_3 - y_1 - y_3)}{(x_1 - y_1)(x_3 - y_3) - (x_2 - y_2)^2} + \frac{c+d}{cd - e^2}; \quad (4.14)$$

where, $c = x_1 + (m-1)y_1$, $e = x_2 + (m-1)y_2$ *and* $d = x_3 + (m-1)y_3$.

Proof: It is not difficult to show that L has the eigenvalues κ_i(i=1,2,...,2m), given in Table 4.1. Substituting eigenvalues from the table into $tr(L^{-1}) = \sum_{i=1}^{2m} \kappa_i^{-1}$, we will get the solution and the lemma is proved.♣

Table 4.1: Eigenvalues of L

Eigenvalue(κ_i)	multiplicities
$\frac{(x_1-y_1)+(x_3-y_3)+\sqrt{((x_1-y_1)-(x_3-y_3))^2+4(x_2-y_2)^2}}{2}$	m-1
$\frac{(x_1-y_1)+(x_3-y_3)-\sqrt{((x_1-y_1)-(x_3-y_3))^2+4(x_2-y_2)^2}}{2}$	m-1
$\frac{c+d+\sqrt{(c-d)^2+4e^2}}{2}$	1
$\frac{c+d-\sqrt{(c-d)^2+4e^2}}{2}$	1

Corollary 4.2 *If L is a positive definite matrix then* $(x_1 - y_1) + (x_3 - y_3)$, $(x_1 - y_1)(x_3 - y_3) - (x_2 - y_2)^2$, $c + d$ *and* $cd - e^2$ *are all positive.*

Proof: Each of the four expressions can be obtained as either a sum of a pair of eigenvalues of L or a product. Hence provided L is positive definite, they are positive.♣

In order to express $tr(\bar{M}^{-1})$ in terms of combinatorial features of the design, we employ the following further notation:

$$D_A = \sum_{i=1}^{n-1}\sum_{j=1}^{b} n_{Aij}^2,\ D_D = \sum_{i=1}^{n-1}\sum_{j=1}^{b} n_{Dij}^2,\ D_{AD} = \sum_{i=1}^{n-1}\sum_{j=1}^{b} n_{Aij}n_{Dij},$$

$$S_A = \sum_{j=1}^{b} T_{Aj}^2\ ,\ S_D = \sum_{j=1}^{b} T_{Dj}^2\ ,\ S_B = \sum_{j=1}^{b} T_{Bj}^2,$$

$$S_{AD} = \sum_{j=1}^{b} T_{Aj}T_{Dj}\ ,\ S_{AB} = \sum_{j=1}^{b} T_{Aj}T_{Bj},$$

$$d_A = \frac{T_A}{n-1} - \frac{D_A}{k(n-2)} + \frac{S_A}{k(n-1)(n-2)}, \tag{4.15}$$

$$d_D = \frac{T_D}{n-1} - \frac{D_D}{k(n-2)} + \frac{S_D}{k(n-1)(n-2)},$$

$$d_{AD} = \frac{D_{AD}}{k(n-2)} - \frac{S_{AD}}{k(n-1)(n-2)},$$

$$q_A = \frac{T_A}{n-1} - \frac{S_A}{k(n-1)}\ ,\ q_D = \frac{T_D}{n-1} - \frac{S_D}{k(n-1)}\ ,\ q_B = \frac{T_B}{n-1} - \frac{S_B}{k(n-1)},$$

$$q_{AD} = \frac{S_{AD}}{k(n-1)}\ ,\ q_{AB} = \frac{S_{AB}}{k(n-1)}.$$

The following result expresses the design-dependent bound $tr(\bar{M}^{-1})$ as a function of the elements of the incidence matrix of the design.

Lemma 4.4 *Let $\bar{M}$ be the matrix given in Lemma 4.2, then*

$$tr(\bar{M}^{-1}) = (n-2)f_1(n_{Aij}, n_{Dij}) + f_0(T_{Aj}, T_{Bj}), \tag{4.16}$$

where

$$f_1(n_{Aij}, n_{Dij}) = \frac{2d_A + d_D - 2d_{AD}}{d_A d_D - d_{AD}^2}, \tag{4.17}$$

and

$$f_0(T_{Aj}, T_{Bj}) = \frac{q_A + q_B}{q_A q_B - q_{AB}^2}, \tag{4.18}$$

where d_A, d_D, d_{AD}, q_A, q_B and q_{AB} are defined in (4.15).

Proof: From Corollary 4.1 and Lemma 4.3 the result follows.♣

Corollary 4.3 *If design d in Theorem 4.1 is a PBDS design, then the inequality in (4.5) become equality.*

Proof: By Corollary 2.1(page 44), since d is a PBDS design, the structure of its information matrix for the estimators of the contrast of interest, M, is the same as the structure of L given in Lemma 4.3. The proof follows from here.♣

We now seek the minimum value of the design-dependent bound $tr(\bar{M}^{-1})$ over all designs having particular values for b, k and t. This will give a very tight bound for $k \geq 4$(see Table 4.2) and, more importantly, a means of identifying efficient designs, since any design which achieves this minimum value must be highly efficient.

4.3 Finding Minimum Values for the $tr(\bar{M}^{-1})$:

In order to find the A-optimal designs in the class of $n \times 2$ CFBD(00) designs, we need to characterize those designs which minimize $tr(\bar{M}^{-1})$, given in (4.16). In this section we try to minimize this design-dependent bound over all possible designs in $n \times 2$ CFBD(00). In other words our task in this section is to find those values of n_{Aij}'s, n_{Dij}'s, T_{Bj}'s and T_{Aj}'s which minimize $f_0(T_{Aj}, T_{Bj})$ and $f_1(n_{Aij}, n_{Dij})$, given in (4.17) and (4.18) respectively. Unfortunately $tr(\bar{M}^{-1})$ is a nonlinear multivariate function of discrete variables and no computer package was found which was able to minimize it. Now we give some analytical results which in some cases simplify our object function.

Lemma 4.5 *For any block design $d \in n \times 2$ CFBD(00) the following expressions, formed from the above functions are always positive:*

$$d_A,\ \ d_D,\ \ q_A,\ \ q_B,\ \ q_Aq_B - q_{AB}^2, \tag{4.19}$$

$$d_Ad_D - d_{AD}^2,\ \ d_A + d_D - 2d_{AD},\qquad 2d_A + d_D - 2d_{AD}.$$

Proof: The diagonal elements of the A-matrix of the design for treatment i belonging to set A satisfies:

$$r_{Ai} - \frac{1}{k}\sum_{j=1}^{b} n_{Aij}^2 \geq r_{Ai} - \sum_{j=1}^{b} n_{Aij} = 0. \tag{4.20}$$

This implies that

$$\sum_{i=1}^{n-1}(r_{Ai} - \frac{1}{k}\sum_{j=1}^{b} n_{Aij}^2) = T_A - \frac{1}{k}\sum_{i=1}^{n-1}\sum_{j=1}^{b} n_{Aij}^2 \geq 0. \tag{4.21}$$

But after some algebra d_A can be written as follows:

$$d_A = \frac{1}{p}\left\{T_A - \frac{1}{k}\sum_{i=1}^{n-1}\sum_{j=1}^{b} n_{Aij}^2\right\} + \frac{1}{kp(n-2)}\sum_{j=1}^{b}\left\{T_{Aj}^2 - \sum_{i=1}^{n-1} n_{Aij}^2\right\}, \tag{4.22}$$

where p=n-1 and the first term on the RHS is positive by (4.21). The second term is also positive, since we have

$$T_{Aj}^2 = \left\{\sum_{i=1}^{n-1} n_{Aij}\right\}^2 = \sum_{i=1}^{n-1} n_{Aij}^2 + \sum_{i=1}^{n-1}\sum_{l\neq i}^{n-1} n_{Aij}n_{Alj} \geq \sum_{i=1}^{n-1} n_{Aij}^2. \tag{4.23}$$

By the same approach we can prove that $d_D > 0$.

It can be shown that

$$q_A = \frac{1}{k(n-1)}\sum_{j=1}^{b} T_{Aj}(k - T_{Aj}). \tag{4.24}$$

Since $0 \leq T_{Aj} \leq k$, it follows that $q_A > 0$. To prove $q_B > 0$ the same approach can be utilized. To establish that the other expressions in the statement of the lemma are positive, notice that $d_A d_D - d_{AD}^2$, $d_A + d_D - 2d_{AD}$ and $q_A q_B - q_{AB}^2$ are all either products or sum of the eigenvalues of the positive definite matrix, $\bar{M}$. Then by Corollaries 4.1 and 4.2, the lemma is proved.♣

In the following two sections we first assume that the T_{Aj}'s and T_{Dj}'s are fixed and consider the behaviour of $f_1(n_{Aij}, n_{Dij})$. Then we assume T_A and T_D are fixed and minimize $f_0(T_{Aj}, T_{Bj})$.

4.3.1 Minimizing $f_1(n_{Aij}, n_{Dij})$:

In this section we assume that the T_{Aj}'s and T_{Bj}'s are fixed(and hence $T_{Bj} = k - T_{Aj} - T_{Dj}$ is also fixed)(j=1,2,...,b), then try to obtain the minimum value of $f_1(n_{Aij}, n_{Dij})$, defined in (4.17). First, we prove that if either the T_{Aj}'s(j=1,2,...,b) or the T_{Bj}'s(j=1,2,...,b) are divisible by p=n-1, f_1 is minimized when the replications of the treatment combinations belonging to set A are as near equal as possible in each block, i.e. $|n_{Aij} - n_{Ai'j}| \leq 1$ for $i \neq i'$ and j=1,2,...,b and the same is true for the treatment combinations belonging to set D. We then state the conjecture that if neither the T_{Aj}'s nor the T_{Dj}'s are divisible by n-1, the same conditions on the treatment replications ensure the minimization of f_1. Therefore to minimize f_1 we consider 3 separate cases:

1. Each T_{Aj}, T_{Dj}(j=1,2,...,b) is divisible by p.
2. Exactly one of the sets $\{T_{Aj}; j = 1,2,...,b\}$ and $\{T_{Dj}; j = 1,2,...,b\}$ has every element divisible by p.
3. Neither set in 2 has every element divisible by p.

- **CASE I**

For minimizing $f_1(n_{Aij}, n_{Dij})$, in this case the following lemma is needed.

Lemma 4.6 *Suppose we have the following function:*

$$g(x_{ij}, y_{ij}) = \frac{2d_x - 2d_{xy} + d_y}{d_x d_y - d_{xy}^2}, \tag{4.25}$$

in which $(d_x d_y - d_{xy}^2 \neq 0)$, where x_{ij} and y_{ij} are independent variables, such that

$$\textstyle\sum_{i=1}^p x_{ij} = 0, \quad \sum_{i=1}^p y_{ij} = 0, \quad d_{xy} = z\sum_{j=1}^b \sum_{i=1}^p x_{ij} y_{ij}, \tag{4.26}$$
$$\textstyle d_x = d_1 - z\sum_{j=1}^b \sum_{i=1}^p x_{ij}^2, \quad d_y = d_2 - z\sum_{j=1}^b \sum_{i=1}^p y_{ij}^2,$$

where d_1, d_2 and z are positive constants, then $g(x_{ij}, y_{ij})$ is minimized when $x_{ij} = y_{ij} = 0$, for i=1,2,...,p and j=1,2,...,b.

Proof: Note that the function $g(x_{ij}, y_{ij})$ is well-defined since $d_x d_y - d_{xy}^2 \neq 0$. To prove the lemma we first show that $x_{ij} = y_{ij} = 0$ is the only critical point of $g(x_{ij}, y_{ij})$. Then we establish that the Hessian(see Lang,1983,p376) of $g(x_{ij}, y_{ij})$ for the critical point is always positive.

In order to find the critical point of $g(x_{ij}, y_{ij})$, we employ the Lagrange Multipliers λ_{xj}, λ_{yj}(j=1,2,...,b), and define:

$$\phi = g(x_{ij}, y_{ij}) + \sum_{j=1}^{b}(\lambda_{xj}\sum_{i=1}^{p} x_{ij} + \lambda_{yj}\sum_{i=1}^{p} y_{ij}). \tag{4.27}$$

Then we have

$$\partial\phi/\partial x_{ij} = \frac{-2z(2x_{ij}+y_{ij})w}{w^2} + \frac{2z(2d_x - 2d_{xy} + d_y)(d_{xy}y_{ij} + d_y x_{ij})}{w^2} + \lambda_{xj}, \tag{4.28}$$

and

$$\partial\phi/\partial y_{ij} = \frac{-2z(x_{ij}+y_{ij})w}{w^2} + \frac{2z(2d_x - 2d_{xy} + d_y)(d_{xy}x_{ij} + d_y y_{ij})}{w^2} + \lambda_{yj},$$

where $w = d_x d_y - d_{xy}^2$.

By setting these two derivatives to zero and summing over i, we obtain $\lambda_{xj} = \lambda_{yj} = 0$ for j=1,2,...,b. Since $d_x d_y - d_{xy}^2 \neq 0$, the resulting equations are:

$$\begin{aligned} -2z(2x_{ij}+y_{ij})w + 2z(2d_x - 2d_{xy} + d_y)(d_{xy}y_{ij} + d_y x_{ij}) &= 0, \\ -2z(x_{ij}+y_{ij})w + 2z(2d_x - 2d_{xy} + d_y)(d_{xy}x_{ij} + d_y y_{ij}) &= 0, \end{aligned} \tag{4.29}$$

for i=1,2,...,p and j=1,2,...,b.

In matrix form these equations are:

$$\begin{bmatrix} d_x d_y + d_{xy}^2 - 2d_x d_{xy} - d_{xy}d_y & -d_{xy}^2 - 2d_x^2 + 2d_x d_{xy} \\ -2d_{xy}^2 + 2d_{xy}d_y - d_y^2 & d_x d_y + d_{xy}^2 - 2d_x d_{xy} - d_{xy}d_y \end{bmatrix} \begin{bmatrix} x_{ij} \\ y_{ij} \end{bmatrix} = \underline{0}_2. \tag{4.30}$$

If the matrix of coefficients is nonsingular, then $x_{ij} = y_{ij} = 0$ is the unique solution to (4.30). It can be shown that the determinant of this matrix is $-(d_x d_y - d_{xy}^2)^2 \neq 0$. Therefore the proof of the first part is established. Also it can be shown that the Hessian(see Lange,1983,p376) of function g at the critical point is

$$H(g)(00...0) = 2zI_u \otimes W,$$

where

$$W = \begin{pmatrix} d_1^{-2} & -d_1^{-1}d_2^{-1} \\ -d_1^{-1}d_2^{-1} & 2d_2^{-1} \end{pmatrix},$$

and u=b(n-1). By assuming that z, d_1 and q_1 are all positive, it can be shown that W is a positive definite matrix. This implies that $H(g)(00...0)$ is a positive definite matrix. Therefore by Corwin and Szczarba(1982,p194) the critical point (00...0) is a global minimum. This completes the proof.♣

Theorem 4.2 *For fixed values of T_{Aj} and T_{Dj}(j=1,2, ..., b), if $T_{Aj} \equiv 0 \bmod(p)$ and $T_{Dj} \equiv 0 \bmod(p)$, then the function $f_1(n_{Aij}, n_{Dij})$ given in (4.17) is minimized if*

$$n_{Aij} = \frac{T_{Aj}}{p} \quad and \quad n_{Dij} = \frac{T_{Dj}}{p}. \tag{4.31}$$

Proof: In the expression for $f_1(n_{Aij}, n_{Dij})$, d_A, d_D and d_{AD} can be reformulated as follows:

$$d_A = \frac{T_A}{p} - \frac{1}{k(n-2)} \sum_{j=1}^{b} \sum_{i=1}^{p} (\frac{T_{Aj}}{p} - n_{Aij})^2,$$

$$d_D = \frac{T_D}{p} - \frac{1}{k(n-2)} \sum_{j=1}^{b} \sum_{i=1}^{p} (\frac{T_{Dj}}{p} - n_{Dij})^2, \tag{4.32}$$

$$d_{AD} = \frac{1}{k(n-2)} \sum_{j=1}^{b} \sum_{i=1}^{p} (\frac{T_{Aj}}{p} - n_{Aij})(\frac{T_{Dj}}{p} - n_{Dij}),$$

where p=n-1.

Now let $x_{ij} = \frac{1}{p}T_{Aj} - n_{Aij}$ and $y_{ij} = \frac{1}{p}T_{Dj} - n_{Dij}$. Then by applying Lemma 4.6, the only critical point for the function f_1 is (0,0), i.e. $n_{Aij} = T_{Aj}/p$ and $n_{Dij} = T_{Dj}/p$. Hence if $T_{Aj} \equiv 0 \ mod(p)$ and $T_{Dj} \equiv 0 \ mod(p)$, the theorem is proved.♣

Corollary 4.4 *If the conditions in the statement of Theorem 4.2 are satisfied, i.e. $T_{Aj} \equiv 0 \bmod(n-1)$ and $T_{Dj} \equiv 0 \bmod(n-1)$, then*

$$\min \ f_1(n_{Aij}, n_{Dij}) = (n-1)(1/T_A + 2/T_D). \tag{4.33}$$

Proof: Follows from Theorem 4.2.♣

- **CASE II**

Theorem 4.3 *If in an $n \times 2$ CFBD(00) design d, the T_{Aj}/p's(or T_{Dj}/p's) are integers for j=1,2,...,b and if $n_{Aij} = T_{Aj}/p$(or $n_{Dij} = T_{Dj}/p$) for i=1,2,...,p and j=1,2,...,b, where p=n-1. Then by assuming T_{Aj} and T_{Dj} are fixed, f_1 is minimized if*

$$\begin{aligned} n_{Dij} &= \left[\frac{T_{Dj}}{p}\right] \quad or \quad \left[\frac{T_{Dj}}{p}\right] + 1, \\ (\ or\ n_{Aij} &= \left[\frac{T_{Aj}}{p}\right] \quad or \quad \left[\frac{T_{Aj}}{p}\right] + 1) \end{aligned} \tag{4.34}$$

Proof: If $n_{Aij} = T_{Aj}/p$, where T_{Aj}/p is an integer for i=1, 2, ..., p and j=1, 2, ..., b, then $d_A = T_A/p$ is a constant and $d_{AD} = 0$. Therefore $f_1 = 1/d_A + 2/d_D$. In order to minimize f_1 we must maximize d_D. From (4.15), since T_{Dj}'s are fixed, then $\sum_{i=1}^{p} n_{Dij}^2$ must be minimized subject to the condition T_{Dj} is fixed. By Cheng and Wu(1980, Lemma 2.3) the result follows. Similarly it can be proved for n_{Aij}'s.♣

- **CASE III**

As we mentioned earlier, the conditions $T_{Aj} \equiv 0 \ mod(p)$ and $T_{Dj} \equiv 0 \ mod(p)$ given in Theorem 4.2 cannot be met for $k < 2(n-1)$. Then the question is: if T_{Aj} and T_{Dj} are assumed to be fixed, which values of n_{Aij}'s and n_{Dij}'s(i=1, 2,... , p; j=1, 2,..., b) minimize f_1? Roughly speaking, Theorems 4.2 and 4.3 suggest that the values of n_{Aij}'s should be as equal as possible, i.e. $n_{Aij} = [T_{Aj}/p]$ or $[T_{Aj}/p] + 1$, where [.] denotes the integer part. The same suggestion can be made for n_{Dij}'s. Strictly speaking, we need to show that the function g given in Lemma 4.6 is a convex function, i.e. it must be shown that the Hessian of g, i.e. H(g) is a nonnegative definite matrix(see Roberts and Varberg,1973,p103). This is a difficult task, since H(g) is a parametric matix of order 2b(n-1). However, numerical computation indicates that this is the case. We give this intuitive result, backed up by computing results as the following conjecture.

Conjecture 4.1 *If in the statement of Theorem 4.2, both T_{Aj}/p and T_{Dj}/p (j=1,2,...,b) are not integers, then f_1 is minimized if*

$$\begin{aligned} n_{Aij} &= [T_{Aj}/p] \quad or \quad [T_{Aj}/p] + 1, \\ and \quad n_{Dij} &= [T_{Dj}/p] \quad or \quad [T_{Dj}/p] + 1, \end{aligned} \tag{4.35}$$

where p=n-1 and [.] denotes the "integer part of.".

Support for the conjecture has been found by examining the structure of A-optimal designs and observing that they have the conjectured replications for the treatments. This is illustrated in the following example.

Example 4.1 *For n=4, b=4 and k=3, the following design is the most efficient design generated by JE:*

Block1	*01*	*10*	*11*
Block2	*01*	*20*	*21*
Block3	*01*	*30*	*31*
Block4	*11*	*21*	*31*

In this highly efficient PBDS design(see Table 4.2 for an assessment of efficiency) we can see that $T_{D1} = T_{D2} = T_{D3} = 1$, $T_{D4} = 3$, $T_{A1} = T_{A2} = T_{A3} = 1$ *and* $T_{A4} = 0$. *In line with the conjecture we observe that* $n_{D11} = 1$, $n_{Di1} = 0$ *for i=2,3 and so on.*

If we assume that Conjecture 4.1 is true, then we can establish he following theorem which shows that for small block sizes($k \leq n-1$), the binary designs for the treatment combinations belonging to set $A \cup D$ are more efficient than the non-binary designs.

Theorem 4.4 *If d is an* $n \times 2$ *CFBD(00) design with block size* $k \leq n-1$ *which is non-binary for the treatment combinations in* $A \cup D$, *then there exists a design,* d^* *which is binary in* $A \cup D$ *with smaller total variance on the dual versus single treatment contrasts.*

Proof: Suppose that d$\in$ $n \times 2$ CFBD(00) has $k \leq n-1$, and suppose design d is not binary for treatment combinations belonging to $A \cup D$. Then if treatment combination i0, belonging to set A, appears more than once in a block, we substitute another treatment combination of set A which does not appear in the block, and keep the treatment combination i0 only once in the block. Suppose we repeat this substitution for each treatment combination belonging to set A and simultaneously, we do the same substitution for each treatment combination belonging to set D, and call the resulting design d^*. Obviously design d^* will be binary in terms of the treatment combinations belonging to set A and D. Since $T_{Aj} \leq k \leq n-1$ and $T_{Dj} \leq k \leq n-1$, the substitution guarantees that design d^* is binary. In making this substitution, the values of q_A, q_D and q_{AD} for both d and d^* remain the same. But in design d^*, the treatment combinations in each set A and D are replicated equally often in each block. Hence by Conjecture 4.1 it is more efficient relative to design d.♣

This result and hence the conjecture are supported by an example of a design with $k \leq n-1$

Example 4.2 *For n=6, b=10 and k=5(k≤n-1), the following design is the most efficient design which has been generated by JE:*

*Block*1	01	10	20	11	21	*Block*6	01	10	30	11	31
*Block*2	01	20	30	21	31	*Block*7	01	20	40	21	41
*Block*3	01	30	40	31	41	*Block*8	01	30	50	31	51
*Block*4	01	40	50	41	51	*Block*9	01	10	40	11	41
*Block*5	01	10	50	11	51	*Block*10	01	20	50	21	51,

This is binary in terms of treatment combinations 10, 20, 30, 40 and 50 and also 11, 21, 31, 41 and 51 with tr(V)=4.445.

The theorem is not true for $k > n - 1$, as demonstrated by the following example:

Example 4.3 *For n=3, b=3 and k=6, from JE, the A-optimal design in the PBDS class which has total variance 2.225 for the contrasts of interest is not binary(see Table 4.2). If we replace the treatment combination 11 in the first block by 01 and the treatment combination 21 in the second block by 01, the design changes to:*

*Block*1	01	01	11	21	10	20
*Block*2	01	01	11	21	10	20
*Block*3	01	01	11	21	10	20

which is binary for the sets A and D. However it has total variance 2.3333 for the contrasts of interest which shows it is not as efficient as the design in Table 4.2.

Now we are in position to give a theorem which gives a reformulation of d_A, d_D and the domain of d_{AD} when the treatment combinations belonging to sets A and D are replicated equally often in each block. The proof of this theorem is given in Appendix A at the end of the thesis.

Theorem 4.5 *Let $a_{Aj} = [T_{Aj}/p]$ and $a_{Dj} = [T_{Dj}/p]$, denote the integer parts of T_{Aj}/p and T_{Dj}/p respectively. Also let $b_{Aj} = T_{Aj} - pa_{Aj}$ and $b_{Dj} = T_{Dj} - pa_{Dj}$, the n_{Aij}'s be either a_{Aj} or $a_{Aj} + 1$ and the n_{Dij}'s be either a_{Dj} or $a_{Dj} + 1$, where $\sum_{i=1}^{n-1} n_{Aij} = T_{Aj}$ and $\sum_{i=1}^{n-1} n_{Dij} = T_{Dj}$. Then:*

$$d_A = \tfrac{T_A}{n-1} - \tfrac{1}{k(n-1)(n-2)} \sum_{j=1}^{b} b_{Aj}(n-1-b_{Aj}),$$

$$d_D = \tfrac{T_D}{n-1} - \tfrac{1}{k(n-1)(n-2)} \sum_{j=1}^{b} b_{Dj}(n-1-b_{Dj}), \tag{4.36}$$

$$d_{AD} \in (u, v),$$

where

$$v = \frac{1}{k(n-2)} \sum_{j=1}^{b} \{min(b_{Aj}, b_{Dj}) - \frac{1}{n-1} b_{Aj} b_{Dj}\}, \tag{4.37}$$

and

$$u = \frac{1}{k(n-2)} \sum_{j=1}^{b} \{max(0, b_{Aj} + b_{Dj} - n + 1) - \frac{1}{n-1} b_{Aj} b_{Dj}\}. \tag{4.38}$$

Conclusion 4.1 *Provided the Conjecture 4.1 is true, we conclude that, subject to assuming T_{Aj} and T_{Dj} are fixed, the function $f_1(n_{Aij}, n_{Dij})$ is minimized if $n_{Aij} = a_{Aj} + 1$ or a_{Aj}, and $n_{Dij} = a_{Dj} + 1$ or a_{Dj}. It is clear that if T_{Aj} and T_{Dj} are fixed, then a_{Aj}, b_{Aj}, a_{Dj} and b_{Dj} are all constants. This implies that d_A and d_D are constants while, as has been shown in Theorem 4.5, d_{AD} is varying across a domain whose boundaries depend on T_{Aj} and T_{Dj}.*

Now we want to consider the behaviour of the function

$$f(d_{AD}) = \frac{2d_A - 2d_{AD} + d_D}{d_A d_D - d_{AD}^2}$$

for fixed values of T_{Aj}'s and T_{Dj}'s under the assumptions that the conditions on n_{Aij}'s and n_{Dij}'s in the statement of the Theorem 4.5 are satisfied. It must be reiterated here that, under these conditions, d_A and d_D are fixed, while d_{AD} is not fixed. We have:

$$\partial f(d_{AD})/\partial d_{AD} = \frac{-2\{d_{AD}^2 - d_{AD}(2d_A + d_D) + d_A d_D\}}{(d_A d_D - d_{AD}^2)^2}. \tag{4.39}$$

We need to find the sign of this function in terms of d_{AD} in the domain which is given in Theorem 4.5. The sign of this function is equivalent to the sign of

$$-d_{AD}^2 + d_{AD}(2d_A + d_D) - d_A d_D. \tag{4.40}$$

It can be shown that v in (4.37) is always positive, while u in (4.38) can be positive or negative. Hence d_{AD} can take both positive and negative values. In order to determine the sign of the expression in (4.40) two cases have to be considered. If d_{AD} is negative, the sign is negative. If this is the case d_{AD} must be maximized in order to minimize f_1. But if d_{AD} is positive, we have not been able to determine the sign of (4.40) analytically, since it is a complicated function. This is not a major problem in establishing a bound and an A-optimal design, since it can be solved by using a computer algorithm numerically. We will discuss this further later in the chapter.

Our next task is to pursue analytically the minimization of $f_0(T_{Aj}, T_{Bj})$.

4.3.2 Minimizing $f_0(T_{Aj}, T_{Bj})$:

In this section we will consider the behaviour of $f_0(T_{Aj}, T_{Dj})$. To minimize $f_0(T_{Aj}, T_{Bj})$, 3 separate cases are considered:

1. Both T_A and T_B are divisible by b.
2. Exactly one of T_A and T_B is divisible by b.
3. Neither T_A nor T_B is divisible by b.

- Case I

  The following lemma is needed.

Lemma 4.7 *Suppose we have the following function:*

$$g(x_j, y_j) = \frac{d_x + d_y}{d_x d_y - d_{xy}^2}, \tag{4.41}$$

in which $d_x d_y - d_{xy}^2 > 0$, where x_j and y_j are independent variables, such that

$$\textstyle\sum_{j=1}^{p} x_j = 0, \quad \sum_{j=1}^{p} y_j = 0, \quad d_x = d_1 - z\sum_{j=1}^{b} x_j^2 \tag{4.42}$$
$$d_{xy} = d_3 + z\textstyle\sum_{j=1}^{b} x_j y_j, \quad d_y = d_2 - z\sum_{j=1}^{b} y_j^2,$$

d_1, d_2, d_3, z are positive constants, d_x and d_y are positive. Then $g(x_j, y_j)$ is minimized when $x_j = y_j = 0$, for j=1,2,...,b.

Proof: Note that the function $g(x_j, y_j)$ is well-defined since $d_x d_y - d_{xy}^2 \neq 0$. To prove the lemma we first show that $x_j = y_j = 0$ is the only critical point of $g(x_j, y_j)$. Then we show that the Hessian of $g(x_j, y_j)$ for the critical point is always positive definite.

In order to find the critical point of $g(x_j, y_j)$, we employ Lagrange Multipliers λ_x and λ_y, and define:

$$\phi = g(x_j, y_j) + \lambda_x(\sum_{j=1}^{b} x_j) + \lambda_y(\sum_{j=1}^{b} y_j). \tag{4.43}$$

Then we have

$$\begin{aligned} \partial\phi/\partial x_j &= \frac{2z\{x_j(d_{xy}^2 + d_y^2) + y_j d_{xy}(d_x + d_y)\}}{(d_x d_y - d_{xy}^2)^2} + \lambda_x \\ \partial\phi/\partial y_j &= \frac{2z\{y_j(d_{xy}^2 + d_x^2) + x_j d_{xy}(d_x + d_y)\}}{(d_x d_y - d_{xy}^2)^2} + \lambda_y. \end{aligned} \tag{4.44}$$

By setting these two derivatives to zero and summing over j, we obtain $\lambda_x = \lambda_y = 0$. Since by assumption $z > 0$ and $d_x d_y - d_{xy}^2 > 0$, the resulting equations are:

$$\begin{aligned} (d_y^2 + d_{xy}^2)x_j + d_{xy}(d_x + d_y)y_j &= 0, \\ d_{xy}(d_x + d_y)x_j + (d_x^2 + d_{xy}^2)y_j &= 0. \end{aligned} \tag{4.45}$$

In matrix form these equations are:

$$\begin{pmatrix} d_y^2 + d_{xy}^2 & d_{xy}(d_x + d_y) \\ d_{xy}(d_x + d_y) & d_x^2 + d_{xy}^2 \end{pmatrix} \begin{pmatrix} x_j \\ y_j \end{pmatrix} = \underline{0}_2. \tag{4.46}$$

If the matrix of coefficients is nonsingular, then $x_j = y_j = 0$ is the unique solution to that equations. It can be shown that the determinant of this matrix is $-(d_x d_y - d_{xy}^2)^2 \neq 0$. Therefore the proof of the first part is established. Also it can be shown that the Hessian of function g at the critical point is

$$H(g)(00...0) = 2zI_b \otimes W,$$

where

$$W = \frac{1}{(d_1 d_2 - d_3^2)^4} \begin{pmatrix} d_2^2 + d_3^2 & d_3(d_1 + d_2) \\ d_3(d_1 + d_2) & d_1^2 + d_3^2 \end{pmatrix}.$$

Further it can be shown that W is a positive definite matrix. This implies that $H(g)(00...0)$ is a positive definite matrix. Therefore by Corwin and Szczarba(1982,p194) the critical point (00...0) is a global minimum. This completes the proof.♣

Theorem 4.6 *For fixed values of T_A and T_D (and consequently a fixed value of $T_B = bk - T_A - T_D$), if T_A/b and T_B/b are integers, the function $f_0(T_{Aj}, T_{Bj})$ given in (4.18) is minimized if:*

$$T_{Aj} = \frac{T_A}{b} \quad and \quad T_{Bj} = \frac{T_B}{b}. \tag{4.47}$$

Proof: We can show that

$$\begin{aligned} \textstyle\sum_{j=1}^b T_{Aj}^2 &= \textstyle\sum_{j=1}^b (T_{Aj} - \frac{T_A}{b})^2 + \frac{T_A^2}{b}, \\ \textstyle\sum_{j=1}^b T_{Bj}^2 &= \textstyle\sum_{j=1}^b (T_{Bj} - \frac{T_B}{b})^2 + \frac{T_B^2}{b}, \\ \textstyle\sum_{j=1}^b T_{Aj}T_{Bj} &= \textstyle\sum_{j=1}^b (T_{Aj} - \frac{T_A}{b})(T_{Bj} - \frac{T_B}{b}) + \frac{T_A T_B}{b}. \end{aligned} \tag{4.48}$$

Based on these we have

$$\begin{aligned} q_A &= \tfrac{T_A}{p}(1 - \tfrac{T_A}{bk}) - \tfrac{1}{kp}\textstyle\sum_{j=1}^b (T_{Aj} - \frac{T_A}{b})^2, \\ q_B &= \tfrac{T_B}{p}(1 - \tfrac{T_B}{bk}) - \tfrac{1}{kp}\textstyle\sum_{j=1}^b (T_{Bj} - \frac{T_B}{b})^2, \\ q_{AB} &= \tfrac{T_A T_B}{bkp} + \tfrac{1}{kp}\textstyle\sum_{j=1}^b (T_{Aj} - \frac{T_A}{b})(T_{Bj} - \frac{T_B}{b}). \end{aligned} \tag{4.49}$$

Now let $x_j = \frac{1}{b}T_A - T_{Aj}$ and $y_j = \frac{1}{b}T_B - T_{Bj}$. Then by applying Lemma 4.7, the only critical point for the function f_0 is (0,0), i.e. $T_{Aj} = T_A/b$ and $T_{Bj} = T_B/b$. Hence if $T_A \equiv 0 \ mod(b)$ and $T_B \equiv 0 \ mod(b)$, then f_0 is minimized and the theorem is proved.♣

Corollary 4.5 *If the conditions in the statement of Theorem 4.6 are satisfied and if T_A and T_B are both divisible by b, then*

$$\min f_0(T_{Aj}, T_{Dj}) = (n-1)(1/T_A + 1/T_B + 2/T_D). \tag{4.50}$$

Proof: The proof follows immediately from the proof of Theorem 4.6.♣

- **Case II**

In this case if T_A is divisible by b, then the following theorem shows that if the numbers of units assigned to A within each block are equal, then in order to minimize $f_0(T_{Aj}, T_{Dj})$, the treatment combination 01 should be replicated as near equally as possible between the blocks. The same result is true when A is replaced by B.

Theorem 4.7 *If, in an $n \times 2$ CFBD(00) design, T_A and T_B are assumed to be constants and $T_{Aj} = T_A/b$ (or $T_{Bj} = T_B/b$) for j=1,2,...,b, where T_A/b (or T_B/b) is integer, then f_0 is minimized if*

$$T_{Bj} = \left[\tfrac{T_B}{b}\right] \quad or \quad \left[\tfrac{T_B}{b}\right] + 1, \qquad (\ or \quad T_{Aj} = \left[\tfrac{T_A}{b}\right] \quad or \quad \left[\tfrac{T_A}{b}\right] + 1) \tag{4.51}$$

for j=1,2,...,b.

