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OPTIMALITY OF CHEMICAL BALANCE WEIGHING DESIGNS.

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University of Windsor

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LA THÈSE A ÉTÉ MICROFILMÉE TELLE QUE NOUS L'AVONS RECUE
OPTIMALITY OF CHEMICAL BALANCE
WEIGHING DESIGNS

by

Joseph Costantino Masaro

A Dissertation
submitted to the Faculty of Graduate Studies
and Research through the Department of Mathematics,
in Partial Fulfillment of the requirements for the
Degree of Doctor of Philosophy at
The University of Windsor

Windsor, Ontario, Canada
1983
To Ann Marie, Jessica, Ronnie,

Robert and Joey.
ABSTRACT

OPTIMALITY OF CHEMICAL BALANCE
WEIGHING DESIGNS

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Joseph Costantino Masaro

Let \( N \geq n \) and let \( \mathcal{E}(N,n) \) denote the set of all \( N \times n \) matrices \( X = (x_{ij}) \) with \( x_{ij} = -1, 0 \) or 1. Let \( \mathcal{G}(N,n) \) be the set of all matrices in \( \mathcal{G}(N,n) \) with entries -1,1. Each such matrix in \( \mathcal{G}(N,n) \) or \( \mathcal{G}'(N,n) \) will be called a weighing design matrix. If \( X_0 \) minimizes \( \Phi(X^TX) \) over \( \mathcal{G}(N,n) \) for some real valued function \( \Phi \), then \( X_0 \) is said to be \( \Phi \)-optimum over \( \mathcal{G}(N,n) \). The characterization of such \( X_0 \) arises from the statistical problems of weighing designs, certain block designs and \( 2^n \) fractional factorial designs. The well-known D-, A- and E-optimality criteria are obtained by taking \( \Phi(X^TX) = \det(X^TX)^{-1} \), \( \text{tr}(X^TX)^{-1} \) and the maximum of the eigenvalue of \( (X^TX)^{-1} \) respectively. All these criteria are functions of the spectrum of \( X^TX \). Let \( \lambda_1, \lambda_2, \ldots, \lambda_n \) be the eigenvalues of \( X^TX \). Then a more general family of criteria are the following \( \Phi_p \)-criteria:

\[
\Phi_p(X^TX) = \left( \frac{1}{n} \sum_{i=1}^{n} \lambda_i^{-p} \right)^{\frac{1}{p}}, \quad 0 < p < \infty.
\]

The A-criterion is the \( \Phi_1 \)-criterion, the E-criterion is the limit of the \( \Phi_p \)-criterion as \( p \to \infty \) and the D-criterion is the limit of the \( \Phi_p \)-criterion as \( p \to 0^+ \).

In this thesis techniques are developed for proving the optimality of designs with respect to the A- and \( \Phi_p \)-criteria, \( 0 \leq p \leq 1 \). In particular, A-optimal designs in \( \mathcal{E}(N,n) \) are classified for \( n = 6 \).
and $N$ arbitrary. In addition, for the cases $N \equiv 2(\text{mod } 4)$ and $N \equiv 3(\text{mod } 4)$, certain designs are shown to be $\Phi_p$-optimal in $\mathcal{B}(N,n)$ if $N$ is sufficiently larger than $n$. In the latter case, it is also shown that $A$-optimality of certain designs in $\mathcal{B}(N,n)$ implies optimality with respect to the $\Phi_p$-criteria $0 \leq p \leq 1$. Analogous results are shown to hold for designs in $\mathcal{B}'(N,n)$. Further, in the case $N \equiv 2(\text{mod } 4)$, designs in $\mathcal{B}'(N,n)$ are shown to be optimal with respect to a large class of criteria which includes the $\Phi_p$-criteria, $0 \leq p \leq \infty$, for all $n$ and $N$. 
PREFACE

The study of optimal chemical balance weighing designs was initiated by Hotelling in 1944. Since then scattered results have appeared in this area. Ehlich (1964), Kiefer (1975), Galil and Kiefer (1980) and Cheng (1978, 1980) strengthened and unified many of these earlier results. In September of 1981 we began to study this problem. The main purpose of this thesis is to add to the existing knowledge on A-optimal weighing designs.

We would like to express our gratitude to Professor C.S. Cheng of the University of California at Berkeley for his useful comments and contributions. With his permission portions of our joint paper "Optimal Weighing Designs" are included in this dissertation (section 4.3). We would also like to thank Professor Mike Jacroux of Washington State University who independently found Theorem 3.3.1 and has generously agreed to publish this result jointly.

The author wishes to express his deepest gratitude to Professor Chi Song Wong for his advice, guidance and support and above all for his encouragement and determination, without which, this thesis would never have been written.

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CHAPTER I

INTRODUCTION


In conducting an experiment one often assumes the following linear model:

\[ y = X_d \beta + e \]

where \( y = (y_1, y_2, \ldots, y_N)^T \) is the vector of observations,
\( \beta = (\beta_1, \beta_2, \ldots, \beta_n)^T \) is the vector of unknown model parameters to be estimated, \( X_d \) is an \( N \times n \) matrix, \( N \geq n \), called the design matrix and \( e \) is an \( N \times 1 \) random vector with expectation zero and dispersion matrix \( \Sigma_e = \sigma^2 I_N \). If \( N = n \), we say that \( X_d \) is saturated in the sense that there are no degrees of freedom left for estimating \( \sigma^2 \).

The \( \beta_i \)'s are estimable if and only if the rank of \( X_d \) is \( n \), i.e. \( X_d^T X_d \) is nonsingular. Suppose that this is the case. The least squared estimate (or equivalently, blue) \( \hat{\beta}_d \) of \( \beta \) is \( (X_d^T X_d)^{-1} X_d^T y \) and has dispersion matrix \( \sigma^2 (X_d^T X_d)^{-1} \).

Financial or other considerations may require us to take a fixed \( N \) which is not too large. Under these circumstances, it is logical for one to choose the design \( d \) (i.e. the design matrix \( X_d \)) which would produce the "most accurate" estimate \( \hat{\beta}_d \) of \( \beta \). The definition of "most accurate" depends, of course, on the needs of the experimenter. Let \( \mathcal{L} \) be the class of all designs under consideration.
and \( \mathcal{M} = \{ \Lambda_d \} \) the corresponding family of information matrices

\[ M_d = X_d^T X_d \]

Three basic criteria in common use for choosing and optimal design in \( \mathcal{D} \) are:

(i) D-optimality: minimize \( \text{det}(M_d^{-1}) \) over \( \mathcal{M} \)

(ii) A-optimality: minimize \( \text{tr}(M_d^{-1}) \) over \( \mathcal{M} \)

(iii) E-optimality: minimize \( \lambda_1(M_d^{-1}) \) over \( \mathcal{M} \)

where \( \lambda_1(M_d^{-1}) \) is the maximum eigenvalue of \( M_d^{-1} \).

To understand the meaning of these criteria, let us return to the linear model \( y = X_d \beta + e \). Under the assumption that \( e \) is normally distributed with mean zero and covariance matrix \( \sigma^2 I_N \), \( \hat{\beta}_d \) is normally distributed with mean \( \beta \) and dispersion matrix \( \sigma^2 (X_d^T X_d)^{-1} \). Thus a \((1-\alpha)100\%\) confidence ellipsoid \( \mathcal{E}_{d,\alpha} \) for \( \beta \) can be constructed for each design \( d \) in \( \mathcal{D} \). In Figure 1 below the ellipsoid \( \mathcal{E}_{d,\alpha} \) is presented for the two-dimensional case (i.e. \( n = 2 \)).

Figure 1.
For a given level of significance one would like the confidence region to be as "small" as possible. The fact that the confidence ellipsoid \( \mathcal{E}_{d,\alpha} \) depends on \( d \) but the level of significance \( 1 - \alpha \) does not implies that one may choose a design \( d \) which minimizes the "size" of the confidence region while the level of significance remains constant. It is the interpretation of "size" which leads to the three optimality criteria mentioned above.

A D-optimal design minimizes the generalized variance of \( \hat{\beta}_d \) and thus, under normality, minimizes the expected volume (or volume if \( s^2 \) is known) of \( \mathcal{E}_{d,\alpha} \) over \( \mathcal{D} \).

The A-criterion minimizes the average variance of the parameter estimates \( \hat{\beta}_{id} \) over \( \mathcal{D} \) ("A" means average) or equivalently the expected mean square error \( L^2(\hat{\beta}_d) \) given by \( L^2(\hat{\beta}_d) = (\hat{\beta}_d - \beta)^T(\hat{\beta}_d - \beta) \).

From a geometric viewpoint an A-optimal design minimizes the expected length of the diagonal of any rectangle circumscribing the confidence ellipsoid \( \mathcal{E}_{d,\alpha} \). Hence an A-optimal design provides a rectangular confidence region, with confidence level at least \( 1 - \alpha' \), which is smallest in the sense indicated above.

An E-optimal design minimizes the expected length of the first principal axis of the confidence ellipsoid \( \mathcal{E}_{d,\alpha} \) over \( \mathcal{D} \). So in this case \( \mathcal{E}_{d,\alpha} \) is not long and narrow. Alternatively an E-optimal design minimizes the maximum variance among all normalized linear combinations of the parameter estimates \( \hat{\beta}_{id}, i = 1,2,\ldots,n \).

To illustrate the difference among the above criteria consider the following ellipsoidal regions in \( \mathbb{R}^2 \) (see Figure 2.)
Figure 2.
\[ \mathcal{E}_1 : \frac{x_1^2}{1^2} + \frac{2}{50^2} \leq 1, \]
\[ \mathcal{E}_2 : \frac{x_1^2}{6^2} + \frac{x_2^2}{15^2} \leq 1, \]
\[ \mathcal{E}_3 : \frac{x_1^2}{12^2} + \frac{x_2^2}{12^2} \leq 1. \]

Among the three, \( \mathcal{E}_1 \) has minimum volume, \( \mathcal{E}_2 \) possesses the circumscribing rectangle with smallest diagonal and \( \mathcal{E}_3 \) has the smallest major axis. Thus each of the above regions is "small" in its own special way. In particular, given a choice of the above regions as confidence regions for \( \beta = (\beta_1, \beta_2)^T \), one could choose \( \mathcal{E}_1 \) if \( \beta_1 \) is the parameter of interest, \( \mathcal{E}_2 \) if minimizing \( (\hat{\beta} - \beta)^T (\hat{\beta} - \beta) \) is required and \( \mathcal{E}_3 \) if estimating \( a_1^2 \beta_1 + a_2^2 \beta_2 \), \( a_1^2 + a_2^2 = 1 \) is a primary importance.

The above discussion has focused on the notion of optimal design as a means of improving the accuracy of the parameter estimates in a given experiment. For a discussion of other aspects of optimal design theory (e.g. applications to testing hypothesis), see Kiefer [21], [22] and [23], and Yadav [15].

1.2 General Optimality Criteria.

The intuitive appeal and computational tractability of the \( D-, A- \) and \( E- \) optimality criteria have made them the main topics of concentration. However in many cases the experimenter may choose his design to satisfy other optimality criteria. This leads to the
following definitions.

Let $\mathcal{D}$ be a class of designs for a given experiment and $\mathcal{M} = \{M_d\} \subseteq \mathcal{D}$ the corresponding family of information matrices. Let $\Phi$ be a function on $\mathcal{M}$ with values in $\mathbb{R} \cup \{\pm \infty\}$. A design $d_1$ is said to be $\Phi$-better than a design $d_2$ if $\Phi(M_{d_1}) < \Phi(M_{d_2})$. A design $d_0$ is said to be $\Phi$-optimal in $\mathcal{D}$ if $d_0$ minimizes $\Phi(M_d)$ over $\mathcal{D}$. The function $\Phi$ is called an optimality criterion.

To illustrate, Kiefer [24] introduced the following family of criteria:

$$\Phi_p(M) = \left[\frac{1}{n} \text{tr} M^{-p}\right]^\frac{1}{p}$$

$$= \left[\frac{1}{n} \sum_{i=1}^{n} \lambda_i^{-p}\right]^\frac{1}{p}, \quad 0 < p < \infty,$$

where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ are the eigenvalues of $M$. Clearly the $A$-criterion is equivalent to the $\Phi_1$-criterion. Furthermore, the $D$-criterion is the limit of the $\Phi_p$-criteria as $p \to 0^+$ and the $E$-criterion is the limit of the $\Phi_p$-criteria as $p \to +\infty$. Thus the class of criteria $\{\Phi_p\}_{0 < p < \infty}$ contains the three main ones.

As an example where the $\Phi_p$-criteria may be of interest, consider the full rank linear model $y = X_\beta + e$ where $e$ is normal with mean zero and variance $\sigma^2 I_N$. As mentioned in Section 1.1 an $A$-optimal or $\Phi_1$-optimal design minimizes the expected mean squared error of $\hat{\beta}$. If controlling the size of the variance of $L^2(\hat{\beta})$ is of interest a $\Phi_2$-optimal design would be appropriate since

$$\text{var}(L^2(\hat{\beta})) = 2n \sigma^4 \left[\Phi_2(M_d)\right]^2.$$
We remark that the $\Phi_p$-criteria, for different values of $p$, may give rise to different designs. We refer the reader to Srivastava and Anderson [31] where examples of $\Phi_p$-optimal designs, $p = 0, 1, 2, \infty$, among the balanced resolution IV* designs of the $2^m$ series are presented and compared.

Examples of other optimality criteria are

(i) $\Phi_S(M) = \text{tr}(M^2)$ (S-optimality)

(ii) $\Phi_{L_p}(M) = \frac{1}{n} \text{tr}(CM^{-1})$ (L-optimality).

For a discussion of these and other criteria see Kiefer [23] and Hedayat [15].

A general procedure for constructing optimality criteria over $\mathcal{F}$ is:

Let $a \mathcal{F} = \max \{ \text{tr} M_d \}$. Then for any function $f$ on $[0, a \mathcal{F}]$ with values in $\mathbb{R} \cup \{ \infty \}$, define

$$\Phi_f(M) = \sum_{i=1}^{n} f(\lambda_i)$$

where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ are the eigenvalues of $M$.

One can easily see that, by taking $f(x) = -\log x$ and $f(x) = x^{-p}$, the $D$ and $\Phi_p$-criteria $0 < p < \infty$ are obtained. The $E$-criterion can be realized as the limit of $\Phi_p$-criteria as $p \to \infty$.

The fundamental problem of optimal design theory is:

(1.2.1) Given a class of functions $C$ determine a design $d \in \mathcal{D}$ which is $\Phi_f$-optimal for all $f \in C$, $d \in \mathcal{D}$. 

1.3. Optimal Weighing Designs: History and Open Problems.

Let $N$ and $n$ be positive integers with $N \geq n$ and let
\( \mathcal{O}(N,n) \) denote the set of all \( N \times n \) matrices \( X = (x_{ij}) \) with \( x_{ij} = -1, 0 \) or \( 1 \). Each such matrix will be called a weighing design matrix. These matrices arise, e.g., in the following statistical setting.

Suppose that we want to estimate the weights of \( n \) objects by weighing them \( N \) times on a chemical balance. Let \( x_{ij} = -1, 1 \) or \( 0 \) according as the \( j \)th object is on the left or right scale, or is not present at the \( i \)th weighing. Then the \( N \times n \) matrix \( X = (x_{ij}) \) is called the design matrix for the underlying design of experiments.

For clarity, we denote the design matrix of a weighing design \( d \) by \( X_d \). Let \( y_1, y_2, \ldots, y_N \) be the readings in \( N \) weighing with the total weight on the left scale subtracted from the total weights on the right scale. Let \( w_1, w_2, \ldots, w_n \) be the actual weights of the \( n \) objects. Then with the usual assumption of equal variances and independence of \( y_1, y_2, \ldots, y_N \), we have the following linear model

\[ y = X_d w + e, \text{ where } y = (y_1, y_2, \ldots, y_N)^T, \quad w = (w_1, w_2, \ldots, w_n)^T \text{ and } e \text{ is an } N \times 1 \text{ random vector with expectation zero and dispersion matrix } \Sigma_e = \sigma^2 I_N. \]

As discussed in Section 1.1, the \( w_i \)'s are estimable if and only if \( (X_d^T X_d)^{-1} \) exists and in this case the least squared estimate \( \hat{w} \) of \( w \) is \( (X_d^T X_d)^{-1} X_d^T y \) and has dispersion matrix \( \sigma^2 (X_d^T X_d)^{-1} \).

In this context the class of all designs \( \mathcal{O} \) under consideration will be identified with \( \mathcal{O}(N,n) \) and the corresponding family of information matrices will be denoted by \( C(N,n) \). The fundamental problem then is
(1.3.1) Given a class of functions $C$ determine a design $d$ in $\mathcal{L}(N,n)$ which is $\Phi_f$-optimal for all $f \in C$, $d \in \mathcal{L}(N,n)$.

Raghavarao [27] and [28], and Bhaskararao [3] had studied this problem, but they only considered designs $d$ such that $X_d^TX_d$ is of the form $aI_n + bJ_n$, where $I_n$ is the $n \times n$ identity matrix and $J_n$ is the $n \times n$ matrix with all entries equal to 1. This is a very stringent restriction. Let $\mathcal{L}^S(N,n)$ be the set of all such designs. Then there is no guarantee that the best design in $\mathcal{L}^S(N,n)$ is really optimal over $\mathcal{L}(N,n)$. Counterexamples do exist (see Cheng [5]). Furthermore, they only considered the $A$-, $D$- and $E$-criteria.

To summarize, the more recent contributions toward solving problem (1.3.1) it is convenient to divide the value of $N$ into four cases.

Case 0 : $N \equiv 0 \pmod{4}$. Let $X_0$ be a member of $\mathcal{L}(N,n)$ such that $X_0^TX_0 = NI_n$. It has been shown (see Kiefer [24]) that $X_0$ is $\Phi$-optimal over $\mathcal{L}(N,n)$ for every nonincreasing-convex orthogonally invariant extended real-valued function $\Phi$ defined on the nonnegative definite $n \times n$ matrices. In particular $X_0$ is $\Phi_f$-optimal for every continuous decreasing convex function $f$. Hotelling [17] also showed that $X_0$ minimizes the individual variances of the best unbiased estimators of the $\omega_i$. Thus since, for $N \leq 264$, an abundance of matrices such as $X_0$ exist, problem (1.3.1) is solved for the case $N \equiv 0 \pmod{4}$.

Case 1 : $N \equiv 1 \pmod{4}$. Let $X_1$ be a matrix in $\mathcal{L}(N,n)$ such that $X_1^TX_1 = (N-1)I_n + J_n$. Ehlich [9] showed that $X_1$ is
D-optimal in the saturated case (i.e. N = n) and Payne [26] extended this result to the unsaturated case. Cheng [5] improved this result substantially by showing that X₁ is optimal over $\mathcal{D}(N,n)$ with respect to a very general class of criteria which includes the A-, D- and E-criteria. We remark that in the case $N > n$, such an X₁ can always be obtained when the design $X_0$ of Case 0 in $\mathcal{D}(n-1,n)$ exists, by adjoining a row of 1's to that design. Unfortunately, in the saturated case, Raghavarao [27] showed that such an X₁ exists only if $n = (\alpha^2 + 1)/2$ for some integer $\alpha$. Such designs are known for $n = 1, 5, 13, 25$. Ehlich and Zeller [11] state that for $N = n = 9$ the design matrix obtained by them, for which the above diagonal elements of $X_1^T X$ are all 1 except for a single 5, can be proved D-optimum. Hence, the problem of classifying optimal designs in $\mathcal{D}(N,N)$ with $N \equiv 1 (\text{mod } 4)$ is wide open.

Case 2 : $N \equiv 2 (\text{mod } 4)$. Let $X_2, Z_2$ be members of $\mathcal{D}(N,n)$ such that

$$X_2^T X_2 = \begin{bmatrix} L & 0 \\ 0 & M \end{bmatrix}$$

where $L = M = (N-2) I_n + 2J_n$ for $n$ even and $L$ and $M$ are

$$\frac{(N-2) I_n + 2J_n}{2}$$

for $n$ odd, and

$$Z_2^T Z_2 = (N-1) I_n$$

It has been shown (see Ehlich [9], Wojtas [32] and Payne [26]) that $X_2$ is D-optimal in $\mathcal{D}(N,n)$. M. Jacroux recently proved that $X_2$ is uniquely D-optimal (see Jacroux, Wong and Masaro [18]).
Galil and Kiefer [13] remark that it is not known what other optimality properties \( X_2 \) possesses. In the aforementioned paper M. Jacroux also showed that \( Z_2 \) is uniquely E-optimal over \( \mathcal{D}(N,n), \ n \geq 3 \).

Cheng (private communication) noted that when \( N = n, X_2 \) and \( Z_2 \) have the same performance under the A-criterion and \( X_2 \) is \( \Phi_p \)-better than \( Z_2 \) for \( 0 \leq p \leq 1 \). More generally, evidence suggests the following conjecture.

For \( N \geq n, \ N \equiv 2(\text{mod } 4) \) there exists a number \( \alpha(N,n) \geq 1 \) such that \( \alpha(N,n) = 1 \) and
\[
X_2 \text{ is } \Phi_p \text{-optimal for } 0 \leq p \leq \alpha(N,n) \text{ and } \]
\[
Z_2 \text{ is } \Phi_p \text{-optimal for } p \geq \alpha(N,n).
\]

Case 3 : \( N \equiv 3(\text{mod } 4) \). This is the most difficult case. Let \( X_3 \) be a matrix in \( \mathcal{D}(N,n) \) such that \( X_3^T X_3 = (N+1)I_n - J_n \). Then Galil and Kiefer [13] showed that \( X_3 \) is D-optimal if \( N \geq 2n - 5 \).

In the case \( N < 2n - 5 \) the situation is less pretty. For example in the case \( N = n = 11 \) there are at least three different forms of \( X^T X \) which are D-optimal. For a discussion of this and other cases see Galil and Kiefer [13] and [14]. We remark that Galil and Kiefer do not discuss D-optimal matrices with zero entries. Concerning E-optimality, Jacroux (see Jacroux, Wong and Masaro [18]) has shown that if \( Z_2 \) in \( \mathcal{D}(N-1, n), \ n \geq 4 \), is as defined in Case 2, then any matrix of the form
\[
\begin{bmatrix}
Z \\
V^T
\end{bmatrix}
\]
with entries -1, 0 or 1 is E-optimal over \( \mathcal{D}(N,n) \). The study of other optimality properties seems to have been neglected. In this
dissertation we make a contribution in this direction.

1.4. Design Matrices with Entries \(-1 \text{ or } 1\).

Let \( \mathcal{D}'(N,n) \) denote the set of all \( N \times n \) matrices, \( N \geq n \), with entries \(-1 \text{ or } 1\) and let \( \mathcal{C}'(N,n) \) be the family of all matrices of the form \( X^TX \) where \( X \) ranges over \( \mathcal{D}'(N,n) \).