Proof: If $T_{Aj} = T_A/b$ is an integer for j=1,2,...,b, then $q_A = T_A(bk - T_A)/(pbk)$ and $q_{AB} = T_A T_B/(pbk)$ are constants since T_A and T_B are constants. Therefore f_0 is only a function of a single variable q_B. Hence

$$\frac{\partial f_0}{\partial q_B} = \frac{-q_A^2 - q_{AB}^2}{(q_A q_B - q_{AB}^2)^2}. \tag{4.52}$$

This derivative is always negative, i.e. f_0 is minimized if q_B is maximized, and q_B is maximized if $\sum_{j=1}^{b} T_{Bj}^2$ is minimized. Since T_B is assumed fixed, then by Lemma 2.3 of Cheng and Wu(1980) the result follows. The result for T_{Aj}(j=1,2,...,b) is proved in a similar way.♣

- **Case III**

Now suppose the conditions of Theorems 4.6 and 4.7 cannot be satisfied. We then ask the question: which values of the T_{Aj}'s and the T_{Bj}'s minimize f_0, if T_A and T_B are assumed to be fixed? The same argument which was made for the n_{Aij}'s and n_{Dij}'s on page 97, can be made for the T_{Aj}'s and T_{Dj}'s. Based on this argument we give the following conjecture which is analogous to Conjecture 4.1.

Conjecture 4.2 *If we assume that T_A and T_B are fixed, then f_0 is minimized if*

$$T_{Aj} = [T_A/b] \quad or \quad [T_A/b] + 1,$$
$$and \quad T_{Bj} = [T_B/b] \quad or \quad [T_B/b] + 1. \tag{4.53}$$

Let a_A and a_B denote the integer part of T_A/b and T_B/b respectively, $b_A = T_A - ba_A$ and $b_B = T_B - ba_B$. Then in the following corollary, we prove that when T_A and T_B are fixed, if $T_{Aj} = a_A + 1$ or a_A and $T_{Bj} = a_B + 1$ or a_B, then q_A and q_B are fixed, while q_{AB} is not fixed. Then we show that, provided that Conjecture 4.2 is true, $f_0(T_{Aj}, T_{Bj})$ is minimized if q_{AB} is minimized.

Corollary 4.6 *Suppose T_A and T_B are fixed, then provided Conjecture 4.2 is true,*

$$q_A = \frac{a_A(bk - T_A - b_A) + b_A(k-1)}{k(n-1)}, q_B = \frac{a_B(bk - T_B - b_B) + b_B(k-1)}{k(n-1)}, \tag{4.54}$$

and $q_{AB} \in (z, w)$, where

$$w = \frac{a_A T_B + a_B b_A + min(b_A, b_B)}{k(n-1)}, z = \frac{a_A T_B + a_B b_A + max(0, b_A + b_B - b)}{k(n-1)}, \tag{4.55}$$

and f_0 is minimized when $q_{AB} = z$.

Proof: Provided Conjecture 4.2 is true, then it can be shown that

$$S_A = \textstyle\sum_{j=1}^{b} T_{Aj}^2 = a_A(T_A + b_A) + b_D,$$
$$\text{and} \quad S_B = \textstyle\sum_{j=1}^{b} T_{Bj}^2 = a_B(T_B + b_B) + b_B. \tag{4.56}$$

Substituting from this into (4.15) for S_A and S_B we will obtain (4.54). By Marshall and Olkin(1979) it can be shown that

$$q_{AB} \leq \tfrac{a_A T_B + a_B b_A + min(b_A, b_B)}{k(n-1)},$$
$$q_{AB} \geq \tfrac{a_A T_B + a_B b_A + max(0, b_A + b_B - b)}{k(n-1)}. \tag{4.57}$$

Since under the given conditions q_A and q_B are fixed, it follows that f_0 is minimized if q_{AB} is minimized. The proof follows from here.♣

Conclusion 4.2 *By assuming T_A and T_B are fixed, the minimum value of $f_0(T_{Aj}, T_{Dj})$ is a function of T_A and T_B only, provided the Conjecture 4.2 is true.*

4.3.3 Minimizing $f_1 + f_0$:

In this section we assume T_A and T_D are fixed and consider the minimum of $tr(\bar{M}^{-1})$. Then give a theorem which is a result derived from Theorems 4.2 and 4.6 and does not require the above conjectures.

Theorem 4.8 *For any $n \times 2$ CFBD(00) design, d, if $n_{Aij} = n_A$, $n_{Dij} = n_D$ (i=1, 2, ..., n-1; j=1, 2, ..., b) and*

$$f(n_A, n_D) = \min \{f(x,y); (x,y) \in \Xi\}; \tag{4.58}$$

where

$$f(x,y) = \frac{2}{x} + \frac{1}{y} + \frac{1}{k - p(x+y)},$$

and

$$\Xi = \{(x,y), (x,y) \in (N^+, N^+); p(x+y) < k\},$$

then design d is overall A-optimal.

<u>Proof</u>: In Theorem 4.1 we show that for any $n \times 2$ CFBD(00) design, we have:

$$tr(C\Omega C') \geq (n-2) f_1(n_{Aij}, n_{Dij}) + f_0(T_{Aj}, T_{Bj}).$$

From Theorem 4.2 if all the n_{Aij}'s and n_{Dij}'s are equal then $f_1(n_{Aij}, n_{Dij})$ is minimized with

$$\min f_1(n_{Aij}, n_{Dij}) = (n-1)(\frac{2}{T_D} + \frac{1}{T_A}). \tag{4.59}$$

Also by Theorem 4.6 and Corollary 4.5, we have $T_{Aj} = (n-1)n_A$, $T_{Bj} = k - (n-1)(n_A + n_D)$ for j=1,2,...,b and

$$\min f_0(T_{Aj}, T_{Bj}) = (n-1)(\frac{1}{T_A} + \frac{2}{T_D} + \frac{1}{T_B}). \tag{4.60}$$

Therefore

$$tr(\bar{M}^{-1}) \geq \frac{p}{b}\left\{\frac{2}{n_D} + \frac{1}{n_A} + \frac{1}{k - p(n_A + n_D)}\right\}. \tag{4.61}$$

Hence design d which achieves $f(n_A, n_D)$ is overall A-optimal design.♣

Example 4.4 *For n=3, b=2 and k=5, a completely randomized block design*(n_{Aij} $= n_{Dij} = 1$) *is overall A-optimal.*

Example 4.5 *For n=3,* $3 \leq b \leq 6$ *and k=13, those designs with* $n_{Bj} = 3$, $n_{Aij} = 2$ *and* $n_{Dij} = 3$ *are overall A-optimal.*

The following lemma which does not depend on the conjecture is needed to prove the next theorem, which gives a short cut to compute the bound whenever it is applicable.

Lemma 4.8 *Suppose in design d,* q_A, q_B, q_D, q_{AB}, q_{AD} *are defined as in (4.15), then*

$$\frac{q_A + q_B}{q_A q_B - q_{AB}^2} = \frac{2q_A + q_D - 2q_{AD}}{q_A q_D - q_{AD}^2}. \tag{4.62}$$

Proof: See Appendix A at the end of the thesis.

Discussion 4.1 *Provided that Conjecture 4.1 is true, we have shown that, by assuming* T_{Aj} *and* T_{Dj} *are fixed, the minimum of* $f_1(n_{Aij}, n_{Dij})$ *is not a constant but depends on* T_{Aj} T_{Dj} *and* $\sum_{i=1}^{n-1}\sum_{j=1}^{b} n_{Aij}n_{Dij}$. *Since the latter term is located in a set bounded by functions of* T_{Aj} *and* T_{Dj}, *we can denote the function* f_1 *by* $F_1(T_{Aj}, T_{Dj})$, *say. As discussed in Conclusion 4.1 this is a very complicated function. But by using a computer algorithm we can find those values of* $\sum_{i=1}^{n-1}\sum_{j=1}^{b} n_{Aij}n_{Dij}$ *which minimize* f_1. *Therefore we can assume that* $F_1(T_{Aj}, T_{Dj})$ *is fixed for fixed values of* T_{Aj} *and* T_{Dj}. *Therefore under this condition,* $F_1(T_{Aj}, T_{Dj}) + f_0(T_{Aj}, T_{Dj})$ *is a bound which does depend on* T_{Aj} *and* T_{Dj}. *By assuming* T_A *and* T_B *are fixed we then considered the behaviour of* $f_0(T_{Aj}, T_{Bj})$ *under the assumption that Conjecture 4.2 is true. The problem which remains to be solved is to consider the behaviour of* $F_1(T_{Aj}, T_{Dj})$ *when* T_A *and* T_D *are taken as fixed. This is a very complicated problem. It should be noted here that the members of staff of the department who deal with the minimization of nonlinear objective functions with integers, knew of no computer package which can be used to minimize* $tr(\bar{M}^{-1})$ *for integer values of* n_{Aij} *and* n_{Dij}. *However numerical computation suggests that the behaviour of* $F_1(T_{Aj}, T_{Dj})$ *is in the same direction as the behaviour of* $f_0(T_{Aj}, T_{Bj})$ *given in Conjecture 4.2. This led to the following conjecture.*

Conjecture 4.3 *Assume that T_A and T_B are fixed. Then $F_1(T_{Aj}, T_{Bj})$ in Discussion 4.1 is minimized if*

$$(i) \quad T_{Aj} = a_A + 1 \text{ or } a_A,$$

$$(ii) \quad T_{Bj} = a_B + 1 \text{ or } a_B, \tag{4.63}$$

$$(iii) \quad S_{AB} = a_A T_B + a_B b_A + \max(0, b_A + b_B - b),$$

where a_A, a_B denote the integer part of T_A/b and T_B/b respectively, $b_A = T_A - ba_A$ and $b_B = T_B - ba_B$.

Based on all three conjectures an algorithm described below was written to minimize $tr(\bar{M}^{-1})$. For at least twenty sets of different parameter values this algorithm has been compared with the minimum value of $tr(C\Omega C')$ obtained from JE. In all cases the bound was found to be very close to the minimum trace and did not exceed the trace. These results support all three conjectures, and are illustrated in the following examples.

Example 4.6 *For n=4, b=8 and k=4, the conjectured bound gives value 2.7163 for the total variance of the contrasts of interest. The most efficient design generated by JE has the value 2.7687 for the trace while the bound given in Chapter 3 is 2.5560, which is poor relative to the conjectured bound.*

Example 4.7 *For n=4, b=3 and k=6, the conjectured bound is 4.5909. The most efficient design given by JE gives value 4.5909 for $tr(C\Omega C')$ while the bound given in Chapter 3 is 4.5000.*

It should be noted here that the conjectured bound is tighter than the bound b_m given in Section 3.5 in Chapter 3, except when the condition $N'r^{-\delta}C' = 0$ is satisfied and both T_A and T_D which minimize (3.13) are divisible by b(n-1). In this case the two bounds are identical. In the previous example the size of the discrepancies between the trace and each of bound b_m and the conjectured bound are respectively 2% and 0% of the bound.

Before giving the algorithm for finding the minimum of $tr(\bar{M}^{-1})$ we give a theorem which when applicable, gives a short cut in computation.

Theorem 4.9 *Suppose we have a design d in which the treatment combinations in sets A and D are replicated equally often in each block and $n_{Aij} \geq n_{Dij}$, for* *i=1,2,...,n-1 and j=1,2,...,b. Then, provided Conjecture 4.1 is true, there exists a design having* $n_{Aij} \leq n_{Dij}$ *which has higher efficiency than design d.*

Proof: See Appendix A at the end of the thesis.

4.4 Algorithm I

Finding the Bound and the Replications:

The algorithm described in this section not only finds the value of the conjectured bound, for specified size of experiments but also gives the total number of units which should be assigned to each of the treatment combinations belonging to sets A, B and D in each block of the design. This information is needed in a construction algorithm presented in Section 4.6.

The computer algorithm in FORTRAN was used to find the conjectured bound for different values of n, b, k and specified total replications, $(t_A, t_D) \in \Xi$, where

$$\Xi = \{(t_A, t_D); t_A \geq n-1, t_D \geq n-1; t_A + t_D \leq bk - 1; t_A, t_D \in N^+\}$$

and N^+ denotes the set of integers, positive numbers.

A listing of the algorithm is given in Appendix B and has the following steps:

STEP 1 : Fix $(t_A, t_B) \in \Xi$, where Ξ is defined above, and compute q_A, q_B and S_{AB} as given in the Conjecture 4.3, by utilizing Corollary 4.6.

STEP 2 : Assign T_{Aj}'s and T_{Bj}'s in block j for j=1,2,...,b, such that S_{AB} of the design equals S_{AB} found in STEP 1 by utilizing Conjecture 4.2. This step specifies the optimal allocations of units in each block for sets A, B and consequently D.

STEP 3 : Having specified T_{Aj}, T_{Bj} and consequently T_{Dj} in STEP 2, by utilizing Conjecture 4.1 and applying Theorem 4.5 and Conclusion 4.1, we obtain the minimum value for $F_1(T_{Aj}, T_{Bj})$.

STEP 4 : Change T_A, T_B and consequently T_D over all possible values in Ξ and utilizing Theorem 4.9, when it is appropriate, to shorten computation time.

Having specified the total number of units assigned to sets A and B, namely T_A and T_B respectively, then based on these numbers we assign either $[T_A/b]$ or

$[T_A/b]+1$ units and $[T_B/b]$ or $[T_B/b]+1$ units to the treatment combinations belonging to sets A and B respectively in each block .

Since the bound obtained by the above algorithm is a conjectured bound, we now give a definition of those designs which achieve this bound.

Definition 4.1 *Any design which achieves the conjectured bound obtained from Algorithm I outlined above will be called a C-design.*

Those designs which do not achieve the bound but give values for $tr(C\Omega C')$ very close to the conjectured bound will be called near C-designs.

The structure of C-designs is examined in the next section. By studying the structure, the designs in Table 4.2 at the end of chapter were derived. As Table 4.2 shows, these designs are all highly efficient compared with b_m and the best design obtained by JE.

The advantage of this approach compared with running JE is that it takes much less computation time and also is applicable for values of $n \geq 10$ and b or k or both bigger than 18. For instance for parameters (n,b,k)=(3,18,4) and (4,12,4) the cpu times used by JE are 3 and 5 respectively, while correponding cpu times used by Algorithm I is .5 and .26 respectively. However, JE always gives a highly efficient design for any combinations of the parameter values $b \leq 18$, $t \leq 18$ and $k \leq 18$.

In order to construct designs we need to study the structure and existence of the most efficient designs which will accommodate the replications produced by the algorithm. These structures are established in the next section and, in the following section, an algorithm for checking the existence of these designs is given.

4.5 Layout of C-designs:

For a set of parameter values n, b and k, let T_A, T_B and T_D be those values which minimize $tr(\bar{M}^{-1})$ as provided by the algorithm of Section 4.4. Assume a PBDS design does exist for the specified values then, if Conjectures 4.1-4.3 are true, the C-designs have one of the following layouts, where u_i denotes the integer part of T_i/b for i=A, B and D.

R-type : If T_A/b, T_B/b and T_D/b are integer values then the design is said to be R-type and the layout of the design is shown in Figure 4.1.

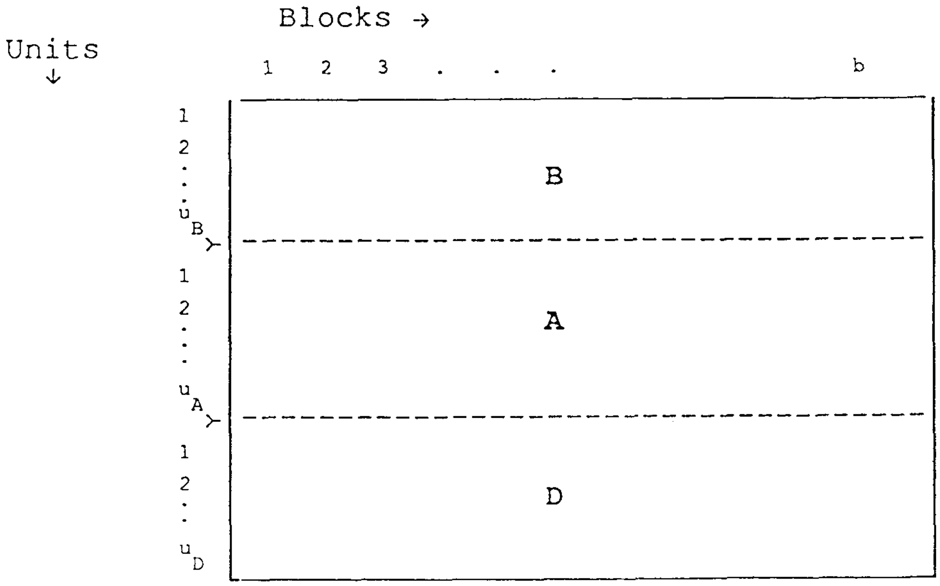

Figure 4.1: An R-type design; where $u_i = T_i / b$ is integer for i=A, B and D.

(R,S)-type : three cases have to be considered here:

1. R-type in terms of treatment 01(set B) and S-type in terms of two other sets. This is the case if T_B/b is integer and T_A/b and T_D/b are not integers. The layout of the design is shown in Figure 4.2.

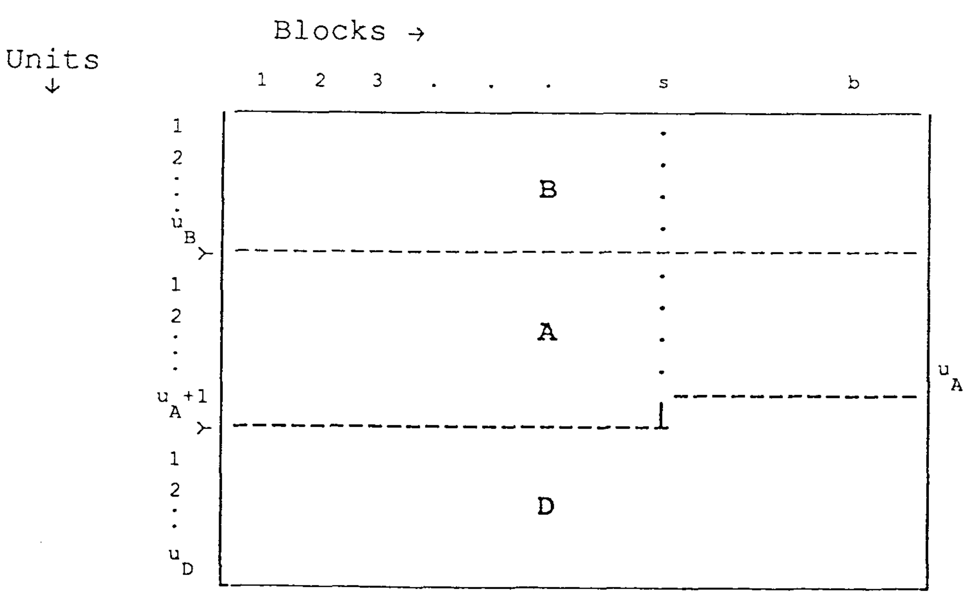

Figure 4.2: An (R,S)-type design, when T_A / b is not an integer and $s = T_A - bu_A$.

2. R-type in terms of set A and S-type in terms of two other sets. This is the case if T_A/b is integer, while T_B/b and T_D/b are not integers. The layout of the design is given in Figure 4.3.

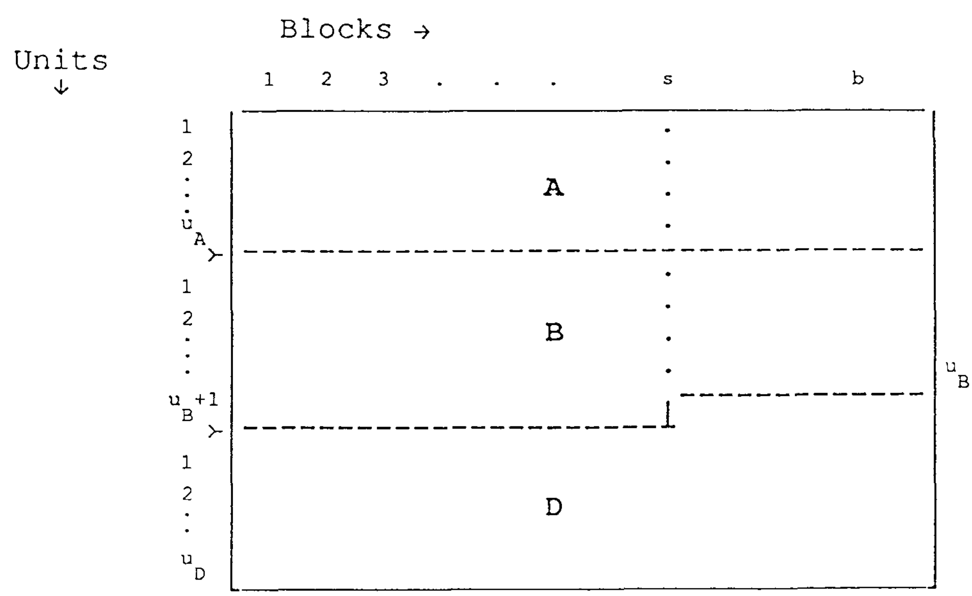

Figure 4.3: An (R,S)-type design, when T_B/b is not an integer and $s=T_B-bu_B$.

3. R-type in terms of set D and S-type in terms of two other sets. This is the case if T_D/b is integer, while T_B/b and T_A/b are not integers. The layout of the design is given in Figure 4.4.

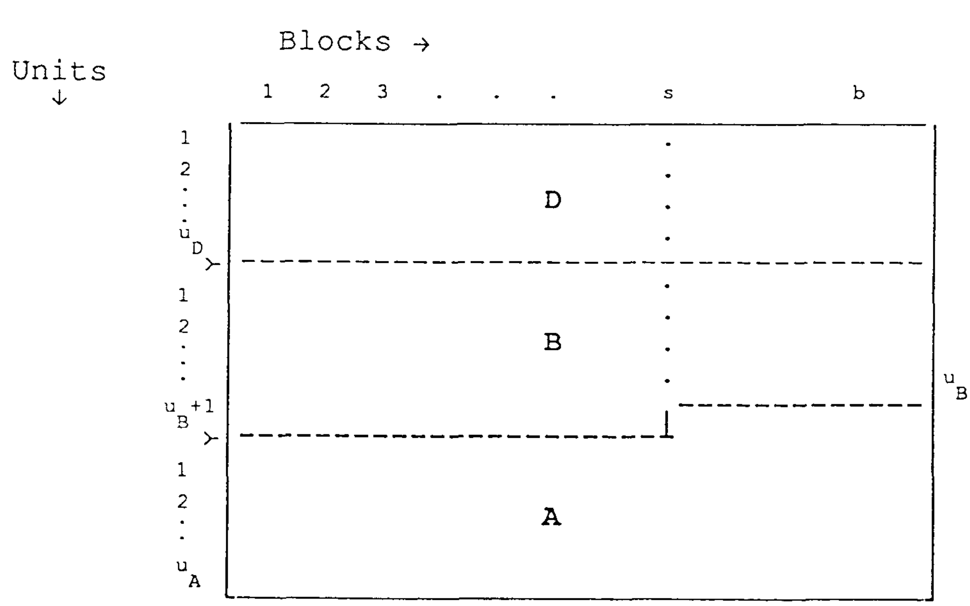

Figure 4.4: An (R,S)-type design, when T_B/b is not an integer and $s=T_B-bu_B$.

(S,S)-type : If none of T_A/b, T_B/b and T_D/b is an integer, then the design is said to be (S,S)-type and the layout of the design is shown in Figure 4.5.

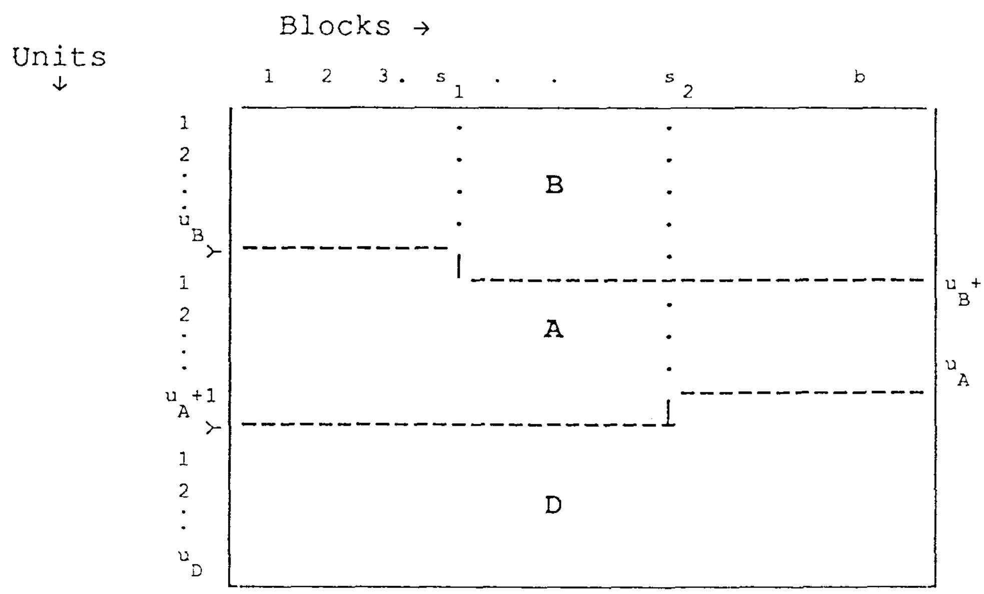

Figure 4.5: An (S,S)-type design, when $T_A - bu_A > b - T_B + bu_B$, $s_1 = b - T_B + bu_B$ and $s_2 = T_A - bu_A$.

4.6 Constructing C-designs:

The construction of a C-design will, in general, be a difficult task. From Figures 4.2-4.5, it is clear that the (R,S)- and (S-S)-type designs can be viewed respectively as a combination of two or three R-type designs.

In the following we give an algorithmic method of constructing C-designs in conjunction with the algorithm of Section 4.4. But first we need a lemma.

Lemma 4.9 *Suppose an $n \times 2$ CFBD(00) design consists of b blocks of size k. Let k_B, k_A and k_D units in each block be assigned to the treatment combinations in sets B, A and D respectively. Then a sufficient condition for a design to be an R-type PBDS design is*

- *BBD(n-1,b,k_A) and BBD(n-1,b,k_D) exist,*
- *either $k_D = k_A + 0 \ mod(n-1)$, or $k_A = k_D + 0 \ mod(n-1)$, or $k_D = 0 \ mod(n-1)$, or $k_A = 0 \ mod(n-1)$.*

It should be mentioned here that there might be other sufficient conditions under which a PBDS design exists. This is a problem for further investigation. But in this study we construct only those designs which satisfy the conditions of the above lemma. These conditions are built into the following algorithm.

Algorithm II:

STEP 1 : Check whether the integers T_A and T_D are divisible by n-1.

STEP 2 : For given T_A, T_B and T_D, partition the layout of the design as given in Figures 4.1 to 4.5. The design consists of one, two or three R-types sets of blocks depending on whether the design is an R-, (R,S)- or (S,S)-type respectively.

STEP 3 : For each R-type set of blocks check whether the appropriate BBD does exist by checking Conditions (2.2) of Ting and Notz(1988, p32).

STEP 4 : For each R-type set of blocks check whether the conditions of Lemma 4.9 are satisfied.

Obviously, this algorithm is unable to identify a C-design for every parameter combination of n, b and k. In an attempt to fill these gaps, we search for C-designs within the class of PBDS designs by finding the next values of T_A and T_B which minimize the conjectured bound via algorithm I and then checking whether the PBDS design does exist by using algorithm II.

In the next section we give another approach for the special cases k=2 and 3, which enables us to identify A-optimal designs within the PBDS class of designs. This approach does not rest on the conjectures. The designs obtained by this approach for $2 \leq b \leq 10$ are included in Table 4.2.

4.7 A-optimal PBDS Designs for k=2 and 3:

For k=2 and 3 we specify the arrangement of treatments in blocks in such a way that the design is a PBDS design and we formulate $tr(C\Omega C')$ in the resulting PBDS design. Then, by a simple computer algorithm, we have derived the A-optimal designs within the class of PBDS designs. The designs are tabulated in Table 4.2.

4.7.1 A-optimal PBDS Designs for k=2:

For this case the following arrangement of treatment combinations in the blocks gives a PBDS design:

Table 4.4: Arrangement of treatment combinations in a PBDS design with k=2.

arrangement of treatments		number of blocks
01	i0	$(n-1)n_a$
01	i1	$(n-1)n_b$
i0	i1	$(n-1)n_c$
i0	$j0(i \neq j)$	$\frac{(n-1)(n-2)n_d}{2}$
i1	$j1(i \neq j)$	$\frac{(n-1)(n-2)n_e}{2}$
i0	$j1(i \neq j)$	$(n-1)(n-2)n_f$

Then by Corollary 4.3 the trace of the variance-covariance matrix of the dual versus single contrast estimators is:

$$tr(C\Omega C') = \frac{(n-2)(2d_A - 2d_{AD} + d_D)}{d_A d_D - d_{AD}^2} + \frac{q_A + q_B}{q_A q_B - q_{AB}^2}, \tag{4.64}$$

where d_A, d_D, d_{AD}, q_A, q_D and q_{AD} were defined in (4.15), in which

$$T_A = D_A = (n-1)\{n_a + n_c + (n-2)(n_d + n_f)\},$$

$$T_D = D_D = (n-1)\{n_b + n_c + (n-2)(n_e + n_f)\},$$

$$S_A = (n-1)\{n_a + n_c + (n-2)(2n_d + n_f)\},$$

$$S_D = (n-1)\{n_b + n_c + (n-2)(2n_e + n_f)\},$$

$$D_{AD} = (n-1)n_c,$$

$$S_{AD} = (n-1)\{n_c + (n-2)n_f\}.$$

After some algebra we obtain:

$$tr(C\Omega C') = 2\left\{\frac{(n-2)X}{Y} + \frac{U}{W}\right\}, \tag{4.65}$$

where

$$X = 2n_a + 2(n-1)n_d + n_b + n_c + (n-1)n_e + (3n-4)n_f,$$

$$Y = \{n_a + (n-1)(n_d + n_f)]\,[n_b + (n-1)(n_e + n_f)\} +$$

$$(n_c - n_f)\left\{n_a + n_b + (n-1)(n_e + n_d + 2n_f)\right\},$$

$$U = 2n_a + n_b + n_c + (n-2)n_f,$$

and

$$W = n_a \times n_b + (n_a + n_b)\left\{n_c + (n-2)n_f\right\}.$$

The A-optimal PBDS design is obtained by minimizing the above expression subject to the following constraint:

$$(n-1)\left\{2n_a + 2n_b + 2n_c + (n-2)(n_d + n_e + 2n_f)\right\} = 2b = fixed. \tag{4.66}$$

Let n_a^*, n_b^*, n_c^*, n_d^*, n_e^* and n_f^*, be those integers which minimize the trace, then any design with such a number of blocks is A-optimal design within the class of PBDS designs for k=2. This has been done by a simple computer algorithm(Appendix B).

4.7.2 A-optimal PBDS Designs for k=3:

For k=3, the PBDS design has the following structure:

1. For n=3 the arrangement of treatment combinations in Table 4.5 gives PBDS design. Then it is possible to show that the trace of the variance-covariance matrix of the dual versus single contrasts is:

$$tr(C\Omega C') = \frac{(n-2)(2d_A - 2d_{AD} + d_D)}{d_A d_D - d_{AD}^2} + \frac{q_A + q_B}{q_A q_B - q_{AB}^2}, \tag{4.67}$$

where, d_A, d_D, d_{AD}, q_A, q_D and q_{AD} were defined in (4.15), in which for this case we have

$$T_A = 2(n_a + n_b + n_e + n_f + n_i + 2n_g + 2n_h + 3n_k),$$

$$D_A = 2(n_a + n_b + n_e + n_f + n_i + 2n_g + 4n_h + 5n_k),$$

$$S_A = 2(2n_a + n_b + n_e + n_f + n_i + 4n_g + 4n_h + 9n_k),$$

$$T_D = 2(n_c + n_d + n_e + n_f + 2n_i + n_g + 2n_j + 3n_l),$$

$$D_D = 2(n_c + n_d + n_e + n_f + 2n_i + n_g + 4n_j + 5n_l),$$

$$S_D = 2(2n_c + n_d + n_e + n_f + 4n_i + n_g + 4n_j + 9n_l),$$

$$D_{AD} = 2(n_e + n_g + n_i),$$

$$S_{AD} = 2(n_e + n_f + 2n_g + 2n_i).$$

Table 4.5: Arrangement of treatment combinations in a PBDS design with k=3 and n=3.

arrangement of treatments			number of blocks
01	i0	j0($i \neq j$)	n_a
01	01	i0	$2n_b$
01	i1	ij($i \neq j$)	n_c
01	01	i1	$2n_d$
01	i1	i0	$2n_e$
01	i0	j1($j \neq i$)	$2n_f$
i0	j0($i \neq j$)	l1(l=i or j)	$2n_g$
01	i0	i0	$2n_h$
i1	j1($i \neq j$)	il(l=i or j)	$2n_i$
01	i1	i1	$2n_j$
i0	i0	j0($j \neq i$)	$2n_k$
i1	i1	j1($j \neq i$)	$2n_l$

The A-optimal PBDS design is obtained by minimizing the above expression subject to the following constraint:

$$b = n_a + n_c + 2(n_b + n_d + n_e + n_f + n_g + n_h + n_i + n_j + n_k + n_l) = fixed. \quad (4.68)$$

This can be done by a simple computer algorithm(Appendix B).

2. For n$\geq$ 4, then the arrangement of treatment combinations is given in Table 4.6. Then it is possible to show that the trace of the variance-covariance matrix of the dual versus single contrasts is:

$$tr(C\Omega C') = \frac{(n-2)(2d_A - 2d_{AD} + d_D)}{d_A d_D - d_{AD}^2} + \frac{q_A + q_B}{q_A q_B - q_{AB}^2}, \quad (4.69)$$

where, d_A, d_D, d_{AD}, q_A, q_D and q_{AD} were defined in (4.15), in which for this case we have

$$T_A = t_A + (n-1)\{2n_m + n_q + 2n_o + (n-2)(2n_p + n_r + 3n_s)\},$$

$$D_A = t_A + (n-1)\{4n_m + 4n_o + n_q + (n-2)(4n_p + n_r + 5n_s)\},$$

$$S_A = s_A + (n-1)\{4n_m + 4n_o + n_q + (n-2)(4n_p + n_r + 9n_s)\},$$

$$T_D = t_D + (n-1)\{2n_n + 2n_q + n_o + (n-2)(2n_r + n_p + 3n_t)\},$$

$$D_D = t_D + (n-1)\{4n_n + 4n_q + n_o + (n-2)(4n_r + n_p + 5n_t)\},$$

Table 4.6: Arrangement of treatment combinations in a PBDS design with k=3 and $n \geq 4$.

arrangement of treatments			number of blocks
01	i0	$j0(i \neq j)$	$\frac{(n-1)(n-2)n_a}{2}$
01	01	i0	$(n-1)n_b$
01	i1	$j1(i \neq j)$	$\frac{(n-1)(n-2)n_c}{2}$
01	01	i1	$(n-1)n_d$
01	i0	i1	$(n-1)n_e$
01	i0	$j1(j \neq i)$	$(n-1)(n-2)n_f$
i0	$j0(i \neq j)$	$l1(l$=i or j)	$(n-1)(n-2)n_g$
i0	$j0(i \neq j)$	$l1(l \neq$ i,j)	$\frac{(n-1)(n-2)(n-3)n_h}{2}$
i1	$j1(i \neq j)$	$l0(l$=i or j)	$(n-1)(n-2)n_i$
i1	$j1(i \neq j)$	$l0(l \neq i,j)$	$\frac{(n-1)(n-2)(n-3)n_j}{2}$
i0	$j0(j \neq i)$	$l0(l \neq i,j)$	$\frac{(n-1)(n-2)(n-3)n_k}{6}$
i1	$j1(j \neq i)$	$l1(l \neq i,j)$	$\frac{(n-1)(n-2)(n-3)n_l}{6}$
01	i0	i0	$(n-1)n_m$
01	i1	i1	$(n-1)n_n$
i0	i0	i1	$(n-1)n_o$
i0	i0	$j1(j \neq i)$	$(n-1)(n-2)n_p$
i0	i1	i1	$(n-1)n_q$
i0	j1	$j1(j \neq i)$	$(n-1)(n-2)n_r$
i0	i0	$j0(j \neq i)$	$(n-1)(n-2)n_s$
i1	i1	$j1(j \neq i)$	$(n-1)(n-2)n_t$

$$S_D = s_D + (n-1)\{4n_n + 4n_q + n_o + (n-2)(4n_r + n_p + 9n_t)\},$$

$$S_{AD} = s_{AD} + 2(n-1)\{n_o + n_q + (n-2)(n_p + n_r)\},$$

$$D_{AD} = d1_{AD} + 2(n-1)(n_o + n_q)\},$$

where

$$t_A = (n-1)\{(n_b + n_e) + (n-2)(n_a + n_f + n_i + 2n_g) + \frac{1}{2}(n-2)(n-3)(n_j + n_k + 2n_h)\},$$

$$s_A = (n-1)\{(n_b + n_e) + (n-2)(2n_a + n_f + n_i + 4n_g) + \frac{1}{2}(n-2)(n-3)(n_j + 3n_k + 4n_h)\},$$

$$t_D = (n-1)\{(n_d + n_e) + (n-2)(n_c + n_f + 2n_i + n_g) + \frac{1}{2}(n-2)(n-3)(2n_j + n_l + n_h)\},$$

$$s_D = (n-1)\{(n_d + n_e) + (n-2)(2n_c + n_f + 4n_i + n_g) + \frac{1}{2}(n-2)(n-3)(4n_j + 3n_l + n_h)\},$$

$$d1_{AD} = (n-1)\{n_e + (n-2)(n_g + n_i)\},$$

$$s_{AD} = (n-1)\{n_e + (n-2)(n_f + 2n_i + 2n_g) + (n-2)(n-3)(n_j + n_h)\}.$$

The A-optimal PBDS design is obtained by minimizing the above expression subject to the following constraint:

$$6b = (n-1)\{6(n_b+n_d+n_e+n_m+n_n+n_o+n_q)+3(n-2)(n_a+n_c+2n_f+2n_g+2n_i)+ (n-2)[6(n_p + n_r + n_s + n_t) + (n-3)(3n_h + 3n_j + n_k + n_l)]\} = fixed. \quad (4.70)$$

A computer algorithm for this case is given in Appendix B.