Design matrices such as those in \( \mathcal{D}'(N,n) \) occur in the setting of \( 2^k \) fractional factorial designs of resolution \( 2t+1 \) (i.e. odd resolution). This type of design allows for the estimation of all effects up to the \( t \)-factor interactions assuming the \((t+1)\)-factor and higher interactions zero. The linear model for this type of design is

\[
y_{j_1j_2\ldots j_k} = \beta_0 + \sum_{i=1}^N \beta_i' x_i + \sum_{1 \leq i < j \leq k} \beta_{ij} x_i x_j + \ldots
\]

\[
+ \sum_{1 \leq i_1 < i_2 < \ldots < i_t \leq k} \beta_{i_1i_2\ldots i_t} x_{i_1} x_{i_2} \ldots x_{i_t} + \ldots + \epsilon_{j_1j_2\ldots j_k}
\]

where \( x_i = 1 \text{ or } -1 \) according as \( j_i = 1 \text{ or } 0 \), \( E(\epsilon_{j_1j_2\ldots j_k}) = 0 \) and \( \text{var}(\epsilon_{j_1j_2\ldots j_k}) = \sigma^2 \). In matrix notation the model can be written as \( y = X_d \beta^* + e \) where \( X_d \) is an \( N \times n \) matrix with entries \(-1 \text{ or } 1\),

\[
\beta^T = (\beta_0', \beta_1', \beta_2', \ldots, \beta_k', \beta_1^2, \beta_2^2, \beta_3^2, \beta_4^2, \ldots, \beta_{k-1}^2, \ldots)
\]

\[
\beta_{12}^t, \ldots, \beta_{k-t+1}^t, \ldots, \beta_{k-1}^t
\]

and \( e \) is an \( N \times 1 \) random vector with mean zero and dispersion matrix \( \sigma^2 I_N \). Here the number of parameters to be estimated is
n = 1 + \binom{k}{1} + \binom{k}{2} + \ldots + \binom{k}{t}. The number of runs \( N \) is called a fraction.

The set of design matrices for a \( 2^k \) fractional factorial experiment of odd resolution with \( n \) parameters to be estimated and \( N \) runs is, in general, a proper subset of \( \mathcal{B}'(N,n) \). Thus the results in Section 1.3 where the optimal designs belong to \( \mathcal{B}'(N,n) \) are perfect for the problem of \( 2^k \) fractional factorial designs. In addition Cheng [5] proved that if \( X_3 \) is as defined in Case 3 of Section 1.3 then \( X_3 \) is optimal in \( \mathcal{B}'(N,n) \) with respect to a large class of criteria called the generalized Type 2 criteria. Cheng also mentions a variety of results on E-optimal designs in \( \mathcal{B}'(N,n) \).

Very few results have appeared concerning A-optimal (or more generally, \( \phi^p \)-optimal) designs in \( \mathcal{B}'(N,n) \) with \( N \equiv 2 \pmod{4} \) and \( N \equiv 3 \pmod{4} \). Some are provided in this paper. Our results, however, are only applicable to designs of resolution III.

Finally, we remark that there is a large literature on factorial designs. For a systematic development of the basic concepts of the theory and for further references, we refer the reader to Raktoe, Hedayat and Federer [29].

1.5 Contributions of this Dissertation.

It is well known that, in general, proving a design optimal with respect to a given criterion \( \phi \) can be extremely difficult. One only has to look at the history of D-optimality (e.g. Ehlich [9] and [10], Payne [26] and Calil and Kiefer [13] and [14]) to see the effort (both mathematical and computer aided) put forth. The
difficulty, of course, is the enormous number of cases to be considered. Indeed the number of designs in $\mathcal{D}(N,n)$ is \( \binom{3^n}{N} \) and in $\mathcal{D}'(N,n)$ is \( \binom{2^{N-1}}{N} \). For example, $\mathcal{D}'(6,6)$ has 906,192 members, 556,192 of which have full rank (see Raktoe, Hedayat and Federer [29]). Furthermore, the search for optimal designs in $\mathcal{D}(N,n)$ with respect to criteria, other than D-optimality, is expected to be more difficult. Indeed the D-criterion has the nice property that there always exists a matrix in $\mathcal{D}'(N,n)$ which is D-optimal over $\mathcal{D}(N,n)$. This as we shall see is not always true of the other optimality criteria.

In this dissertation A-optimal designs in $\mathcal{D}(N,n)$ are classified for $n = 6$ and $N$ arbitrary. In addition, for the cases $N \equiv 2 \pmod{4}$ and $N \equiv 3 \pmod{4}$, $\phi_p$-optimal designs $0 \leq p \leq 1$ are found when $N$ is large relative to $n$. In the latter case, it is also shown that A-optimality implies optimality with respect to a large class of criteria which includes the $\phi_p$-criteria $0 \leq p \leq 1$. Further, designs in $\mathcal{D}'(N,n)$, $N \geq n$, $N \equiv 2 \pmod{4}$ arbitrary, are proved optimal with respect to all relevant criteria. Also some $\phi_p$-optimal designs, $0 \leq p \leq 1$, are found in $\mathcal{D}(N,n)$, $N \equiv 3 \pmod{4}$, and $n \leq 7$.

Finally, we remark that problems and techniques in optimal design theory are often related to problems and techniques in other fields. For example in graph theory there is a problem of finding a graph which has a maximum number of spanning trees among all graphs with a given number of vertices and edges (see Keimans and Chelnokov [20] and Shier [30]). N. Gaffke [12] in his doctoral dissertation,
noted that the above problem in graph theory is related to the problem of finding a D-optimal incomplete block design. A common technique in optimal design theory as well as in other related areas is to embed the class of designs of interest in a larger family in which it is (mathematically) easier to find a best design. One then hopes that this best design belongs to the original class. Cheng [4] successfully applied this technique to optimal design theory, then, in Cheng [6], used the same technique to show that a regular complete multipartite graph has the maximum number of spanning trees among all simple graphs with the same number of vertices and edges. Techniques developed in this thesis can be used to obtain results in graph theory. As an example, we remark first that the conjecture

"A graph maximizing the total number of spanning trees over all graphs with a given number of edges and vertices is nearly balanced"

is related to the so-called Mitchell-John conjecture (see John and Mitchell [19]) in statistical design:

"If an incomplete block design is D-optimal (or A-optimal) it is a regular graph design".

Using the methods in the dissertation, it can be shown that, at least in a large system, the above conjectures are true (see Cheng, Masaro and Wong [8]).

The relations among optimal designs in graph theory, statistical theory, etc., can be further seen from the viewpoint that it is possible for two or more different sets $\mathcal{D}_1$ of designs to be embedded in the same larger set of designs $\mathcal{D}$ and a best design $d$
exists in $\mathcal{P}$ such that $d \in \mathcal{P}_i$ for all $i$. This means that a
family of problems may be solved simultaneously and in a unified way.

For brevity, throughout this thesis results and examples taken
from [33], [34] and [35] will not be mentioned.
CHAPTER II
PRELIMINARY DEFINITIONS AND RESULTS

2.1 Majorization.

Majorization is a useful tool in optimality theory and for this reason we include a brief discussion. For a more in depth treatment, we refer the reader to Marshall and Olkin [25].

Let \( x = (x_1, x_2, \ldots, x_n)^T \) be a vector in \( \mathbb{R}^n \). The symbol \( x[i] \) will denote the \( i^{th} \) largest component of \( x \), so that \( x[1] \geq x[2] \geq \cdots \geq x[n] \). If \( x \) and \( y \) are elements of \( \mathbb{R}^n \), we say that \( x \) is majorized by \( y \), and write \( x \prec y \), if

\[
\sum_{i=1}^{k} x[i] \leq \sum_{i=1}^{k} y[i], \quad k = 1, 2, \ldots, n - 1 \quad \text{and} \quad \sum_{i=1}^{n} x[i] = \sum_{i=1}^{n} y[i].
\]


The following theorem (see Marshall and Olkin [25]) is the main reason majorization plays a fundamental role in finding optimal designs:

Theorem 2.1.1. Let \( x, y \in \mathbb{R}^n \). Then \( x \prec y \) if and only if

\[
\sum_{i=1}^{n} f(x_i) \leq \sum_{i=1}^{n} f(y_i)
\]

for all continuous convex functions \( f \).

Now let \( M \) be an \( n \times n \) symmetric matrix. Let \( \lambda_i(M) \) be the \( i^{th} \) largest eigenvalue of \( M \) and let \( \lambda(M) = (\lambda_1(M), \lambda_2(M), \ldots, \lambda_n(M))^T \).

The following theorems (see Marshall and Olkin [25]) will be used in the sequel.

Theorem 2.1.2. (Ky Fan). Let \( M \) and \( \overline{M} \) be \( n \times n \) symmetric matrices of the form

\[
\begin{align*}
\sum_{i=1}^{n} f(x_i) \leq \sum_{i=1}^{n} f(y_i)
\end{align*}
\]
\[ M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}, \quad \overline{M} = \begin{bmatrix} M_{11} & 0 \\ 0 & M_{22} \end{bmatrix}, \]

where \( M_{11} \) is \( \ell \times \ell \) and \( M_{22} \) is \( m \times m \), \( \ell + m = n \).

Then \( \lambda(\overline{M}) \prec \lambda(M) \).

Theorem 2.1.3. (Schur). Let \( M \) be an \( n \times n \) symmetric matrix and \( d = (m_{11}, m_{22}, \ldots, m_{nn})^T \) the vector of diagonal elements of \( M \). Then \( d \prec \lambda(M) \).

2.2 Preliminary Results.

We begin with an application of majorization to optimal design theory. The following result is due to Kiefer [24].

Theorem 2.2.1. Let \( N \equiv 0 \mod 4 \) and let \( X_0 \) be a member of \( \mathcal{O}(N,n) \) such that \( X_0^T X_0 = N I_n \). Then \( X_0 \) is \( \Phi_f \)-optimal in \( \mathcal{O}(N,n) \) for every continuous decreasing convex function \( f \) on \([0, nN]\).

Proof. Let \( X_0 \) and \( f \) be as stated above and let \( X \in \mathcal{O}(N,n) \).

Let \( d = (d_{11}, \ldots, d_{nn})^T \) be the vector of diagonal elements of \( X^T X \) and let \( \lambda = (\lambda_1, \lambda_2, \ldots, \lambda_n) \) be the vector of eigenvalues of \( X^T X \).

By Theorem 2.1.3, \( d \prec \lambda \); hence Theorem 2.1.1 implies that

\[
\sum_{i=1}^{n} f(d_{ii}) \leq \sum_{i=1}^{n} f(\lambda_i).
\]

Since \( N \geq d_{ii}, i = 1, 2, \ldots, n \) and \( f \) is decreasing, we have

\[
\sum_{i=1}^{n} f(N) \leq \sum_{i=1}^{n} f(d_{ii}) \leq \sum_{i=1}^{n} f(\lambda_i).
\]

Whence \( \Phi_f(X_0^T X_0) \leq \Phi_f(X^T X) \). This completes the proof.

In general, given a class of functions \( C \), one hopes to find an
optimal design in \( \mathcal{L}(N,n) \) which is \( \Phi_f \) optimal for all \( f \) in \( C \).

For \( N \equiv 0(\text{mod} \ 4) \), Theorem 2.2.1 shows that we can take \( C \) to be the family of all continuous decreasing convex functions on \([0,nN] \).

Unfortunately when \( N \) is not \( \equiv 0(\text{mod} \ 4) \) the class \( C \) must be reduced in size in order to solve the problem. Such a reduction was made by Cheng [4] in the following definitions.

(a) An optimality criterion \( \Phi_f \) is of Type 1 if

1. \( f \) is continuous, strictly convex and strictly decreasing on \([0,nN] \). (We allow \( f(0^+) = +\infty \)).

2. \( f \) is continuously differentiable on \((0,nN) \) and \( f' \) is strictly concave on \((0,nN) \).

That is: \( f' < 0, f'' > 0 \) and \( f''' < 0 \) on \((0,nN) \).

(b) \( \Phi_f \) is a criterion of Type 2 if \( f \) is as in (a) except that strict concavity of \( f' \) is replaced by strict convexity, i.e. \( f''' > 0 \) on \((0,nN) \).

(c) \( \Phi \) is a generalized criterion of Type \( i \) \((i = 1,2) \) if it is the pointwise limit of a sequence of Type \( i \) criteria.

Note that the \( A-, D- \) and \( \Phi_p \)-criteria are of Type 1 and the \( E \)-criterion is generalized Type 1 criterion (being the limit of \( \Phi_p \)-criteria as \( p \to \infty \)). An example of a Type 2 criterion is \( \Phi_f \) where \( f(x) = \varepsilon x^3 - bx \) where \( \varepsilon > 0, b > 0 \) and \( \varepsilon \) is small compared with \( b \).

The following theorem, due to Cheng [4], is a useful tool for proving optimality of designs.

Theorem 2.2.2. Let \( \mathcal{M} = \{M_d \}_{d \in \mathbb{D}} \) be a class of \( n \times n \) symmetric
nonnegative definite matrices.

(a) Suppose that $M_{d^*} \in \mathcal{M}$ is either a multiple of $I_n$ or has two distinct nonzero eigenvalues $\lambda > \mu$ such that the multiplicity of $\mu$ is $n - 1$ and

\begin{align*}
(2.2.1) & \quad M_{d^*} \text{ maximizes } \text{tr}M_d \text{ over } \mathcal{M} \\
(2.2.2) & \quad \text{tr}(M_{d^*}^2) < \left(\text{tr}M_{d^*}\right)^2/(n-1) \\
(2.2.3) & \quad M_{d^*} \text{ maximizes } \text{tr}M_d - \left\{ n/(n-1) \right\}^{1/2} \times \\
& \quad \left[ \text{tr}(M_d^2) - (\text{tr}M_d)^2/n \right]^{1/2} \text{ over } \mathcal{M}.
\end{align*}

Then $M_{d^*}$ is optimal over $\mathcal{M}$ with respect to any generalized criterion of Type 1.

(b) Suppose $M_{d^*} \in \mathcal{M}$ is either a multiple of $I_n$ or has two distinct nonzero eigenvalues $\lambda > \mu$ such that $\lambda$ has multiplicity $n - 1$, and

\begin{align*}
(2.2.4) & \quad M_{d^*} \text{ maximizes } \text{tr}M_d \text{ over } \mathcal{M} \\
(2.2.5) & \quad M_{d^*} \text{ maximizes } \text{tr}M_d - \{n(n-1)[\text{tr}M_d^2 - (\text{tr}M_d)^2/n]\}^{1/2}
\end{align*}

over $\mathcal{M}$. Then $M_{d^*}$ is optimal over $\mathcal{M}$ with respect to any generalized criterion of Type 2.

In settings where $\text{tr}M_d$ is constant for all $d \in \mathcal{D}$, (2.2.1) and (2.2.3) (or (2.2.4) and (2.2.5)) can be replaced by

\begin{align*}
(2.2.6) & \quad M_{d^*} \text{ minimizes } \text{tr}M_d^2 \text{ over } \mathcal{M}, \text{ and the condition } \\
& \quad "f' < 0" \text{ in the definitions of Type 1 and Type 2 criteria can be dropped. Further, if } f(0^+) = +\infty \text{ then condition (2.2.2) is unnecessary.}
\end{align*}

Using Theorem 2.2.2, Cheng [5] proved the following results:

Theorem 2.2.3. Let $N \equiv 1(\text{mod } 4)$ and let $X_1 \in \mathcal{D}(N,n)$ be such that
\( X_1^T X_1 = (N-1)I_n + J_n \). Then \( X_1 \) is optimal over \( \mathcal{G}(N,n) \) with respect to any generalized criteria of Type 1.

Theorem 2.2.4. Let \( N \equiv 3(\text{mod } 4) \) and let \( X_3 \in \mathcal{G}(N,n) \) be such that \( X_3^T X_3 = (N+1)I_n - J_n \). Then \( X_3 \) is optimal over \( \mathcal{G}(N,n) \) with respect to any generalized Type 2 criterion.

In Chapter III we will prove a result analogous to Theorem 2.2.3 for designs in \( \mathcal{G}(N,n) \), \( N \equiv 2(\text{mod } 4) \). However, for designs in \( \mathcal{G}(N,n) \) and \( N \equiv 2(\text{mod } 4) \) or \( N \equiv 3(\text{mod } 4) \) no similar result is known at the present time.

### 2.3 Some Useful Lemmas

The results of this section will be useful in reducing the number of designs among which one must search in order to find an optimum one. We will need the notion of equivalence. Two matrices \( X \) and \( Y \) in \( \mathcal{G}(N,n) \) (\( \mathcal{G}'(N,n) \)) are said to be equivalent if \( Y \) can be obtained from \( X \) by a finite number of transformations of the form: multiplication of any row by \( -1 \), interchanging any two rows, or transposition. It is straightforward to show that if \( X \) and \( Y \) are equivalent and \( X^T X \) is nonsingular then \( X^T X \) and \( Y^T Y \) are similar. So, for design purposes, equivalent matrices have the same optimality properties.

The following lemma is due to Ehlich [9].

Lemma 2.3.1. Let \( X \in \mathcal{G}'(N,n) \), \( N \equiv 2(\text{mod } 4) \). Then \( X \) is equivalent to a matrix \( Y \) in \( \mathcal{G}'(N,n) \) such that

\[
Y^T Y = \begin{bmatrix}
A & B \\
B^T & C
\end{bmatrix}
\]

where \( a_{ij} \equiv 2(\text{mod } 4) \), \( c_{ij} \equiv 2(\text{mod } 4) \) and \( b_{ij} \equiv 0(\text{mod } 4) \).
The following technical lemmas will be useful.

Lemma 2.3.2. (Ehlich [9]). Let $x_1, x_2, x_3$ be vectors in $\mathbb{R}^n$, $n \equiv 2 \pmod{4}$, with entries $\pm 1$. If $x_1 \cdot x_2 \equiv 0 \pmod{4}$ and $x_1 \cdot x_3 \equiv 0 \pmod{4}$ then $x_2 \cdot x_3 \equiv 2 \pmod{4}$.

Lemma 2.3.3. Let $X \notin \mathcal{O}(7,5)$ be such that

$$X^TX = \begin{bmatrix}
1 & 6 & 1 \\
1 & -6 & 1 \\
1 & 1 & -7 \\
\end{bmatrix}$$

Then $|b_{ij}| \geq 2$ for at least one pair $(i,j)$.

Proof. Suppose $b_{ij} = 0$ for all $i, j$. We may assume

$$X = [x_1, x_2, x_3, x_4, x_5],$$

where $x_1^T = (1, 0, 1, 1, 1, 1)$ and $x_2^T = (0, 1, 1, 1, -1, -1)$. Write $x_1^T = (1, 0, u_1^T)$, $x_2^T = (0, 1, u_2^T)$ and $x_3^T = (a, b, u_3^T)$. Then $u_1^T = (1, 1, 1, 1, 1, 1)$, $u_2^T = (1, 1, 1, -1, -1)$ and the entries of $x_3$ are $1$ or $-1$. By assumption, $x_1 \cdot x_3 = 0$ and $x_2 \cdot x_3 = 0$. Thus,

$$a + u_1 \cdot u = 0 \quad \text{and} \quad b + u_2 \cdot u = 0.$$

Therefore

$$a + b + (u_1 + u_2) \cdot u = 0.$$

Since $u_1^T + u_2^T = (2, 2, 2, 0, 0)$, $a + b$ cannot be zero. Hence

$$a = b = \pm 1.$$

Applying similar arguments to the other columns of $X$, we conclude that $X$ must have the form:
where $|a_i| = 1$ and the $v_i$'s are $5 \times 1$ column vectors with entries $\pm 1$. By multiplying columns $x_3$, $x_4$, $x_5$ by $-1$ if necessary, we may assume that $a_i = -1$, $i = 1, 2, 3$. Thus since $x_i \cdot x_j = 0$, $i = 1, 2, j = 3, 4, 5$, $u_1 \cdot v_j = u_2 \cdot v_j = 1$, $j = 1, 2, 3$. Also $|x_i \cdot x_j| = 1$ for $i \neq j$, $i,j = 3, 4, 5$. Thus $v_i \cdot v_j = -3$ or $-1$. Since

\[ u_1^T = (1, 1, 1, 1, 1) \quad \text{and} \quad u_2^T = (1, 1, 1, -1, -1), \]

each $v_j$ must be of the form $v_j^T = (p^T, q^T)$ where $p$ is the $3 \times 1$ and has exactly two entries equal to $1$ and $q$ is $2 \times 1$ and has exactly one entry equal to $1$. There are only six possible choices for the $v_j$. They are listed as columns of the following matrix:

\[
V = \begin{bmatrix}
1 & 1 & 1 & 1 & -1 & -1 \\
1 & 1 & -1 & -1 & 1 & 1 \\
-1 & -1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & -1 \\
-1 & 1 & -1 & 1 & -1 & 1 \\
\end{bmatrix}
\]

Since

\[
V^T V = \begin{bmatrix}
5 & 1 & 1 & -3 & 1 & -3 \\
1 & 5 & -3 & 1 & -3 & 1 \\
1 & -3 & 5 & 1 & 1 & -3 \\
-3 & 1 & 1 & 5 & -3 & 1 \\
1 & -3 & 1 & -3 & 5 & 1 \\
-3 & 1 & -3 & 1 & 1 & 5 \\
\end{bmatrix},
\]

it is clear that the set \{ $v_{i_1}$, $v_{i_2}$, ..., $v_{i_k}$ \} satisfies ...
\( v_i \cdot v_j = -3 \) for \( i \neq j \). But our assumption that all \( b_{ij} = 0 \) requires \( k = 3 \). This contradiction proves the lemma.

We note that Lemma 2.3.3 is the best we can do. For example, let

\[
X = \begin{bmatrix}
1 & 0 & 1 & 1 & 1 \\
0 & 1 & 1 & 1 & -1 \\
1 & -1 & 1 & -1 & 1 \\
1 & -1 & -1 & 1 & -1 \\
1 & 1 & -1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 \\
1 & 1 & 1 & -1 & -1
\end{bmatrix}.
\]

Then

\[
X^TX = \begin{bmatrix}
6 & 1 & 0 & 0 & 2 \\
6 & 0 & 0 & 0 & \ast \\
7 & -1 & -1 & \ast & \ast \\
7 & -1 & \ast & \ast & \ast \\
7 & \ast & \ast & \ast & \ast
\end{bmatrix}.
\]

2.4 Hadamard Matrices.

Let \( N \equiv 0 \text{(mod 4)} \). An \( N \times N \) matrix \( H_N \) is said to be a Hadamard matrix of order \( N \) if each entry of \( H_N \) is \(-1\) or \(1\) and \( H_N^T H_N = I_N \). Theorem 2.2.1 shows that if \( X_0 \) is any \( N \times n \) matrix consisting of \( n \) distinct columns of \( H_N \), then \( X_0 \) is \( \Phi_f \)-optimal in \( \mathcal{O}(N,n) \) for all continuous decreasing convex functions \( f \). Thus Hadamard matrices play an important role in the search for optimal designs. At the moment, 268 is the smallest \( N \) for which we do not know if a Hadamard matrix of order \( N \) exists.