4.8 The Tabulated Designs:

The algorithms given in Sections 4.4 and 4.6 can be used to find the C-designs or "near" C-designs which are PBDS designs. As an illustration the designs have been tabulated in Table 4.2 for $3 \leq n \leq 6$, $2 \leq b \leq 10$ and $k \leq 9$. For each design its discrepancies with b_m and with the conjectured bound are given in Table 4.2. For those designs having discrepancies exceeding 5% of b_m, the discrepancies with $tr(C\Omega C')$ of the best design obtained by JE is also given in the table. In 132 out of 159 designs tabulated the discrepancy is within 10% of the smaller bound.

The following examples show how to use the table for given parameter values.

Example 4.8 *For n=3, b=4 and k=5, Table 4.2 shows that an efficient C-design is composed of four copies of the set of blocks indexed 1. From Table 4.3, index 1 consists of one block of size 5 which accommodates each of the treatment combinations once. Therefore the highly efficient C-design is a randomized block design with four blocks. The discrepancy of this design is 2% and .5% compared with b_m and the conjectured bound respectively.*

Example 4.9 *For n=5, b=8 and k=7, from Table 4.2, the efficient C-design consists of 2 copies of index 2 set of blocks. From Table 4.3, the index 2 consists of 4 blocks each of size 7, in which the arrangement of the treatment combinations is*

Block 1	*01*	*10*	*20*	*30*	*11*	*21*	*31*
Block 2	*01*	*10*	*20*	*40*	*11*	*21*	*41*
Block 3	*01*	*10*	*30*	*40*	*11*	*31*	*41*
Block 4	*01*	*20*	*30*	*40*	*21*	*31*	*41*

Therefore the design is $2 \cup 2$ *which has discrepancies of 3.7 and 1.8% of* b_m *and the conjectured bound respectively.*

Note that for some values of n, b and k designs are not tabulated. For some parameter values PBDS designs do not exist because they violate combinatorial restrictions on the designs(given in Section 2.4.3). For other parameter values the designs were not efficient, having a discrepancy greater than 20% compared with the conjectured bound.

4.9 Conclusion:

As we have seen in this chapter, the minimization of $tr(\bar{M}^{-1})$ is very complicated. If we had been able analytically to give a minimum value for the trace in terms of the parameter values and the number of replications of the treatment combinations, then any design which hits that bound would be overall A-optimal. Analytical tools have been used earlier in this chapter to reduce the minimization problem to some extent, but due to the discrete nature of the problem, the reduction becomes unappreciable. However, our attempt was partially successful, since the problem in some cases, reduced to minimizing a simple function in terms of T_A, T_B and T_D(Theorem 4.8). Based on numerical results we made three conjectures. Intuitively an A-optimal design within the class of PBDS designs, might be regarded as a highly efficient design for comparing the dual versus single treatments, but it is not always the case. This can be seen from Table 4.2. Roughly speaking the A-optimal design within this class has average variance not far from that of the design which is A-optimal across all possible designs for specific values of the parameters. In addition the class of PBDS designs gives equal precision and correlations for each set of the contrast estimators corresponding to dual versus A and dual versus B which often corresponds to an experimenter's requirements.

Tables of Efficient C-designs:

For given $2 \le k \le 9$ $2 \le b \le 10$ and $3 \le n \le 6$, Table 4.2 gives a summary of the design as $(i_1, i_2, ..., i_m;\ f_1, f_2, ..., f_m)$, where i_j is a set of blocks given in Table 4.3 and f_i is the number of duplicates of the set of blocks in the design. Below this summary is entered the percentage discrepancy between the total variance of the estimators of the dual versus single treatment contrasts and the bound b_m(see Section 3.5), and conjectured bound(see Section 4.3) respectively. Where the discrepancy between the total variance and b_m exceeds 5% (i.e. small b and small k), the discrepancy between the total variance for the design and the total variance for the best design obtained from JE, is given as the third figure.

Table 4.2 Index and performance of C- and near C-designs in PBDS for n=3.

b\k	2	3	4	5	6	7	8	9
2	–	(1;1) 13,2,0	(1;1) 7,0,0	(1;2) 0,0	(1;1) 1.2,1	(1;1) 1.2,1	(1;2) 0,1.5	(1;1) .5,0
3	–	(1,2;1,1) 13,8,.1	(1,2;1,1) 6,2,0	(1;3) 0,.5	(1,2;1,1) 3,0	(1,2;1,1) 2,.4	(1,2;1,1) 1,.3	(1,1;1,1) 1,1
4	(1,2;1,1) 13,0,0	(1,3;1,1) 11,7,2	(1,3;1,1) 7,3,1	(1;4) 2,.5	(1,2;1,2) 3,.5	(1,3;1,1) 2,.4	(1,2;2,1) 1,0	(1;2) .6,0
5	(1,2,3;1,1,1) 13,8,0	(1,3,4;1,1,1) 8,4,1	(1,2;2,1) 5,0	(1,2;3,1) 2,.5	(1,2;2,1) 2,.2	(1,2;2,1) 2,.5	(1,2;3,1) 1,0	(1,2;2,1) .8,.4
6	(1,2,4;1,1,1) 13,10,1	(1,3;2,1) 5,0	(1,3;2,1) 6,1,.3	(1,2;4,1) 2,.2	(1,2;2,2) 3,.2	(1,3;2,1) 2,.01	(1,2;4,1) 1,.2	(1;3) .6,0
7	(1,2,4,5;1,1,1,1) 9,6,0	(1,2,3;2,1,1) 5,.1	(1,2;3,1) 6,1,0	(1,2;5,1) 2,.05	(1,2;2,3) 7,.4,0	(1,2,3;2,1,1) 2,0	(1,2;3,2) 1,.2	(1,2;3,1) .8,.2
8	(1,2,3,4,5;1,1,1,1,1) 13,12,5	(1,3;3,1) 4,0	(1,3;3,1) 6,1,0	(1,2;6,1) 2,0	(1,2;3,2) 3,.2	(1,3;3,1) 2,.1	(1,2;4,2) 1,.1	(1;4) .5,0
9	(1,2,4,5;1,2,1,1) 4,3	(1,2,3;3,1,1) 4,0	(1,2,3;3,1,1) 6,.1,0	(1,2;7,1) 2,0	(1,2;3,3) 3,.2	(1,2,3;3,1,1) 2,0	(1,2;5,2) 1,.07	(1,2;4,1) .8,.2
10	(1,2,6;2,2,1) 5,4	(1,4;4,1) 4,.3	(1,2;4,2) 6,1,0	(1,2;8,1) 2,0	(1,2,3;3,2,1) 3,.2	(1,2,3;3,2,1) 2,.3	(1,2;6,2) 1,.1	(1;5) .7,0

For given index and k from Table 4.2, the following table gives the required designs, in which the blocks are represented by columns.

Table 4.3 Constituent blocks of C- and near C-designs in PBDS for n=3.

index\k	2	3	4	5	6	7	8	9
1	01 01 11 21	01 01 10 20 11 21	01 01 10 20 11 11 21 21	01 10 20 11 21	01 01 10 10 20 20 11 11 11 21 21 21	01 01 01 01 10 10 20 20 11 11 11 21 21 21	01 01 10 20 11 11 21 21	01 01 01 01 10 10 10 20 20 20 11 11 11 11 21 21 21 21
2	10 20 11 21	01 11 21	10 20 11 21	01 01 10 20 11 11 11 21 21 21	01 01 10 20 11 21	01 10 20 11 11 21 21	01 01 01 01 10 10 10 20 20 20 11 11 11 21 21 21	01 01 01 10 20 11 11 21 21
3	10 20	10 20 11 11 21 21	01 01 10 10 20 20 11 21	–	01 01 01 01 10 20 11 11 11 21 21 21	01 01 10 10 10 20 20 20 11 11 11 21 21 21	–	–
4	01 01 10 20	10 10 20 20 11 21	–	–	–	–	–	–
5	11 21	–	–	–	–	–	–	–
6	10 20 21 11	–	–	–	–	–	–	–

Table 4.2 Index and performance of C- and near C-designs in PBDS for n=4.

b\k	2	3	5	6	7	8	9
2	–	–	–	–	(1;2) 0,2.2	(1;2) 1.6,2.2	(1;2) 11,10,1
3	–	(1;1) 17,14,0	(1;1) 2,1	(1;1) 2,0	(1;3) 2.1,2.3	(1;3) 2.4,2.5	(2;1) 1,.03
4	–	(1,2;1,1) 13,9,0	(1,2;1,1) 5,3	(1,2;1,1) 5,4	(1,2;1,1) 2.5,1.3	(1,2;1,1) 2.3,1.2	(1,2;1,1) 3,2
5	–	(1,2,3;1,1,1) 18,15,3	(1,2;1,2) 13,10,9	(1,2;1,2) 13,11,10	(1,2;2,1) 2,.5	(1,2;2,1) 2,.6	(1,2;2,1) 5,3
6	(1,2;1,1) 17,13,0	(1,4;1,1) 13,10,2	(1,2;1,3) 4,1.3	(1;2) 2.2,0	(1,2;3,1) 1.5,.2	(1,2;3,1) 2,.5	(2;1) 1.4,.2
7	–	(1,2;2,1) 8,5,2	(1,2;2,1) 4,1.4	(1,2;2,1) 4,1.7	(1,2;4,1) 1.6,.01	(1,2;4,1) 2.3,.6	(1,2;1,2) 2.4,1.1
8	–	1,2,3;2,1,1) 11,8,4	(1,2;2,2) 6,3.3,3	(1,2;2,2) 7,4,4	(1,2;5,1) 2,.08	(1,2;5,1) 2.4,.7	(1,2;2,2) 3,2
9	(1,2,3;1,1,1) 17,14,3	(1,4;2,1) 7,4,0	(1,2;2,3) 3.3,1.3	(1;3) 2.4,0	(1,2;6,1) 2,.13	(1,2;6,1) 2.4,.8	(2;1) 1.4,.2
10	–	(1,2;3,1) 9,5,4	(1,2;3,1) 4,1	(1,2;3,1) 3.4,1	(1,3;7,1) 2,.17	(1,2;4,2) 2.3,.7	(1,2;1,3) 2.2,.8

Table 4.3 Constituent blocks of C- and near C-designs in PBDS for n=4.

index\k	2	3	5	6
1	01 01 01 11 21 31	01 01 01 10 20 30 11 21 31	01 01 01 10 10 20 20 30 30 11 11 21 21 31 31	01 01 01 10 10 20 20 30 30 11 11 11 21 21 21 31 31 31
2	10 20 30 11 21 31	11 21 31	01 01 11 21 31	10 20 30 11 21 31
3	01 01 01 10 20 30	10 20 30	–	–
4	–	10 20 30 21 11 11 31 31 21	–	–

Table 4.3 Constituent blocks of C- and near C-designs in PBDS for n=4.

index\k	7	8	9
1	01 10 20 30 11 21 31	01 01 10 20 30 11 21 31	01 01 01 10 20 30 11 21 31
2	01 01 01 01 01 01 10 10 20 20 30 30 11 11 11 21 21 21 31 31 31	01 01 01 10 10 10 20 20 20 30 30 30 11 11 11 11 21 21 21 21 31 31 31 31	01 01 01 01 01 01 10 10 10 20 20 20 30 30 30 11 11 11 11 21 31 21 21 21 31 31 31
3	01 01 01 10 20 30 11 11 11 11 21 21 21 21 31 31 31 31	–	01 01 01 10 10 10 20 20 20 30 30 30 11 11 11 11 11 21 21 21 21 21 31 31 31 31 31
4	–	10 20 30 21 11 11 31 31 21	–

Table 4.2 Index and performance of C- and near C-designs in PBDS for n=5.

b\k	2	3	4	5	6	7	8	9
2	–	–	–	–	–	–	–	(1;2) 2.1,4.2
3	–	–	–	–	–	–	–	(1;3) 3.9,4.4
4	–	(1;1) 20,17,0	–	–	–	(1;1) 1.7,1.6	(1;1) 1.8,1	(2;1) 2,1
5	–	–	–	–	–	–	(1,2;1,1) 7,5,5	(1,2;1,1) 1.3,.3
6	–	–	–	(1;1) 4.7,1.7	(3;1) 18,15,13	(4;1) 6,4,4	(3;1) 9,7,7	(1,2;2,1) 1,.01
7	–	–	–	–	–	–	–	(1,2;3,1) 1.2,.1
8	(1,2;1,1) 20,18,0	(1;2) 20,17,7	–	–	(1,4;1,1) 18,15,10	(2;2) 3.7,1.8	(1,4;1,1) 2.2,.7	(1,2;4,1) 1.6,.3
9	–	–	–	–	–	–	(1,2;2,1) 5,3.2	(1,2;5,1) 1.8,.4
10	–	–	(1,2;1,1) 18,12,10	(1,2;1,1) 17,12,12	–	(1,4;1,1) 2.7,.5	(3,5;1,1) 2.3,.6	(1,2;2,2) 1.6,.3

Table 4.3 Constituent blocks of C- and near C-designs in PBDS for n=5.

index\k	2	3	4
1	01 01 01 01 11 21 31 41	01 01 01 01 10 20 30 40 11 21 31 41	01 01 01 01 11 11 11 21 21 21 31 31 31 41 41 41
2	10 20 30 40 11 21 31 41	–	10 10 10 20 20 30 20 30 40 30 40 40 11 11 11 21 21 31 21 31 41 31 41 41

Table 4.3 Constituent blocks of C- and near C-designs in PBDS for n=5.

index\k	5	6	7
1	01 01 01 01 01 01 10 10 10 20 20 30 20 30 40 30 40 40 11 11 11 21 21 31 21 31 41 31 41 41	01 01 01 01 10 20 30 40 11 11 11 11 21 21 21 21 31 31 31 31 41 41 41 41	01 01 01 01 01 01 10 10 10 20 20 30 20 30 40 30 40 40 11 11 11 11 11 11 21 21 21 21 21 21 31 31 31 31 31 31 41 41 41 41 41 41
2	01 01 01 01 01 01 01 01 11 11 11 21 21 21 31 31 31 41 41 41	01 01 11 21 31 41	01 01 01 01 10 10 10 20 20 20 30 30 30 40 40 40 11 11 11 21 21 21 31 31 31 41 41 41
3	–	01 01 01 01 01 01 01 01 01 01 01 01 10 10 10 20 20 30 20 30 40 30 40 40 11 11 11 21 21 31 21 31 41 31 41 41	–
4	–	10 10 10 20 20 20 30 30 30 40 40 40 11 11 11 21 21 21 31 31 31 41 41 41	–

Table 4.3 Constituent blocks of C- and near C-designs in PBDS for n=5.

index\k	8	9
1	01 01 01 01 10 10 10 20 20 20 30 30 30 40 40 40 11 11 11 11 21 21 21 21 31 31 31 31 41 41 41 41	01 10 20 30 40 11 21 31 41
2	10 20 30 40 11 21 31 41	01 01 01 01 01 01 01 10 10 10 10 20 20 20 30 30 30 40 40 40 11 11 11 11 21 21 21 21 31 31 31 31 41 41 41 41
3	01 01 01 01 01 01 01 01 01 01 01 01 10 10 10 20 20 30 20 30 40 30 40 40 11 11 11 11 11 11 21 21 21 21 21 21 31 31 31 31 31 31 41 41 41 41 41 41	–
4	01 01 01 01 01 01 01 01 10 10 10 20 20 20 30 30 30 40 40 40 11 11 11 21 21 21 31 31 31 41 41 41	–
5	01 01 01 01 10 10 10 10 20 20 20 20 30 30 30 30 40 40 40 40 11 11 11 21 21 21 31 31 31 41 41 41	–

Table 4.2 Index and performance of C- and near C-designs in PBDS for n=6.

b\k	2	3	5	6	7	8	9
5	–	(1;1) 23,20,0	–	–	–	–	(1;1) 4.3,3.1
10	(1,2;1,1) 23,21,0	(1;2) 23,20,8	(1;1) 8,3,3	(1;1) 22,17,17	(1;1) 4.3,1.7	(1;1) 9,7,6	(2;1) 2.4,1.4

Table 4.3 Constituent blocks of C- and near C-designs in PBDS for n=6.

index\k	2	3	5
1	01 01 01 01 01 11 21 31 41 51	01 01 01 01 01 10 20 30 40 50 11 21 31 41 51	01 01 01 01 01 01 01 01 01 01 10 10 10 10 20 20 20 30 30 40 20 30 40 50 30 40 50 40 50 50 11 11 11 11 21 21 21 31 31 41 21 31 41 51 31 41 51 41 51 51
2	10 20 30 40 50 11 21 31 41 51	–	–

Table 4.3 Constituent blocks of C- and near C-designs in PBDS for n=6.

index\k	6	7
1	01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 10 10 10 10 20 20 20 30 30 40 20 30 40 50 30 40 50 40 50 50 11 11 11 11 21 21 21 31 31 41 21 31 41 51 31 41 51 41 51 51	01 01 01 01 01 01 01 01 01 01 10 10 10 10 10 10 20 20 20 30 20 20 20 30 30 40 30 30 40 40 30 40 50 40 50 50 40 50 50 50 11 11 11 11 11 11 21 21 21 31 21 21 21 31 31 41 31 31 41 41 31 41 51 41 51 51 41 51 51 51

Table 4.3 Constituent blocks of C- and near C-designs in PBDS for n=6.

index\k	8	9
1	01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 01 10 10 10 10 10 10 20 20 20 30 20 20 20 30 30 40 30 30 40 40 30 40 50 40 50 50 40 50 50 50 11 11 11 11 11 11 21 21 21 31 21 21 21 31 31 41 31 31 41 41 31 41 51 41 51 51 41 51 51 51	- 01 01 01 01 01 10 10 10 10 20 20 20 20 30 30 30 30 40 40 40 40 50 50 50 50 11 11 11 11 21 21 21 21 31 31 31 31 41 41 41 41 51 d1 51 51
2	–	01 01 01 01 01 01 01 01 01 01 10 10 10 10 10 10 20 20 20 30 20 20 20 30 30 40 30 30 40 40 30 40 50 40 50 50 40 50 50 50 11 11 11 11 11 11 11 11 11 11 21 21 21 21 21 21 21 21 21 21 31 31 31 31 31 31 31 31 31 31 41 41 41 41 41 41 41 41 41 41 51 51 51 51 51 51 51 51 51 51

Chapter 5

Designs for Two Factors with More than Two Levels

5.1 Introduction:

In the previous chapters we considered $n \times m$ blocked experiments with 00 excluded for m=2 and n any positive integer. In this chapter we extend some of the findings to the case of $n \times m$ experiments for any $m > 2$. In Section 5.2 we employ the permutation method in an attempt to obtain a design-dependent bound(a generalization of Section 4.2) . In Section 5.3 we specify a class of designs which achieves the design-dependent bound and consider some of its properties. We characterize a series of overall A-optimal designs for the case $k > t$ in Section 5.4, and give a critical assessment of these designs. In Section 5.5 we give some methods of constructing designs which belong to the class of designs defined in Section 5.3 and give recommendations on their use in practice.

The formulation of the bound in terms of the elements of the concurrence matrix of the design has proved a very difficult task, and is a topic for future work. This will enable the characterization of further efficient designs for any number of units within each block when both factors have more than two levels.

5.2 A Design-Dependent Bound:

In this section we apply the permutation matrix technique described in Section 4.2 of Chapter 4, i.e. we use a set of permutation matrices, under which our contrasts of interest are invariant, and apply it to the A-matrix of design to obtain a bound which is design-dependent.

Let the treatment combinations be ordered as follows

$$\tau_{01}, \tau_{02}, \ldots, \tau_{0q}, \tau_{10}, \tau_{20}, \ldots, \tau_{p0}, \tau_{11}, \tau_{12}, \ldots, \tau_{1q}, \tau_{21}, \tau_{22}, \ldots, \tau_{2q},$$

$$\ldots, \ldots, \tau_{p1}, \tau_{p2}, \ldots, \tau_{pq}, \tag{5.1}$$

where t=mn-1, p=n-1, and q=m-1.

We put the ordering of treatments in a $t \times 1$ column vector $\underline{\tau}$. The contrasts of interest are $C_1\underline{\tau}$ and $C_2\underline{\tau}$ where the contrast matrices are:

$$\begin{aligned} C_1 &= (\ -\mathrm{I}_q \otimes \underline{1}_p \quad 0_{l \times p} \quad E\ ), \\ C_2 &= (\ 0_{l \times q} \quad -\mathrm{I}_p \otimes \underline{1}_q \quad \mathrm{I}_\ell\ ), \\ C &= (\ C_1' \quad C_2'\ )', \end{aligned} \tag{5.2}$$

where I_n is an identity matrix of order n, $O_{u \times v}$ is a zero matrix of u rows and v columns, $\underline{1}_n$ is an $n \times 1$ column vector with all entries 1, $\otimes$ denotes Kronecker product, $\ell = pq$ and

$$E = \begin{bmatrix} E_{11} & E_{12} & E_{13} & \ldots\ldots & E_{1p} \\ E_{21} & E_{22} & E_{23} & \ldots\ldots & E_{2p} \\ E_{31} & E_{32} & E_{33} & \ldots\ldots & E_{3p} \\ \ldots & \ldots & \ldots & \ldots\ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots\ldots & \ldots \\ E_{q1} & E_{q2} & E_{q3} & \ldots\ldots & E_{qp} \end{bmatrix}, \tag{5.3}$$

where the E_{ij}'s are $p \times q$ matrices with a 1 in the (j,i)th position and zero elsewhere. Let the A-matrix of the design be partitioned as follows:

$$A = \begin{bmatrix} D & B & F \\ & & \\ B' & G & H \\ & & \\ F' & H' & L \end{bmatrix} \tag{5.4}$$

where D is an $q \times q$ symmetric matrix, B is a $q \times p$ matrix, $F = [F_1, F_2 \ldots, F_p]$ in which F_i is $q \times q$ matrix, for i=1,2,...,p, G is a $p \times p$ symmetric matrix, $H = [H_1, H_2, \ldots, H_p]$ in which H_j is a $p \times q$ matrix for i=1,2,...,p, and $L = (L_{ij})$, where each L_{ij} is a $q \times q$ matrix(i,j=1,2,...,p), p=n-1 and q=m-1.

Suppose $\{q_i; i = 1, 2, ..., q!\}$ and $\{p_j; j = 1, 2, ..., p!\}$ are sets of permutation matrices of order q and p respectively, where p=n-1 and q=m-1.

Also let

$$\prod = \{(\pi_{ij})\}, \tag{5.5}$$

where

$$\pi_{ij} = \begin{bmatrix} q_i & 0 & 0 \\ 0 & p_j & 0 \\ 0 & 0 & p_j \otimes q_i \end{bmatrix}.$$

The set $\prod$ is a set of permutation matrices such that the function $\Phi(A) = tr(C\Omega C')$ is invariant, where Ω is a g-inverse of A. In other words $\Phi(\pi_{ij} A \pi'_{ij}) = \Phi(A)$. Define $\bar{A}$ as the average of A over all the permutations in $\prod$, i.e.

$$\bar{A} = \frac{1}{p!q!} \sum_{i=1}^{q!} \sum_{j=1}^{p!} \pi_{ij} A \pi'_{ij}. \tag{5.6}$$

Now we are in a position to give the main theorem of this chapter.

Theorem 5.1 *For any design $d \in n \times m$ CFBD(00), suppose A is the A-matrix of design d and $\bar{A}$ is the matrix defined in (5.6). Suppose Ω and $\bar{\Omega}$ are the respective g-inverses of A and $\bar{A}$, then:*

$$tr(C\Omega C') \geq tr(C\bar{\Omega}C') \tag{5.7}$$

Proof: If A denotes the A-matrix of any connected design, then r(A)=t-1. Define $\Phi(A) = tr(C\Omega C')$, then by Majumdar(1986) Φ is a convex function. This implies that

$$\Phi(\bar{A}) \leq \sum_{i=1}^{q!} \sum_{j=1}^{p!} \frac{1}{p!q!} \Phi(\pi_{ij} A \pi'_{ij}). \tag{5.8}$$

By definition $\Phi(\pi_{ij} A \pi'_{ij}) = tr(C\pi_{ij}\Omega\pi'_{ij}C')$. Since each permutation matrix π_{ij} is such that the contrasts are invariant, then $tr(C\pi_{ij}\Omega\pi'_{ij}C') = tr(C\Omega C')$. Therefore the RHS of (5.8) is $tr(C\Omega C')$. Hence the theorem is proved.♣

For $\bar{\Omega}$ any g-inverse of $\bar{A}$, a design-dependent bound for the contrasts of interest is given by $tr(C\bar{\Omega}C')$. If we minimize $tr(C\bar{\Omega}C')$ over all possible designs for given parameter values n, m, b and k, this gives a bound to assess the performance of designs.

Following the approach of Chapter 4, we should like to formulate the design-dependent bound as a function of the elements of the incidence matrix of the design, i.e. as a function of the number of concurrences of each treatment combination in each block. This will then facilitate the calculation of the bound. In addition it provides a means of identifying designs which are overall A-optimal. The key to this approach is to evaluate a g-inverse of $\bar{A}$ by finding $(\bar{A} + xJ_t)^{-1}$ for some $x \neq 0$. In order to evaluate the bound in (5.7) we need to calculate $tr\{C(\bar{A} + xJ_t)^{-1}C\}$. This is a generalization of the approach in Sections 4.2 and 4.3 in Chapter 4. However, the approach proved mathematically intractable. Our attempts included employing an algebraic computer algorithm, REDUCE, which is a system for carrying out algebraic operations accurately, no matter how complicated the expressions become(see user's Manual,1985). However this gave a two-page expression for $tr(C\bar{\Omega}C')$ which is too difficult to handle. However, Theorems 5.1 reveals that even for small k, the class of GPBDS designs is a source of some efficient designs. Some methods of constructing such designs will be described in Sections 5.5 and 5.6.

5.3 A Class of Efficient Designs:

In the following we characterize a class of designs which is a generalization of the PBDS class of designs defined in Chapter 1. By examining the variance-covariance matrix of this class we shall see that the designs estimate the contrasts within the dual versus A and dual versus B sets($C_2\underline{\tau}$ and $C_1\underline{\tau}$) with equal precision.

We begin by deriving the structure of the A-matrix via the permutation method.

5.3.1 Structure of the A-matrix:

In this section first we give a lemma which specifies the structure of the $\bar{A}$ matrix given in (5.6), then we formally define the class of efficient designs. Finally we show how designs within this class achieve the design-dependent bound given in (5.7).

Lemma 5.1 *Matrix $\bar{A}$ given in (5.6) has the following structure*

$$\bar{A} = \begin{bmatrix} a_1 I_q + b_1 J_q & c J_{q\times p} & \underline{1}'_p \otimes (a_2 I_q + b_2 J_q) \\ & a_3 I_p + b_3 J_p & (a_4 I_p + b_4 J_p) \otimes \underline{1}'_q \\ & & I_p \otimes (a_5 I_q + b_5 J_q) + J_q \otimes (a_6 I_q + b_6 J_q) \end{bmatrix}. \tag{5.9}$$

Also, one possible g-inverse of $\bar{A}$, called $\bar{\Omega}$, has the following structure:

$$\bar{\Omega} = \begin{bmatrix} x_1 I_q + y_1 J_q & z J_{q\times p} & \underline{1}'_p \otimes (x_2 I_q + y_2 J_q) \\ & x_3 I_p + y_3 J_p & (x_4 I_p + y_4 J_p) \otimes \underline{1}'_q \\ & & I_p \otimes (x_5 I_q + y_5 J_q) + J_p \otimes (x_6 I_q + y_6 J_q) \end{bmatrix}, \tag{5.10}$$

where x_1, x_3, y_1, y_3, z, x_2, x_4, y_2, y_4, x_5, x_6, y_5 and y_6 are functions of a_1, a_1, a_3, a_4, a_5, a_6, c, b_1, b_2, b_3, b_4, b_5 and b_6.

Proof: See Appendix A at the end of the thesis.

Now we define a general class of partly balanced dual versus single treatment designs.

Definition 5.1 *A design $d \in n \times m$ CFBD(00), is a* **Generalized** *PBDS design if its A-matrix has the structure (5.9). This class will be denoted by* **GPBDS** *hereafter.*

It will be shown in Section 5.3.2 that the designs in the GPBDS class of designs estimate the dual versus A and dual versus B contrasts with equal precision.

In the following we give a corollary which shows that if a design is a GPBDS design then the total variance of the contrasts in (5.2) is $tr(C\bar{\Omega}C')$. This indicates that the class of GPBDS designs might prove a source of efficient designs.

Corollary 5.1 *If in the statement of Theorem 5.1, d is in the class of GPBDS designs, then inequality in (5.7) changes to equality.*

Proof: If d is in the class of GPBDS designs, then $A = \bar{A}$, which implies that $(A + xJ)^{-1} - (\bar{A} + xJ)^{-1} = 0$. The result follows from here.♣

The following examples illustrate that this class of designs does contain highly efficient designs for the dual versus single treatment problem.

Example 5.1 *For m=n=3, b=8 and k=3, the design*

*Block*1	*Block*2	*Block*3	*Block*4	*Block*5	*Block*6	*Block*7	*Block*8
20	10	01	02	01	02	02	01
21	11	11	12	20	20	10	10
22	12	21	22	21	22	12	11

has the A-matrix

$$A = \begin{bmatrix} 2I_2 & -0.33J_2 & -0.67\underline{1}_2' \otimes I_2 \\ -0.33J_2 & 2I_2 & -0.67I_2 \otimes \underline{1}_2' \\ -0.67\underline{1}_2 \otimes I_2 & -0.67I_2 \otimes \underline{1}_2 & I_2 \otimes (2.67I_2 - 0.33J_2) - 0.33J_2 \otimes I_2 \end{bmatrix},$$

which has the same structure as $\bar{A}$ in (5.9). Hence it is a GPBDS design. The design has $tr(C\Omega C')$=6.429 and bound b_m=6.319. Hence the discrepancy between $tr(C\Omega C')$ and b_m is 1.7% of b_m, showing the design is highly efficient.

Example 5.2 *For n=4, m=3, b=2 and k=12, the design*

*Block*1	01	02	02	10	20	30	11	12	21	22	31	32
*Block*2	01	01	02	10	20	30	11	12	21	22	31	32

is an efficient design belonging to the class of GPBDS designs with a discrepancy 0.3% of b_m.

The next step is to locate the highly efficient designs within this class, exploiting the form of the A-matrix. This has proved difficult to do in general, but efficient designs for some special cases have been found and are given in Sections 5.5 and 5.6.

5.3.2 Variance-Covariance Matrix of the Class of GPBDS Designs:

In this section we derive the structure of the variance-covariance matrix for the estimators of dual treatment versus A alone contrasts and dual treatment versus B alone contrasts in any GPBDS design.

The following lemma is required to specify the structure of the variance-covariance matrix. Its proof follows by direct substitution of E from equation (5.3).

Lemma 5.2 *Let E denote the matrix defined in (5.3), then we have*

$$\{\underline{1}_p' \otimes (aI_q + bJ_q)\}E' = (aI_q + bJ_q) \otimes \underline{1}_p',$$

$$(I_q \otimes \underline{1}_p)\{\underline{1}_p' \otimes (aI_q + bJ_q)\} = \underline{1}_p' \otimes (aI_q + bJ_q) \otimes \underline{1}_p,$$

$$E\{I_p \otimes (aI_q + bJ_q) + J_p \otimes (cI_q + dJ_q)\}E' = \tag{5.11}$$

$$I_q \otimes (aI_p + cJ_p) + J_q \otimes (bI_p + dJ_p),$$

$$E\{\underline{1}_p \otimes (aI_q + bJ_q)\} = (aI_q + bJ_q) \otimes \underline{1}_p,$$

$$E\{(aI_p + bJ_p) \otimes \underline{1}_q\} = \underline{1}_q \otimes (aI_p + bJ_p).$$

The following theorem examines parts of the variance-covariance matrix corresponding to the dual treatment versus A and the dual treatment versus B contrasts and shows that the variances are equal within the two sets of contrasts.

Theorem 5.2 *Let design $d \in GPBDS$, with $\bar{\Omega}$ as a g-inverse of its A-matrix as given in (5.10), then we have:*

$$C_1\bar{\Omega}C_1' = \tag{5.12}$$

$$I_q \otimes \{x_5 I_p + (x_1 + x_6 - 2x_2)J_p\} + J_q \otimes \{y_5 I_p + (y_1 + y_6 - 2y_2)J_p\},$$

$$C_2\bar{\Omega}C_2' = \tag{5.13}$$

$$I_p \otimes \{x_5 I_q + (x_3 + y_5 - 2x_4)J_q\} + J_p \otimes \{x_6 I_q + (y_3 + y_6 - 2y_4)J_q\},$$

where C_1 and C_2 are given in (5.2).

Proof: If we premultiply and postmultiply $\bar{\Omega}$ respectively by C_1 and its transpose, and apply Lemma 5.1, we obtain

$$C_1\bar{\Omega}C_1' = \left\{ \begin{array}{ccc} A_1 & B_1 & D_1 \end{array} \right\} C_1' = A_1(-I_q \otimes \underline{1}_p') + D_1 E', \tag{5.14}$$

where

$$A_1 = \{(x_2 - x_1)I_q + (y_2 - y_1)J_q\} \otimes \underline{1}_p,$$

$$B_1 = \underline{1}_q \otimes \{x_4 I_p + (y_4 - z)J_p\},$$

and

$$D_1 = -\underline{1}_p' \otimes (x_2 I_q + y_2 J_q) \otimes \underline{1}_p +$$

$$E\{I_p \otimes (x_5 I_q + y_5 J_q) + J_p \otimes (x_6 I_q + y_6 J_q)\}.$$

Substituting from these into (5.14) we obtain the required expression in (5.12). Similarly

$$C_2 \bar{\Omega} C_2' = \left\{ \begin{array}{ccc} A_2 & B_2 & D_2 \end{array} \right\} C_2' = B_2(-I_p \otimes \underline{1}_q') + D_2, \tag{5.15}$$

where

$$A_2 = \underline{1}_p \otimes \{x_2 I_q + (y_2 - z) J_q\},$$

$$B_2 = \{(x_4 - x_3) I_p + (y_4 - y_3) J_p\} \otimes \underline{1}_q,$$

and

$$D_2 = I_p \otimes \{x_5 I_q + (y_5 - x_4) J_q\} + J_p \otimes (x_6 I_q + (y_6 - y_4) J_q\}.$$

Substituting from these into (5.15) we obtain the required expression for (5.13).♣

Corollary 5.2 *If we have an $n \times m$ CFBD(00) design d, in which one of the g-inverse of its A-matrix is given in (5.10), then:*

$$tr(C\bar{\Omega}C') = \tag{5.16}$$

$$pq\left\{x_1 + x_3 + y_1 + y_3 + 2(x_5 + x_6 + y_5 + y_6) - 2(x_2 + x_4 + y_2 + y_4)\right\}.$$

Proof: It is not difficult to show that:

$$tr(C\bar{\Omega}C') = tr(C_1\bar{\Omega}C_1') + tr(C_2\bar{\Omega}C_2') \tag{5.17}$$

where C_1 and C_2 are given in (5.2). But from Theorem 5.2 we have:

$$tr(C_1\bar{\Omega}C_1') = pq\{x_1 + y_1 + x_5 + y_5 + x_6 + y_6 - 2(x_2 + y_2)\}, \tag{5.18}$$

and

$$tr(C_2\bar{\Omega}C_2') = pq\{x_3 + y_3 + x_5 + y_5 + x_6 + y_6 - 2(x_4 + y_4)\}. \tag{5.19}$$

Hence the result follows.♣

In the following we give a corollary whose proof follows directly from Theorem 5.2.