Galil and Kiefer [13] remark that for fixed \( n \) it is unnecessary to demand the existence of a Hadamard matrix \( H_n \) for all \( N \). Instead
the following proposition may be used.

Proposition 2.4.1. For \( n \geq 4 \), let \( N_n = \min\{j : j \geq n, j \equiv 0 \pmod{4}\} \).

Suppose \( H_j \) exists for all \( j \equiv 0 \pmod{4} \) satisfying \( N_n \leq j < 2N_n \).

Then, for all \( N \geq n \) with \( N \equiv 0 \pmod{4} \), there is an \( X_0 \) in \( \mathcal{G}(N,n) \) with \( X_0^TX_0 = NI_n \).

Thus, for example, when \( n = 6 \), the existence of \( H_8 \) and \( H_{12} \) implies that \( X_0 \) exists for \( n = 6 \) and all \( N \geq n \), \( N \equiv 0 \pmod{4} \).

For more on Hadamard matrices we refer the reader to Hedayat and Wallis [16]. Finally, we remark that Hadamard matrices are also useful in constructing optimal designs in \( \mathcal{G}(N,n) \) even if \( N \) is not congruent to \( 0 \pmod{4} \).
CHAPTER III

OPTIMAL N x n WEIGHING DESIGN MATRICES

WITH N \equiv 2 (\text{MOD} 4)

3.1 Optimal Designs in $\mathcal{B}'(N,n)$.

Throughout this chapter $N$ will be congruent to $2 (\text{MOD} 4)$ and $X_2$ will be a matrix in $\mathcal{B}'(N,n)$ such that

\begin{equation}
X_2^T X_2 = \begin{bmatrix}
L & 0 \\
0 & M
\end{bmatrix},
\end{equation}

where $L = M = (N-2) \frac{I_n}{2} + 2 \frac{J_n}{2}$ if $n$ is even and $L$ and $M$ are

\begin{equation}
(N-2) \frac{I_{n+1}}{2} + 2 \frac{J_{n+1}}{2}
\end{equation}

if $n$ is odd.

Ehlich [9] and Payne [26] proved that $X_2$ is D-optimal in $\mathcal{B}'(N,n)$ and recently Cheng [5] proved that $X_2$ is E-optimal over $\mathcal{B}'(N,n)$. In this section it is proved in a unified way that $X_2$ is optimal with respect to a large subclass of the Type 1 criteria. This approach gives a new proof of the result of Ehlich and Payne mentioned above.

We require the following lemma.

Lemma 3.1.1. Let $\mathcal{B}$ be the family of $n \times n$ matrices of the form:

\[ B(s,t) = \begin{bmatrix}
(N-2)I_s + 2J_s & 0 \\
0 & (N-2)I_t + 2J_t
\end{bmatrix}, \]

where $s + t = n$. Let $s_0 = t_0 = n/2$ if $n$ is even,

$s_0 = t_0 + 1 = (n+1)/2$ if $n$ is odd. Then the eigenvalues of $B(s_0,t_0)$ are majorized by the eigenvalues of all other matrices.
B(s,t) in \( \mathcal{B} \).

Proof. Suppose \( N \) is odd, then \( s_0 = (n+1)/2 \) and \( t_0 = (n-1)/2 \).

The vector of eigenvalues of \( B(s_0, t_0) \) arranged in decreasing order is \( x = (N+n-1, N+n-3, N-2, \ldots, N-2)^T \). For \( B(s,t) \), \( s \geq t \geq 0 \) the corresponding vector is \( y = (N+2s-2, N+2t-2, N-2, \ldots, N-2)^T \).

Since \( n \) is odd, \( s \geq (n+1)/2 \), so \( 2s - 2 \geq n - 1 \). Hence

\[
\sum_{i=1}^{n-1} x_i \leq \sum_{i=1}^{n-1} y_i \quad \text{and} \quad \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i. \quad \text{Thus } x \preceq y. \quad \text{The proof is similar for } n \text{ even.}
\]

We now prove our main result (M. Jacroux independently found this result. See Jacroux, Wong and Masaro [18]).

**Theorem 3.1.** Let \( X_2 \) be as in (3.1.1). Then \( X_2 \) is optimal in \( \mathcal{B}'(N,n) \) with respect to any Type 1 criterion \( \Phi_t \) such that

\[
\lim_{x \to +\infty} f(x) = +\infty. \quad \text{Further up to similarity of } X_2^T X_2, \quad X_2 \text{ is unique.}
\]

Proof. Let \( X \in \mathcal{B}'(N,n) \). By Lemma 2.3.1 we may assume that

\[
X^T X = \begin{bmatrix}
A_{s \times s} & B \\
B^T & C_{t \times t}
\end{bmatrix}
\]

where \( |a_{ij}| \geq 2, \quad |c_{ij}| \geq 2 \). Thus,

\[
(3.1.2) \quad \text{tr} A^2 \geq \text{tr} [(N-2)I_s + 2J_s]^2
\]

and

\[
(3.1.3) \quad \text{tr} B^2 \geq \text{tr} [(N-2)I_t + 2J_t]^2.
\]

Hence by Theorem 2.2.2 (since \( f(0^+) = +\infty \)) we have

\[
(3.1.4) \quad \Phi_t(A) \geq \Phi_t((N-2)I_s + 2J_s)
\]
and

\[(3.1.5) \quad \phi_f(B) \geq \phi_f((N-2)I_t + 2J_t).\]

So by Ky Fan's result (Theorem 2.1.2) and Lemma 3.1.1,

\[\phi_f(X^TX) = \phi_f \begin{bmatrix} A & 0 \\ 0 & C \end{bmatrix} = \phi_f(A) + \phi_f(C) \geq \phi_f((N-2)I_s + 2J_s) + \phi_f((N-2)I_t + 2J_t)\]

\[(3.1.6) \quad = \phi_f(B(s,t)) \geq \phi_f(B(s_0, t_0)) \geq \phi_f(X_2^TX_2).\]

For uniqueness, suppose that \(\phi_f(X^TX) = \phi_f(X_2^TX_2)\). Then all inequalities in (3.1.4), (3.1.5) and (3.1.6) become equalities.

Letting \(f(x) = -\log x\), we see that \(\det(X^TX) = \det(A) \det(C)\). Hence

\[X^TX = \begin{bmatrix} A & 0 \\ 0 & C \end{bmatrix}.\]

Further, since \(\phi_f(A) = \phi_f((N-2)I_s + 2J_s)\), then from the proof of Theorem 2.2 of Cheng [4], \(A\) must have the same eigenvalues as \((N-2)I_s + 2J_s\). Similarly \(C\) has the same eigenvalues as \((N-2)I_t + 2J_t\). Finally, since \(\phi_f(B(s,t)) = \phi_f(X_2^TX_2)\), then

\[f(N+2s-2) + f(N+2t-2) = \begin{cases} f(N+n-1) + f(N+n-2) & \text{if } n \text{ is odd} \\ 2f(N+n-2) & \text{if } n \text{ is even} \end{cases}\]

Letting \(f(x) = 1/x\) and solving for \(s\) and \(t\) we find that \(s = s_0\), \(t = t_0\). Thus \(B(s,t) = B(s_0, t_0) = X_2^TX_2\). Thus \(X^TX\) and \(X_2^TX_2\) have the same eigenvalues and therefore are similar. This
completes the proof.

We remark that in general, \( X_2 \) is not \( \Phi_f \)-optimal for every continuous convex function \( f \). For example, let \( N = n = 6 \),

\[
X_2 = \begin{bmatrix}
1 & 1 & -1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 & -1 & 1 \\
1 & 1 & 1 & 1 & -1 & -1 \\
1 & 1 & 1 & -1 & 1 & -1 \\
1 & -1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & -1 & -1 & -1
\end{bmatrix}
\]

Then by Theorem 3.1.1, \( X_2 \) is optimal with respect to any Type 1 criteria \( \Phi_f \) such that \( f(0^+) = +\infty \). However, the eigenvalues 10, 10, 4, 4, 4, 4 of \( X_2^T X_2 \) are not majorized by the eigenvalues of all matrices in \( \mathcal{O}'(N,n) \). Indeed, if we take

\[
X = \begin{bmatrix}
1 & -1 & -1 & -1 & -1 & 1 \\
1 & -1 & 1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1 & 1 & -1 \\
-1 & -1 & 1 & 1 & -1 & -1 \\
1 & -1 & 1 & 1 & -1 & 1 \\
1 & 1 & -1 & -1 & -1 & -1
\end{bmatrix}
\]

then

\[
X^T X = \begin{bmatrix}
6 & -2 & -2 & -2 & 0 & 0 \\
-2 & 6 & -2 & -2 & 0 & 0 \\
-2 & -2 & 6 & 2 & 0 & 0 \\
-2 & -2 & 2 & 6 & 0 & 0 \\
0 & 0 & 0 & 0 & 6 & -2 \\
0 & 0 & 0 & 0 & -2 & 6
\end{bmatrix}
\]

The eigenvalues of \( X^T X \) are 10, 4.721, 8, 8, 4, 4, 1.5279 which do not majorize the eigenvalues of \( X_2^T X_2 \).

It should be noted that designs \( X_2 \) satisfying condition (3.1.1)
can be found for many classes \( \mathcal{G}(N,n) \). Indeed, let \( n \leq N - 2 \)
and \( X_0 \in \mathcal{G}'(N-2,n) \) such that \( X_0^T X_0 = (N-2)I_n \) (from section 2.4
many such \( X_0 \) exist). Then an \( X_2 \), as above, can be obtained by
adjoining to \( X_0 \) two rows, one consisting entirely of 1's and the
other consisting of \([n/2]\) 1's and \( n-[n/2] \) -1's. If \( n = N \)
designs such as \( X_2 \) have been constructed, using circulant matrices,
by Pfliegh [9] in all cases \( n \leq 38 \) except \( n = 22 \) and 34. Other
designs in these cases were obtained by Yang [36], who in the references
cited by him there also constructed \( X_2 \) for \( n = 42, 46, 48, 52 \). For
\( n = N - 1 \) the appropriate matrix \( X_2 \) in \( \mathcal{G}'(N,N-1) \) can be obtained
by removing any column from the corresponding \( X_2 \) in \( \mathcal{G}'(N,N) \).

3.2. A-optimal Designs in \( \mathcal{G}(N,n) \).

Let \( X_2 \) be as in (3.1.1). We conjecture that

(1) \( X_2 \) is A-optimal in \( \mathcal{G}(N,n) \).

In support of (1), we note that (Theorem 3.3.1) for any \( n \),
\( X_2 \) above is A-optimal for sufficiently large \( N \). The problem is left
for small \( N \) which can be done with little help from computers. For
example, when \( N = n = 6 \), \( \mathcal{G}(N,n) \) has \( \binom{36}{6} \) elements. By using
Ky Fan's result on majorization (Theorem 2.1.2) we shall prove that
for \( n = 6 \) and \( N \geq 6 \), \( X_2 \) is A-optimal. Our technique can be used
to prove other results. It is our hope that a refined use of such
methods can be applied in a more general setting.