Corollary 5.3 *A necessary condition for a design to have structures (5.12) and (5.13) for the variance-covariance matrices for the estimators of the dual versus B contrasts and the dual versus A contrasts respectively, is that the design belongs to the GPBDS class.*

5.4 Towards A-optimal $n \times m$ Designs with $k > t$:

In Section 3.2 of Chapter 3 we applied Wu(1980) to obtain bound b_1 on the total variance of estimators of the contrasts for the dual versus single factor. In Corollary 3.2 we showed that this bound can be achieved if $N'r^{-\delta}C' = 0$.

Now we are in position to characterize a series of overall A-optimal designs. This is a generalization of Theorem 4.8 in Chapter 4.

Theorem 5.3 *Let $n = 2p_1^2 + 1$ and $m = 2q_1^2 + 1$, where p_1 and q_1 are positive integers. Suppose a design for block size $k \equiv 0 \ mod\{2p_1q_1(p_1 + q_1 + 2p_1q_1)\}$ has the following respective numbers of replications of any treatment combination belonging to sets B, A and D in each block:*

$$n_B = \frac{k}{2q_1(p_1 + q_1 + 2p_1q_1)},$$

$$n_A = \frac{k}{2p_1(p_1 + q_1 + 2p_1q_1)}, \tag{5.20}$$

and

$$n_D = \frac{k}{2p_1q_1(p_1 + q_1 + 2p_1q_1)},$$

where sets A, B and D were defined on page 70. Then the resulting design is overall A-optimal.

<u>Proof</u>: For any $d \in n \times m$ CFBD(00) if $N'r^{-\delta}C' = 0$, then from Wu(1980) we have:

$$tr(C\Omega C') = tr(Cr^{-\delta}C') = p\sum_{j=1}^{q}\frac{1}{r_{Bj}} + q\sum_{i=1}^{p}\frac{1}{r_{Ai}} + 2\sum_{i=1}^{p}\sum_{j=1}^{q}\frac{1}{r_{Dij}}, \tag{5.21}$$

where r_{Bj}, r_{Ai} and r_{Dij} were defined on page 70.

But we have

$$tr(C\Omega C') = tr(Cr^{-\delta}C') = 2(p_1^2\sum_{j=1}^{q}\frac{1}{r_{Bj}} + q_1^2\sum_{i=1}^{p}\frac{1}{r_{Ai}} + \sum_{i=1}^{p}\sum_{j=1}^{q}\frac{1}{r_{Dij}}). \tag{5.22}$$

The problem is to minimize:

$$p_1^2\sum_{j=1}^{q}\frac{1}{r_{Bj}} + q_1^2\sum_{i=1}^{p}\frac{1}{r_{Ai}} + \sum_{j=1}^{q}\sum_{i=1}^{p}\frac{1}{r_{Dij}}, \tag{5.23}$$

subject to the condition:

$$\sum_{j=1}^{q} r_{Bj} + \sum_{i=1}^{p} r_{Ai} + \sum_{i=1}^{p}\sum_{j=1}^{q} r_{Dij} = bk = fixed. \tag{5.24}$$

Applying a Lagrange Multiplier, λ, we obtain the required result. ♣

Example 5.3 *For m=n=3 we have $p_1 = q_1 = 1$, Theorem 5.3 gives overall A-optimal designs for $k \equiv 0mod(8)$. If k=8, then the design with $n_A = n_B = n_D = 1$ (i.e. a randomized block design) with any number of blocks is A-optimal. Also if k=16, the design with $n_A = n_B = n_D = 2$ in each block is overall A-optimal.*

Example 5.4 *For m=3 and n=9 we have $p_1 = 2$ and $q_1 = 1$. To employ the theorem we require $k \equiv 0mod(28)$. If k=28, then $n_B = 2$, $n_A = n_D = 1$ and the resulting design is A-optimal.*

Comment: The series of overall A-optimal designs given by Theorem 5.3 has limited practical application because the block sizes quickly become large, as is clear from Examples 5.3 and 5.4. For instance, for m=3 and n=9 the theorem does not give A-optimal designs for $k < 28$ or for $29 \leq k < 56$. Even for small values of m and n, as in Example 5.3, the designs for which A-optimality is established have block sizes of 8, 16, 24 and so on.

5.5 Some Methods of Constructing GPBDS Designs:

In this section we give two construction methods which produce two series of designs, one for block size 2 and the other for block size 3. The performance of these designs can be assessed by the bound b_m, given in Section 3.5 of Chapter 3.

It should be noted here that, as for $n \times 2$ experiments, we can use the same approach as Chapter 4, Section 4.7, to construct GPBDS designs for k=2 and 3. The difficulty with this approach is that we cannot get a simple expression for the total variance of the contrast estimators. We therefore consider a different approach.

5.5.1 Constructing GPBDS designs for k=2:

Since we are interested in contrasts $\tau_{ij} - \tau_{i0}$ and $\tau_{ij} - \tau_{0j}$, a natural way is to accommodate in each block either ij and $i0$ or ij and $0j$, for i=1,2,...,n-1 and j=1,2,...,m-1. Such a design will have b=2pq blocks, and replications of 2, q and p for treatment combinations ij, $i0$ and $0j$ respectively, where p=n-1 and q=m-1. If we require more replication of the treatments and a greater number of blocks we might consider using duplicates of the above set of blocks. The application of this method is recommended for small values of b, in particular, when b=2pq.

Suppose our design consists of u replicates of the given design, then it can be shown that:

$$C_1 \Omega C_1' = \frac{1}{pqu}\{qI_q \otimes (pI_p + J_p) + J_q \otimes (pI_p - J_p)\}, \tag{5.25}$$

and

$$C_2 \Omega C_2' = \frac{1}{pqu}\{pI_p \otimes (qI_q + J_q) + J_p \otimes (qI_q - J_q)\}. \tag{5.26}$$

Therefore for the designs of this kind:

1. For the dual versus B, i.e. contrasts $\tau_{ij} - \tau_{0j}$, we have:

$$V(\hat{\tau}_{ij} - \hat{\tau}_{0j}) = \frac{mn-2}{pqu},$$

$$Cov(\hat{\tau}_{ij} - \hat{\tau}_{0j}, \hat{\tau}_{lj} - \hat{\tau}_{0j}) = \frac{m-2}{pqu}, \tag{5.27}$$

$$Cov(\hat{\tau}_{ij} - \hat{\tau}_{0j}, \hat{\tau}_{kl} - \hat{\tau}_{0l}) = \begin{cases} \frac{n-2}{pqu} & \text{if i=k and } j \neq l \\ -\frac{1}{pqu} & \text{if } i \neq k \text{ and } j \neq l \end{cases}$$

for $k, i(i \neq l)$=1,2,...,p and j=1,2,...,q($l \neq j$).

2. For the dual versus A contrasts, i.e. $\tau_{ij} - \tau_{i0}$, we have:

$$V(\hat{\tau}_{ij} - \hat{\tau}_{i0}) = \frac{mn-2}{pqu},$$

$$Cov(\hat{\tau}_{ij} - \hat{\tau}_{i0}, \hat{\tau}_{il} - \hat{\tau}_{i0}) = \frac{n-2}{pqu}, \tag{5.28}$$

$$Cov(\hat{\tau}_{ij} - \hat{\tau}_{i0}, \hat{\tau}_{kl} - \hat{\tau}_{k0}) = \begin{cases} \frac{m-2}{pqu} & \text{if i=k and } j \neq l \\ -\frac{1}{pqu} & \text{if } i \neq k \text{ and } j \neq l \end{cases}$$

for $k, i(i \neq l)$=1,2,...,p and j=1,2,...,q($l \neq j$).

3. The trace of the variance-covariance matrix which gives the sum of the variances of the estimators of the dual versus single treatment contrasts is 2(mn-2)/u.

A critical assessment of these designs can be summarized as follows:

Advantages:

1. connectedness,
2. highly efficient for small b(u=1),
3. all the required contrasts are made within each block,
4. the designs estimate all the contrasts of interest with equal precision,
5. easy to run practically, since one of the factors is kept at a constant level throughout each block.

Disadvantages:

1. i0 and j0 are replicated a large number of times, especially for $u \geq 2$,
2. the number of blocks is large,
3. the designs are less efficient for large b($u \geq 2$).

The following two examples illustrate these advantages and disadvantages.

Example 5.5 *For m=n=3 and b=8(u=1) we obtain the following design:*

*Block*1	*Block*2	*Block*3	*Block*4	*Block*5	*Block*6	*Block*7	*Block*8
11	12	21	22	11	12	21	22
01	02	01	02	10	10	20	20

For this design:

$$A = \begin{bmatrix} I_2 & 0_2 & -0.5\underline{1}_2' \otimes I_2 \\ 0_2 & I_2 & -0.5 I_2 \otimes \underline{1}_2' \\ -0.5\underline{1}_2 \otimes I_2 & -0.5 I_2 \otimes \underline{1}_2 & I_2 \otimes I_2 \end{bmatrix},$$

which illustrates the structure (5.9). Each of the treatments 01, 02, 10, 20, 11, 12, 21 and 12 is replicated twice. The variance-covariance matrix of the contrasts of interest is given below showing the structure of the variance-covariance matrix of a GPBDS design.

$$V = \begin{bmatrix} W & X \\ X' & W \end{bmatrix},$$

where $W = I_2 \otimes (I_2 - 0.5J_2) + J_2 \otimes (0.5I_2 - 0.25J_2)$ *and*

$$X = \begin{bmatrix} 0.25 & -0.25 & -0.25 & 0.25 \\ -0.25 & 0.25 & 0.25 & -0.25 \\ -0.25 & 0.25 & 0.25 & -0.25 \\ 0.25 & -0.25 & -0.25 & 0.25 \end{bmatrix}.$$

The trace of this matrix which equals the sum of the variances of the contrasts estimators of interests is 14. The bound b_m *is 12.637 and the discrepancy between* b_m *and the trace is* 11% *of the bound. This is the most efficient design which can be generated by JE.*

Example 5.6 *For m=n=3 and b=16(u=2), two copies of the design given in Example 5.5 give value 7 for the total of the variance of the contrasts of interest with 4 replications of each treatment combination. As an assessment of this design, we can compare it with the the most efficient design generated by JE, viz:*

*Block*1	01	11	*Block*9	01	10
*Block*2	01	21	*Block*10	01	20
*Block*3	02	12	*Block*11	02	10
*Block*4	02	22	*Block*12	02	20
*Block*5	10	11	*Block*13	11	12
*Block*6	10	12	*Block*14	11	21
*Block*7	20	21	*Block*15	12	22
*Block*8	20	22	*Block*16	21	22

which also has each treatment combination replicated 4 times, but is not a GPBDS design. The trace of the variance-covariance matrix is 6.761905 which is slightly better than the value 7 achieved by using two copies of the design given in Example 5.5.

Table 5.1 demonstrates that for u=1 the designs with $b \leq 18$ obtained by this approach are very efficient through a comparison with the bound from JE. Note that the high discrepancy with bound b_m is due to the poor performance of b_m for k=2(see Section 3.4). For $b > 18$, it is not practical to use JE for comparisons.

For 3 × 3 designs with u=2 the discrepancy with JE indicates that the designs constructed are less efficient for u=2 than u=1. Therefore, the application of this method is recommended only for small values of u, in particular, when u=1.

Table 5.1: Assessment[1] of designs for k=2^2.

$n \times m$	u=1		u=2	
	b_m	JE	b_m	JE
3 × 3	11.0%	0%	11.0%	4.2%
3 × 4	11.7%	0%	11.7%	†
4 × 4	11.5%	0%	11.5%	†
3 × 5	13.0%	0%	13.0%	†
4 × 5	18.5%	0%	18.5%	†

5.5.2 Constructing GPBDS Designs with k=3:

Since we are interested in contrasts $\tau_{ij} - \tau_{i0}$ and $\tau_{ij} - \tau_{0j}$, a natural construction method is to accommodate in each block treatment combinations ij, $i0$ and $0j$, for i=1,2,...,n-1 and j=1,2,...,m-1. Such a design will have b=pq blocks, and replications of 1, q and p for treatment combinations ij, $i0$ and $0j$ respectively, where p=n-1 and q=m-1. If we require more replication of the treatments and a greater number of blocks we might consider using duplicates of the above set of blocks.

Suppose our design consists of u replicates of the given design, then it can be shown that:

$$C_1 \Omega C_1' = \frac{1}{2pqu}\{qI_q \otimes (3pI_p + J_p) + J_q \otimes (pI_p - J_p)\}, \tag{5.29}$$

and

$$C_2 \Omega C_2' = \frac{1}{2pqu}\{pI_p \otimes (3qI_q + J_q) + J_p \otimes (qI_q - J_q)\}. \tag{5.30}$$

Therefore for the designs of this kind:

1. For the dual versus B, i.e. contrasts $\tau_{ij} - \tau_{0j}$, we have:

$$V(\hat{\tau}_{ij} - \hat{\tau}_{0j}) = \frac{3mn - 2m - 2n}{2pqu},$$

[1]JE denotes the discrepancy between the total variance of the design and the minimum value of $tr(C\Omega C')$ obtained by the algorithm of Jones and Eccleston(1980).

[2]†denotes that the design has more than 18 blocks.

$$Cov(\hat{\tau}_{ij} - \hat{\tau}_{0j}, \hat{\tau}_{lj} - \hat{\tau}_{0j}) = \frac{m-2}{2pqu}, \tag{5.31}$$

$$Cov(\hat{\tau}_{ij} - \hat{\tau}_{0j}, \hat{\tau}_{kl} - \hat{\tau}_{0l}) = \begin{cases} \frac{n-2}{2pqu} & \text{if i=k and } j \neq l \\ -\frac{1}{2pqu} & \text{if } i \neq k \text{ and } j \neq l \end{cases}$$

for $k, i(i \neq l)$=1,2,...,p and j=1,2,...,q($l \neq j$).

2. For the dual versus A contrasts, i.e. $\tau_{ij} - \tau_{i0}$, we have:

$$V(\hat{\tau}_{ij} - \hat{\tau}_{i0}) = \frac{3mn - 2m - 2n}{2pqu},$$

$$Cov(\hat{\tau}_{ij} - \hat{\tau}_{i0}, \hat{\tau}_{il} - \hat{\tau}_{i0}) = \frac{n-2}{2pqu}, \tag{5.32}$$

$$Cov(\hat{\tau}_{ij} - \hat{\tau}_{i0}, \hat{\tau}_{kl} - \hat{\tau}_{k0}) = \begin{cases} \frac{m-2}{2pqu} & \text{if i=k and } j \neq l \\ -\frac{1}{2pqu} & \text{if } i \neq k \text{ and } j \neq l \end{cases}$$

for $k, i(i \neq l)$=1,2,...,p and j=1,2,...,q($l \neq j$).

3. The trace of the variance-covariance matrix which gives the sum of the variances corresponding to the dual versus single treatment contrasts is (3mn-2m-2n)/u.

These designs have the following advantages and disadvantages:

Advantages:

1. connectedness,
2. highly efficient for small b(u=1),
3. all the required contrasts are made within each block,
4. the designs estimate all the contrasts of interest with the same precision,
5. easy to run practically since, within each block, one level for A and one level for B are used alone and in combination.

Disadvantages:

1. treatment combinations i0 and j0 are replicated a large number of times, especially for $u \geq 2$,
2. the number of blocks is large,
3. the designs are less efficient for large b($u \geq 2$).

The following two examples show these advantages and disadvantages.

Example 5.7 *For m=n=3 and u=1 the trace of the variance-covariance matrix is 15. This design is the most efficient design which can be generated by using JE. The variance-covariance matrix is:*

$$V = 2 \times \begin{bmatrix} W & Y \\ Y' & W \end{bmatrix},$$

where $W = I_2 \otimes (0.76I_2 + 0.12J_2) + J_2 \otimes (0.12I_2 - 0.06J_2)$ *and*

$$Y = \begin{bmatrix} 0.56 & -0.06 & -0.06 & 0.06 \\ -0.06 & 0.06 & 0.56 & -0.06 \\ -0.06 & 0.56 & 0.06 & -0.06 \\ 0.06 & 0.06 & -0.06 & 0.56 \end{bmatrix}.$$

Example 5.8 *For u=2 in Example 5.7, the method gives the value 7.5 for tr(C Ω C'). While the most efficient design generated by JE gives the value 6.75 for the tr($C\Omega C'$). The discrepancy between tr($C\Omega C'$) of the constructed design and that of JE is 11%.*

Table 5.2 shows that for u=1 the designs obtained by this approach are highly efficient. As it is clear from the table the designs are poorer for u=2 and it appears that for bigger values of u the discrepancy with the bound given by JE becomes worse. Therefore, the application of this method is recommended for small values of u only, in particular, when u=1.

Table 5.2: Discrepancies[3] of designs for k=3[4].

$n \times m$	u=1	u=2
3×3	0%	11.0%
3×4	0%	15.0%
4×4	0%	21.0%
3×5	0%	21.0%
4×5	0%	31.%†

5.6 Designs for Symmetric Factorial Experiments:

We now consider the case when m=n. We obtain a simplification of Theorem 5.1 which leads to a simpler evaluation of a bound on the trace of the variance-covariance matrix for the contrasts of interest.

To establish this we can apply the permutation method using a larger set of permutations on A. This is equivalent to operating on the matrix $\bar{A}$ defined in (5.6) in the following way.

Let $\bar{A}$ be the average of the A-matrix over all permutation matrices as described in (5.6). Then define

$$\bar{A}_1 = \begin{bmatrix} 0 & I_p & 0 \\ I_p & 0 & 0 \\ 0 & 0 & E \end{bmatrix} \bar{A} \begin{bmatrix} 0 & I_p & 0 \\ I_p & 0 & 0 \\ 0 & 0 & E' \end{bmatrix}, \tag{5.33}$$

where E is given in (5.3), and define

$$\bar{A}_2 = \frac{1}{2}(\bar{A} + \bar{A}_1). \tag{5.34}$$

Observe that $tr(\bar{A}_1) = tr(\bar{A}) = tr(\bar{A}_2)$.

Corollary 5.4 *For any connected design, when n=m,*

$$\Phi(A) \geq \Phi(\bar{A}) \geq \Phi(\bar{A}_2). \tag{5.35}$$

Proof: If we define Φ as in (5.8), then by the convexity of Φ(Majumdar, 1986), we obtain the required inequalities.♣

[3]Compared with JE.

[4]†This design has more than 18 blocks. The bound shown is b_m.

This corollary gives a simplification of Theorem 5.1, when n=m. The structure of $\bar{A}_2$, as we will show in the following lemma, is much simpler than the structure of $\bar{A}$ and the evaluation of $tr(C\bar{\Omega}_2C')$ is much easier than that of $tr(C\bar{\Omega}C')$.

Lemma 5.3 *Matrix $\bar{A}_2$ given in (5.34) has the following structure*

$$\bar{A}_2 = \begin{bmatrix} a_1^*I_p + b_1^*J_p & c^*J_{p\times p} & \underline{1}_p' \otimes (a_2^*I_p + b_2^*J_p) \\ & a_1^*I_p + b_1^*J_p & (a_2^*I_p + b_2^*J_p) \otimes \underline{1}_p' \\ & & I_p \otimes (a_5^*I_p + b_5^*J_p) + J_p \otimes (b_5^*I_p + b_6^*J_p) \end{bmatrix}, \tag{5.36}$$

where

$$\begin{array}{ll} a_1^* = (a_1 + a_3)/2 & b_1^* = (b_1 + b_3)/2, \\ a_2^* = (a_2 + a_4)/2 & b_2^* = (b_2 + b_4)/2, \\ a_5^* = a_5 & b_5^* = (a_6 + b_5)/2, \\ c^* = c & b_6^* = b_6 \end{array} \tag{5.37}$$

Proof: The result follows directly from Lemma 5.1 and from evaluating $\bar{A}_1$ in (5.33).♣

Example 5.9 *For m=n=3, b=8 and k=3, Example 5.1 shows how the design with the A-matrix similar to the structure of $\bar{A}_2$ is a very efficient design.*

In the following section, we give two methods of constructing GPBDS designs for m=n. The first method is similar to the method when k=2 or k=3. The second approach is based on group divisible designs.

5.6.1 Designs Arranged in Blocks of Size k=n:

When n=m GPBDS designs with block size n can be constructed by taking the union of the following two sets of blocks:

SET 1 : Accommodate ij(j=0,1,.. .,p) in the ith block for i=1,2,...,p.

SET 2 : Accommodate ij(i=0,1,.. .,p) in the jth block for j=1,2,...,p.

The resulting design will be a GPBDS design.

Example 5.10 *For m=n=k=3 the design consists of:*

SET 1		SET 2
10 11 12	and	01 11 21
20 21 22		02 12 22

has concurrence matrix:

$$NN' = \begin{bmatrix} I & 0 & \underline{1}' \otimes I \\ 0 & I & I \otimes \underline{1}' \\ \underline{1} \otimes I & I \otimes \underline{1} & I \otimes J + J \otimes I \end{bmatrix},$$

showing that it is a GPBDS design.

This design is the most efficient design which can be generated by JE. The total variance for this design is 15.04. The structure of the variance-covariance matrix is very similar to the structure of the A-matrix of the design and it is totally variance-balanced.

For n=3, the combination of the blocks in Example 5.10 with those in the design for k=3 in Section 5.5.2 gives the following highly efficient GPBDS design whose variance properties was discussed in Example 5.1:

Example 5.11 *For m=n=k=3 and b=8, the following design which consists of two sets each of 4 blocks; one set is constructed by the approach in Section 5.5.2 and the other set is given in Example 5.10, is a GPBDS design and the most efficient design which can be obtained by JE. The design is:*

SET 1				SET 2		
11	10	01		10	11	12
12	10	02	+	20	21	22
21	20	01		01	11	21
22	20	02		02	12	22

The total variance for the resulting design is 6.429 which is less than half of the total variance for each SET 1 and SET 2 which both give the value 15.04(15.04/2= 7.52). The discrepancy between b_m and this value is 1.3% of the bound which shows that the design is very efficient.

Numerical computations shows that for m=n=k=3 and b=4u, where u is an integer, then if u is even, the design composed of u/2 copies of each of the above

SETS 1 and 2 is very efficient. If u is odd, then [u/2] copies of SET 1 together with [u/2]+1 copies of SET 2 is very efficient, where [.] denotes "integer part of ". A design of equal efficiency is obtained from [u/2]+1 copies of SET 1 together with [u/2] copies of SET 2. The results for u=1, 2, 3 and 4 are given in Table 5.3.

Table 5.3 Designs and their discrepancies.

u	design	discrepancy	
		JE	b_m
1	1 copy of Set 1 or 1 copy of Set 2	0%	19%
2	1 copy of Set 1 + 1 copy of Set 2	0%	1.7%
3	1 copy of Set 1 + 2 copies of Set 2	0%	3.3%
	or		
	2 copies of Set 1 + 1 copy of Set 2	0%	"
4	2 copies of Set 1 + 2 copies of Set 2	0%	1.7%

5.6.2 Designs Arranged in Two Group Divisible Designs:

Suppose there exists a Group Divisible design with the parameters t=n(n-1), b, k, r, m_1=n-1, m_2=n, λ_1 and λ_2. Then if we construct the following two sets of blocks and combine them together, the resulting design is totally variance-balanced and belongs to the GPBDS class of designs:

SET 1 : Let i0,i1, i2,...,ip be the first associates and the other treatment combinations, excluding {0j;j=1,2,...,p}, be the second associates(i=1,2,...,p).

SET 2 : Let 0j,1j,2j,...,pj be the first associates and the other treatment combinations, excluding {i0;i=1,2,...,p}, be the second associates(j=1,2,...,p).

Example 5.12 *For n=3, t=6, b=12, k=4, using the group divisible design R94 of Clatworthy(1973,p200) we obtain a design with total variance of 3.504. The discrepancy between this and* b_m *given in Section 3.5 of Chapter 3 is* 25% *of the bound. The design has totally variance-balanced property. However, a better design generated by JE is not totally variance-balanced and has total variance of 2.904 with discrepancy* 4%.

The variance-covariance matrix of the design consisting of SETS 1 and 2 is:

$$V = 2 \times \begin{bmatrix} W & Z \\ Z' & W \end{bmatrix},$$

where $W = I_2 \otimes (0.066I_2 + 0.136J_2) + J_2 \otimes (0.003I_2 + 0.014J_2)$ *and*

$$Z = \begin{bmatrix} 0.047 & -0.017 & 0.017 & -0.014 \\ -0.017 & -0.014 & 0.047 & -0.017 \\ -0.017 & 0.047 & -0.014 & -0.017 \\ -0.140 & -0.017 & -0.017 & 0.047 \end{bmatrix}.$$

We have considered Clatworthy(1973) to find how many designs can be constructed by this approach. There are 39 designs which can be generated from Clatworthy. The following table gives these GD designs and their discrepancies with the bound b_m(see Chapter 3, Section 3.5). For only four designs constructed by this technique, JE can be applied($k \leq 18$). The discrepancy of these designs with the bound obtained by the algorithm is given as a second value in Table 5.4.

Table 5.4 : Assessments of designs constructed from group divisible designs of Clatworthy[5].

n	Design reference and corresponding discrepancies
3	SR6(50,40) SR7(50), SR8(50), R20(23), R25(20), R43(25), R45(23), R47(21), R49(20), R52(31), R53(19), R94(25,21), R95(25).
4	S53(26,21), S54(28,21), S55(28), S56(28), S57(28), SR26(46), SR27(46), SR68(39), R38(46), R72(32), R76(29), R111(39), R143(29), R146(29), R167(31), R174(30), R193(28).
5	S106(33), S107(34), S108(34), SR46(48), SR47(48), R124(38), R179(41).
8	SR88(54).
9	SR98(100).

Comment: As is clear from Table 5.4, these designs are not very efficient compared with b_m and are not recommended. However their construction is very easy and all the contrasts of interest are estimated with the same precision.

[5]SR6 is the reference from Clatworthy and 50 denotes the percentage discrepancy between b_m and the design constructed from SR6 by the above method.

Conclusions: In this chapter we have given a series of overall A-optimal designs when each of the two factors has more than two levels and $k \geq t$ and 00 cannot be used. Our attempt to find general results on A-optimal designs included the case $k < t$, but it was not successful due to calculation difficulties described in Section 5.3. Pursuit of this general problem is a topic for future work. However, for the sake of practical needs we have given some construction methods producing designs in the GPBDS class some of which are shown to be highly efficient.

Chapter 6

Completely Randomized Designs and Weighted A-optimal Designs:

6.1 Introduction:

In previous chapters we considered block designs which are efficient for estimating the dual versus single treatment contrasts. In the present chapter we first consider the A-optimal completely randomized design for the contrasts of interest for a general $n \times m$ censored factorial experiment in which treatment combination 00 is excluded from the experiment. Then we consider completely randomized designs and block designs which are efficient for cases in which the two sets of contrasts dual versus A and dual versus B are not of equal interest. Finally, we establish a design-dependent bound on the weighted sum of the total variances of each set of these contrasts.

6.2 A-optimal Completely Randomized Designs for $n \times m$ Censored Factorial Experiments:

In this section we consider an $n \times m$ censored factorial experiment conducted in a completely randomized design and characterize A-optimal designs in terms of the numbers of replications of each treatment combination involved in the design.

6.2.1 Contrasts and Goal of Experiments:

Suppose an $n \times m$ censored factorial experiment is conducted in a completely randomized design consisting of N homogeneous units with treatment combination 00 being excluded or censored. Suppose that the contrasts of interest are the dual versus A and the dual versus B contrasts defined in Chapter 1(1.12). Then we want to characterize those designs which minimize

$$\sum_{i=1}^{n-1}\sum_{j=1}^{m-1}\{V(\hat{\tau}_{ij}-\hat{\tau}_{i0})+V(\hat{\tau}_{ij}-\hat{\tau}_{0j})\} \tag{6.1}$$

among all possible competing designs.

Let $D(t,N)$ denotes the class of all possible completely randomized designs with t=mn-1 treatments arranged in N units. Also let:

$$A=\{10,20,...,p0\},$$

$$B=\{01,02,...,0q\}, \tag{6.2}$$

$$D=\{11,12,...,1q,21,22,...,2q,.....,p1,p2,...,pq\};$$

where $p=n-1$ and $q=m-1$.

Also for $d \in D(t,N)$, let n_{Ai}, n_{Bj} and n_{Dij} denote the respective number of replications of treatment combinations i0, 0j and ij in the design, where i=1,2,...,p, j=1,2,...,q, and T_B, T_A and T_D denote the total numbers of units receiving treatments from sets B, A and D respectively in the design d, i.e.

$T_B=\sum_{j=1}^{m-1} n_{Bj}$, $T_A=\sum_{i=1}^{n-1} n_{Ai}$ and $T_D=\sum_{i=1}^{n-1}\sum_{j=1}^{m-1} n_{Dij}$.

6.2.2 Sum of the Variances of the Contrasts:

It can be shown that for a completely randomized design:

$$\sum_{i=1}^{p}\sum_{j=1}^{q}\{V(\hat{\tau}_{ij}-\hat{\tau}_{i0})+V(\hat{\tau}_{ij}-\hat{\tau}_{0j})\}=p\sum_{j=1}^{q}\frac{1}{n_{Bj}}+q\sum_{i=1}^{p}\frac{1}{n_{Ai}}+2\sum_{j=1}^{q}\sum_{i=1}^{p}\frac{1}{n_{Dij}}, \tag{6.3}$$

where p=n-1 and q=m-1. Our aim is to find those designs which minimize (6.3).

6.2.3 Towards A-optimal Designs:

In this section we characterize A-optimal completely randomized designs for the estimators of the contrasts of interest, in terms of the replications of the treatment combinations involved in the design. In other words by, (6.3), a design $d \in D(t, N)$ is A-optimal if it minimizes the function:

$$p\sum_{j=1}^{q}\frac{1}{n_{Bj}} + q\sum_{i=1}^{p}\frac{1}{n_{Ai}} + 2\sum_{j=1}^{q}\sum_{i=1}^{p}\frac{1}{n_{Dij}} \tag{6.4}$$

over all possible designs in D(t,N).

Assume the total number of units of the design, N, is fixed. Then the problem is to minimize the expression in (6.4) subject to the condition:

$$\sum_{j=1}^{q} n_{Bj} + \sum_{i=1}^{p} n_{Ai} + \sum_{j=1}^{q}\sum_{i=1}^{p} n_{Dij} = N. \tag{6.5}$$

Now we can prove a theorem which enables us to find A-optimal designs.

Theorem 6.1 *If for $d \in D(t, N)$, t_B, t_A and t_D are fixed integers denoting the total number of units receiving a B alone, a A alone and a dual treatment respectively such that $t_B + t_A + t_D = N$, then minimizing the expressions*

(i) $\sum_{j=1}^{m-1}\frac{1}{n_{Bj}}$ *subject to the condition that t_B is fixed,*

(ii) $\sum_{i=1}^{n-1}\frac{1}{n_{Ai}}$ *subject to the condition that t_A is fixed,* (6.6)

(iii) $\sum_{j=1}^{m-1}\sum_{i=1}^{n-1}\frac{1}{n_{Dij}}$ *subject to the condition that t_D is fixed,*

is equivalent to minimizing:

$$p\sum_{j=1}^{q}\frac{1}{n_{Bj}} + q\sum_{i=1}^{p}\frac{1}{n_{Ai}} + 2\sum_{j=1}^{q}\sum_{i=1}^{p}\frac{1}{n_{Dij}}, \tag{6.7}$$

subject to condition (6.5).

Proof: If t_B, t_A and t_D are fixed then (i)-(iii) can be regarded as independent. Therefore the global minimum of (6.5) under the given condition will be obtained by minimizing each expressions in (i)-(iii) individually. Hence minimizing (i)-(iii) independently subject to the required condition is equivalent to minimizing:

$$p\sum_{j=1}^{q}\frac{1}{n_{Bj}} + q\sum_{i=1}^{p}\frac{1}{n_{Ai}} + 2\sum_{j=1}^{q}\sum_{i=1}^{p}\frac{1}{n_{Dij}}. \tag{6.8}$$

Hence the Theorem is proved.♣

Now we give a theorem which characterizes A-optimal designs in terms of t_B, t_A and t_D.

Theorem 6.2 *For $d \in D(t, N)$, let T_B, T_A and T_D denote the total numbers of units in d which are assigned to treatment combinations in sets B, A and D respectively. Then design d is A-optimal if:*

$$f(T_B, T_A, T_D) = \min f(t_B, t_A, t_D), \tag{6.9}$$

for all $(t_B, t_A, t_D) \in \Xi$, where

$$f(t_B, t_A, t_D) = \frac{p(2q\bar{r}_B + q - t_B)}{\bar{r}_B(\bar{r}_B + 1)} + \frac{q(2p\bar{r}_A + p - t_A)}{\bar{r}_A(\bar{r}_A + 1)} + \frac{2(2pq\bar{r}_D + pq - t_D)}{\bar{r}_D(\bar{r}_D + 1)}, \tag{6.10}$$

where $\bar{r}_i = [\frac{t_i}{m_i}]$ for i=B, A and D, $m_B = q$, $m_A = p$, $m_D = pq$, [.] denotes "the integer part of " and

$$\Xi = \{(t_B, t_A, t_D); t_B \geq q, t_A \geq p, t_D \geq pq; t_B + t_A + t_D = N\}.$$

Proof: By assuming t_B, t_A, and t_D fixed and by applying Theorem 6.1 and Lemma 3.2 on page 72, we will get the required expression for $f(t_B, t_A, t_D)$. Then if we let t_B, t_A and t_D vary over all Ξ, the global minimum of $f(t_B, t_A, t_D)$ will be $f(T_B, T_A, T_D)$, which is the minimum value for the total variance of the contrasts of interest. Since design d achieves this minimum value, d is A-optimal.♣

The following theorem gives a particular series of A-optimal completely randomized designs for the contrasts of interest, by establishing the number of units to be allocated to each of the (t-1) treatment combinations.

Theorem 6.3 *Consider a completely randomized design d$\in D(t, N)$, where $N \equiv 0 \bmod\{2p_1q_1(p_1+q_1+2p_1q_1)\}$ for $p_1 = \sqrt{(n-1)/2}$ and $q_1 = \sqrt{(m-1)/2}$ integers. Then if the numbers of replications in d of each treatment combination belonging to the respective sets B, A and D are:*

$$\begin{aligned} n_B &= \frac{N}{2q_1(p_1 + q_1 + 2p_1q_1)}, \\ n_A &= \frac{N}{2p_1(p_1 + q_1 + 2p_1q_1)} \\ \text{and } n_D &= \frac{N}{2p_1q_1(p_1 + q_1 + 2p_1q_1)}, \end{aligned} \tag{6.11}$$

then d is overall A-optimal.

Proof: For any d$\in D(t,N)$ with excluded treatment combination 00, by expression (6.3) we have:

$$\sum_{i=1}^{p}\sum_{q}^{m-1}\{V(\hat{\tau}_{ij}-\hat{\tau}_{i0})+V(\hat{\tau}_{ij}-\hat{\tau}_{0j})\} = p\sum_{j=1}^{q}\frac{1}{n_{Bj}}+q\sum_{i=1}^{p}\frac{1}{n_{Ai}}+2\sum_{j=1}^{q}\sum_{i=1}^{p}\frac{1}{n_{Dij}}. \quad (6.12)$$

But under the given condition we have:

$$\sum_{i=1}^{p}\sum_{j=1}^{q}\{V(\hat{\tau}_{ij}-\hat{\tau}_{i0})+V(\hat{\tau}_{ij}-\hat{\tau}_{0j})\} = 2({p_1}^2\sum_{j=1}^{q}\frac{1}{n_{Bj}}+{q_1}^2\sum_{i=1}^{p}\frac{1}{n_{Ai}}+\sum_{j=1}^{q}\sum_{i=1}^{p}\frac{1}{n_{Dij}}). \quad (6.13)$$

Then the problem is to minimize (6.13) subject to the condition:

$$\sum_{j=1}^{q}n_{Bj}+\sum_{i=1}^{p}n_{Ai}+\sum_{j=1}^{q}\sum_{i=1}^{p}n_{Dij}=N. \quad (6.14)$$

Employing a Lagrangian Multiplier, λ , we obtain n_B, n_A and n_D as in the theorem.♣

Example 6.1 *For m=n=3 we have $p_1 = q_1 = 1$. Hence for $N \equiv 0(mod8)$, i.e. $N = 8u(u \geq 1)$, the design with $n_B = n_A = n_D = u$ is A-optimal. Thus, for example, the A-optimal design for a 3×3 experiment in 16 units with 00 excluded has every treatment combination replicated twice.*

A computer algorithm in Fortran has been written to find those values of $(T_B, T_A, T_D) \in \Xi$ which minimize $f(t_B, t_A, t_D)$ over all possible $(t_B, t_A, t_D) \in \Xi$. This algorithm is given in Appendix B at the end of the thesis.

To illustrate the use of this algorithm a selection of A-optimal designs is given in Table 6.1 at the end of this chapter. The designs selected are all those having parameter values in the range $3 \leq m, n \leq 10$ and $N \leq 100$ and which have equal treatment replication within sets A, B and D. It should be noted that, in general, the A-optimal designs are not equi-replicate. The algorithm can be used to provide designs for parameter values leading to nonequi-replicate A-optimal designs, but these have not been tabulated here.

6.3 Weighted A-optimal Designs:

So far we have considered those designs which are efficient for the cases in which the estimation of both sets of contrasts, dual versus A and dual versus

B, were of equal of importance. However, experiments are often carried out in which one set of contrasts is more important than the other. Different criteria will, therefore, be needed for choosing designs appropriate for such experiments. Pearce(1975) proposes maximizing the weighted mean of the efficiency factors of interest. Freeman(1976b) suggests minimizing the weighted mean(sum) given by $\sum_{i=1}^{\ell} w_i V(C_i'\hat{\underline{\tau}})$, where $C_i'\underline{\tau}$ represents a contrast of interest and $w_i \geq 0$ is the weight to be attached to this contrast. In other words if w^{δ} denotes a diagonal matrix with weights on its diagonal and C is the contrast matrix of interest, the criterion is one of minimizing

$$tr(w^{\delta/2} C \Omega C' w^{\delta/2}) = tr(\Omega C' w^{\delta} C). \tag{6.15}$$

The difficulty is choosing appropriate weights, as the choice in practice is most likely to be a highly subjective one. Jones and Eccleston(1980) have given a computer algorithm to derive optimal block designs using criterion (6.15). We will use the criterion suggested by Freeman(1976b), since it has statistical meaning in our case.

Let w_A and w_B denote the weights (representing the degrees of importance) for the dual versus A and dual versus B contrast estimators respectively, then the sum of the weighted variances is:

$$\sum_{i=1}^{p} \sum_{j=1}^{q} \{w_A V(\hat{\tau}_{ij} - \hat{\tau}_{i0}) + w_B V(\hat{\tau}_{ij} - \hat{\tau}_{0j})\}. \tag{6.16}$$

Definition 6.1 *If a design d has minimum value for*

$$\sum_{i=1}^{p} \sum_{j=1}^{q} \{w_A V(\hat{\tau}_{ij} - \hat{\tau}_{i0}) + w_B V(\hat{\tau}_{ij} - \hat{\tau}_{0j})\} \tag{6.17}$$

over all possible designs, where w_A and $w_B \geq 0$, then d is **Weighted A-optimal** *with respect to the weights w_A and w_B and will be denoted by* **WA(w_A, w_B)-optimal.**

In the next section we derive results which enable the overall WA(w_A, w_B)-optimal completely randomized design to be specified for a limited selection of weights. In the later sections we investigate the same problem for block designs.

6.3.1 WA(w_A, w_B)-optimal Design Arranged in a Completely Randomized Design:

For any completely randomized design it can be shown, by expanding (6.16), that the sum of the weighted variances of the estimators of the dual versus single treatment contrasts is:

$$pw_B \sum_{j=1}^{q} \frac{1}{n_{Bj}} + qw_A \sum_{i=1}^{p} \frac{1}{n_{Ai}} + (w_A + w_B) \sum_{j=1}^{q} \sum_{i=1}^{p} \frac{1}{n_{Dij}}, \tag{6.18}$$

where p=n-1, q=m-1 and n_{Bj}, n_{Ai} and n_{Dij} are defined in Section 6.2.1.

The following theorem specifies the treatment replications for WA-optimal completely randomized designs.

Theorem 6.4 *The design d∈ $D(t, N)$ is WA(w_A, w_B)-optimal if $\sqrt{pw_B}$,$\sqrt{qw_A}$ and $\sqrt{w_A + w_B}$ are integer values, $N \equiv 0(mod N_1)$ and*

$$\begin{aligned} n_{Bj} &= \frac{N\sqrt{pw_B}}{N_1}, \\ n_{Ai} &= \frac{N\sqrt{qw_A}}{N_1}, \\ n_{Dij} &= \frac{N\sqrt{w_A + w_B}}{N_1}, \end{aligned} \tag{6.19}$$

where $N_1 = q\sqrt{pw_B} + p\sqrt{qw_A} + pq\sqrt{w_A + w_B}$ and n_{Bj}, n_{Ai} and n_{Dij} give the replications of the treatment combinations 0j, i0 and ij respectively(i=1,2,...,p; j=1,2,...,q).

Proof: The problem is to find integer values n_{Bj}, n_{Ai} and n_{Dij} which minimize the function:

$$pw_B \sum_{j=1}^{q} \frac{1}{n_{Bj}} + qw_A \sum_{i=1}^{p} \frac{1}{n_{Ai}} + (w_A + w_B) \sum_{j=1}^{q} \sum_{i=1}^{p} \frac{1}{n_{Dij}} \tag{6.20}$$

subject to the condition that

$$\sum_{j=1}^{q} n_{Bj} + \sum_{i=1}^{p} n_{Ai} + \sum_{j=1}^{q} \sum_{i=1}^{p} n_{Dij} = N. \tag{6.21}$$

By applying a Lagrange Multiplier, (6.20) is minimized if:

$$n_{Bj} = \frac{N\sqrt{pw_B}}{N_1},$$

$$n_{Ai} = \frac{N\sqrt{qw_A}}{N_1}$$

and

$$n_{Dij} = \frac{N\sqrt{w_A + w_B}}{N_1}$$

for $i = 1, 2, ..., p$ and $j = 1, 2, ..., q$.♣

The following corollary is a special case of Theorem 6.4.

Corollary 6.1 *For $w_B = p$, $w_A = q$ and $p + q = x^2$, where $x > 0$ is an integer, the treatment replications which minimize the sum of the weighted variances(6.18) in a completely randomized design of size N, where $N \equiv 0\{modpq(2 + x)\}$, are obtained by substituting $w_B = p$, $w_A = q$.*

Example 6.2 *For a 3×3 experiment, p=q=2 giving x=2 and $N_1 = 16$. If we let N=16l, for l any positive integer, then the values $n_{Bj} = n_{Ai} = n_{Dij} = 2l$ give the WA(2,2)-optimal design. The same numbers of replications have been given in Table 6.1 for the A-optimal completely randomized designs for these parameter values, since in this example $w_A = w_B$.*

Example 6.3 *For a 6×5 experiment, p=5 and q=4 giving $x^2 = p + q = 9$ and x=3. If N=100, then $n_{Bj} = 5$, $n_{Ai} = 4$ and $n_{Dij} = 3$ give the replications for the WA(4,5)-optimal design.*

For the same parameter values if $w_A = w_B$ then $n_{Bj} = 4$, $n_{Ai} = 5$ and $n_{Dij} = 3$ give the A-optimal replications(see Table 6.1).

6.3.2 WA(w_A, w_B)-optimal $n \times 2$ Censored Factorial Experiments Arranged in Block Designs:

As we have seen in Chapter 5, a characterization of the unweighted A-optimal design in a general $n \times m$ censored factorial experiment arranged in blocks with treatment combination 00 censored is very complicated. However, for big values of k compared with t=mn-1, there are cases in which we can characterize a family of A-optimal designs for comparing dual treatments with single treatments. In this section we first consider weighted A-optimal block design for the $n \times 2$ factorial experiment. Then a general $n \times m$ censored factorial experiment arranged in block designs will be considered for some specific circumstances.

6.3.2.1 Weighted A-optimal Designs for $n \times 2$ Factorial Experiments:

Let M denote the information matrix for the estimators of the dual treatment versus single treatment contrasts as defined in Chapter 2(2.12) and $\bar{M}$ denote the average of M over all permutations given in (4.3) in Chapter 4. Also let

$$w^{\delta} = \begin{pmatrix} w_B I_p & 0 \\ 0 & w_A I_p \end{pmatrix}, \tag{6.22}$$

where p=n-1.

Now we are in a position to give a theorem which leads us to characterize WA-optimal designs in our context. But first we need to give some lemmas.

Lemma 6.1 *If $Y = aI_m + bJ_m$ is a nonsingular matrix, then*

$$tr(Y^{-1}) = \frac{1}{a+mb} + \frac{m-1}{a}. \tag{6.23}$$

Proof: It can be shown that Y has eigenvalues a+mb and a with multiplicities 1 and m-1 respectively. Also we have

$$tr(Y^{-1}) = \sum_{i=1}^{m} \lambda_i^{-1},$$

where λ_i is the eigenvalue of Y. The proof follows immediately from here.♣

Lemma 6.2 *Let*

$$X = \begin{pmatrix} x_1 I_m + y_1 J_m & x_2 I_m + y_2 J_m \\ x_2 I_m + y_2 J_m & x_3 I_m + y_3 J_m \end{pmatrix}$$

be a nonsingular matrix. Also let

$$X^{-1} = \begin{bmatrix} X^{11} & X^{12} \\ X^{21} & X^{22} \end{bmatrix},$$

where $X^{21} = X'^{12}$.

Then we have

$$tr(X^{11}) = \frac{(m-1)x_3}{x_1x_3 - x_2^2} + \frac{d_3}{d_1d_3 - d_2^2},$$

and

$$tr(X^{22}) = \frac{(m-1)x_1}{x_1x_3 - x_2^2} + \frac{d_1}{d_1d_3 - d_2^2},$$

where $d_1 = x_1 + my_1$, $d_2 = x_2 + my_2$ and $d_3 = x_3 + my_3$.

Proof: Let $X_{11} = x_1 I_m + y_1 J_m$, $X_{12} = x_2 I_m + y_2 J_m$ and $X_{22} = x_3 I_m + y_3 J_m$. Then we have(Ref: Graybill,1983,p184)

$$(X^{11})^{-1} = X_{11} - X_{12}(X_{22})^{-1}X_{21}.$$

But

$$(X_{22})^{-1} = \frac{1}{x_3}\{I_m - \frac{y_3}{d_3}J_m\}.$$

On substitution after some algebra we obtain

$$(X^{11})^{-1} = aI_m + bJ_m,$$

where

$$a = \frac{x_1x_3 - x_2^2}{x_3},$$

$$b = y_1 - \frac{d_2(y_2x_3 - x_2y_3) + x_2y_2d_3}{x_3d_3}.$$

By applying Lemma 6.1 we get the required expression for $tr(X^{11})$. The proof of the second part follows similarly.♣

Theorem 6.5 *Suppose $\bar{M}$ is the average of M over all permutations as given in Chapter 4(4.3) and its elements are as given in Lemma 4.2. Then for the partition*

$$\bar{M}^{-1} = \begin{bmatrix} \bar{M}^{11} & \bar{M}^{12} \\ \bar{M}'^{12} & \bar{M}^{22} \end{bmatrix}, \tag{6.24}$$

we have

$$tr(\bar{M}^{11}) = \frac{(n-2)d_A}{d_Ad_D - d_{AD}^2} + \frac{q_A}{q_Aq_B - q_{AB}^2}, \tag{6.25}$$

$$tr(\bar{M}^{22}) = \frac{(n-2)(d_A + d_D - 2d_{AD})}{d_Ad_D - d_{AD}^2} + \frac{q_B}{q_Aq_B - q_{AB}^2},$$

where d_A, d_D, d_{AD}, q_A, q_B and q_{AB} were given in Chapter 4(4.15).

Proof: Since $\bar{M}$ has the same structure as X in Lemma 6.2, by using Lemmas 6.2 and 4.2, we obtain

$$\begin{aligned} x_1 &= d_A + d_D - 2d_{AD}, \\ d_1 &= q_A + q_D - 2q_{AD}, \\ x_2 &= -d_A + d_{AD}, \\ d_2 &= -q_{AB}, \\ x_3 &= d_A, \\ d_3 &= q_A. \end{aligned} \tag{6.26}$$

From here by using Lemma 6.2 and some algebra we get the required expressions.♣

Theorem 6.6 *Let w^{δ} be as defined in (6.22), then for any design $d \in n \times 2$ CFBD(00) we have:*

$$tr(w^{\delta/2}C\Omega C'w^{\delta/2}) \geq \frac{(n-2)\{(w_A + w_B)d_A + w_A d_D - 2w_A d_{AD}\}}{d_A d_D - d_{AD}^2} + \frac{w_B q_A + w_A q_B}{q_A q_B - q_{AB}^2}, \tag{6.27}$$

where d_A, d_D, d_{AD}, q_A, q_B and q_{AB} were given in Chapter 4(4.15).

Proof: Let for any positive definite matrix, X, define $\Phi(X) = tr(w^{\delta/2}X^{-1}w^{\delta/2})$, then Φ is a convex functin, i.e.

$$\frac{1}{(n-1)!}\sum_{i=1}^{(n-1)!} tr\{w^{\delta/2}(\pi_i M \pi_i')^{-1}w^{\delta/2}\} \geq tr(w^{\delta/2}\bar{M}^{-1}w^{\delta/2}),$$

where $\bar{M}$ is defined in (4.3). But we have

$$tr\{w^{\delta/2}(\pi_i M \pi_i')^{-1}w^{\delta/2}\} = tr\{w^{\delta/2}M^{-1}w^{\delta/2}\},$$

since if we partition M^{-1} as follows

$$M^{-1} = \begin{bmatrix} M^{11} & M^{12} \\ M^{21} & M^{22} \end{bmatrix},$$

then from (6.22) we obtain

$$w^{\delta/2}(\pi_i M \pi_i')^{-1}w^{\delta/2} = \begin{pmatrix} w_B p_i M^{11} p_i' & (w_B w_A)^{1/2} p_i M^{12} p_i' \\ (w_B w_A)^{1/2} p_i M^{21} p_i' & w_A p_i M^{22} p_i' \end{pmatrix}.$$

This implies that

$$tr\{w^{\delta/2}(\pi_i M \pi_i')^{-1}w^{\delta/2}\} = w_B tr(M^{11}) + w_A tr(M^{22}) = tr(w^{\delta/2}M^{-1}w^{\delta/2}).$$

Also we have

$$tr\{w^{\delta/2}\bar{M}^{-1}w^{\delta/2}\} = w_B tr(\bar{M}^{11}) + w_A tr(\bar{M}^{22}).$$

Applying Lemma 6.2 we will get the required expression in (6.27). Hence the result follows.♣

Corollary 6.2 *If in the statement of the Theorem 6.6, M denotes the information matrix of the contrasts of interest in a PBDS design, the inequality in (6.27) changes to equality.*

Proof: If the design is PBDS, then $M = \bar{M}$, and the proof follows.♣

6.3.2.2 Weighted A-optimal Designs for $n \times m$ Factorial Experiment:

In this section we try to characterize WA(w_A, w_B)-optimal designs for a general $n \times m$ censored factorial block design with 00 censored.

The generalization of Theorem 6.6 to $m > 2$ is very complicated because, as in Theorem 5.1, it is very difficult to calculate the bounds. However, there are cases in which the problem can be simplified. This simplification normally happens for those cases in which $k \geq t = mn - 1$. In this section we utilize all the notation which has been used so far, especially the notation of Chapter 3. The matrix of weights for this case is:

$$w^{\delta} = \begin{pmatrix} w_B I_\ell & 0 \\ 0 & w_A I_\ell \end{pmatrix}, \tag{6.28}$$

where ℓ=(n-1)(m-1), w_A and w_B are positive real values.

Theorem 6.7 *For an $n \times m$ CFBD(00) design we have*

$$tr(w^{\delta}C\Omega C') \geq p w_B \sum_{j=1}^{q} \frac{1}{r_{Bj}} + q w_A \sum_{i=1}^{p} \frac{1}{r_{Ai}} + (w_A + w_B) \sum_{i=1}^{p}\sum_{j=1}^{q} \frac{1}{r_{Dij}}, \tag{6.29}$$

where w^{δ} is given in (6.28) and C is defined in Chapter 1(1.12).

Proof: If r^{δ} denotes the diagonal replication matrix as given in (3.3) in Chapter 3, then by Lemma 3.1 there exists a g-inverse, Ω, such that $\Omega - r^{\delta}$ is non-negative definite. Then by Graybill(1983,p396) $w^{\delta}C(\Omega - r^{-\delta})C'$ is also a non-negative definite matrix. This implies that

$$tr(w^\delta C\Omega C') \geq tr(w^\delta Cr^{-\delta}C') = tr(C'w^\delta Cr^{-\delta}). \quad (6.30)$$

It can be shown that

$$C'w^\delta C = \begin{bmatrix} pw_B I_q & 0 & -w_B 1_p' \otimes I_q \\ 0 & qw_A I_p & -w_A I_p \otimes 1_q' \\ -w_B 1_p \otimes I_q & -w_A I_p \otimes 1_q & (w_A + w_B) I_l \end{bmatrix}. \quad (6.31)$$

Therefore we can show that

$$tr(C'w^\delta Cr^{-\delta}) = pw_B tr(r^{-B}) + qw_A tr(r^{-A}) + (w_A + w_B) tr(r^{-D}), \quad (6.32)$$

where r^B, r^A and r^D were defined in Chapter 3(3.3) and r^{-x} denotes the inverse of r^x. The result follows immediately from here.♣

Corollary 6.3 *If d is an $n \times m$ CFBD(00) design, such that $N'r^{-\delta}C' = 0$, then the inequality (6.29) becomes equality.*

Proof: Since $N'r^{-\delta}C' = 0$, it follows that

$$Ar^{-\delta}C' = (r^\delta - \frac{1}{k}NN')r^{-\delta}C' = C' - \frac{1}{k}NN'r^{-\delta}C' = C'. \quad (6.33)$$

On premultiplying (6.33)by $C\Omega$ and using the estimability condition $C\Omega A = C$, we obtain:

$$C\Omega C' = C\Omega Ar^{-\delta}C' = Cr^{-\delta}C'. \quad (6.34)$$

Thus $w^\delta C\Omega C' = w^\delta Cr^{-\delta}C'$. The result follows immediately.♣

Theorem 6.8 *In an $n \times m$ CFBD(00) design, let $T_B = \sum_{i=1}^q r_{Bi}$, $T_A = \sum_{i=1}^p r_{Ai}$ and $T_D = \sum_{i=1}^p \sum_{j=1}^q r_{Dij}$ be regarded as fixed and such that $T_B \geq q$, $T_A \geq p$, $T_D \geq pq$ and $T_A + T_D \leq bk - q$. Also let $\bar{r}_A = [T_A/p]$, $\bar{r}_B = [T_B/q]$ and $\bar{r}_D = [T_D/pq]$, then*

$$tr(w^\delta Cr^{-\delta}C') \geq pw_B \left\{ \frac{2q\bar{r}_B + q - T_B}{\bar{r}_B(\bar{r}_B + 1)} \right\} + qw_A \left\{ \frac{2p\bar{r}_A + p - T_A}{\bar{r}_A(\bar{r}_A + 1)} \right\} +$$

$$(w_A + w_B) \left\{ \frac{2pq\bar{r}_D + pq - T_D}{\bar{r}_D(\bar{r}_D + 1)} \right\}. \quad (6.35)$$

Proof: Follows from the fact that if T_A and T_D are regarded as fixed, then $T_B = bk - T_A - T_D$ is fixed, and the minimization of $tr(w^\delta C r^{-\delta} C')$ follows from Lemma 3.2.♣

The minimum value for $tr(w^\delta C r^{-\delta} C')$ in Theorem 6.8 is a function in terms of T_A and T_D only since p and q are fixed and $\bar{r}_A$, $\bar{r}_B$ and $\bar{r}_D$ are functions in terms of T_A, T_B and T_D respectively. Therefore let

$$F(T_A, T_D; w_A, w_B) = pw_B \left\{ \frac{2q\bar{r}_B + q - T_B}{\bar{r}_B(\bar{r}_B + 1)} \right\} + qw_A \left\{ \frac{2p\bar{r}_A + p - T_A}{\bar{r}_A(\bar{r}_A + 1)} \right\} +$$

$$(w_A + w_B) \left\{ \frac{2pq\bar{r}_D + pq - T_D}{\bar{r}_D(\bar{r}_D + 1)} \right\}. \tag{6.36}$$

Let $T_B = q\bar{r}_B + a_B$, where $0 \le a_B < q$, $T_D = pq\bar{r}_D + a_D$; $0 \le a_D < pq$ and $T_A = p\bar{r}_A + a_A$; $0 \le a_A < p$. Then if we substitute T_A, T_B and T_D from here into $F(T_A, T_D; w_A, w_B)$, we will obtain the function in terms of a_A, $\bar{r}_A$, a_B, $\bar{r}_B$ and a_D, $\bar{r}_D$, viz

$F(T_A, T_D; w_A, w_B)$

$$pq\left(\frac{w_B}{\bar{r}_B} + \frac{w_A}{\bar{r}_A} + \frac{w_A + w_B}{\bar{r}_D}\right) - \left\{ \frac{pw_B a_B}{\bar{r}_B(\bar{r}_B + 1)} + \frac{qw_A a_A}{\bar{r}_A(\bar{r}_A + 1)} + \frac{(w_A + w_B)a_D}{\bar{r}_D(\bar{r}_D + 1)} \right\}. \tag{6.37}$$

For given weights w_A and w_B a simple computer algorithm could be used to obtain weighted A-optimal designs with equal replication for the treatment combinations within each set in each block, by the following steps:

STEP 1 : Finding those values of T_A and T_B which minimize (6.37).

STEP 2 : Checking that T_A/p, T_D/pq and $(bk - T_A - T_D)/q$ are integers.

STEP 3 : Checking that $n_{Aij} = T_A/bp$, $n_{Di\ell j} = T_D/bpq$ and $n_{B\ell j} = (bk - T_A - T_D)/bq$ are integers.

STEP 4 : Checking that the incidence matrix N with $n_{B\ell j}$, n_{Aij} and $n_{Di\ell j}$ satisfies the condition $N' r^{-\delta} C = 0$. Then, if this condition is satisfied the design is weighted A-optimal.

The following theorem characterizes a family of weighted A-optimal designs.

Theorem 6.9 *Consider a design for an $n \times m$ experiment with block size $k \equiv 0\{mod\, pq(2 + x)\}$, where p=n-1, q=m-1 and $p + q = x^2$, for $x > 0$ an integer.*

If the design has the following numbers of replications within each block for any treatment combination belonging to sets B, A and D respectively:

$$n_B = \frac{k}{q(2+x)},$$

$$n_A = \frac{k}{p(2+x)}, \tag{6.38}$$

$$\textit{and } n_D = \frac{kx}{pq(2+x)},$$

then the design is WA(q,p)-optimal.

Proof: For any $d \in n \times m$ CFBD(00) if $N'r^{-\delta}C = 0$, then from Wu(1980) we have:

$$tr(w^{\delta}C\Omega C') = tr(Cr^{-\delta}C') = pw_B \sum_{j=1}^{q} \frac{1}{r_{Bj}} + qw_A \sum_{i=1}^{p} \frac{1}{r_{Ai}} + (w_A + w_B) \sum_{i=1}^{p} \sum_{j=1}^{q} \frac{1}{r_{Dij}}. \tag{6.39}$$

The problem is to minimize (6.39) subject to the condition:

$$\sum_{j=1}^{q} r_{Bj} + \sum_{i=1}^{p} r_{Ai} + \sum_{i=1}^{p} \sum_{j=1}^{q} r_{Dij} = bk, \tag{6.40}$$

where bk is the fixed total number of units.

Applying a Lagrange Multiplier, λ, we will get the required result. For those designs with n_A, n_B and n_D given in (6.38) as the respective number of replications for any treatment combination belonging to sets A, B and D, the condition $N'r^{-\delta}C = 0$ is satisfied. Hence the theorem is proved.♣

Example 6.4 *For a* 2×4 *experiment, we have p=1, q=3 and hence x=2. Then for k=12, the design which accommodates the following set of treatments in each block is WA(3,1)-optimal:*

01 02 03 10 10 10 11 11 12 12 13 13

Example 6.5 *For a* 3×3 *experiment we have p=q=2 and hence x=2. Then for k=16, the design with the following set of treatments in each block is WA(2,2)-optimal:*

01 01 02 02 10 10 20 20 11 11 12 12 21 21 22 22

6.4 Conclusions:

In this chapter sufficient conditions are established for a completely randomized design to be A-optimal for the estimation of the dual versus single contrasts. It is found that a completely randomized design is optimal if the treatment combinations within each of the sets A and D are replicated equally often throughout the design. A selection of A-optimal designs which have this property are summarized in Table 6.1 for $3 \leq n, m \leq 10$ and a total number of units at most 100.

The result is then generalized to establishing conditions for a completely randomized design to be weighted A-optimal in the sense of minimizing a weighted sum of the variances of the estimators of the dual versus single contrasts.

Finally, the problem of finding block designs which are weighted A-optimal is considered. A design-dependent bound on the weighted sum of the variances is derived for given weights. This could be used to find a bound, which is not design-dependent via the approach of Chapter 4 and hence could lead to characterizing weighted A-optimal designs.

Table 6.1: Number of replications r_B, r_A and r_D of the treatment combination belonging to the respective sets B, A and D in an A-optimal completely randomized design of N units.

n	m	N	r_B	r_A	r_D
3	3	8	1	1	1
		10	1	2	1
		14	1	2	2
		16	2	2	2
		24	3	3	3
		32	4	4	4
		34	4	5	4
		40	5	5	5
		42	5	6	5
		46	5	6	6
		48	6	6	6
		56	7	7	7
		64	8	8	8
		72	9	9	9
		78	9	10	10
		80	10	10	10
		88	11	11	11
		90	11	12	11
		94	11	12	12
		96	12	12	12
		98	12	13	12
	4	11	1	1	1
		13	1	2	1
		19	1	2	2
		22	2	2	2
		24	2	3	2
		33	3	3	3
		35	3	4	3
		44	4	4	4
		46	4	5	4
3	4	57	5	6	5
		59	5	7	5
		65	5	7	6
		68	6	7	6
		70	6	8	6
		79	7	8	7
		81	7	9	7
		87	7	9	8
		90	8	9	8
		92	8	10	8
	5	14	1	1	1
		16	1	2	1
		24	1	2	2
		28	2	2	2
		30	2	3	2
		44	3	4	3
		46	3	5	3
		54	3	5	4
		58	4	5	4
		60	4	6	4
		72	5	6	5
		74	5	7	5
		76	5	8	5
		84	5	8	6
		88	6	8	6
		90	6	9	6
		98	6	9	7
	6	17	1	1	1
		19	1	2	1
		29	1	2	2

Table 6.1: continued...

n	m	N	r_B	r_A	r_D	n	m	N	r_B	r_A	r_D
3	6	34	2	2	2	3	8	66	2	5	3
		36	2	3	2			73	3	5	3
		38	2	4	2			75	3	6	3
		48	2	4	3			98	4	7	4
		53	3	4	3			100	4	8	4
		55	3	5	3		9	26	1	1	1
		57	3	6	3			28	1	2	1
		72	4	6	4			30	1	3	1
		74	4	7	4			46	1	3	2
		89	5	7	5			54	2	3	2
		91	5	8	5			56	2	4	2
		93	5	9	5			58	2	5	2
	7	20	1	1	1			74	2	5	3
		22	1	2	1			82	3	5	3
		24	1	3	1			84	3	6	3
		36	1	3	2			86	3	7	3
		42	2	3	2		10	29	1	1	1
		44	2	4	2			31	1	2	1
		62	3	4	3			33	1	3	1
		64	3	5	3			51	1	3	2
		66	3	6	3			60	2	3	2
		84	4	6	4			62	2	4	2
		86	4	7	4			64	2	5	2
		88	4	8	4			91	3	5	3
		100	4	8	5			93	3	6	3
	8	23	1	1	1			95	3	7	3
		25	1	2	1	4	4	15	1	1	1
		27	1	3	1			18	1	2	1
		41	1	3	2			21	2	2	1
		48	2	3	2			30	2	2	2
		50	2	4	2			33	2	3	2
		52	2	5	2			36	3	3	2

Table 6.1: continued...

n	m	N	r_B	r_A	r_D	n	m	N	r_B	r_A	r_D
4	4	45	3	3	3	4	6	80	4	5	3
		48	3	4	3			98	4	6	4
		51	4	4	3		7	27	1	1	1
		60	4	4	4			30	1	2	1
		63	4	5	4			36	2	2	1
		66	5	5	4			39	2	3	1
		78	5	6	5			57	2	3	2
		81	6	6	5			60	2	4	2
		87	7	7	5			66	3	4	2
		96	7	7	6			84	3	4	3
	5	19	1	1	1			87	3	5	3
		22	1	2	1			93	4	5	3
		26	2	2	1			96	4	6	3
		38	2	2	2		8	31	1	1	1
		41	2	3	2			34	1	2	1
		45	3	3	2			41	2	2	1
		60	3	4	3			44	2	3	1
		64	4	4	3			65	2	3	2
		67	4	5	3			68	2	4	2
		79	4	5	4			75	3	4	2
		83	5	5	4			78	3	5	2
		86	5	6	4			99	3	5	3
		98	5	6	5		9	35	1	1	1
	6	23	1	1	1			38	1	2	1
		26	1	2	1			46	2	2	1
		31	2	2	1			49	2	3	1
		46	2	2	2			73	2	3	2
		49	2	3	2			76	2	4	2
		54	3	3	2			84	3	4	2
		57	3	4	2			87	3	5	2
		72	3	4	3		10	39	1	1	1
		75	3	5	3			42	1	2	1

Table 6.1: continued...

n	m	N	r_B	r_A	r_D	n	m	N	r_B	r_A	r_D
4	10	45	1	3	1	5	8	39	1	1	1
		54	2	3	1			43	1	2	1
		81	2	3	2			50	2	2	1
		84	2	4	2			54	2	3	1
		93	3	4	2			82	2	3	2
		96	3	5	2			89	3	3	2
5	5	24	1	1	1			93	3	4	2
		28	1	2	1			97	3	5	2
		32	2	2	1		9	44	1	1	1
		48	2	2	2			48	1	2	1
		56	3	3	2			56	2	2	1
		76	3	4	3			60	2	3	1
		80	4	4	3			92	2	3	2
		84	4	5	3		10	49	1	1	1
		88	5	5	3			53	1	2	1
	6	29	1	1	1			62	2	2	1
		33	1	2	1			66	2	3	1
		38	2	2	1	6	6	35	1	1	1
		58	2	2	2			40	1	2	1
		62	2	3	2			45	2	2	1
		67	3	3	2			70	2	2	2
		71	3	4	2			80	3	3	2
		91	3	4	3			90	4	4	2
		96	4	4	3		7	41	1	1	1
		100	4	5	3			46	1	2	1
	7	34	1	1	1			52	2	2	1
		38	1	2	1			57	2	3	1
		44	2	2	1			87	2	3	2
		48	2	3	1			93	3	3	2
		72	2	3	2			98	3	4	2
		78	3	3	2		8	47	1	1	1
		82	3	4	2			52	1	2	1

Table 6.1: continued...

n	m	N	r_B	r_A	r_D
6	8	59	2	2	1
		64	2	3	1
		99	2	3	2
	9	53	1	1	1
		58	1	2	1
		66	2	2	1
		71	2	3	1
	10	59	1	1	1
		64	1	2	1
		73	2	2	1
		78	2	3	1
7	7	48	1	1	1
		54	1	2	1
		60	2	2	1
		66	2	3	1
	8	55	1	1	1
		61	1	2	1
		68	2	2	1
		74	2	3	1
	9	62	1	1	1
		68	1	2	1
		76	2	2	1

n	m	N	r_B	r_A	r_D
7	9	82	2	3	1
	10	69	1	1	1
		75	1	2	1
		84	2	2	1
		90	2	3	1
8	8	63	1	1	1
		70	1	2	1
		77	2	2	1
		91	3	3	1
	9	71	1	1	1
		78	1	2	1
		86	2	2	1
		93	2	3	1
	10	79	1	1	1
		86	1	2	1
		95	2	2	1
9	9	80	1	1	1
		88	1	2	1
		96	2	2	1
	10	89	1	1	1
		97	1	2	1
10		99	1	1	1

Chapter 7

Related Problems and Conclusions

7.1 Introduction:

In this chapter two problems related to those of the earlier chapters are discussed, and issues for future work are described. In Sections 7.2 and 7.3 we consider the estimation of factorial effects in completely randomized and randomized block designs when a particular treatment combination is excluded from the experiment and some of the effects are assumed to be negligible. We concentrate on the case when the treatment combinations are equally replicated, and show that the greater the dependence of the set of negligible contrasts on the excluded treatment combination, the smaller the increase in variance due to excluding it. Also it is shown that low involvement of the excluded treatment combination in the contrasts to be estimated leads to low loss of precision in estimating the contrasts. Further, a linear combinations of the set of negligible contrasts which maximizes the precision of the estimators of the contrasts of interest is found. The main practical application of this work is when it is possible only to use a single replicate of the treatment combinations due to cost constraints.

In Section 7.4 we consider briefly how to generalize the results to choose the possibly unequal replications in a completely randomized design so that the factorial contrasts of interest can be estimated with high precision.

In Section 7.5 we consider for a variety of problems, the similarity between the structure of $C'C$(the coefficient matrix corresponding to the contrasts of interest), and the structure of the A-matrix of the class of designs which is sought to be a source of efficient designs.

7.2 Estimation of Factorial Effects:

We again consider experiments with a single excluded treatment combination, but now investigate the estimation of the factorial effects, in particular the main effects and low order interactions. We consider n factors F_1, F_2,...,F_n at m_1, m_2,...,m_n levels respectively giving $t = \prod_{i=1}^{n} m_i$ treatment combinations in all. Suppose the particular treatment combination which is not allowed in the experiment is $i_1i_2...i_n$, in which factor F_j has level labelled $i_j(i_j = 0, 1, 2, \ldots, m_j - 1)$. For example $i_1i_2...i_n$ could be an unsuitable treatment in a medical trial.

We restrict consideration to the following classes of designs:

1. Completely randomized designs under an additive model for treatments and errors.

2. Block designs in which treatments are orthogonal to blocks and an additive model is assumed for treatments, blocks and errors.

In general for an experiment in which $i_1i_2...i_n$ is excluded it will not be possible to estimate each factorial contrast separately, and a quantity calculated to estimate, for example, a particular main effect will in general depend also on the true value of one or more other factorial contrasts. An appropriate design is one which estimates each main effect and, if possible, each low-order interaction, in such a way that these effects are entangled or aliased only with high-order interactions. If it is valid to assume these high order interactions are negligible then estimation of the main effects and low order interactions is possible. In addition, assumptions of negligible high order interactions are sometimes made in order to estimate error in fractional factorials. This practice also arises in single replicate factorial experiments but needs to be used with caution(see Cochran and Cox,1953,p189).