The following well-known result gives a lower bound for
\( \text{tr}(X^TX)^{-1} \) over \( \mathcal{G}(N,n) \). With such a lower bound, one gets a feeling
in comparing one \( \text{tr}(X^TX)^{-1} \) with another.
Theorem 3.2.1. Let \( X \in \mathcal{B}(N,n) \). Then

\[
\text{tr}(X^T X)^{-1} \geq n^2 / \text{tr}(X^T X) \geq n/N .
\]

In particular \( \text{tr}(X^T X)^{-1} \geq 1 \) if \( X \) is saturated. Moreover

\[
\text{tr}(X^T X)^{-1} = n^2 / \text{tr}(X^T X) \text{ if and only if } X^T X \text{ is a scalar multiple of } \frac{I_n}{n} .
\]

Proof. With the trace inner product, we have, by the Schwarz inequality,

\[(X^T X)^{-1/2} , (X^T X)^{1/2} \leq \| (X^T X)^{-1/2} \| \| (X^T X)^{1/2} \| ,\]

i.e.

\[n \leq (\text{tr}(X^T X)^{-1})^{1/2} (\text{tr}(X^T X))^{1/2} ,\]

proving the result. [Another proof: Let \( W = (\text{tr} X^T X/n)I_n \). Then the eigenvalues of \( W \) are majorized by the diagonal elements of \( X^T X \) which are in turn majorized by the eigenvalues of \( X^T X \) (see Theorem 2.1.3). Hence \( \text{tr}(X^T X)^{-1} \geq \text{tr} W^{-1} = n^2 / \text{tr} X^T X \).]

The above result can be generalized to the following:

Theorem 3.2.2. Let \( C \) be a positive definite \( n \times n \) matrix, \( t = \text{tr} C \), \( a > 0 \), and

\[b(t,a) = \frac{(n-2)(at-n^2) + \sqrt{n^4 a^2 - 2n^2 (n-2) at + n^4 (n-2)^2}}{4n(n-1)a^2} + \frac{t^2}{n} .\]

Suppose that \( \text{tr} C^2 \geq b(t,a) \). Then \( \text{tr} C^{-1} \geq a \). Moreover, \( \text{tr} C^{-1} > a \) if \( \text{tr} C^2 > b(t,a) \) and \( at \neq (n-2)^2 \).

Proof. Let \( S = \{ (\lambda_1, \lambda_2, \ldots, \lambda_n) : \sum \lambda_i = t, \sum \lambda_i^2 = \text{tr} C^2 \}, \lambda_i \geq 0, i = 1, 2, \ldots, n \} \) and \( f, g \) be defined by

\[f((\lambda_i)) = \sum_{i=1}^{n} g(\lambda_i), \text{ for } (\lambda_i) \in S , \quad g(x) = \frac{1}{x}, \text{ for } x > 0, \quad g(0) = +\infty .\]
Then \((\lambda_1) \in S\) where the \(\lambda_i\)'s are the eigenvalues of \(C\). So \(S\) is a nonempty compact subset of \(\mathbb{R}^n\) and \(f\) is a continuous function of \(S\) into \([0, \infty]\). Thus there exists \((\mu_i) \in S\) such that 
\[ f((\mu_i)) = \min f(S). \]
Obviously each \(\mu_i > 0\) (otherwise \(f((\mu_i)) = +\infty\) which cannot be \(\min f(S)\)). By Lemmas A2, A3 and A6 of Cheng [4] we may assume that \(\mu_1 = \mu_2 = \ldots = \mu_{n-1} \leq \mu_n\). Write \(u = \mu_1\) and 
\[ \lambda = \mu_n. \]
Since \((\mu_i) \in S\), 
\[ u = \frac{t - \sqrt{n(n-1)}}{\sqrt{n-1}} P, \quad \lambda = \frac{t + \sqrt{n(n-1)}}{\sqrt{n-1}} P \quad \text{with} \quad P = \frac{1}{\sqrt{\text{tr} C^2 - \frac{t^2}{n}}}. \]
\(\text{tr} C^{-1} \in f(S)\). So \(\text{tr} C^{-1} \geq f((\mu_i))\). It then suffices to prove that 
\[ f((\mu_i)) > a, \quad \text{i.e.} \]
\[ \frac{n(n-1)}{\sqrt{n-1}} + \frac{n}{\sqrt{n(n-1)}} > \frac{a}{P} \]
or 
\[ n(n-1)a P^2 + \left[ n^2(n-2)\sqrt{n(n-1)} - (n-2)\sqrt{n(n-1)} \right] aP + n^2(n-1)t - (n-1)t a^2 \geq 0. \]
Let \(h(P)\) be the left side of this inequality. It suffices to prove that \(P \geq P_0\), where \(P_0\) is the positive root of \(h(P) = 0\). Using the quadratic formula, we obtain 
\[ P_0 = \frac{(n-2)(at - n^2) + \sqrt{n^2 at^2 + 2n^2(n^2 - n^2)at + n^4(n-2)^2}}{2a\sqrt{n(n-1)}}. \]
Thus \(P_0^2 = b(t, a) - \frac{t^2}{n}\). So 
\[ P = \sqrt{\text{tr} C^2 - \frac{t^2}{n}} > b(t, a) - \frac{t^2}{n} = P_0. \]
Suppose now that \(\text{tr} C^2 > b(t, a)\) and \(at \neq (n-2)^2\). Since \(b(t, \cdot)\) is continuous on \(\left(\frac{(n-2)^2}{t}, \frac{n^2}{t}\right)\), \(\text{tr} C^2 > b(t, a')\) for some
a' > a . By the result just proved, \( \text{tr} \ C^{-1} \geq a' > a \).

Instead of \( \text{tr} \ C^{-1} \), the above useful result can be stated and proved for \( |C^{-1}| \), etc.

We remark that if we set \( a = n^2/t \) in Theorem 3.2.2, then \( b(t,a) = 0 \), and Theorem 3.2.2 is reduced to Theorem 3.2.1.

We will make much use of Theorem 3.2.2. Consequently we will need to refer to Table 3.2.1 below. In this table, \( a = \text{tr}(X_2^T X_2)^{-1} \), where \( X_2 \) is as in (3.1.3), \( t = \text{tr}(X^T X) \) where \( X \in \mathcal{O}(N,n) \), \( k \) is the number of zero entries in \( X \) and \( b(t,a) \) is as in Theorem 3.2.2.

We note that the absence of a value for \( [b(t,a)] + 1 \) in Table 3.2.1 indicates that \( b(t,a) \) is undefined (this is easily seen to be equivalent to \( at < n^2 \)).

To illustrate the use of Table 3.2.1 and Theorem 3.2.2, let \( X \in \mathcal{O}(6,6) \) have two zero entries and satisfy \( \text{tr}(X^T X)^2 \geq 235 \). Then Theorem 3.2.2 and line 3 of Table 3.2.1 show that \( \text{tr}(X^T X)^{-1} \geq 1.2 \).
### Table 3.2.1

<table>
<thead>
<tr>
<th>N = 6</th>
<th>n</th>
<th>k</th>
<th>(a)</th>
<th>([b(t,a)] + 1)</th>
<th>([a(t)] + 1)</th>
</tr>
</thead>
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<tr>
<td>6</td>
<td>6</td>
<td>1</td>
<td>1.2</td>
<td>261</td>
<td>43</td>
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<tr>
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<td>6</td>
<td>2</td>
<td>1.2</td>
<td>235</td>
<td>41</td>
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<td>3</td>
<td>1.2</td>
<td>209</td>
<td>40</td>
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<tr>
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<td>6</td>
<td>4</td>
<td>1.2</td>
<td>187</td>
<td>39</td>
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<td>6</td>
<td>5</td>
<td>1.2</td>
<td>167</td>
<td>38</td>
</tr>
<tr>
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<td></td>
<td>9</td>
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<tr>
<td>3</td>
<td>3</td>
<td>2</td>
<td></td>
<td></td>
<td>9</td>
</tr>
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<td>387</td>
<td>17</td>
</tr>
<tr>
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<td>4</td>
<td>2</td>
<td></td>
<td></td>
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<tr>
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<td>4</td>
<td>3</td>
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<td>26</td>
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<td>2</td>
<td></td>
<td>471</td>
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<td>5</td>
<td>3</td>
<td></td>
<td></td>
<td>25</td>
</tr>
<tr>
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<td>625</td>
<td>38</td>
</tr>
<tr>
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<td></td>
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<td>38</td>
</tr>
<tr>
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<td>6</td>
<td>3</td>
<td></td>
<td>.554</td>
<td>37</td>
</tr>
</tbody>
</table>
We are now ready to prove:

Theorem 3.2.3. Let \( X_2 \) be as in (3.2.1). Then \( X_2 \) is A-optimal in \( \mathcal{G}(N,n) \) for \( n \leq 6 \) and \( N \) arbitrary.

Proof. Part A: \( N = 6, n \leq 6 \).

We shall prove only the case where \( n = 6 \). (The case \( n < 6 \) is similar and easier. When \( n \leq 2 \), the desired result is obvious by Theorem 2.2.2.

A simple calculation gives \( \text{tr}(X_2^TX_2)^{-1} = \frac{6}{5} = 1.2 \). Let \( X \in \mathcal{G}(6,6) \). We must show that \( \text{det}(X^TX)^{-1} \geq 1.2 \). Let \( t = \text{tr}(X^TX), \)
\( a = 1.2, C = X^TX \). Suppose that some column, say \( \bar{X}_1 \), of \( X \) has two or more zero entries. Then by the majorization of Ky Fan (Theorem 2.1.2),

\[
\text{tr}C^{-1} \geq \text{tr}(\bar{X}_1^T\bar{X}_1)^{-1} + \text{tr}(Z^TZ)^{-1}, \quad Z \in \mathcal{G}(6,5).
\]

By this theorem with \( n = 5 \),

\[
\text{tr}(Z^TZ)^{-1} \geq \text{tr}
\begin{bmatrix}
6 & 2 & 2 & 0 \\
2 & 6 & 2 & 0 \\
2 & 2 & 6 & 0 \\
0 & 6 & 2 & 0
\end{bmatrix}^{-1}
\]

\[
= \frac{32}{6 - 2} + \frac{1}{6 + 2} + \frac{1}{6 - 2} + \frac{1}{6 + 2} = \frac{39}{40}
\]

whence

\[
\text{tr}C^{-1} \geq \frac{1}{4} + \frac{39}{40} = \frac{49}{40} > 1.2.
\]

So we may assume that no column of \( X \) has more than one zero entry.

Let \( Z(X) \) denote the number of zero entries in \( X \).

Case 1. \( Z(X) = 0 \). By Theorem 3.1.1, \( \text{tr}C^{-1} \geq 1.2 \).

Case 2. \( Z(X) = 1 \). We may assume that the zero entry is in the first column of \( X \). By rearranging columns \( \bar{X}_2, \bar{X}_3, \ldots, \bar{X}_6 \) of
[\bar{X}_2, \bar{X}_3, \ldots, \bar{X}_6], we may by Ehlich's result (Lemma 2.3.1) assume that

\[ [\bar{X}_2^T, \bar{X}_3, \ldots, \bar{X}_6^T] = \begin{bmatrix} A & B \\ B^T & D \end{bmatrix} \]

where \( A \in M_{s \times s}, s \leq 2 \), \( D \in M_{(n-s) \times (n-s)} \), \( a_{ij} \equiv 2 \pmod{4} \),
\( d_{ij} \equiv 2 \pmod{4} \), \( b_{ij} \equiv 0 \pmod{4} \). Since \( \bar{X}_1 \) has a zero entry
\[ |c_{i,j}| \geq 1 \]. Thus

\[ \text{tr} C^2 \geq 10 \times 1 + 5^2 + \text{tr} \begin{bmatrix} A & B \\ B^T & D \end{bmatrix}^2 \]
\[ \geq 35 + 5 \times 6^2 + 4s(s-1) + 4(5-s)(4-s) \]
\[ = 8(s - \frac{5}{2})^2 + 245 \].