In a factorial experiment involving n factors let $C^x\underline{\tau}$ denote a set of n_x independent normalized contrasts within a particular factorial effect. Let $C^y\underline{\tau}$ be a set of n_y independent normalized contrasts which can be assumed negligible and which belong to a different factorial effect. Further let both $C^x\underline{\tau}$ and $C^y\underline{\tau}$ involve the effect of $i_1i_2...i_n$. It is possible to estimate $C^x\underline{\tau}$ from the design by using the fact that any linear combination of the contrasts in $C^y\underline{\tau}$, say $\underline{l}'C^y\underline{\tau}$, can be assumed zero and hence can be used to eliminate the effect of $i_1i_2...i_n$

from $C^x\underline{\tau}$. This is analogous to the estimation of contrasts in classical fractional factorial experiments. Thus we obtain the following set of contrasts which can be estimated from the data on the (t-1) treatment combinations alone:

$$C^{x^*}\underline{\tau} = (C^x - \underline{f} \otimes \underline{l}'C^y)\underline{\tau}, \tag{7.1}$$

where f is an $n_x \times 1$ vector defined in (7.2) below. By assuming the negligibility of $\underline{l}'C^y\underline{\tau}$, it follows that in the design with only (t-1) treatments $C^{x^{**}}\hat{\underline{\tau}}^*$ can be used as an estimator of $C^x\underline{\tau}$ even though one of the treatment combinations has not been observed, where $C^{x^{**}}$ is C^{x^*} after eliminating the column involving the excluded treatment combination, $\underline{\tau}^*$ is obtained from $\underline{\tau}$ by removing the effect of the excluded treatment combination and $\hat{\underline{\tau}}^*$ is the least squares estimator of $\underline{\tau}^*$. The vector of real numbers, $\underline{f}$, must be chosen in such a way that the coefficient involving the excluded treatment combination in $C^{x^*}\underline{\tau}$ is zero. This is achieved by giving the ith element of f the following value:

$$f_i = \frac{C^x_{i(i_1 i_2 \ldots i_n)}}{\underline{l}'\underline{C}^y_{i_1 i_2 \ldots i_n}}, \tag{7.2}$$

for $i = 1, 2, \ldots, n_x$, where $C^x_{i(i_1 i_2 \ldots i_n)}$ denotes the coefficient of the effect of the excluded treatment combination $i_1 i_2 \ldots i_n$ in the ith contrast belonging to set $C^x\underline{\tau}$, and $\underline{C}^y_{i_1 i_2 \ldots i_n}$ is an $n_y \times 1$ vector whose entries are the coefficients of the excluded treatment combination of the contrasts belonging to the set $C^y\underline{\tau}$. The set of the contrasts $C^{x^*}\underline{\tau}$ will be called the contrasts of interest **adjusted** for $\underline{l}'C^y\underline{\tau}$. Without loss of generality, we restrict consideration to a normalized vector $\underline{l}$, that is having $\underline{l}'\underline{l} = 1$.

Example 7.1 *In an* 3×3 *factorial experiment, let treatment combination 00 be excluded and suppose we want to compare the first and the third levels of the first factor, i.e. we want to estimate the single contrast:*

$$C^x\underline{\tau} = \frac{1}{\sqrt{6}}(\ -1\ \ -1\ \ -1\ \ 0\ \ 0\ \ 0\ \ 1\ \ 1\ \ 1\ )\underline{\tau}.$$

We assume the following contrasts from the interaction are negligible:

$$C^y\underline{\tau} = \frac{1}{\sqrt{12}}\begin{bmatrix} -1 & 0 & 1 & 2 & 0 & -2 & -1 & 0 & 1 \\ -1 & 2 & -1 & 0 & 0 & 0 & 1 & -2 & 1 \end{bmatrix}\underline{\tau}.$$

As an illustration we use the linear combination $\underline{l}'C^y\underline{\tau} = (1/\sqrt{5})(1\ \ -2)C^y\underline{\tau}$ *to facilitate the estimation of* $C^x\underline{\tau}$, *giving:*

$$\underline{l}'C^y = \frac{1}{\sqrt{60}}(\ 1\ \ -4\ \ 3\ \ 2\ \ 0\ \ -2\ \ -3\ \ 4\ \ -1\ ).$$

Since the values of the coefficients of the excluded treatment combination in $C^x\underline{\tau}$ *and* $C^y\underline{\tau}$ *are given by*

$$C^x_{1(00)} = -1/\sqrt{6} \text{ and } C^y_{00} = -1/\sqrt{12}\,\underline{1},$$

respectively, it follows from (7.2) that $f = (-1/\sqrt{6})/(1/\sqrt{60}) = -\sqrt{10}$. *Hence, on substituting in (7.1), we obtain*

$$C^{x^*} = \frac{1}{\sqrt{6}}(\ 0\ \ -5\ \ 2\ \ 2\ \ 0\ \ -2\ \ -2\ \ 5\ \ 0\ )$$

and $C^{x^*}\hat{\underline{\tau}}$ *estimates* $C^x\underline{\tau}$.

7.3 Experiments Arranged in a Completely Randomized Design and in a Randomized Block Design:

In practice there is often a choice of negligible interactions, $C^y\underline{\tau}$, which can be used for estimation purposes. In addition we can also choose the particular linear combination $\underline{l}'C^y$ to employ in (7.1). In order to decide on the best choices for any particular experiment in a completely randomized design or a randomized block design we consider the loss of information due to the exclusion of the particular treatment combination and how it depends on $\underline{l}$ and C^y. We assume that σ^2 is the same in the experiment with the treatment combination excluded and the hypothetical experiment with the treatment combination included.

Definition 7.1 *In a factorial experiment, let* $C^x\underline{\tau}$ *and* $C^y\underline{\tau}$, *be the set of contrasts. Then* $tr\left\{V(C^{x^{**}}\hat{\underline{\tau}}^*) - V(C^x\hat{\underline{\tau}})\right\}$ *will be called the* **total loss of information** *on the contrasts* $C^x\underline{\tau}$, *due to excluding treatment combination* $i_1i_2...i_n$ *and assuming* $\underline{l}'C^y\underline{\tau} = \underline{0}$. *We assume that* σ^2 *is the same for the experiment with the excluded treatment combination as it is in the hypothetical experiment employing all the treatment combinations, and, for simplicity, we take* $\sigma^2 = 1$. *Thus* $tr\left\{V(C^{x^{**}}\hat{\underline{\tau}}^*) - V(C^x\hat{\underline{\tau}})\right\}$ *represents the loss in precision per unit variance due to the excluded treatment combination It will be denoted by* $Loss(C^x; i_1i_2...i_n, \underline{l}, C^y)$.

Example 7.2 *Suppose Example 7.1 is conducted in a completely randomized design, in which each allowable treatment combination is replicated r times . Then* $V(C^x\hat{\underline{\tau}}) = r^{-1}C^x(C^x)' = r^{-1}$. *Also,* $V(C^{x^*}\hat{\underline{\tau}}) = r^{-1}C^{x^*}(C^{x^*})' = 11r^{-1}$. *Therefore, by Definition 7.1, loss* $= (11-1)r^{-1} = 10r^{-1}$.

In the remainder of this section we examine the conditions on C^y and $\underline{l}$ which give minimum loss of information in the estimation of $C^x\underline{\tau}$ when one treatment combination is excluded. In order to do this we require the following definition and lemma.

Definition 7.2 *Let $\underline{v}$ be an $n \times 1$ vector in R^n. The* **norm** *of $\underline{v}$, $||\underline{v}||$, is defined by:*

$$||\underline{v}|| = (\underline{v}'\underline{v})^{1/2}. \tag{7.3}$$

Lemma 7.1 *For any non-negative definite matrix X of the form $\underline{x}\ \underline{x}'$; where $\underline{x}$ is a column vector having at least one of its elements non zero, the maximum eigenvalue of X is $||\underline{x}||^2$, with corresponding eigenvector $\underline{z} = \alpha\underline{x}$(for any $\alpha \neq 0$).*

Proof: Since $\underline{x} \neq \underline{0}$, it follows that $r(X) = r(\underline{x}) = 1$. The matrix has only one non-zero eigenvalue which is positive. Because the matrix is non-negative definite, the other eigenvalues are zero, and the non-zero eigenvalue equals $tr(X) = tr(\underline{x}\ \underline{x}') = ||\underline{x}||^2$. Let $\underline{s}$ be the eigenvector corresponding to this eigenvalue, then we must have:

$$\underline{x}\ \underline{x}'\underline{s} = ||\underline{x}||^2\underline{s}. \tag{7.4}$$

Clearly vector $\underline{s} = \alpha\underline{x}$ satisfies the above equation for any $\alpha \neq 0$. Therefore $\underline{s} = \alpha\underline{x}$ is the eigenvector corresponding to the unique non zero eigenvalue of X. Hence the Lemma is proved.♣

Lemma 7.2 *(Rao,1973,page 62) Let X be a $m \times m$ matrix, $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_m$ be its eigenvalues, then for any vector $\underline{w} \neq \underline{0}$,*

$$\max_{\underline{w}} \frac{\underline{w}'X\underline{w}}{\underline{w}'\underline{w}} = \lambda_1.$$

Theorem 7.1 *Consider an equireplicate completely randomized design or a randomized block design under an assumed additive model for the observations. If we assume that $||\underline{l}|| = 1$ and that σ^2 is the same for the hypothetical experiment involving all treatment combinations and for the experiment with a single excluded treatment combination, then*

$$Loss(C^x; i_1i_2...i_n, \underline{l}, C^y) = r^{-1}(\underline{l}'C^yC'^y\underline{l})\underline{f}'\underline{f} \geq r^{-1}(\underline{l}'C^yC'^y\underline{l})\frac{||\underline{C}^x_{i_1i_2\ldots i_n}||^2}{||\underline{C}^y_{i_1i_2\ldots i_n}||^2}, \tag{7.5}$$

where $\underline{C}^x_{i_1 i_2 \ldots i_n}$ is an $n_x \times 1$ vector in which its ith element is the coefficient of the excluded treatment combination of the ith contrast belonging to the set $C^x \underline{\tau}$ and $\underline{C}^y_{i_1 i_2 \ldots i_n}$ is an $n_y \times 1$ vector in which its jth element is the coefficient of the excluded treatment combination of the jth contrast belonging to the set $C^y \underline{\tau}$.

Proof: In an equireplicate completely randomized design or a randomized block design with member of the full set of t treatment combinations replicated r times:

$$V(C^x \hat{\underline{\tau}}) = r^{-1} C^x C'^x. \tag{7.6}$$

When all replications of $i_1 i_2 \ldots i_n$ are excluded, we have:

$$V(C^{x^*} \hat{\underline{\tau}}) = r^{-1} C^{x^*} C'^{x^*}, \tag{7.7}$$

where C^{x^*} is defined in (7.1). It can be shown that:

$$C^{x^*} C'^{x^*} = C^x C'^x + \underline{f}\, \underline{f}' \otimes (\underline{l}' C^y C'^y \underline{l}) - C^x \{\underline{f}' \otimes C'^y \underline{l}\} - (\underline{f} \otimes \underline{l}' C^y) C'^x. \tag{7.8}$$

Since C^x and C^y are contrast matrices for different factorial effects, we know that $C^x C'^y = 0$. Hence (7.8) becomes

$$C^{x^*} C'^{x^*} = C^x C'^x + (\underline{l}' C^y C'^y \underline{l}) \underline{f}\, \underline{f}'. \tag{7.9}$$

Therefore by assuming σ^2 is the same in both included and excluded cases, we have:

$$Loss(C^x; i_1 i_2 \ldots i_n, \underline{l}, C^y) = r^{-1} (\underline{l}' C^y C'^y \underline{l}) tr(\underline{f}\, \underline{f}') = r^{-1} (\underline{l}' C^y C'^y \underline{l}) \underline{f}' \underline{f},$$

where:

$$\underline{f}' \underline{f} = \frac{\|\underline{C}^x_{i_1 i_2 \ldots i_n}\|^2}{\underline{l}' \underline{C}^y_{i_1 i_2 \ldots i_n} \underline{C}'^y_{i_1 i_2 \ldots i_n} \underline{l}}. \tag{7.10}$$

We can find the maximum value of the denominator by taking $\underline{x} = \underline{C}^y_{i_1 i_2 \ldots i_n}$ and applying Lemmas 7.1 and 7.2. This maximum is $tr(\underline{C}^y_{i_1 i_2 \ldots i_n} \underline{C}'^y_{i_1 i_2 \ldots i_n}) = \|\underline{C}^y_{i_1 i_2 \ldots i_n}\|^2$.♣

Corollary 7.1 *If in the statement of Theorem 7.1 the rows of $C^y \underline{\tau}$ are orthogonal, then*

$$Loss(C^x; i_1 i_2 \ldots i_n, \underline{l}, C^y) \geq r^{-1} \frac{\|\underline{C}^x_{i_1 i_2 \ldots i_n}\|^2}{\|\underline{C}^y_{i_1 i_2 \ldots i_n}\|^2}, \tag{7.11}$$

and the minimum is achieved when

$$\underline{l} = (||\underline{C}^y_{i_1 i_2 \ldots i_n}||)^{-1} \underline{C}^y_{i_1 i_2 \ldots i_n}. \tag{7.12}$$

Proof: From Theorem 7.1, we have:

$$Loss(C^x; i_1 i_2 \ldots i_n, \underline{l}, C^y) \geq r^{-1}(\underline{l}' C^y C'^y \underline{l}) \frac{||\underline{C}^x_{i_1 i_2 \ldots i_n}||^2}{||\underline{C}^y_{i_1 i_2 \ldots i_n}||^2}.$$

On substituting $C^y C'^y = I$, the result follows, since $\underline{l}'\underline{l} = 1$.♣

Example 7.3 *In Example 7.1, $||\underline{C}^x_{00}||^2 = ||\underline{C}^y_{00}||^2 = 1/6$. In order to obtain the minimum loss for the particular choice of $C^y\underline{\tau}$ we should take $\underline{l} = (1/\sqrt{2})\ \underline{1}$, giving loss $= r^{-1}$ which is very small compared with the loss in Example 7.2.*

Discussion 7.1 *Corollary 7.1 tells us that to obtain the minimum increase in variance on sets of orthogonal contrasts within the factorial effects of interest, we should choose that matrix C^y which has maximum value for $||\underline{C}^y_{i_1 i_2 \ldots i_n}||^2$ and use this, together with the consequent l, for all the factorial effects. Further $||\underline{C}^y_{i_1 i_2 \ldots i_n}||^2$ is a maximum when the absolute values of the elements of $\underline{C}^y_{i_1 i_2 \ldots i_n}$ are as big as possible. This simply means that the greater the dependence on the excluded treatment combination in the set of negligible contrasts, the smaller the increase in variance due to excluding it.*

From Corollary 7.1 we can also see which factorial effects will suffer the least loss in precision due to excluding the treatment combination as follows:

The minimum value for the loss function is minimized if $||\underline{C}^x_{i_1 i_2 \ldots i_n}||$ is minimized, that is if the absolute values of the elements of $\underline{C}^x_{i_1 i_2 \ldots i_n}$ are as small as possible(in the sense of small absolute coefficients). This simply means that low involvement of the excluded treatment combination in the contrasts to be estimated leads to low loss of precision on them. In the extreme case when a set of contrasts does not include the effect of the excluded treatment combination the variance of the estimator does not change, whether the treatment combination, $i_1 i_2 \ldots i_n$ is involved in the design or not.

Corollary 7.2 *Let $C^{\varpi}\underline{\tau}$ be the maximal set of neglected factorial effects with the properties that:*

1. *for each $C^y\underline{\tau} \subset C^{\varpi}\underline{\tau}$, $\underline{C}^y_{i_1 i_2 \ldots i_n}$ contains nonzero elements only,*

2. rows of C^y are orthogonal,

and let C^φ be a proper subset of C^ϖ, then

$$\min\ Loss(C^x; i_1i_2...i_n, \underline{l}, C^\varpi) < \min\ Loss(C^x; i_1i_2...i_n, \underline{l}, C^\varphi). \tag{7.13}$$

Proof: From Corollary 7.1, we have:

$$\min\ Loss(C^x; i_1i_2...i_n, \underline{l}, C^\varpi) = r^{-1}\frac{||\underline{C}^x_{i_1i_2...i_n}||^2}{||\underline{C}^\varpi_{i_1i_2...i_n}||^2}. \tag{7.14}$$

But by definition:

$$||\underline{C}^\varpi_{i_1i_2...i_n}||^2 = ||\underline{C}^\varphi_{i_1i_2...i_n}||^2 + ||\underline{C}^\delta_{i_1i_2...i_n}||^2,$$

where C^δ is a set of contrasts which is not in C^φ and it is a non-empty subset of C^ϖ. Therefore

$$||\underline{C}^\varpi_{i_1i_2...i_n}||^2 > ||\underline{C}^\varphi_{i_1i_2...i_n}||^2.$$

and the result follows.♣

Corollary 7.2 shows that in order to minimize the loss on factorial contrasts of interest, we should use a linear combination of as large a number of negligible factorial effects as possible. The following two examples illustrate the gains to be made.

Example 7.4 *If in Example 7.1 let :*

$$C^\varpi\underline{\tau} = \frac{1}{\sqrt{12}}\begin{bmatrix} \sqrt{3} & 0 & -\sqrt{3} & 0 & 0 & 0 & -\sqrt{3} & 0 & \sqrt{3} \\ -1 & 0 & 1 & 2 & 0 & -2 & -1 & 0 & 1 \\ -1 & 2 & -1 & 0 & 0 & 0 & 1 & -2 & 1 \end{bmatrix}\underline{\tau},$$

and

$$C^\varphi\underline{\tau} = \frac{1}{\sqrt{12}}\begin{bmatrix} -1 & 0 & 1 & 2 & 0 & -2 & -1 & 0 & 1 \\ -1 & 2 & -1 & 0 & 0 & 0 & 1 & -2 & 1 \end{bmatrix}\underline{\tau}.$$

Then

$$\min\ Loss(C^x; i_1i_2...i_n, \underline{l}, C^\varpi) = 0.4r^{-1}.$$

and

$$\min\ Loss(C^x; i_1i_2...i_n, \underline{l}, C^\varphi) = r^{-1}.$$

Example 7.5 *An 3×4 experiment is conducted in a completely randomized design, in which each treatment combination is replicated r times except for the treatment combination 00 which is excluded from the experiment. Our aim is to estimate the orthogonal polynomial contrasts within the main effects and the linear×linear interaction, by assuming that all the other interactions are negligible. Therefore*

$$C^{\varpi} = \{C^y; C^y \underline{{}_T} \text{consists of all the interactions except linear} \times \text{linear}\}.$$

Then (see Lindman,1974,page 325 for coefficients)

$$\underline{C}^{\varpi}_{00} = (1/\sqrt{120})(\ -\sqrt{15}\ \ -3\ \ \sqrt{3}\ \ \sqrt{5}\ \ -1\ )',$$

and

$$\underline{C}^{x}_{00} = (1/\sqrt{120})(\ -\sqrt{15}\ \ \sqrt{5}\ \ -3\sqrt{2}\ \ \sqrt{10}\ \ -\sqrt{2}\ \ 3\sqrt{3}\ )'.$$

For this case

$$\min\ loss(C^x; 00, C^{\varpi}) = r^{-1}\frac{||\underline{C}^{x}_{00}||^2}{||\underline{C}^{\varpi}_{00}||^2} = 2.33r^{-1}.$$

Now, let

$$C^{\varphi}\underline{{}_T} = \{\ \text{linear} \times \text{cubic, quadratic} \times \text{quadratic and quadratic} \times \text{cubic interactions}\}.$$

Then clearly $C^{\varphi} \subset C^{\varpi}$. It can be shown that

$$\min\ loss(C^x, 00, C^{\varphi}) = 8.55r^{-1}.$$

which is greater than $2.33r^{-1}$.

7.4 Loss Function in Designs with Unequal Replication:

So far in this chapter we have considered designs which are equreplicate. One application of these findings is in single replicate factorial experiment in which each treatment combination is replicated once in the entire design. Now we consider unequal replicate designs. Suppose that, in a completely randomized design, r_i denotes the number of replication of treatment combination i in the design for i=1,2,...,t, and

$$r^{\delta} = diag(r_1, r_2, \ldots, r_t).$$

Our aim is to estimate $C^x\underline{\tau}$ under the condition that the treatment combination labelled u is excluded from the experiment and $C^y\underline{\tau}$ is assumed to be negligible. If there is no exclusion we have

$$tr\{V(C^x\hat{\underline{\tau}})\} = tr(C^x r^{-\delta} C^{x'}) = \sum_{i=1}^{n_x}\sum_{j=1}^{t} \frac{(C_{ij}^x)^2}{r_j}, \tag{7.15}$$

where n_x denotes the number of rows of C^x, and C_{ij}^x denotes the coefficient corresponding to the jth treatment combination in the ith row of C^x. Now if we assume that the treatment combination labelled u is excluded from the experiment and $C^y\underline{\tau}$ is negligible, then as in Section 7.2 we can estimate $C^x\underline{\tau}$ by $C^{*x}\underline{\tau}$ in a design with u excluded, where $C^{*^x}\underline{\tau}$ is defined in (7.1). Therefore

$$tr\{V(C^{*x}\hat{\underline{\tau}})\} = tr(C^{*x} r^{-\delta} C^{*x'}) = \sum_{i=1}^{n_x}\sum_{\substack{j=1\\ j\neq u}}^{t} \frac{(C_{ij}^{*x})^2}{r_j}. \tag{7.16}$$

Hence, by definition

$$Loss(C^x; u, \underline{l}, C^y) = \sum_{i=1}^{n_x}\sum_{\substack{j=1\\ j\neq u}}^{t} \frac{(C_{ij}^{*x})^2}{r_j} - \sum_{i=1}^{n_x}\sum_{j=1}^{t} \frac{(C_{ij}^x)^2}{r_j}. \tag{7.17}$$

After some algebra we obtain

$$Loss(C^x; u, \underline{l}, C^y) = \sum_{i=1}^{n_x}\sum_{\substack{j=1\\ j\neq u}}^{t} \frac{(C_{ij}^{*x})^2 - (C_{ij}^x)^2 - r_j(C_{iu}^x)^2/\{r_u(t-1)\}}{r_j}. \tag{7.18}$$

It is obvious that (7.18) is not necessarily minimized when the r_j's are made equal, unless the condition

$$\sum_{i=1}^{n_x}\left\{(C_{ij}^{*x})^2 - (C_{ij}^x)^2 - \frac{r_j(C_{iu})^2}{r_u(t-1)}\right\} = fixed, \tag{7.19}$$

is satisfied for $j \neq u$; j=1,2,...,t. Under this condition equireplicate designs give small loss in precision on the contrasts of interest. More work is needed to explore which choice of linear combination of negligible factorial contrasts gives the smallest loss in precision on the contrasts of interest.

7.5 Similarity of $C'C$ and A-matrix Structure:

In this section we consider the general problem of how to locate a class of designs which contains highly efficient(including A-optimal) designs for estimating a specified set of treatment contrasts. This is often a valuable short cut to finding good designs since it is easier and quicker to search through a subclass rather than to consider all possible designs. By a further application of Theorem 3.2 on page 76, we show how the structure of the A-matrix of a class of designs for estimating contrasts $C\underline{\tau}$ can be linked to the structure of $C'C$.

It should be noted here that the idea of this section comes from Section 3.3 of Chapter 3. Therefore we shall refer to that section whenever it is needed without mentioning the chapter.

The designs have the following property.

Definition 7.3 *A design has* **property S with respect to a contrast matrix C** *if the A-matrix of the design and $C'C$ have the following features in common:*

1. *a set of orthonormal eigenvectors,*
   and
2. *the multiplicities of the corresponding eigenvalues.*

Corollary 7.3 *If there exists a design with property S with respect to the matrix C, then*

$$tr(C\Omega C') = \sum_{i=1}^{t-1} \frac{\theta_i}{\lambda_i}, \tag{7.20}$$

where C, θ_i and λ_i are defined in the statement of Theorem 3.2.

Proof: From (3.20), $tr(C\Omega C') = \sum_{i=1}^{t-1} \lambda_i^{-1} \underline{\xi}_i' C'C \underline{\xi}_i$. If $\underline{\xi}_i = \underline{\mu}_i$, where $\underline{\mu}_i$ is the ith normalized eigenvector of $C'C$ with corresponding eigenvalue θ_i, then

$$\underline{\xi}_i' C'C \underline{\xi}_i = \underline{\mu}_i' C'C \underline{\mu}_i = \theta_i \underline{\mu}_i' \underline{\mu}_i = \theta_i. \tag{7.21}$$

Therefore we have $tr(C\Omega C') = \sum_{i=1}^{t-1} \theta_i \lambda_i^{-1}$.♣

This corollary simply says that property S designs with respect to C can achieve the bound in Theorem 3.2. However this bound is design-dependent and is not an overall bound for all possible designs. Therefore, for a specific contrast matrix C a design known to have property S will not necessarily be efficient because the bound achieved in (7.20) might be very poor.

However Corollary 7.3 can enable us to find an A-optimal design by the following procedure

1. Calculate $b_2 = \min \sum \theta_i/\lambda_i$ over all possible designs.
2. Search through the class of designs with structure S to locate a design achieving b_2, if one exists.

If a design is located in this way then, by Theorem 3.2, it is A-optimal. If a design cannot be found to achieve b_2, then we can consider that design in the class which has a value for $tr(C\Omega C')$ closest to b_2. However, in general, we have no guarantee that this design will be highly efficient. Nevertheless, for a range of practical problems, that is specific contrast matrices, the best design having property S turns out to be highly efficient. We illustrate this approach through considering the following 3 problems.

- Dual versus single treatment contrasts.
- Test treatments versus
  1. a set of control treatments,
  2. a single control treatment,
- A full set of orthonormalized contrasts.

Clearly location of subclasses containing efficient designs must proceed by separate consideration of the different C-matrices of interest. This is seen from (7.20) since the eigenvalues of $C'C$ are involved in the bound. Hence there will not be a single subclass of designs which hit the design-dependent bound (7.20) for all C-matrices.

For each of the four problems we adopt the same strategy, namely identifying a set of eigenvectors of the $C'C$ matrix and then specifying the structure of the A-matrix in terms of the eigenvectors so that (7.20) is satisfied. We require the following lemma.

Lemma 7.3 *Suppose $\underline{x}_1$, $\underline{x}_2$, ..., $\underline{x}_{\ell-1}$ is a set of orthonormalized column vectors of order $\ell \times 1$, such that $\underline{x}_i'\underline{1}=0$ for $i = 1, 2, \ldots, \ell-1$, then we have:*

$$\sum_{i=1}^{\ell-1} \underline{x}_i \underline{x}_i' = I_\ell - \frac{1}{\ell} J_\ell. \qquad (7.22)$$

Proof: Let $\underline{y} = \ell^{-1/2}\underline{1}_\ell$, then the vectors $\underline{y}$, $\underline{x}_1$, $\underline{x}_2$, ..., $\underline{x}_{\ell-1}$ form a basis for the $\ell \times \ell$ vector space. This implies that:

$$\sum_{i=1}^{\ell-1} \underline{x}_i \underline{x}_i' + \underline{y}\ \underline{y}' = I_\ell. \tag{7.23}$$

But $\underline{yy'} = \ell^{-1} J_\ell$ and the result follows.♣

7.5.1 Dual versus Single Treatment Comparisons:

In this section for simplicity we consider only $n \times 2$ CFBD(00) experiments and prove that the class of designs having structure S is a subset of the PBDS class. From (2.4), we have:

$$C'C = \begin{bmatrix} p & \underline{0}_p' & -\underline{1}_p' \\ \underline{0} & I_p & -I_p \\ -\underline{1}_p & -I_p & 2I_p \end{bmatrix}. \tag{7.24}$$

The eigenvalues of this matrix which are given in Table 7.1 have been deduced from Table 3.1 by taking q=1.

Table 7.1: Eigenvalues of $C'C$ matrix.

Eigenvalues(θ_i)	multiplicities
$\frac{n+2+\sqrt{(n+2)^2-4(2n-1)}}{2}$	1
$\frac{n+2-\sqrt{(n+2)^2-4(2n-1)}}{2}$	1
$\frac{3+\sqrt{5}}{2}$	n-2
$\frac{3-\sqrt{5}}{2}$	n-2
0	1

Lemma 7.4 *The eigenvectors of the $C'C$ matrix given in (7.24) for an $n \times 2$ CFBD(00) experiment are:*

1. $\underline{\xi}_i' = c_1 \left[0,\ \underline{y}_i'\ ,\ (1-\theta_1)\underline{y}_i'\right]$ *for i=1,2,...,n-2, corresponding to* $\theta_1 = (3-\sqrt{5})/2$, *such that* $\underline{y}_i$*'s are* $(n-1) \times 1$ *contrast vectors in which* $\underline{y}_i'\underline{y}_j = \delta^{ij}$, *where* δ^{ij}*=1 if* $i=j$ *and 0 if* $i \neq j$.
2. $\underline{\xi}_i' = c_2 \left[0\ ,\ \underline{y}_{i-n+2}'\ ,\ (1-\theta_2)\underline{y}_{i-n+2}'\right]$ *for i=n-1,n,...,2n-4, corresponding to* $\theta_2 = (3+\sqrt{5})/2$,
3. $\underline{\xi}_{2n-3}' = c_3 \left[1,\ \frac{n-1-\theta_3}{(1-\theta_3)(n-1)}\underline{1}',\ (n-1-\theta_3)(n-1)^{-1}\underline{1}'\right]$ *corresponding to* $\theta_3 = \left[n+2-\sqrt{(n-2)^2-4(2n-1)}\ \right]/2$,

4. $\underline{\xi}'_{2n-2} = c_4 \left[1, \frac{n-1-\theta_4}{(1-\theta_4)(n-1)}\underline{1}', (n-1-\theta_4)(n-1)^{-1}\underline{1}'\right]$ *corresponding to* $\theta_4 = \left[n+2+\sqrt{(n-2)^2-4(2n-1)}\,\right]/2$, *and*

5. $\underline{\xi}_{2n-1} = t^{-1/2}\underline{1}_t$, *corresponding to* $\theta_5 = 0$, *where* c_j*'s(j=1,2,3,4) are normalizing coefficients.*

Proof: The proof follows by showing that $C'C\underline{\xi}_i = \theta_i\underline{\xi}_i$ in each case.♣

As we have shown in Chapter 2, an $n \times 2$ CFBD(00) design is PBDS design if and only if it has the A-matrix of the structure W given in (2.20) of Chapter 2.

Now we are in a position to give a theorem which specifies the structure of the A-matrix for a design with property S with respect to the dual versus single treatment contrasts.

Theorem 7.2 *If a design has property S for the dual versus single treatment contrasts, then it is a PBDS design.*

Proof: Let

$$\Gamma = (\underline{\xi}_1, \underline{\xi}_2, \ldots, \underline{\xi}_t), \tag{7.25}$$

where the $\underline{\xi}_i$'s are given in Lemma 7.4.

Suppose design d has property S, then we have

$$\Gamma' A \Gamma = \begin{bmatrix} \alpha_1 I_{n-2} & & & & 0 \\ & \alpha_2 I_{n-2} & & & \\ & & \alpha_3 & & \\ & & & \alpha_4 & \\ 0 & & & & 0 \end{bmatrix}. \tag{7.26}$$

where the α_i's are the distinct eigenvalues of the A-matrix. Since the columns of Γ form an orthonormal basis for a $t \times t$ vector space, Γ is a nonsingular matrix such that $\Gamma'\Gamma = \Gamma\Gamma' = I_t$. Therefore from (7.26) we have:

$$A = \Gamma \begin{bmatrix} \alpha_1 I_{n-2} & & & & 0 \\ & \alpha_2 I_{n-2} & & & \\ & & \alpha_3 & & \\ & & & \alpha_4 & \\ 0 & & & & 0 \end{bmatrix} \Gamma'.$$

By applying the spectral decomposition(see Mardia, Kent and Bibby,1979, p469) we obtain:

$$A = \alpha_1 \sum_{i=1}^{n-2} \underline{\xi}_i \underline{\xi}_i' + \alpha_2 \sum_{i=n-1}^{2n-4} \underline{\xi}_i \underline{\xi}_i' + \alpha_3 \underline{\xi}_{2n-3} \underline{\xi}_{2n-3}' + \alpha_4 \underline{\xi}_{2n-2} \underline{\xi}_{2n-2}' + \alpha_5 \underline{\xi}_{2n-1} \underline{\xi}_{2n-1}'. \quad (7.27)$$

Then by substituting for $\underline{\xi}_i$'s from Lemma 7.4 and applying Lemma 7.3 it follows that the A-matrix has structure W. Therefore design d is a PBDS design. This completes the proof.♣

Discussion 7.2 *Theorem 7.2 illustrates how identifying property S designs leads us to a class which contains highly efficient designs. We have established in Chapter 2 that the PBDS class contains efficient designs. It also includes some A-optimal designs(as was shown in Chapter 4).*

7.5.2 All Sets of (t-1) Orthogonal Contrasts:

In some experiments a specific set of contrasts for investigation is not known prior to the experiment; for example if we want to identify the treatment giving the 'best' response in some sense we analyse the experiment by using multiple comparison tests. In these circumstances a design is required which is efficient for estimating any set of orthogonal contrasts. We now identify the S property designs for this problem. First we consider the bound.

Corollary 7.4 *If $C_{\underline{T}}$ is any set of t-1 orthonormalized contrasts, then we have*

$$tr(C\Omega C') = \sum_{i=1}^{t-1} \frac{1}{\lambda_i}, \quad (7.28)$$

where the λ_i's were given in the statement of Theorem 3.2.

Proof: Let Ω is the Moore-Penrose g-inverse of the A-matrix of the design, then

$$tr(C\Omega C') = tr(\Omega C'C).$$

By Lemma 7.3 we have $C'C = I_t - 1/tJ_t$. Therefore

$$tr(C\Omega C') = tr(\Omega(I_t - 1/tJ_t) = tr(\Omega) - tr(1/t\Omega J_t).$$

But the second term in the RHS of the above expression is zero and by the property of Ω the first term in the RHS gives the required expression in (7.28).♣

Theorem 7.3 *A design has property S for any set of t-1 orthonormalized contrasts between the treatments if and only if it is a BIBD or BBD design.*

Proof: In this case C is a set of t-1 orthonormal contrasts, therefore by Lemma 7.3 we have $C'C = I_t - (1/t)J_t$. It can be shown that the columns of $\Gamma = (\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_{t-1}, t^{-1/2}\underline{1})$ are eigenvectors of $C'C$ matrix, where the x_i's are $t \times 1$ column vectors such that, (a): $\underline{x}_i'\underline{x}_j = \delta^{ij}$, where $\delta^{ij} = 1$ if i=j and 0 otherwise, and (b): $\underline{x}_i'\underline{1} = 0$ for i=1,2,...,t-1, then

1. Suppose the design is BIBD or BBD, i.e. its A-matrix can be denoted by $A = aI_t + bJ_t$, then

$$\Gamma' A \Gamma = a\Gamma'\Gamma + b\Gamma' J_t \Gamma. \tag{7.29}$$

But by Lemma 7.3 we have $\Gamma'\Gamma = I_t$ and $\Gamma' J_t \Gamma = diag(0, 0, ..., 0, t)$. Substituting from here into above expression we obtain

$$\Gamma' A \Gamma = \begin{bmatrix} aI_{t-1} & 0 \\ 0 & 0 \end{bmatrix}. \tag{7.30}$$

This means that the columns of Γ are eigenvectors of the A-matrix of design d. This gives the proof of the first part.

2. Suppose we have a design d with A-matrix satisfying the condition (7.30), then we show that this design is either a BIBD or a BBD design. In other words we show that the A-matrix of the design has structure $cI_t + dJ_t$. By the spectral decomposition we have:

$$A = \lambda \sum_{i=1}^{t-1} \underline{x}_i \underline{x}_i' + (0)t^{-1} J_t = \lambda(I_t - \frac{1}{t} J_t). \tag{7.31}$$

This completes the proof of the second part. Hence the theorem is proved.♣

Discussion 7.3 *From Corollary 7.4 it is clear that the bound in (7.28) is achieved by those designs with equal eigenvalues. The class of BIBD or BBD have this property. Therefore the corollary simply says that if the contrasts among all the treatments involved in the design are of equal importance, then if for the given parameter values a BIBD or BBD does exist, it will be the most efficient design within the entire class of designs(the A-optimality criterion). This is the well-known property which was derived by Kiefer(1958).*

Note that even if a specific set of t-1 orthogonal contrasts of interest is defined then by applying the above arguments the S-property designs with these specified contrasts are still BIBD or BBD. This is because $C'C$ is invariant to the particular C-matrix, provided its rows form a complete set of orthogonal contrasts.