We shall use Theorem 3.2.2 and its notations. Now \( n = 6 \) and
\( \beta(t,a) = 260.8 \) or more precisely \( \beta(t,a) < 261 \). By Theorem 3.2.2, we may assume that \( \text{tr} C^2 \leq 260 \). If \( s < 2 \) then \( \text{tr} C^2 \geq 8 \left( \frac{3}{2} \right)^2 + 245 = 263 \).

So let \( s = 2 \). By multiplying the columns of \( X \) by \(-1\), we may assume that all \( a_{ij} = 2 = d_{ij} \). (Recall that rearranging the columns of \( X \) or multiplying the columns of \( X \) by \(-1\) will not affect the eigenvalues of \( X^T X \) and for brevity, will be referred to as 'some basic operations' on the columns of \( X \)). Since \( s = 2 \),

\[ (3.2.1) \quad \text{tr} C^2 \geq 8(2 - \frac{5}{2})^2 + 245 = 247 \].

If some \( b_{ij} \neq 0 \), then \( b_{ij}^2 = 4^2 \) and
\[ \text{tr} C^2 \geq 247 + 2 \times 4^2 = 279 > 260 \].

So we may assume that \( b_{ij} = 0 \) for all \( i,j \). Thus
\[
C = \begin{bmatrix}
5 & a_1 & a_2 & a_3 & a_4 & a_5 \\
a_1 & 6 & c_1 & 0 & 0 & 0 \\
a_2 & c_1 & 6 & 0 & 0 & 0 \\
a_3 & 0 & 0 & 6 & 2 & 2 \\
a_4 & 0 & 0 & 2 & 6 & c_2 \\
a_5 & 0 & 0 & 2 & c_2 & 6
\end{bmatrix}
\]

where \(|c_1| = 2\), \(|a_1| \geq 1\). If one of \(|a_1| \neq 1\) then

\[2a_1^2 \geq 2 \times 3^2 = 2(8+1)\] and therefore by (3.2.1),

\[\text{tr } C^2 \geq 247 + 2 \times 8 = 263 > 260\, .\] So we may assume that all \(|a_1| = 1\).

(Note now that \(\text{tr } C^2 = 247\), i.e. \(\text{tr } C^2\) is minimum and this is the only case which cannot be taken care of by Theorem 3.2.2 above). By multiplying \(\bar{X}_2, \bar{X}_3\) by -1, if necessary, we may further assume that

\[a_1 = a_2 = 1\, .\] Let

\[
A_1 = \begin{bmatrix}
5 & 1 & 1 \\
1 & 6 & c_1 \\
1 & c_1 & 6
\end{bmatrix} \quad A_2 = \begin{bmatrix}
6 & 2 & 2 \\
2 & 6 & c_2 \\
2 & c_2 & 6
\end{bmatrix} \quad B^T = \begin{bmatrix}
a_3 & 0 & 0 \\
a_4 & 0 & 0 \\
a_5 & 0 & 0
\end{bmatrix} \, .
\]

For symmetric \((a_{ij}) \in M_{3 \times 3}\) such that \((a_{ij})^{-1}\) exists,

\[(3.2.2) \quad \text{tr}(a_{ij})^{-1} = \sum_{i \leq j} a_{ii} a_{jj} - \sum_{i \leq j} a_{ij}^2 \]

\[= \frac{a_{11} a_{22} a_{33} + 2a_{12} a_{13} a_{23} - a_{11} a_{22}^2 - a_{22} a_{11}^2 - a_{33} a_{11}^2}{a_{11} a_{22} a_{33} + 2a_{12} a_{13} a_{23} - a_{11} a_{22}^2 - a_{22} a_{11}^2 - a_{33} a_{11}^2} \, .\]

Thus \(\text{tr } A_1^{-1} = \frac{45}{74 + c_1}\), \(\text{tr } A_2^{-1} = \frac{12}{8 + c_2}\). Suppose that \(c_2 = -2\).

Thus \(\text{tr } A_1^{-1} + \text{tr } A_2^{-1} \geq \frac{45}{76} + \frac{12}{16} = \frac{51}{38} > 1.2\).

By the (above) majorization theorem of Ky Fan, \(X^T X\) majorizes
\[ \text{diag}(A_1, A_2) \]. So
\[ \text{tr } C^{-1} \geq \text{tr} (\text{diag } (A_1, A_2))^{-1} = \text{tr } A_1^{-1} + \text{tr } A_2^{-1} > 1.2. \]

Thus we may assume \( c_2 = 2 \). Suppose that \( c_1 = -2 \). Then
\[ \text{tr } A_1^{-1} + \text{tr } A_2^{-1} = \frac{45}{72} + \frac{12}{20} = \frac{49}{40} > 1.2. \]

By the majorization theorem of Ky Fan \( \text{tr } C^{-1} > 1.2 \). So we may assume \( c_1 = 2 \), i.e.
\[
C = \begin{bmatrix}
5 & 1 & 1 & a_3 & a_4 & a_5 \\
1 & 6 & 2 & 0 & 0 & 0 \\
1 & 2 & 6 & 0 & 0 & 0 \\
a_3 & 0 & 0 & 6 & 2 & 2 \\
a_4 & 0 & 0 & 2 & 6 & 2 \\
a_5 & 0 & 0 & 2 & 2 & 6
\end{bmatrix}, \quad a_i = \pm 1.
\]

Applying some basic operations on columns of \( X \), we may assume that \((a_3, a_4, a_5) = (1, 1, -1)\) or \((1, 1, 1)\). Let \( f(a_1, a_2, a_3) = \text{tr } C^{-1} \).

Note that for \( C = \begin{bmatrix} A_1 & B \\ B^T & A_2 \end{bmatrix} \), if \( A_1^{-1} \) and \( A_2^{-1} \) exists then
\[
(3.2.3) \quad \text{tr } C^{-1} = \text{tr } A_1^{-1} + \text{tr } E^{-1} E^T + \text{tr } D^{-1},
\]
where \( D = A_2 - B^T A_1^{-1} B \) and \( E = A_1^{-1} B \). Thus (3.2.3) gives
\[
f(1, 1, -1) = 1.2716 > 1.2 \quad \text{and} \quad f(1, 1, 1) = 1.213 > 1.2.
\]

Case 3. \( Z(X) = 2 \). Let \( V \) be the matrix obtained from \( X \) by replacing the two zeros in \( X \) by 1. By the (above) result of Ehlich, we may assume that
\[
(3.2.4) \quad V^T V = \begin{bmatrix} P & Q \\ Q^T & R \end{bmatrix},
\]
where \( P \in M_{s \times s} \), \( R \in M_{(n-s) \times (n-s)} \), \( P_{ij} \equiv 2 \pmod{4}, \quad r_{ij} \equiv 2 \pmod{4} \).
\( q_{ij} \equiv 0 (\text{mod} \ 4) \). Now \( t = 34 \), \( b(t,a) = 234.147 \).

Case 3.0. \( s = 0 \). Applying some basic operations on columns of \( X \), we may assume that

\[
C = \begin{bmatrix}
5 & * \\
\text{} & a \\
\text{} & 6 \\
\text{} & e_{ij} \\
\text{} & d_{ij}
\end{bmatrix}
\]

(3.2.5)

where \( a \equiv 0 (\text{mod} \ 4) \), \( |e_{ij}| \geq 1 \), \( |d_{ij}| \geq 2 \). Thus

\[
\text{tr} \ C^2 = 2 \times 5^2 + 4 \times 6^2 + 12 \times 2^2 = 258 > 234.
\]

By Theorem 3.2.2, \( \text{tr} \ C^{-1} \geq 1.2 \).

Case 3.1. \( s' = 1 \).

Case 3.1.1. Suppose that the two zero entries of \( X \) lie on the same row of \( X \) (and do not lie on column \( X_1 \)). Applying some basic operations on the columns of \( X \), we may assume that

\[
C = \begin{bmatrix}
6 & * & * & * \\
\text{} & 5 & * \\
\text{} & b_{ij} & c_{ij} & 5 \\
\text{} & e_{ij} & d_{ij} \\
\text{} & q_{ij} & 6
\end{bmatrix}
\]

(3.2.6)

where \( |b_{ij}| \geq 1 \), \( |c_{ij}| \geq 1 \), \( |e_{ij}| \geq 1 \), \( q_{ij} \equiv 0 (\text{mod} \ 4) \), \( |d_{ij}| \geq 2 \).

Therefore,

\[
\text{tr} \ C^2 = 4 \times 6^2 + 2 \times 5^2 + 18 \times 1 + 6 \times 2^2 = 236 > 234.
\]

By Theorem 3.2.2, \( \text{tr} \ C^{-1} \geq 1.2 \).
Case 3.1.2. Suppose that the two zero entries of $X$ lie in
different rows of $X$ (and do not lie on column $X_1$). Repeating the
argument in Case 3.1.1, we obtain (3.2.6), except all $|c_{ij}| > 0$ and
therefore $\text{tr} \ C^2 > 234$. Theorem 3.2.2 allows us to assume $\text{tr} \ C^2 = 234$
the minimum $\text{tr} \ C^2$ in this setting. By applying some basic operations
on the columns of $X$,

(3.2.7) \[ C = \begin{bmatrix}
 A_1 & & & & \\
 0 & d_1 & d_4 & & \\
 0 & d_2 & d_5 & A_2 & \\
 0 & d_3 & d_6 & &
\end{bmatrix} \]

where

\[ A_1 = \begin{bmatrix}
 6 & 1 & 1 \\
 1 & 5 & 0 \\
 1 & 0 & 5
\end{bmatrix}, \quad A_2 = \begin{bmatrix}
 6 & 2 & 2 \\
 2 & 6 & c \\
 2 & c & 6
\end{bmatrix}, \quad c = \pm 2, \quad |d_4| = 1 \]

By (3.2.2), $\text{tr} \ A_1^{-1} = \frac{83}{140}$, $\text{tr} \ A_2^{-1} = \frac{12}{18 + c}$. If $c = -2$, then

$\text{tr} \ A_1^{-1} + \text{tr} \ A_2^{-1} = \frac{83}{140} + \frac{3}{4} = \frac{47}{35} > 1.2$

and therefore Ky Fan's majorization theorem $\text{tr} \ C^{-1} > 1.2$. So we may
assume that $c = 2$. Thus

(3.2.8) \[ C = \begin{bmatrix}
 6 & 1 & 1 & 0 & 0 & 0 \\
 1 & 5 & 0 & d_1 & d_2 & d_3 \\
 1 & 0 & 5 & d_4 & d_5 & d_6 \\
 0 & d_1 & d_4 & 6 & 2 & 2 \\
 0 & d_2 & d_5 & 2 & 6 & 2 \\
 0 & d_3 & d_6 & 2 & 2 & 6
\end{bmatrix}, \quad |d_4| = 1 \]

Suppose that $d_4, d_5, d_6$ are not all equal. Let
\[ A_1 = \begin{bmatrix} 6 & 1 \\ 1 & 5 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 5 & d_4 & d_5 & d_6 \\ d_4 & 6 & 2 & 2 \\ d_5 & 2 & 6 & 2 \\ d_6 & 2 & 2 & 6^* \end{bmatrix}. \]

Up to similarity (and symmetry) of \( C \) we may assume \( d_4^* d_5 = 1, \ d_6^* = -1. \)

By Ky Fan's majorization theorem
\[
\text{tr} \ C^{-1} \geq \text{tr} \ A_1^{-1} + \text{tr} \ A_2^{-1} = \frac{11}{31} + \frac{75}{86} > 1.2.
\]

So we may assume that \( d_4 = d_5 = d_6^* \). Let
\[
A_1 = \begin{bmatrix} 5 & 0 & d_1 & d_2 \\ 0 & 5 & d_4 & d_5 \\ d_1 & d_4 & 6 & 2 \\ d_2 & d_5 & 2 & 6 \\ d_3 & d_6 & 2 & 2 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 5 & 0 & 1 & 1 \\ 0 & 5 & 1 & 1 \\ 1 & 1 & 6 & 2 \\ 1 & 1 & 2 & 6 \\ s & 1 & 2 & 2 \end{bmatrix}.
\]

Up to similarity of \( C \), we may assume
\[
A_2 = \begin{bmatrix} 5 & 0 & 1 & 1 \\ 0 & 5 & 1 & 1 \\ 1 & 1 & 6 & 2 \\ 1 & 1 & 2 & 6 \\ s & 1 & 2 & 2 \end{bmatrix}, \quad s = \pm 1.
\]

Then
\[
\text{tr} \ C^{-1} \geq \text{tr} \ A_1^{-1} + \text{tr} \ A_2^{-1} = \begin{cases} 797/660 & \text{if } s = 1 \\ 3050/2424 & \text{if } s = -1 \end{cases} > 1.2.
\]

Case 3.1.3. Suppose that one of the zero entries of \( X \) lies in \( \tilde{X}_1 \). Applying some basic operations on the columns of \( X \) we may assume (3.2.5) and carry on arguments from there.
Case 3.2. $s = 2$.