7.5.3 Test Treatments versus Control Treatment(s):

In this section we first consider the general problem of comparing a set of w test treatments with a set of u controls. Without loss of generality we assume that $u \leq w$. We identify the structure S designs and show that these are the same as the class of designs identified by Majumdar(1986) via the permutation method as containing A-optimal or highly efficient designs. This class of designs has been characterized by their A-matrix as having the following structure:

$$A = \begin{bmatrix} aI_u + bJ_u & eJ_{u\times w} \\ eJ_{w\times u} & cI_w + dJ_w \end{bmatrix}. \tag{7.32}$$

The contrast matrix C, is given by:

$$C = \begin{pmatrix} -I_u \otimes \underline{1}_w & \underline{1}_u \otimes I_w \end{pmatrix}. \tag{7.33}$$

For this case we have:

$$C'C = \begin{bmatrix} wI_u & -J_{u\times w} \\ -J_{w\times u} & uI_w \end{bmatrix}. \tag{7.34}$$

The eigenvalues of $C'C$ are given in Table 7.2.

Table 7.2: Eigenvalues of $C'C$ matrix.

Eigenvalues(θ_i)	multiplicities
u+w	1
w	u-1
u	w-1
0	1

Lemma 7.5 *The eigenvectors of the $C'C$ matrix given in (7.34) for w test treatments versus u controls are:*

1. $\underline{\xi}_1' = 1/\sqrt{uw(u+w)}(-w\underline{1}_u' \;,\; u\underline{1}_w')$, *corresponding to* $\theta = u + w$,
2. $\underline{\xi}_i' = (\underline{x}_i' \;,\; \underline{0}_w')$, *for i=2,3,...,u, corresponding to* $\theta = w$, *where* $\underline{x}_i$*'s are* $u\times 1$ *vectors such that* $\underline{x}_i'\underline{x}_j = \delta^{ij}$ *and* $\underline{x}_i'\underline{1}_u = 0$.
3. $\underline{\xi}_i' = (\underline{0}_u' \;,\; \underline{y}_{i-u}')$, *for i=u+1,u+2,...,u+w-1, corresponding to* $\theta = u$, *where* $\underline{y}_j$*'s are* $w\times 1$ *vectors such that* $\underline{y}_\ell'\underline{y}_j = \delta^{\ell j}$ *and* $\underline{x}_\ell'\underline{1}_w = 0$, *where* ℓ*=1,2,...,w. and*
4. $\underline{\xi}_t = t^{-1/2}\underline{1}_t$, *corresponding to* $\theta = 0$, *where t=u+w.*

Proof: The proof is straightforward by showing that $C'C\underline{\xi}_i = \theta_i\underline{\xi}_i$.♣

We now identify the S-property designs for this problem. First we consider the bound.

Corollary 7.5 *If* $C\tau$ *is a set of uw contrasts which compare each of w test treatments with each of u control treatments, then*

$$tr(C\Omega C') \geq \frac{t}{\lambda_1} + w\sum_{i=2}^{u}\frac{1}{\lambda_i} + u\sum_{i=u+1}^{t-1}\frac{1}{\lambda_i}, \tag{7.35}$$

where t=u+w.

Proof: The result follows from Table 7.2 by applying Theorem 3.2 and assuming $u \leq w$.♣

Theorem 7.4 *A design has property S for comparing a set of w test treatments with a set of u controls if and only if its A-matrix has the structure given in (7.32).*

Proof: Let

$$\Gamma = (\underline{\xi}_1, \underline{\xi}_2, \cdots, \underline{\xi}_t), \tag{7.36}$$

where $\underline{\xi}_i$'s are given in Lemma 7.5. Then

1. suppose design d has A-matrix with structure (7.32), then it can be easily shown that:

$$\Gamma' A \Gamma = \begin{bmatrix} x & & & 0 \\ & aI_{u-1} & & \\ & & cI_{w-1} & \\ 0 & & & 0 \end{bmatrix}; \; x = a + c + ub + wd. \tag{7.37}$$

This simply says that the eigenvectors of the A-matrix of design d with structure given in (7.32) are the same as those of $C'C$ given in Lemma 7.5 and have same multiplicities of eigenvalues. This proves the first part.

2. From equation (7.37) by the spectral decomposition we have:

$$A = x\underline{\xi}_1 \underline{\xi}_1' + a\sum_{i=2}^{u} \underline{\xi}_i\underline{\xi}_i' + c\sum_{i=u+1}^{u+w-1} \underline{\xi}_i\underline{\xi}_i' + (0)\underline{\xi}_{u+w}\underline{\xi}_{u+w}'. \tag{7.38}$$

Then by applying Lemma 7.3, we have:

(a)

$$\underline{\xi}_1\underline{\xi}_1' = \frac{uw}{u+w}\begin{bmatrix} \frac{1}{u^2}J_u & -\frac{1}{uw}J_{u\times w} \\ -\frac{1}{uw}J_{w\times u} & \frac{1}{w^2}J_w \end{bmatrix}, \tag{7.39}$$

(b)

$$\sum_{i=2}^{u}\underline{\xi}_i\underline{\xi}_i' = \begin{bmatrix} \sum_{i=1}^{u-1} x_i x_i' & 0_{u\times w} \\ 0_{w\times u} & 0_w \end{bmatrix} = \begin{bmatrix} I_u - \frac{1}{u}J_u & 0_{u\times w} \\ 0_{w\times u} & 0_w \end{bmatrix},$$

(c)

$$\sum_{i=u+1}^{u+w-1}\underline{\xi}_i\underline{\xi}_i' = \begin{bmatrix} 0_u & 0_{u\times w} \\ 0_{w\times u} & \sum_{j=1}^{w-1} y_j y_j' \end{bmatrix} = \begin{bmatrix} 0_u & 0_{u\times w} \\ 0_{w\times u} & I_w - \frac{1}{w}J_w \end{bmatrix}.$$

This shows that the structure of the A-matrix of design d is the same as the structure given in (7.32). This completes the proof of the second part. Hence the theorem is proved.♣

A special case of the above problem is when u=1. This problem is known as the test treatments versus control problem in the literature.

Discussion 7.4 *Theorem 7.4 again illustrates how identifying property S designs leads us to a class of designs containing highly efficient designs. The class of partially balanced designs with the structure (7.32) for their A-matrices has been identified by Majumdar(1986) as containing efficient designs for u $\geq$ 2. For u=1, the theorem leads us to the BTIB or the BTB designs. These designs were identified by Bechhofer and Tamhane(1981) and shown by Majumdar and Notz(1983) to contain highly efficient and some A-optimal designs.*

Conclusion: From this section we concluded that for a specific sets of contrasts of interest, C_T, the structure of the A-matrix of the observed class of designs having efficient designs, is linked to $C'C$. This includes three well-known problems. Generalization of this link to consider a general contrast matrix is a topic for further research.

7.6 Conclusions and Directions for Further Research:

In the final section, there are two questions which might be answered. Firstly, what conclusions can be drawn from the research presented in this thesis and secondly, how might this research be improved and extended? We shall start by summarizing the main results of the thesis.

7.6.1 Conclusions:

The aim of conducting an experiment is to estimate or test hypotheses about some specified unknown parameters. Different considerations leads us to different criteria for the choice of an "efficient" design.

Our experiment involves two factors, namely A and B at n and m levels respectively, where treatment combination 00 is excluded from the experiment. Our aim is to consider whether the effects of using both factors together is better than using only a single factor. In order to do this we need designs which estimate these contrasts with the highest precision; that is we employ the A-optimality criterion. To find such designs we have done two things: Firstly, a tight lower bound has been derived on the total variance of the estimators of the contrasts which enables us to assess the performance of the designs. Secondly, designs with high performance have been characterized by determining a class of designs which is a source of good designs, in the sense of giving small total variance on the estimators of the contrasts of interest.

In Chapter 1 we briefly reviewed the literature related to our problem as well as giving related concepts and definitions. Our considerations concentrated on 2×2 experiments for which series of A-optimal and highly efficient designs have already been tabulated. A successful attempt was made to fill the gaps in the practical range of parameter combinations. The results are given in Tables 1.1

and 1.2.

Then we considered $n \times 2$ factorial experiments and introduced a class of designs which contain efficient designs and give equal precision within the dual versus A contrasts and within the dual versus B contrasts. These designs are called PBDS designs and were studied in Chapters 2-4. In Chapter 2 we introduced a method of constructing PBDS designs based on the group divisible designs, called RGDD, which can be constructed easily. Further, we investigated some properties of these designs and characterized the most efficient. Designs having total balance, that is giving equal variance for all the estimated contrasts of interest were studied. It was concluded that, due to combinatorial restrictions, the designs were not useful in practice.

Establishment of two bounds on the total variance of the estimators of the contrasts of interest is the main topic of Chapter 3. This two different bounds were found by applying different methods. It was shown numerically that in the designs with $k > t$ one bound(b_1) is uniformally tighter than the other(b_2). However, for the cases where $k < t$ this is not true and one bound is not uniformally tighter than the other. Therefore we take the maximum value of these bounds as a lower bound(b_m). The performance of the RGDD's which can be constructed via the catalogue of Clatworthy was assessed at the end of Chapter 3.

In Chapter 4 it was shown that the most efficient designs in the PBDS class are highly efficient in the entire class of designs by utilizing the permutation technique. The efficient designs were characterized by the number of units which is assigned to each set of treatment combinations A, B and D within each block. Some methods of constructing PBDS designs(excluding RGDD's) were introduced. Finally, efficient designs for $3 \leq n \leq 6$, $2 \leq k \leq 9$ and $2 \leq b \leq 10$, which covers most practical cases arising in clinical trials, are summarized in Table 4.2.

In Chapter 5 n×m experiments were considered by using a more general permutation technique than employed in Chapter 4. A generalization of PBDS designs was specified, called GPBDS designs. We obtained a design-dependent bound for the total variance of the estimators of the contrasts of interest but failed to calculate it in terms of the elements of the concurrence matrix of the design. However, a series of overall A-optimal designs were obtained for the cases when $k \geq t$. Some methods of constructing GPBDS designs were introduced with emphasis on the practical cases arising in clinical trials, that is $3 \leq n, m \leq 5$. The performances of these designs were assessed and recommendations made on their use.

In Chapter 6 we considered experiments conducted in a completely randomized designs and characterized those designs which are A-optimal. A series of A-optimal designs obtained from these results was summarized in Table 6.1. Later we allowed different sets of contrasts to have different degrees of importance and defined a Weighted A-optimal criterion. Then, we characterized those completely randomized designs which are weighted A-optimal designs for specific weights on the dual versus A and the dual versus B contrasts. The idea of weighted A-optimal design was then generalized to block designs and a design-dependent bound on the weighted total variance of the contrasts of interest was established.

In Chapter 7, firstly we considered one way of estimating a specific set of factorial effects when a certain treatment combination is excluded from the experiment and another set of factorial effects was assumed to be negligible. This has been done in randomized block designs and completely randomized designs with equal treatment replications via assuming the negligibility of a linear combination of the negligible factorial effects. Next we established a rule to enable us to choose the particular linear combination of negligible factorial effects which enables the factorial effects of interest to be estimated with maximum precision. Consideration of completely randomized designs with unequal treatment replications proved more difficult than the equireplicate cases.

We examined, through Theorem 3.2, the similarity between the structure of the A-matrix of the class of designs which is a source of efficient designs and the structure of $C'C$, where C is the contrast matrix corresponding to the contrasts of interest. We observed, for three types of problem that Theorem 3.2 provides the structure of the A-matrix of a class of designs which have been shown to be a source of efficient designs for example balanced block designs.

7.6.2 Further Research:

The following questions remain unanswered and are topics for future work.

1. Is there any means of minimizing our objective function $tr(C\bar{\Omega}C')$ given in (4.5) in Chapter 4?

2. Is it possible to prove that Conjectures 4.1–4.3 are true?

3. What are other sufficient conditions for a design to be PBDS and do these enable further efficient designs to be obtained?

4. Can we express $tr(C\bar{\Omega}C')$ in Chapter 5 as a function of the elements of the concurrence matrix of the design? If we can obtain such a function which designs minimize the value of the function?

5. Suppose our experiment is conducted in a block design other than a randomized block design, then how can we estimate a set of factorial effects by neglecting another set of factorial effects(see Section 7.3)?

6. Can we extend the idea of similarity between the structure of the A-matrix of the class containing efficient designs and $C'C$ from specific C's to more general cases than those described in Chapter 7?

Appendix A

Proofs of theorems and lemmas:

A.1 Proofs Related to Chapter 4

A.1.1 Proof of Theorem 4.5:

From the assumptions in the statement of theorem we have:

$$n_{Aij} = \begin{cases} a_{Aj} + 1 & \text{for } i = 1, 2, \ldots, b_{Aj}, \\ \\ a_{Aj} & \text{for } i = b_{Aj} + 1, \ldots, n-1. \end{cases}$$

$$n_{Dij} = \begin{cases} a_{Dj} + 1 & \text{for } i = 1, 2, \ldots, b_{Dj}, \\ \\ a_{Dj} & \text{for } i = b_{Dj} + 1, \ldots, n-1. \end{cases}$$

From these we obtain

$$\sum_{i=1}^{n-1} n_{Aij}^2 = (n-1)a_{Aj}^2 + 2a_{Aj}b_{Aj} + b_{Aj}, \tag{A.1}$$

$$\sum_{i=1}^{n-1} n_{Dij}^2 = (n-1)a_{Dj}^2 + 2a_{Dj}b_{Dj} + b_{Dj},$$

for j=1,2,...,b.

From (A.1)

$$\sum_{j=1}^{b} \sum_{i=1}^{n-1} n_{Aij}^2 = (n-1) \sum_{j=1}^{b} a_{Aj}^2 + 2 \sum_{j=1}^{b} a_{Aj} b_{Aj} + \sum_{j=1}^{b} b_{Aj},$$

$$\sum_{j=1}^{b}\sum_{i=1}^{n-1} n_{Dij}^2 = (n-1)\sum_{j=1}^{b} a_{Dj}^2 + 2\sum_{j=1}^{b} a_{Dj}b_{Dj} + \sum_{j=1}^{b} b_{Dj},$$

$$\sum_{j=1}^{b} T_{Aj}^2 = (n-1)^2\sum_{j=1}^{b} a_{Aj}^2 + 2(n-1)\sum_{j=1}^{b} a_{Aj}b_{Aj} + \sum_{j=1}^{b} b_{Aj}^2, \tag{A.2}$$

$$\sum_{j=1}^{b} T_{Dj}^2 = (n-1)^2\sum_{j=1}^{b} a_{Dj}^2 + 2(n-1)\sum_{j=1}^{b} a_{Dj}b_{Dj} + \sum_{j=1}^{b} b_{Dj}^2,$$

$$\frac{T_{Aj}T_{Dj}}{n-1} = (n-1)a_{Aj}a_{Dj} + (a_{Aj}b_{Dj} + a_{Dj}b_{Aj}) + \frac{b_{Aj}b_{Dj}}{n-1}.$$

Substituting from (A.2) into the expression of d_A and d_D we obtain the required expressions in (4.36).

In order to obtain the required expressions for u and v, by applying Marshall and Olkin(1979, proposition A.3,p 141), four cases have to be considered here:

(i) $b_{Dj} \leq b_{Aj}$, then

$$\begin{aligned}\textstyle\sum_{i=1}^{n-1} n_{Aij}n_{Dij} \leq\ & b_{Dj}(a_{Dj}+1)(a_{Aj}+1)+ \\ & a_{Dj}\left\{(b_{Aj}-b_{Dj})(a_{Aj}+1)+(n-1-b_{Aj})a_{Aj}\right\} \\ & = (a_{Aj}b_{Dj}+a_{Dj}b_{Aj})+(n-1)(a_{Aj}a_{Dj})+b_{Dj}\end{aligned} \tag{A.3}$$

(ii) $b_{Aj} \leq b_{Dj}$, then

$$\begin{aligned}\textstyle\sum_{i=1}^{n-1} n_{Aij}n_{Dij} \leq\ & b_{Aj}(a_{Dj}+1)(a_{Aj}+1)+ \\ & a_{Aj}\left\{(b_{Dj}-b_{Aj})(a_{Dj}+1)+(n-1-b_{Dj})a_{Dj}\right\} \\ & = (a_{Aj}b_{Dj}+a_{Dj}b_{Aj})+(n-1)(a_{Aj}a_{Dj})+b_{Aj}\end{aligned} \tag{A.4}$$

On substitution from (A.3) and (A.4) into the expression for d_{AD} in (4.15) we obtain v in (4.37).

(iii) $b_{Dj} + b_{Aj} - (n-1) \geq 0$, then

$$\begin{aligned}\textstyle\sum_{i=1}^{n-1} n_{Aij}n_{Dij} \geq\ & (n-1-b_{Dj})a_{Dj}(a_{Aj}+1)+ \\ & (a_{Dj}+1)(b_{Aj}+b_{Dj}-n+1)(a_{Aj}+1)+ \\ & (a_{Dj}+1)(n-1-b_{Aj})a_{Aj} \\ & = (a_{Aj}b_{Dj}+a_{Dj}b_{Aj})+(n-1)(a_{Aj}a_{Dj})+ \\ & (b_{Dj}+b_{Aj}-n+1)\end{aligned} \tag{A.5}$$

(iv) $b_{Aj} + b_{Dj} - (n-1) \leq 0$, then

$$\begin{aligned}\sum_{i=1}^{n-1} n_{Aij}n_{Dij} \geq\ & b_{Aj}a_{Dj}(a_{Aj}+1)+ \\ & a_{Aj}\{(n-1-b_{Dj}-b_{Aj})a_{Dj} + b_{Dj}(a_{Dj}+1)\} \\ & = (a_{Aj}b_{Dj} + a_{Dj}b_{Aj}) + (n-1)(a_{Aj}a_{Dj}).\end{aligned} \quad (A.6)$$

On substituting from (A.5) and (A.6) into the expression for d_{AD} given in (4.15) we will obtain u in (4.38). Hece the theorem is proved.♣

A.1.2 Proof of Lemma 4.8:

Based on the definitions of T_{Aj}, T_{Dj} and T_{Bj}, we have $T_{Aj} + T_{Bj} + T_{Dj} = k$. This implies that $T_{Dj} = k - T_{Bj} - T_{Aj}$. Therefore

$$q_D = \frac{T_D}{n-1} - \frac{1}{k(n-1)}\sum_{j=1}^{b}(k - T_{Aj} - T_{Bj})^2.$$

After some algebra we obtain

$$q_D = q_A + q_B - 2q_{AB}. \quad (A.7)$$

Also

$$q_{AD} = \frac{1}{k(n-1)}\sum_{j=1}^{b} T_{Aj}(k - T_{Aj} - T_{Bj}).$$

After some manipulation the expression becomes

$$q_{AD} = q_A - q_{AB}. \quad (A.8)$$

On substitution for q_D and q_{AD} from (A.7) and (A.8) respectively in the RHS of (4.62) we obtain the expression in LHS. Hence the lemma is proved.♣

A.1.3 Proof of Theorem 4.9:

If in each a block of design d, we change treatment combination i0 by i1 and vice versa, and call the resulting design d^*, then in design d^* we have $n_{Aij} \leq n_{Dij}$. In order to show that d^* is more efficient than design d, it is enough to show that from Conjecture 4.1, the bound which can be obtained by design d^* is tighter than that of d. Let B_d and B_{d^*} denote the lower bound which is provided by applying Conjecture 4.1 on designs d and d^* respectively, then we need to show that:

$$B_d - B_{d^*} \geq 0.$$

By using Lemma 4.8, it can be shown that

$$B_d - B_{d^*} = \frac{(n-2)(d_A - d_D)}{d_A d_D - d_{AD}^2} + \frac{q_A - q_D}{q_A q_D - q_{AD}^2}, \tag{A.9}$$

where d_A, d_D, d_{AD}, q_A, q_D and q_{AD} were defined in (4.15). On substitution from (4.15) in the above expression, after some algebra, we can show that:

$$q_A - q_D = \frac{T_A - T_D}{n-1} - \frac{1}{k(n-1)} \sum_{j=1}^{b} (T_{Aj} - T_{Dj})(T_{Aj} + T_{Dj}). \tag{A.10}$$

Since $T_{Aj} + T_{Dj} \leq k$ and $T_{Aj} \geq T_{Dj}$, then

$$q_A - q_D \geq \frac{T_A - T_D}{n-1} - \frac{1}{n-1} \sum_{j=1}^{b} (T_{Aj} - T_{Dj}) = 0. \tag{A.11}$$

From (4.15)

$$d_A - d_D = \frac{T_A - T_D}{n-1} - \frac{D_A - D_D}{k(n-2)} + \frac{S_A - S_D}{k(n-1)(n-2)}. \tag{A.12}$$

It can be shown that

$$D_A - D_D = \sum_{j=1}^{b} \sum_{i=1}^{n-1} (n_{Aij} - n_{Dij})(n_{Aij} + n_{Dij}). \tag{A.13}$$

Since $n_{Aij} + n_{Dij} \leq T_{Aj} + T_{Dj}$ and based on the assumption, $n_{Aij} - n_{Dij} \geq 0$, hence

$$D_A - D_D \leq \sum_{j=1}^{b} \sum_{i=1}^{n-1} (T_{Aj} + T_{Dj})(n_{Aij} - n_{Dij}) = S_A - S_D. \tag{A.14}$$

From (A.12) and (A.14) we obtain

$$d_A - d_D \geq \frac{T_A - T_D}{n-1} - \frac{S_A - S_D}{k(n-2)} + \frac{S_A - S_D}{k(n-1)(n-2)} = \frac{T_A - T_D - \frac{S_A - S_D}{k}}{n-1}. \tag{A.15}$$

From (4.15), it can be shown that

$$\frac{S_A - S_D}{k} = \frac{1}{k} \sum_{j=1}^{b} (T_{Aj} - T_{Dj})(T_{Aj} + T_{Dj}). \tag{A.16}$$

Since $T_{Aj} \geq T_{Dj}$ and $T_{Aj} + T_{Dj} \leq k$, this implies that

$$\frac{S_A - S_D}{k} \leq T_A - T_D. \tag{A.17}$$

Then from (A.17) and (A.15) we obtain

$$d_A - d_D \geq \frac{T_A - T_D}{n-1} - \frac{T_A - T_D}{n-1} = 0. \tag{A.18}$$

Hence from (A.11) and (A.18) the proof follows.♣

A.2 Proof of Lemma 5.1:

From (5.6) we have

$$\bar{A} = \frac{1}{p!q!}\sum_{i=1}^{q!}\sum_{j=1}^{p!}\pi_{ij}A\pi'_{ij} = \begin{bmatrix} \bar{D} & \bar{B} & \bar{F} \\ \bar{B}' & \bar{G} & \bar{H} \\ \bar{F}' & \bar{H}' & \bar{L} \end{bmatrix}, say. \tag{A.19}$$

We now determine the structure of $\bar{A}$ by substituting for A from (5.4). By premultipying and postmultiplying A by π_{ij} and its transpose π'_{ij} respectively, we obtain

$$\pi_{ij}A\pi'_{ij} = \begin{bmatrix} q_iDq'_i & q_iBp'_j & q_iF(p_j \otimes q_i)' \\ p_jB'q'_i & p_jGp'_j & p_jH(p_j \otimes q_i)' \\ (p_j \otimes q_i)F'q'_i & (p_j \otimes q_i)H'p'_j & (p_j \otimes q_i)L(p_j \otimes q_i)' \end{bmatrix}. \tag{A.20}$$

Then, if we let y_{ij} denote the ijth entry in matrix Y, we obtain

1.

$$\bar{D} = \frac{1}{p!q!}\sum_{i=1}^{q!}\sum_{j=1}^{p!} q_iDq'_i = \frac{1}{q!}\sum_{i=1}^{q!} q_iDq'_i = (\bar{d}_{ij}),$$

where by Majumdar and Notz(1983):

$$\bar{d}_{ij} = \begin{cases} \frac{1}{q}\sum_{i=1}^{q} d_{ii} = \bar{d}_1 & \text{if } i = j \\ \frac{1}{q(q-1)}\sum_{i=1}^{q}\sum_{j\neq i}^{q} d_{ij} = \bar{d}_2 & \text{if } i \neq j \end{cases}$$

Therefore

$$\bar{D} = a_1 I_q + b_1 J_q,$$

where $a_1 + b_1 = \bar{d}_1$ and $b_1 = \bar{d}_2$.

2.

$$\bar{G} = \frac{1}{p!q!}\sum_{i=1}^{q!}\sum_{j=1}^{p!} p_i G p_i' = \frac{1}{p!}\sum_{j=1}^{p!} p_i G p_i' = (\bar{g}_{ij}).$$

Similarly

$$\bar{g}_{ij} = \begin{cases} \frac{1}{p}\sum_{i=1}^{p} g_{ii} = \bar{g}_1 & \text{if } i = j \\ \\ \frac{1}{p(p-1)}\sum_{i=1}^{p}\sum_{j\neq i}^{p} g_{ij} = \bar{g}_2 & \text{if } i \neq j \end{cases}$$

and

$$\bar{G} = a_3 I_p + b_3 J_p,$$

where $a_3 + b_3 = \bar{g}_1$ and $b_3 = \bar{g}_2$.

3.

$$\bar{B} = \frac{1}{p!q!}\sum_{i=1}^{q!}\sum_{j=1}^{p!} q_i B p_j',$$

which gives

$$\bar{b}_{ij} = \frac{1}{pq}\sum_{i=1}^{q}\sum_{j=1}^{p} b_{ij} = \bar{b}, say.$$

Therefore $\bar{B} = \bar{b} J_{q\times p}$.

4.

$$\bar{F} = \frac{1}{p!q!}\sum_{i=1}^{q!}\sum_{i=1}^{p!} q_i F (p_j \otimes q_i)',$$

which is

$$\bar{F} = \frac{1}{pq!}\sum_{i=1}^{q!} q_i F (J_p \otimes q_i)'.$$

This gives

$$\bar{F} = \underline{1}_p' \otimes \{\frac{1}{q!}\sum_{i=1}^{q!} q_i \bar{S} q_i'\},$$

where $\bar{S} = \frac{1}{p}\sum_{i=1}^{p} F_i$. This can be shown as

$$\bar{F} = \underline{1}_p' \otimes \bar{\bar{S}},$$

where $\bar{\bar{S}} = (\bar{\bar{s}}_{ij})$ and

$$\bar{\bar{s}}_{ij} = \begin{cases} \frac{1}{q}\sum_{i=1}^{q} \bar{s}_{ii} = \bar{\bar{s}}_1 & \text{if } i = j \\ \\ \frac{1}{q(q-1)}\sum_{i=1}^{q}\sum_{j\neq i}^{q} \bar{s}_{ij} = \bar{\bar{s}}_2 & \text{if } i \neq j \end{cases}$$

Therefore

$$\bar{F} = \underline{1}'_p \otimes (a_2 I_q + b_2 J_q),$$

where $a_2 + b_2 = \bar{\bar{s}}_1$ and $b_2 = \bar{\bar{s}}_2$.

5. Similarly,

$$\bar{H} = (\frac{1}{qp!}) \sum_{j=1}^{p!} p_j(H_1, H_2, \ldots, H_p)(p'_j \otimes J_q),$$

where after some algebra as above, we obtain

$$\bar{H} = (a_4 I_p + b_4 J_p) \otimes \underline{1}'_q,$$

where

$$a_4 + b_4 = \sum_{i=1}^{p} H_{ii}\underline{1}_q/(pq)$$

$$b_4 = \sum_{i=1}^{q} \sum_{j=1}^{p} H_{ij}\underline{1}_q / [p(p-1)q]\,(i \neq j)$$

and H_{ij} is an $1 \times q$ vector corresponding to the ith row of H_j.

6.

$$\bar{L} = \frac{1}{p!q!} \sum_{i=1}^{q!} \sum_{j=1}^{p!} (p_j \otimes q_i) L (p_j \otimes q_i)'.$$

Let

$$\bar{L}_1 = \frac{1}{p} \sum_{i=1}^{p} L_{ii},$$

$$\bar{L}_2 = \frac{1}{p(p-1)} \sum_{i=1}^{p} \sum_{i' \neq i}^{p} L_{ii'},$$

$$\bar{\bar{L}}_1 = \frac{1}{q!} \sum_{i=1}^{q!} q_i \bar{L}_1 q'_i,$$

and

$$\bar{\bar{L}}_2 = \frac{1}{q!} \sum_{i=1}^{q!} q_i \bar{L}_2 q'_i.$$

Then

$$\bar{L} = I_p \otimes (\bar{\bar{L}}_1 - \bar{\bar{L}}_2) + J_p \otimes \bar{\bar{L}}_2.$$

But $\bar{\bar{L}}_1 = \alpha_1 I_q + \beta_1 J_q$; $\alpha_1 + \beta_1 = \bar{\bar{l}}_{1(ii)}$ and $\beta_1 = \bar{\bar{l}}_{1(ii')}(i \neq i')$. Also $\bar{\bar{L}}_2 = \alpha_2 I_q + \beta_2 J_q$; $\alpha_2 + \beta_2 = \bar{\bar{l}}_{2(ii)}$ and $\beta_2 = \bar{\bar{l}}_{2(ii')}(i \neq i')$. From these we obtain

$$\bar{L} = I_p \otimes (a_5 I_q + b_5 J_q) + J_q \otimes (a_6 I_q + b_6 J_q),$$

where $a_5 = \alpha_1 - \alpha_2$, $b_5 = \beta_1 - \beta_2$, $a_6 = \alpha_2$ and $b_6 = \beta_2$.

Therefore the general structure of $\bar{A}$ is as follows:

$$\bar{A} = \begin{bmatrix} a_1 I_q + b_1 J_q & cJ_{q\times p} & \underline{1}'_p \otimes (a_2 I_q + b_2 J_q) \\ & a_3 I_p + b_3 J_p & (a_4 I_p + b_4 J_p) \otimes \underline{1}'_q \\ & & I_p \otimes (a_5 I_q + b_5 J_q) + J_q \otimes (a_6 I_q + b_6 J_q) \end{bmatrix}. \tag{A.21}$$

In order to establish the structure of $\bar{\Omega}$, notice that for any connected GPBDS design, a g-inverse of its A-matrix, $\bar{\Omega}$ is obtained as $(\bar{A}+xJ)^{-1}$ for any real number $x \neq 0$. $\bar{A}$ has the same rank of A because it was obtained by permutation. Hence it is obvious that $\bar{A} + xJ$ is a nonsingular matrix with the same structure as $\bar{A}$. Therefore without loss of generality let us assume that $\bar{A}$ is nonsingular. Now we partition $\bar{A}$ as follows:

$$\bar{A} = \begin{bmatrix} \bar{A}_{11} & \bar{A}_{12} \\ \bar{A}_{21} & \bar{A}_{22} \end{bmatrix},$$

where

$$\bar{A}_{11} = \begin{bmatrix} a_1 I_q + b_1 J_q & cJ_{q\times p} \\ cJ_{p\times q} & a_3 I_p + b_3 J_q \end{bmatrix},$$

$$\bar{A}_{12} = \begin{bmatrix} \underline{1}'_p \otimes (a_2 I_q + b_2 J_q) \\ (a_4 I_p + b_4 J_p) \otimes \underline{1}'_q \end{bmatrix},$$

$\bar{A}_{21} = \bar{A}'_{12}$ and

$$\bar{A}_{22} = I_p \otimes (a_5 I_q + b_5 J_q) + J_p \otimes (a_6 I_q + b_6 J_q).$$

Let $\bar{A}^{-1}$ denote the inverse of $\bar{A}$, and be partitioned as:

$$\bar{A}^{-1} = \begin{bmatrix} \bar{A}^{11} & \bar{A}^{12} \\ \bar{A}^{21} & \bar{A}]^{22} \end{bmatrix}.$$

Then by Graybill(1983,p184);

$$\bar{A}^{11} = (\bar{A}_{11} - \bar{A}_{12}\bar{A}_{22}^{-1}\bar{A}_{21})^{-1},$$

$$\bar{A}^{22} = (\bar{A}_{22} - \bar{A}_{21}\bar{A}_{11}^{-1}\bar{A}_{12})^{-1}$$

and

$$\bar{A}^{12} = -\bar{A}^{11}\bar{A}_{12}\bar{A}_{22}^{-1}.$$

By Graybill(1983,p195) and Lemma 2.3 in Chapter 2, $\bar{A}_{22}$ and $\bar{A}_{22}^{-1}$ have same structure. Pre and Postmultiplying $\bar{A}_{22}^{-1}$ by $\bar{A}_{12}$ and its transpose respectively, shows that $\bar{A}_{12}\bar{A}_{22}^{-1}\bar{A}_{21}$ and hence $\bar{A}_{11} - \bar{A}_{12}\bar{A}_{22}^{-1}\bar{A}_{21}$ have the same structures as $\bar{A}_{11}$.

Similarly, $\bar{A}_{21}\bar{A}_{11}^{-1}\bar{A}_{12}$ and hence $\bar{A}_{22} - \bar{A}_{21}\bar{A}_{11}^{-1}\bar{A}_{12}$ have the same structures as $\bar{A}_{22}$.

By the same method as two above cases we can show that $\bar{A}^{12}$ has the same structure as $\bar{A}_{12}$. This completes the proof.♣

Appendix B

Computer Algorithms

B.1 Algorithms for 2×2 Factorial Experiments:

B.1.1 A-optimal Designs:

```
PROGRAM OPTING1
    C THIS PROGRAMME GIVES THOSE VALUES OF R WHICH MINIMIZES
    C THE FUNCTION F(R), THEN CHECK WHETHER FOR THIS VALUE OF
    C R THE BTBD EXISTS OR NOT.
    DIMENSION FU(1000)
    IP=2
    P=IP
    DO 50 K=5,30
    IF(K.EQ.5)GO TO 100
    IF(K.EQ.6)GO TO 100
    IF(K.EQ.8)GO TO 100
    IF(K.EQ.9)GO TO 100
    IF(K.EQ.11)GO TO 100
    IF(K.EQ.12)GO TO 100
    IF(K.EQ.15)GO TO 100
    IF(K.EQ.16)GO TO 100
    IF(K.EQ.18)GO TO 100
    IF(K.EQ.19)GO TO 100
    IF(K.EQ.23)GO TO 100
    IF(K.EQ.25)GO TO 100
    IF(K.NE.30)GO TO 50
    IXYXY=10
    100 DO 50 IB=2,50
    B=IB
    M=B*K/2
```

```
R0=0
FMIN=999999999
DO 1 I=1,M
IR=I
R=I
NU=IR/IB
U=NU
NX=(IB*K-IR)/IP
X=NX
NY=(NX+1)/IB
Y=NY
NZ=NX/IB
Z=NZ
C=K*B-R+(P-K*B+R+P*X)*Z*(2*X-B-B*Z)+(K*B-R-P*X)*Y*(2*(X+1)-B
*-B*Y)
G=R+(2*R-B)*U-B*U**2
C=C/K
G=G/K
FU(I)=P*(P-1)**2/(P*(B*K-R-C)-(R-G))+P/(R-G)
IF(FU(I).GT.FMIN)GO TO 1
FMIN=FU(I)
R0=I
1 CONTINUE
IR0=R0
C UP TO HERE PROGRAMME FOUND R WHICH MINIMIZS F(R)
C THIS STEP IS TO DETRMINE WHETHER (BK-R)/P IS INTEGER OR NOT.
IF(IB*K-IR0-2*((IB*K-IR0)/2).NE.0)GO TO 50
C THIS STEP IS TO DETRMINE WHETHER R/B IS INTEGER OR NOT.
RR0=R0/B
NR0=IR0/IB
XR0=NR0
IF(RR0.EQ.XR0)GO TO 40
C THIS STEP CHECKS WHTHER BTBD EXISTS WHILE R/B IS NOT INTEGER
IB1=IR0-IB*NR0
K1=K-NR0-1
IB2=IB-IB1
K2=K-NR0
XB1=IB1
XB2=IB2
R1=XB1*K1/P
NR1=(IB1*K1)/IP
XR1=NR1
IF(R1.NE.XR1)GO TO 50
```

```
C.................................
R2=XB2*K2/P
NR2=(IB2*K2)/IP
XR2=NR2
IF(R2.NE.XR2)GO TO 50
C...............................
IQ1=K1-IP*((IB1*K1)/(IP*IB1))
C PRINT *,IR0,IQ1
IF(IQ1.EQ.0)GO TO 105
IF(IQ1.EQ.2)GO TO 105
IF(IQ1.EQ.1)GO TO 130
PRINT *,' ERROR??...'
GO TO 50
130 XXX=XB1/2
NXX=IB1/2
XXXX=NXX
IF(XXX.NE.XXXX)GO TO 50
C..............................
105 IQ2=K2-IP*((IB2*K2)/(IP*IB2))
IF(IQ2.EQ.0)GO TO 110
IF(IQ2.EQ.2)GO TO 110
IF(IQ2.EQ.1)GO TO 120
PRINT *,' ERROR ???...'
GO TO 50
120 XXX=XB2/2
NXX=IB2/2
XXXX=NXX
IF(XXX.NE.XXXX)GO TO 50
110 ICODE=2
ICODE1=1
GO TO 101
C..............................
40 IQ=K-NR0-IP*((K*IB-IR0)/(IP*IB))
IF(IQ.EQ.0)GO TO 111
IF(IQ.EQ.2)GO TO 111
IF(IQ.EQ.1)GO TO 200
PRINT *,' ERROR???...'
GO TO 50
200 XXX=B/2.
NXX=IB/2
XXXX=NXX
IF(XXX.NE.XXXX)GO TO 50
111 ICODE=1
```

```
ICODE1=0
NYY=(K*IB-IR0)/(IP*IB)
101 IF(IXYXY.EQ.ICODE1)GO TO 108
IF(ICODE1.NE.1)GO TO 300
PRINT *,' K B R0 CODE B1 K1 B2 K2'
GO TO 301
300 PRINT *,' K B R0 CODE (BK-R0)/TB IQ '
301 PRINT *,'**********************************************'
108 IF(ICODE1.EQ.1)GO TO 102
WRITE(6,7)K,IB,IR0,ICODE,NYY,IQ
IXYXY=ICODE1
GO TO 50
102 WRITE(6,8)K,IB,IR0,ICODE,IB1,K1,IB2,K2
IXYXY=ICODE1
50 CONTINUE
7 FORMAT(5X,6I6)
8 FORMAT(5X,8I6)
2 STOP
END
```

B.1.2 Near A-optimal Designs:

```
PROGRAM OPTING2
    C
    C THIS PROGRAM GENERATES A-OPTIMAL DESIGNS WITHIN BTBD
    C CLASS OF DESIGNS WHEN AN OVERALL A-OPTIMAL BTBD DESIGN
    C DOES NOT EXIST
    DIMENSION FU(1000)
    IP=2
    P=IP
    DO 50 K=3,30
    DO 50 IB=2,50
    B=IB
    M=B*K/2
    R0=0
    FMIN=999999999
    DO 1 I=1,M
    R=I
    NU=R/B
    U=NU
    NX=(B*K-R)/P
    X=NX
    NY=(X+1)/B
    Y=NY
    NZ=X/B
    Z=NZ
    C=K*B-R+(P-K*B+R+P*X)*Z*(2*X-B-B*Z)+(K*B-R-P*X)*Y*(2*(X+1)-B
    *-B*Y)
    G=R+(2*R-B)*U-B*U**2
    C=C/K
    G=G/K
    FU(I)=P*(P-1)**2/(P*(B*K-R-C)-(R-G))+P/(R-G)
    IF(FU(I).GT.FMIN)GO TO 1
    FMIN=FU(I)
    R0=I
    1 CONTINUE
    MR0=R0
    IF(IB*K-MR0.EQ.2*((IB*K-MR0)/2))GO TO 50
    BOU=FU(MR0)
    IR1=MR0+1
    IF(FU(IR1).LE.FU(MR0-1))GO TO 500
    IR1=MR0-1
    500 E=FU(MR0)/FU(IR1)
    IR0=IR1
```

```
R0=IR0
RR0=R0/B
NR0=IR0/IB
XR0=NR0
IF(RR0.EQ.XR0)GO TO 40
C
C THIS STEP CHECKS WHTHER BTBD EXISTS WHILE R/B IS NOT INTEGER
C
IB1=IR0-IB*NR0
K1=K-NR0-1
IB2=IB-IB1
K2=K-NR0
XB1=IB1
XB2=IB2
R1=XB1*K1/P
NR1=(IB1*K1)/IP
XR1=NR1
IF(R1.NE.XR1)GO TO 50
C.................................
R2=XB2*K2/P
NR2=(IB2*K2)/IP
XR2=NR2
IF(R2.NE.XR2)GO TO 50
C..............................
IQ1=K1-IP*((IB1*K1)/(IP*IB1))
C PRINT *,IR0,IQ1
IF(IQ1.EQ.0)GO TO 105
IF(IQ1.EQ.2)GO TO 105
IF(IQ1.EQ.1)GO TO 130
PRINT *,' ERROR??...'
GO TO 50
130 XXX=XB1/2
NXX=IB1/2
XXXX=NXX
IF(XXX.NE.XXXX)GO TO 50
C..............................
105 IQ2=K2-IP*((IB2*K2)/(IP*IB2))
IF(IQ2.EQ.0)GO TO 110
IF(IQ2.EQ.2)GO TO 110
IF(IQ2.EQ.1)GO TO 120
PRINT *,' ERROR ???...'
GO TO 50
120 XXX=XB2/2
```

```
NXX=IB2/2
XXXX=NXX
IF(XXX.NE.XXXX)GO TO 50
110 ICODE=2
ICODE1=1
GO TO 101
C..............................
40 IQ=K-NR0-IP*((K*IB-IR0)/(IP*IB))
IF(IQ.EQ.0)GO TO 111
IF(IQ.EQ.2)GO TO 111
IF(IQ.EQ.1)GO TO 200
PRINT *,' ERROR???...'
GO TO 50
200 XXX=B/2.
NXX=IB/2
XXXX=NXX
IF(XXX.NE.XXXX)GO TO 50
111 ICODE=1
ICODE1=0
NYY=(K*IB-IR0)/(IP*IB)
101 IF(IXYXY.EQ.ICODE1)GO TO 108
IF(ICODE1.NE.1)GO TO 300
PRINT *,' K B R0 CODE B1 K1 B2 K2'
GO TO 301
300 PRINT *,' K B R0 CODE (BK-R0)/TB IQ '
301 PRINT *,'**********************************************'
108 IF(ICODE1.EQ.1)GO TO 102
WRITE(6,7)K,IB,IR0,ICODE,NYY,IQ,E
IXYXY=ICODE1
GO TO 50
102 WRITE(6,8)K,IB,IR0,ICODE,IB1,K1,IB2,K2,E
IXYXY=ICODE1
50 CONTINUE
7 FORMAT(5X,6I6,F12.4)
8 FORMAT(5X,8I6,F12.4)
2 STOP
END
```

B.2 Algorithm for Designs with Two Factors One with Two Levels; Another with More than Two Levels:

B.2.1 Conjectured Bound, C- and Near C-designs:

```
PROGRAM SPBDS
    C THIS GENERATES THE CONJECTURED BOUND AND C-DESIGNS OR
    C NEAR C-DESIGNS
    DIMENSION IEX(100,2)
    COMMON IEX
    M=2
    DO 5 N= 6, 6
    IP=N-1
    P=IP
    DO 5 K= 6, 6
    XK=K
    WRITE(6,22)
    DO 5 IB=15,15
    B=IB
    NM=IB*K
    F=99999999
    CALL TAA1(N,NM,IP,P,K,XK,IB,B,F,F1)
    PRINT *,N,K,B,F1
    F2=F1
    L=0
    222 F=99999999
    CALL TAA(N,NM,IP,P,K,XK,IB,B,F,IEX,L,F1,IIA,IIB,IID)
    L=L+1
    IEX(L,1)=IIA
    IEX(L,2)=IID
    IIRB=IIB/IB
    IBB=IIB-IIRB*IB
    CALL TESTA(IIRB,IBB,IIA,IB,K,IP,NN,IB1,KA1,KD1,IB2,KA2,KD2,
    *IB3,KA3,KD3)
    IF(NN.EQ.0)GO TO 400
    CALL TESTD(IIRB,IBB,IID,IB,K,IP,NN,IB1,KA1,KD1,IB2,KA2,KD2,
    *IB3,KA3,KD3)
    IF(NN.EQ.1)GO TO 200
    400 DD=(F1-F2 )*100/F2
    KB1=K-KA1-KD1
    KB2=K-KA2-KD2
```

```
KB3=K-KA3-KD3
IF(IB1.EQ.0)KB1=0
IF(IB2.EQ.0)KB2=0
IF(IB3.EQ.0)KB3=0
WRITE(6,15)N,K,IB,IB1,KB1,KA1,KD1,IB2,KB2,KA2,KD2,IB3,KB3,KA3,KD3
PRINT *,' '
GO TO 5
200 IF(L.LT.40)GO TO 222
PRINT *,'THERE IS NO SOLUTION BY THIS ALGORITHM'
PRINT *,' '
5 CONTINUE
6 FORMAT(3I5,5X,3I4,2X,F9.4,F9.2,F9.4)
STOP
15 FORMAT(3I4,3X,3(4I4,2X))
22 FORMAT(' N K B IB1 KB1 KA1 KD1 IB2 KB2 KA2 KD2 IB3 K
*B3 KA3 KD3')
END
SUBROUTINE TAA1(N,NM,IP,P,K,XK,IB,B,F,F1)
DIMENSION IITA(100),IITD(100),IIBA(100),IIBD(100)
DIMENSION IIAA(100),IIAD(100),IITB(100)
DO 1 ITB=1,NM/2
DO 1 ITD=IP,NM-ITB-IP
ITA=NM -ITB-ITD
IF(ITA.GT.ITD)GO TO 1
IAA=ITA/IB
IBA=ITA-IAA*IB
IAD=ITD/IB
IBD=ITD-IAD*IB
IAB=ITB/IB
IBB=ITB-IAB*IB
DO 110 J=1,IB-IBB
110 IITB(J)=IAB
DO 120 J=IB-IBB+1,IB
120 IITB(J)=IAB+1
DO 101 J=1,IBA
101 IITA(J)=IAA+1
DO 102 J=IBA+1,IB
102 IITA(J)=IAA
SA=0
SB=0
SD=0
SAB=0
SAD=0
```

```
DO 130 J=1,IB
IITD(J)=K-IITA(J)-IITB(J)
SA=SA+IITA(J)**2
SB=SB+IITB(J)**2
SD=SD+IITD(J)**2
SAB=SAB+IITA(J)*IITB(J)
130 SAD=SAD+IITD(J)*IITA(J)
DO 105 J=1,IB
IIAA(J)=IITA(J)/IP
IIAD(J)=IITD(J)/IP
IIBA(J)=IITA(J)-IP*IIAA(J)
105 IIBD(J)=IITD(J)-IP*IIAD(J)
DA=0
DD=0
IDADMI=0
IDADMA=0
DO 106 J=1,IB
DA=DA+IIBA(J)*(IIAA(J)+1)+IIAA(J)*IITA(J)
DD=DD+IIBD(J)*(IIAD(J)+1)+IIAD(J)*IITD(J)
INF=IIAA(J)*IITD(J)+IIAD(J)*IIBA(J)+
*MAX(0,IIBA(J)+IIBD(J)-IP)
IDADMI=IDADMI+INF
ISUP=IIAA(J)*IITD(J)+IIAD(J)*IIBA(J)+
*MIN(IIBA(J),IIBD(J))
IF(IIAA(J)+IIAD(J)+2.GT.K)GO TO 116
IDADMA=IDADMA+ISUP
GO TO 106
116 IDADMA=IDADMA+INF
106 CONTINUE
Y1=K*(N-1)
Y2=Y1*(N-2)
Y3=K*(N-2)
TA=ITA
TD=ITD
TB=ITB
D1=TA/P-DA/Y3+SA/Y2
D2=TD/P-DD/Y3+SD/Y2
Q1=TA/P-SA/Y1
Q2=TB/P-SB/Y1
Q3=SAB/Y1
DO 1 J=IDADMI,IDADMA
QQ=J
D3=QQ/Y3-SAD/Y2
```

```
YY=D1*D2-D3**2
IF(YY.EQ.0)GO TO 1
TR1=(P-1.)*(2.*D1-2.*D3+D2)/YY
IF(TR1.LT.0)GO TO 1
YY=Q1*Q2-Q3**2
IF(YY.EQ.0)GO TO 1
TR2= (Q1+Q2)/YY
IF(TR2.LT.0)GO TO 1
TR=TR1+TR2
IF(F.LE.TR)GO TO 1
F=TR
IIB=ITB
IIA=ITA
IID=ITD
1 CONTINUE
F1=F
RETURN
END
SUBROUTINE TAA(N,NM,IP,P,K,XK,IB,B,F,IEX,L,F1,IIA,IIB,IID)
DIMENSION IITA(100),IITD(100),IIBA(100),IIBD(100)
DIMENSION IIAA(100),IIAD(100),IITB(100),IEX(100,2)
DO 1 ITB=1,NM/2
DO 1 ITD=IP,NM-ITB-IP,IP
ITA=NM -ITB-ITD
IF(ITA.GT.ITD)GO TO 1
IF(ITA.NE.IP*(ITA/IP))GO TO 1
IF(L.EQ.0)GO TO 200
DO 500 I=1,L
IF(ITA.EQ.IEX(I,1).AND.ITD.EQ.IEX(I,2))GO TO 1
500 CONTINUE
200 IAA=ITA/IB
IBA=ITA-IAA*IB
IAD=ITD/IB
IBD=ITD-IAD*IB
IAB=ITB/IB
IBB=ITB-IAB*IB
DO 110 J=1,IB-IBB
110 IITB(J)=IAB
DO 120 J=IB-IBB+1,IB
120 IITB(J)=IAB+1
DO 101 J=1,IBA
101 IITA(J)=IAA+1
DO 102 J=IBA+1,IB
```

```
102 IITA(J)=IAA
SA=0
SB=0
SD=0
SAB=0
SAD=0
DO 130 J=1,IB
IITD(J)=K-IITA(J)-IITB(J)
SA=SA+IITA(J)**2
SB=SB+IITB(J)**2
SD=SD+IITD(J)**2
SAB=SAB+IITA(J)*IITB(J)
130 SAD=SAD+IITD(J)*IITA(J)
DO 105 J=1,IB
IIAA(J)=IITA(J)/IP
IIAD(J)=IITD(J)/IP
IIBA(J)=IITA(J)-IP*IIAA(J)
105 IIBD(J)=IITD(J)-IP*IIAD(J)
DA=0
DD=0 IDADMI=0
IDADMA=0
DO 106 J=1,IB
DA=DA+IIBA(J)*(IIAA(J)+1)+IIAA(J)*IITA(J)
DD=DD+IIBD(J)*(IIAD(J)+1)+IIAD(J)*IITD(J)
INF=IIAA(J)*IITD(J)+IIAD(J)*IIBA(J)+
*MAX(0,IIBA(J)+IIBD(J)-IP)
IDADMI=IDADMI+INF
ISUP=IIAA(J)*IITD(J)+IIAD(J)*IIBA(J)+
*MIN(IIBA(J),IIBD(J))
IF(IIAA(J)+IIAD(J)+2.GT.K)GO TO 116
IDADMA=IDADMA+ISUP
GO TO 106
116 IDADMA=IDADMA+INF
106 CONTINUE
Y1=K*(N-1)
Y2=Y1*(N-2)
Y3=K*(N-2)
TA=ITA
TD=ITD
TB=ITB
D1=TA/P-DA/Y3+SA/Y2
D2=TD/P-DD/Y3+SD/Y2
Q1=TA/P-SA/Y1
```

```
Q2=TB/P-SB/Y1
Q3=SAB/Y1
DO 1 J=IDADMI,IDADMA
QQ=J
D3=QQ/Y3-SAD/Y2
YY=D1*D2-D3**2
IF(YY.EQ.0)GO TO 1
TR1=(P-1.)*(2.*D1-2.*D3+D2)/YY
IF(TR1.LT.0)GO TO 1
YY=Q1*Q2-Q3**2
IF(YY.EQ.0)GO TO 1
TR2= (Q1+Q2)/YY
IF(TR2.LT.0)GO TO 1
TR=TR1+TR2
IF(F.LE.TR)GO TO 1
F=TR
IIB=ITB
IIA=ITA
IID=ITD
1 CONTINUE
F1=F
RETURN
END
SUBROUTINE TESTA(IIRB,IBB,IIA,IB,K,IP,NN,IB1,KA1,KD1,IB2,KA2
.,KD2,IB3,KA3,KD3)
NN=0
IIRA=IIA/IB
KB1=IIRB+1
KB2=IIRB
IBA2=IIA-IIRA*IB
KA2=IIRA+1
IBA1=IB-IBA2
KA1=IIRA
IB1=MIN(IBB,IBA1)
IB2=IB-MAX(IBB,IBA1)
IB3=MAX(IBB,IBA1)-IB1
KD1=K-KA1-KB1
KD2=K-KA2-KB2
KB3=KB1
KA3=KA2
IF(IBB.EQ.MIN(IBB,IBA1)) THEN
KB3=KB2
KA3=KA1
```

```
END IF
KD3=K-KB3-KA3
IF(IB1.EQ.0) GO TO 201
IIB=IB1
IRD=(IB1*KD1)/IP
IF(IB1*KD1.NE.IRD*IP)GO TO 200
IRA=(IB1*KA1)/IP
IF(IB1*KA1.NE.IRA*IP)GO TO 200
KA=KA1
KD=KD1
CALL CHECK(IIB,IP,IRA,IRD,KA,KD,NN)
IF(NN.EQ.1)GO TO 200
GO TO 203
201 KA1=0
KD1=0
203 IF(IB2.EQ.0) GO TO 202
IIB=IB2
IRD=(IB2*KD2)/IP
IF(IB2*KD2.NE.IRD*IP)GO TO 200
IRA=(IB2*KA2)/IP
IF(IB2*KA2.NE.IRA*IP)GO TO 200
KA=KA2
KD=KD2
CALL CHECK(IIB,IP,IRA,IRD,KA,KD,NN)
IF(NN.EQ.1)GO TO 210
GO TO 204
202 KA2=0
KD2=0
204 IF(IB3.EQ.0) GO TO 205
IIB=IB3
IRD=(IB3*KD3)/IP
IF(IB3*KD3.NE.IRD*IP)GO TO 200
IRA=(IB3*KA3)/IP
IF(IB3*KA3.NE.IRA*IP)GO TO 200
NN=0
KA=KA3
KD=KD3
CALL CHECK(IIB,IP,IRA,IRD,KA,KD,NN)
GO TO 210
205 KA3=0
KD3=0
GO TO 210
200 NN=1
```

```
210 RETURN
END
SUBROUTINE TESTD(IIRB,IBB,IID,IB,K,IP,NN,IB1,KA1,KD1,IB2,KA2
.,KD2,IB3,KA3,KD3)
NN=0
IIRD=IID/IB
KB2=IIRB
IBD=IID-IIRD*IB
IB1=MIN(IBB,IBD)
KB1=IIRB+1
KD1=IIRD+1
KA1=K-KB1-KD1
IB2=MAX(IBB,IBD)-IB1
KB2=KB1-1
KD2=KD1
IF(IBD.EQ.IB1) THEN
KB2=KB1
KD2=KD1-1
END IF
KA2=K-KB2-KD2
IB3=IB-IB1-IB2
KB3=KB1-1
KD3=KD1-1
KA3=K-KB3-KD3
IF(IB1.EQ.0) GO TO 201
IIB=IB1
IRD=(IB1*KD1)/IP
IF(IB1*KD1.NE.IRD*IP)GO TO 200
IRA=(IB1*KA1)/IP
IF(IB1*KA1.NE.IRA*IP)GO TO 200
KA=KA1
KD=KD1
CALL CHECK(IIB,IP,IRA,IRD,KA,KD,NN)
IF(NN.EQ.1)GO TO 200
GO TO 203
201 KA1=0
KD1=0
203 IF(IB2.EQ.0) GO TO 202
IIB=IB2
IRD=(IB2*KD2)/IP
IF(IB2*KD2.NE.IRD*IP)GO TO 200
IRA=(IB2*KA2)/IP
IF(IB2*KA2.NE.IRA*IP)GO TO 200
```

```
KA=KA2
KD=KD2
CALL CHECK(IIB,IP,IRA,IRD,KA,KD,NN)
IF(NN.EQ.1)GO TO 200
GO TO 204
202 KA2=0
KD2=0
204 IF(IB3.EQ.0) GO TO 205
IIB=IB3
IRD=(IB3*KD3)/IP
IF(IB3*KD3.NE.IRD*IP)GO TO 200
IRA=(IB3*KA3)/IP
IF(IB3*KA3.NE.IRA*IP)GO TO 200
NN=0
KA=KA3
KD=KD3
CALL CHECK(IIB,IP,IRA,IRD,KA,KD,NN)
GO TO 210
205 KA3=0
KD3=0
GO TO 210
200 NN=1
210 RETURN
END
SUBROUTINE CHECK(IIB,IP,IRA,IRD,KA,KD,NN)
I1=IRA/IIB
I2=IRD/IIB
K1=KA-IP*I1
K2=KD-IP*I2
IF(K1.EQ.0.AND.K2.EQ.0)GO TO 2
IF(K1.EQ.0) THEN
IR2=(IIB*K2)/IP
IF(IP*IR2.NE.IIB*K2)GO TO 1
L2=(IR2*(K2-1))/(IP-1)
IF(L2*(IP-1).NE.IR2*(K2-1))GO TO 1
ELSE IF(K2.EQ.0) THEN
IR1=(IIB*K1)/IP
IF(IP*IR1.NE.IIB*K1)GO TO 1
L1=(IR1*(K1-1))/(IP-1)
IF(L1*(IP-1).NE.IR1*(K1-1))GO TO 1
ELSE
IF(K1.NE.K2)GO TO 1
IR1=(IIB*K1)/IP
```

```
IF(IP*IR1.NE.IIB*K1)GO TO 1
L1=(IR1*(K1-1))/(IP-1)
IF(L1*(IP-1).NE.IR1*(K1-1))GO TO 1
IR2=(IIB*K2)/IP
IF(IP*IR2.NE.IIB*K2)GO TO 1
L2=(IR2*(K2-1))/(IP-1)
IF(L2*(IP-1).NE.IR2*(K2-1))GO TO 1
END IF
GO TO 2
1 NN=1
2 RETURN
END
```

B.3 A-optimal PBDS Designs for k=2,3:

B.3.1 A-optimal PBDS Designs for k=2

```
PROGRAM K2PB
    C THIS PROGRAM GENERATES A-OPTIMAL PBDS DESIGN FOR K=2
    INTEGER A,B,C,D,E,F
    DO 100 N=3,10
    N1=N-1
    N2=N-2
    M=(N1*N2)/2
    X1=N1
    X2=N2
    Y=M
    DO 100 IB=2,10
    FF=9999999
    DO 1 NA=0,IB/N1
    ID1=IB-NA*N1
    IF(ID1.LT.0)GO TO 1
    DO 1 NB=0,ID1/N1
    ID2=ID1-N1*NB
    IF(ID2.LT.0)GO TO 1
    DO 1 NC=0,ID2/N1
    ID3=ID2-N1*NC
    IF(ID3.LT.0)GO TO 1
    DO 1 ND=0,ID3/M
    ID4=ID3-M*ND
    IF(ID4.LT.0)GO TO 1
    DO 1 NE=0,ID4/M
    ID5=ID4-M*NE
    IF(ID5.LT.0)GO TO 1
    NF=ID5/(N1*N2)
    LL=1
    IF(ID5.NE.NF*N1*N2)GO TO 1
    LL=0
    DA=NA+NC+N1*ND+N2*NF
    DA=DA/2.0
    DD=NB+NC+N1*NE+N2*NF
    DD=DD/2.0
    DAD=NC-NF
    DAD=DAD/2.0
    XX=DA*DD-DAD**2
    IF(XX.EQ.0)GO TO 1
    QA=NA+NC+N2*NF
```

```
QA=QA/2.0
QD=NB+NC+N2*NF
QD=QD/2.0
QAD=NC+N2*NF
QAD=QAD/2.0
YY=QA*QD-QAD**2
IF(YY.EQ.0)GO TO 1
TR=X2*(2*DA+DD-2*DAD)/XX+(2*QA+QD-2*QAD)/YY
IF(FF.LT.TR)GO TO 1
FF=TR
A=NA
B=NB
C=NC
D=ND
E=NE
F=NF
1 CONTINUE
IF(LL.EQ.1)GO TO 100
WRITE(6,20)N,IB,A,B,C,D,E,F,FF
100 CONTINUE
20 FORMAT(2I4,5X,6I4,6X,F11.5)
STOP
END
```

B.3.2 A-optimal PBDS Designs for k=n=3:

```
PROGRAM K3PBN3
   C THIS PROGRAM GENERATES A-OPTIMAL PBDS DESIGN FOR K=3, N=3
   INTEGER A,B,C,D,E,F,G,H,I,J,K,L
   N=3
   DO 100 IB=2,10
   FF=9999999
   DO 1 NA=0,IB
   ID1=IB-NA
   DO 1 NB=0,ID1/2
   ID2=ID1-2*NB
   IF(ID2.LT.0)GO TO 1
   DO 1 NC=0,ID2
   ID3=ID2-NC
   IF(ID3.LT.0)GO TO 1
   DO 1 ND=0,ID3/2
   ID4=ID3-2*ND
   IF(ID4.LT.0)GO TO 1
   DO 1 NE= 0,ID4/2
   ID5=ID4-2*NE
   IF(ID5.LT.0)GO TO 1
   DO 1 NF=0,ID5/2
   ID6=ID5-2*NF
   IF(ID6.LT.0)GO TO 1
   DO 1 NG=0,ID6/2
   ID7=ID6-2*NG
   IF(ID7.LT.0)GO TO 1
   DO 1 NH=0,ID7/2
   ID8=ID7-2*NH
   IF(ID8.LT.0)GO TO 1
   DO 1 NI=0,ID8/2
   ID9=ID8-2*NI
   IF(ID9.LT.0)GO TO 1
   DO 1 NJ=0,ID9/2
   ID10=ID9-2*NJ
   IF(ID10.LT.0)GO TO 1
   DO 1 NK=0,ID10/2
   ID11=ID10-2*NK
   IF(ID11.LT.0)GO TO 1
   NL=ID11/2
   LL=1
   IF(ID11.NE.2*NL)GO TO 1
   LL=0
```

```
TA=2*(NA+NB+NE+NF+NI+2*NG+2*NH+3*NK)
DA=2*(NA+NB+NE+NF+NI+2*NG+4*NH+5*NK)
SA=2*(2*NA+NB+NE+NF+NI+4*NG+4*NH+9*NK)
TD=2*(NC+ND+NE+NF+2*NI+NG+2*NJ+3*NL)
DD=2*(NC+ND+NE+NF+2*NI+NG+4*NJ+5*NL)
SD=2*(2*NC+ND+NE+NF+4*NI+NG+4*NJ+9*NL)
DAD=2*(NE+NG+NI)
SAD=2*(NE+NF+2*NG+2*NI)
D1=TA/2.-DA/3.+SA/6.
D3=TD/2.-DD/3.+SD/6.
D2=DAD/3.-SAD/6.
Q1=TA/2.-SA/6.
Q3=TD/2.-SD/6.
Q2=SAD/6.
XXX=D1*D3-D2**2
YYY=Q1*Q3-Q2**2
IF(XXX.EQ.0)GO TO 1
IF(YYY.EQ.0)GO TO 1
TR=(2*D1-2*D2+D3)/XXX+(2*Q1-2*Q2+Q3)/YYY
IF(TR.LT.0)GO TO 1
IF(FF.LT.TR)GO TO 1
FF=TR
A=NA
B=NB
C=NC
D=ND
E=NE
F=NF
G=NG
H=NH
I=NI
J=NJ
K=NK
L=NL
ITA=TA
ITD=TD
ITB=IB*3- TA- TD
ISA=SA
ISD=SD
IDAD=DAD
ISAD=SAD
1 CONTINUE
IF(LL.EQ.1)GO TO 100
```

```
WRITE(6,20)N,IB,A,B,C,D,E,F,G,H,I,J,K,L,FF
100 CONTINUE
20 FORMAT(2I4,3X,12I4,3X,F9.3 )
STOP
END
```

B.3.3 A-optimal PBDS Designs for k=3 and $n \geq 4$:

```
PROGRAM K3PB
  C THIS PROGRAM GENERATES A-OPTIMAL PBDS DESIGN FOR K=3
  C AND N>3.
  INTEGER A,B,C,D,E,F,G,H,I,J,K,L,M,NU,O,P,Q,R,S,T
  DO 100 N=4, 9
  N1=N-1
  N2=N-2
  N3=N-3
  M1=(N1*N2)/2
  M2=(N2*N3)/2
  M3=(N1*N2*N3)/2
  M4=(N1*N2*N3)/6
  X1=N1
  X2=N2
  Y1=M1
  DO 100 IB=2 ,10
  FF=9999999
  DO 1 NE=0,IB/N1
  ID1=IB-NE*N1
  IF(ID1.LT.0)GO TO 1
  DO 1 NA=0,ID1/M1
  ID2=ID1-M1*NA
  IF(ID2.LT.0)GO TO 1
  DO 1 NB=0,ID2/N1
  ID3=ID2-N1*NB
  IF(ID3.LT.0)GO TO 1
  DO 1 NC=0,ID3/M1
  ID4=ID3-M1*NC
  IF(ID4.LT.0)GO TO 1
  DO 1 ND=0,ID4/N1
  ID5=ID4-N1*ND
  IF(ID5.LT.0)GO TO 1
  DO 1 NF=0,ID5/(2*M1)
  ID6=ID5-2*M1*NF
  IF(ID6.LT.0)GO TO 1
  DO 1 NG=0,ID6/(2*M1)
  ID7=ID6-2*M1*NG
  IF(ID7.LT.0)GO TO 1
  DO 1 NH=0,ID7/M3
  ID8=ID7-M3*NH
  IF(ID8.LT.0)GO TO 1
  DO 1 NI=0,ID8/(2*M1)
```

```
ID9=ID8-2*M1*NI
IF(ID9.LT.0)GO TO 1
DO 1 NJ=0,ID9/M3
ID10=ID9-M3*NJ
IF(ID10.LT.0)GO TO 1
DO 1 NK=0,ID10/M4
ID11=ID10-M4*NK
IF(ID11.LT.0)GO TO 1
DO 1 NL=0,ID11/M4
ID12=ID11-M4*NL
IF(ID12.LT.0)GO TO 1
DO 1 NM=0,ID12/N1
ID13=ID12-N1*NM
IF(ID13.LT.0)GO TO 1
DO 1 NN=0,ID13/N1
ID14=ID13-N1*NN
IF(ID14.LT.0)GO TO 1
DO 1 NO=0,ID14/N1
ID15=ID14-N1*NO
IF(ID15.LT.0)GO TO 1
DO 1 NP=0,ID15/(N1*N2)
ID16=ID15-N1*N2*NP
IF(ID16.LT.0)GO TO 1
DO 1 NQ=0,ID16/N1
ID17=ID16-N1*NQ
IF(ID17.LT.0)GO TO 1
DO 1 NR=0,ID17/(N1*N2)
ID18=ID17-N1*N2*NR
IF(ID18.LT.0)GO TO 1
DO 1 NS=0,ID18/(N1*N2)
ID19=ID18-(N1*N2)*NS
IF(ID19.LT.0)GO TO 1
NT=ID19/(N1*N2)
LL=1
IF(ID19.NE.N1*N2*NT)GO TO 1
LL=0
TA=N1*(NB+NE)+2*M1*(NA+NF+NI+2*NG)+2*M3*(NJ+NK+2*NH)/2
DA=TA+N1*(4*NM+4*NO+NQ+N2*(4*NP+NR+5*NS))
TA=TA+N1*(2*NM+2*NO+NQ+N2*(2*NP+NR+3*NS))
SA=N1*(NB+NE)+2*M1*(2*NA+NF+NI+4*NG)+M3*(NJ+3*NK+4*NH)
SA=SA+N1*(4*NM+4*NO+NQ+N2*(4*NP+NR+9*NS))
TD=N1*(ND+NE)+2*M1*(NC+NF+2*NI+NG)+M3*(2*NJ+NL+NH)
DD=TD+N1*(4*NN+NO+4*NQ+N2*(NP+4*NR+5*NT))
```

```
TD=TD+N1*(2*NN+NO+2*NQ+N2*(NP+2*NR+3*NT))
SD=N1*(ND+NE)+2*M1*(2*NC+NF+4*NI+NG)+M3*(4*NJ+3*NL+NH)
SD=SD+N1*(4*NN+NO+4*NQ+N2*(NP+4*NR+9*NT))
DAD=N1*NE+2*M1*(NG+NI)
DAD=DAD+2*N1*(NO+NQ)
SAD=N1*NE+2*M1*(NF+2*NI+2*NG)+2*M3*(NJ+NH)
SAD=SAD+2*N1*(NO+NQ+N2*(NP+NR))
D1=TA/X1-DA/(3*X2)+SA/(6*Y1)
D3=TD/X1-DD/(3*X2)+SD/(6*Y1)
D2=DAD/(3*X2)-SAD/(6*Y1)
Q1=TA/X1-SA/(3*X1)
Q3=TD/X1-SD/(3*X1)
Q2=SAD/(3*X1)
XXX=D1*D3-D2**2
YYY=Q1*Q3-Q2**2
IF(XXX.EQ.0)GO TO 1
IF(YYY.EQ.0)GO TO 1
TR=X2*(2*D1-2*D2+D3)/XXX+(2*Q1-2*Q2+Q3)/YYY
IF(TR.LT.0)GO TO 1
IF(FF.LT.TR)GO TO 1
FF=TR
A=NA
B=NB
C=NC
D=ND
E=NE
F=NF
G=NG
H=NH
I=NI
J=NJ
K=NK
L=NL
M=NM
NU=NN
O=NO
P=NP
Q=NQ
R=NR
S=NS
T=NT
ITA=TA
ITD=TD
```

```
ITB=IB*3- TA- TD
ISA=SA
ISD=SD
IDAD=DAD
ISAD=SAD
1 CONTINUE
IF(LL.EQ.1)GO TO 100
WRITE(6,20)N,IB,A,B,C,D,E,F,G,H,I,J,K,L,M,NU,O,P,Q,R,S,T,FF
100 CONTINUE
20 FORMAT(2I4,1X,20I3,1X,F7.2 )
STOP
END
```

B.4 A-optimal Completely Randomized Designs:

```
PROGRAM NMCR
    C THIS PROGRAM GENERATES A-OPTIMAL DESIGN IN THE CLASS
    C OF COMPLETELY RANDOMAIZED DESIGN FOR ANY N AND M AND
    C GIVEN FIXED UNITS AVAILABLE IN THE EXPERIMENT, NN.
    PRINT *,' **************************************'
    PRINT *,' N M NN RB RA RD TRACE'
    PRINT *,' **************************************'
    DO 5 N=3 ,10
    DO 5 M=N,10
    IP=N-1
    IQ=M-1
    P=IP
    Q=IQ
    DO 5 NN=N*M-1,100
    F1=9999999
    DO 1 ITB=IQ,NN-IP*IQ-IP
    DO 1 ITD=IP*IQ,NN-ITB-IP
    ITA=NN -ITB-ITD
    IF(ITA.LT.IP)GO TO 1
    IRB=ITB/IQ
    IRD=ITD/(IP*IQ)
    IRA=ITA/IP
    TB=ITB
    TD=ITD
    TA=ITA
    DB=IRB*(IRB+1)
    DD=IRD*(IRD+1)
    DA=IRA*(IRA+1)
    DBB=IP*(2*IQ*IRB+IQ-TB)
    DBD=2*(2*IP*IQ*IRD+IP*IQ-TD)
    DBA=IQ*(2*IP*IRA+IP-TA)
    DDB=DBB/DB
    DDD=DBD/DD
    DDA=DBA/DA
    TR=DDB+DDD+DDA
    IF(F1.LE.TR)GO TO 1
    F1=TR
    IIB=ITB
    IID=ITD
    IIA=ITA
    BR=F1
```

```
1 CONTINUE
IB=IIB/IQ
IF(IIB-IQ*IB.NE.0)GO TO 5
ID=IID/(IP*IQ)
IF(IID-IP*IQ*ID.NE.0)GO TO 5
IA=IIA/IP
IF(IIA-IP*IA.NE.0)GO TO 5
WRITE(6,6)N,M,NN,IB,IA,ID
5 CONTINUE
6 FORMAT(10X,3I5,3I5)
STOP
END
```

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