Case 3.2.1. Suppose that both zero entries of $X$ lie on $[\bar{X}_3, \bar{X}_4, \bar{X}_5, \bar{X}_6]$. Applying some basic operations on the columns of $X$, we may assume that

$$C = \begin{bmatrix}
6 & 2 & * & * \\
2 & 6 & & \\
& & 5 & h & * \\
& & h & 5 & \\
& & e_{ij} & 6 & 2 \\
& & e_{ij} & 2 & 6 \\
\end{bmatrix}$$

(3.2.9)

where $|b_{ij}| \geq 1$, $|e_{ij}| \geq 1$, $|q_{ij}| \geq 0$. Now,

$$\text{tr } C^2 \geq 2 \times 5^2 + 4 \times 6^2 + 4 \times 2^2 + 16 \times 1 = 226.$$  

If any one of $|b_{ij}|$, $|e_{ij}|$ is not equal to 1, then

$$\text{tr } C^2 \geq 226 + 2(3^2-1) = 242 > 234$$

whence by Theorem 3.2.2, $\text{tr } C^{-1} \geq 1.2$. Similarly, if any one of the $q_{ij}$ is not zero then

$$\text{tr } C^2 \geq 226 + 2(4^2-1) = 256 > 234,$$

and Theorem 3.2.2 again implies $\text{tr } C^{-1} \geq 1.2$. So we may assume that all $|b_{ij}| = 1$, $|e_{ij}| = 1$, $q_{ij} = 0$. Thus applying some basic operations on the columns of $X$, we may write (3.2.9) as

$$C = \begin{bmatrix}
r_1 & 0 & 0 & \\
& A_1 & 0 & 0 \\
& & r_2 & 0 \\
& & & h \\
& & & r_3 \\
& & & & r_4 \\
r_1 & r_2 & h & \\
0 & 0 & r_3 & A_2 \\
0 & 0 & r_4 & \\
\end{bmatrix}$$

(3.2.10)
where
\[
A_1 = \begin{bmatrix} 6 & c_1 & 1 \\ c_1 & 6 & 1 \\ 1 & 1 & 5 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 5 & 1 & 1 \\ 1 & 6 & c_2 \\ 1 & c_2 & 6 \end{bmatrix},
\]
and \( c_1 = \pm 2, \quad r_1 = \pm 1 \). If \(|h| < 3\) then
\[
\text{tr} \ C^2 \geq 225 + 2 \times 3^2 = 244 > 234;
\]
so Theorem 3.2.2 shows \( \text{tr} \ C^{-1} \geq 1.2 \). If \(|h| = 2\) then by Ky Fan's majorization theorem and (3.2.9)
\[
\text{tr} \ C^{-1} \geq \text{tr} \left( \begin{bmatrix} 6 & 2 \\ 2 & 6 \end{bmatrix} \right)^{-1} + \text{tr} \left( \begin{bmatrix} 5 & h \\ h & 5 \end{bmatrix} \right)^{-1} + \text{tr} \left( \begin{bmatrix} 6 & 2 \\ 2 & 6 \end{bmatrix} \right)^{-1}
\]
\[
= \frac{12}{32} + \frac{10}{25-h^2} + \frac{12}{32}
\]
\[
= \frac{103}{84} > 1.2.
\]
So we may assume \( h = 0 \) or \( \pm 1 \). Now as before, \( \text{tr} \ A_1^{-1} = \frac{45}{74 + c_1} \), \( \text{tr} \ A_2^{-1} = \frac{45}{74 + c_2} \). If any one of the \( c_i \)'s is equal to \( -2 \) we have
\[
\text{tr} \ C^{-1} \geq \text{tr} \ A_1^{-1} + \text{tr} \ A_2^{-1} = \frac{45}{74 - 2} + \frac{45}{74 + 2} = \frac{185}{152} > 1.2.
\]
Thus we may assume \( c_1 = c_2 = 2 \) and
\[
(3.2.11) \quad C = \begin{bmatrix} 6 & 2 & 1 & r_1 & 0 & 0 \\ 2 & 6 & 1 & r_2 & 0 & 0 \\ 1 & 1 & 5 & h & r_3 & r_4 \\ r_1 & r_2 & h & 5 & 1 & 1 \\ 0 & 0 & r_3 & 1 & 6 & 2 \\ 0 & 0 & r_4 & 1 & 2 & 6 \end{bmatrix}, \quad |r_i| = 1, \quad |h| = 0 \text{ or } 1.
\]
If \( r_3 = 1 = -r_4 \), then
\[
\text{tr } C^{-1} \geq \text{tr } \begin{bmatrix} 6 & 2 \\ 2 & 6 \end{bmatrix}^{-1} + \text{tr } \begin{bmatrix} 5 & h & 1 & -1 \\ h & 5 & 1 & 1 \\ 1 & 1 & 6 & 2 \\ -1 & 1 & 2 & 6 \end{bmatrix}^{-1} = \begin{cases} 
1.217 & \text{if } h = 0 \\
1.239 & \text{if } h = \pm 1.
\end{cases}
\]

Thus \( \text{tr } C^{-1} > 1.2 \). If \( r_1 = -r_2 = 1 \), a similar argument also gives
\( \text{tr } C^{-1} > 1.2 \). Thus we may assume \( r_1 = r_2 = \pm 1 \) and \( r_3 = r_4 = \pm 1 \).

By multiplying, if necessary, the first three rows and first three columns of \( C \) by \(-1\), we may assume \( r_1 = r_2 = 1 \). Suppose that
\( r_3 = r_4 = 1 \). Then we have

\[
C = \begin{bmatrix}
B_1 & B_2 & B_3 \\
B_2 & B_4 & B_5 \\
B_3 & B_5 & B_6
\end{bmatrix},
\]

where \( B_1 = \begin{bmatrix} 6 & 2 \\ 2 & 6 \end{bmatrix} \), \( B_2 = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \), \( B_3 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \), \( B_4 = \begin{bmatrix} 5 & h \\ h & 5 \end{bmatrix} \), \( h = 0, \pm 1 \), \( B_5 = B_2 \), \( B_6 = B_1 \). The subring \( S \) of \( M_{2\times2} \) generated
by \( I_2 \) and the \( B_i \)'s is commutative. So, one can easily find the
characteristic polynomial \( \phi \) of \( C \) over \( S \):

\[
\phi(\lambda) = (\lambda - B_1)(\lambda - B_4)(\lambda - B_1) - B_2^2 + B_2[-B_2(\lambda - B_6)] \\
= (\lambda - B_1)[\lambda^2 - (B_1 + B_4)\lambda + B_1B_4 - ZB_2^2].
\]

(3.2.13)

So one eigenvalue \( \lambda_1 \) of \( \phi \) is \( B_1 \). The zeros of the characteristic
polynomial of \( B_1 \) (over the real field) give two eigenvalues \( \lambda_1, \lambda_2 \)
for \( C \): \( \lambda_1 = 6 - 2 = 4 \), \( \lambda_2 = 6 + 2 = 8 \). By (3.2.13),
\[ \phi(\lambda)/(\lambda - B_1) = \lambda^2 - \begin{bmatrix} 11 & 2+h \\ 2+h & 11 \end{bmatrix} \lambda + \begin{bmatrix} 26+2h & 6+6h \\ 6+6h & 26+2h \end{bmatrix} \]

\[ = \begin{bmatrix} \lambda^2 - 11\lambda + 26 + 2h & - (2+h)\lambda + 6 + 6h \\ -(2+h)\lambda + 6 + 6h & \lambda^2 - 11\lambda + 26 + 2h \end{bmatrix} \]

Taking the determinant of \( \phi(\lambda)/(\lambda - B_1) \), we obtain the polynomial \( f(\lambda) \) whose zeros \( \lambda_3, \lambda_4, \lambda_5, \lambda_6 \) are the remaining eigenvalues of \( C \):

For real \( \lambda \),

\[ f(\lambda) = \det[\phi(\lambda I)/(\lambda I - B_1)] \]

\[ = \lambda^4 + a\lambda^3 + b\lambda^2 + c\lambda + d, \]

where \( c = 4(3h^2 - 2h - 137), \) \( d = 32(4 + h)(5 - h). \) So

\[ \frac{1}{\lambda_3} + \frac{1}{\lambda_4} + \frac{1}{\lambda_5} + \frac{1}{\lambda_6} = -\frac{c}{d} = \frac{137 + 2h - 3h^2}{8(4 + h)(5 - h)}. \]

Thus,

\[ \text{tr } C^{-1} = \frac{1}{4} + \frac{1}{8} + \frac{137 + 2h - 3h^2}{8(4 + h)(5 - h)} \]

\[ = \begin{cases} 197/160 & \text{if } h = 0 \\ 49/40 & \text{if } h = 1 \\ 31/24 & \text{if } h = -1 \end{cases} > 1.2. \]

So we may assume that \( r_3 = r_4 = -1 \). By multiplying \( \vec{x}_5 \) by \(-1\), we obtain (3.2.13) with

\[ B_1 = \begin{bmatrix} 6 & 2 \\ 2 & 6 \end{bmatrix}, \quad B_2 = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad B_3 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, \quad B_4 = \begin{bmatrix} 5 & h \\ h & 5 \end{bmatrix}, \]

\( h = 0, \pm 1 \). \( B_5 = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad B_6 = \begin{bmatrix} 6 & -2 \\ -2 & 6 \end{bmatrix}. \) The \( B_1 \)'s are commutative with one another. So the preceding method is applicable!

We obtain \( \text{tr } C^{-1} = 1.222 \text{ if } h = 0; \text{ tr } C^{-1} = 1.2468 \text{ if } h = \pm 1 \).
Case 3.3. $s = 3$.

Case 3.3.1. Suppose that both zero entries of $X$ lie in $[\bar{X}_1, \bar{X}_2, \bar{X}_3]$. In terms of arguments and consequences, this is the same as Case 3.1.2.

Case 3.3.2. Suppose that both zero entries of $X$ lie in $[\bar{X}_4, \bar{X}_5, \bar{X}_6]$. By interchanging columns $\bar{X}_1, \bar{X}_2, \bar{X}_3$ with $\bar{X}_4, \bar{X}_5, \bar{X}_6$, this is Case 3.3.1.

Case 3.3.3. Suppose that exactly one zero entry of $X$ lies in $[\bar{X}_1, \bar{X}_2, \bar{X}_3]$. Applying some basic operations on the columns of $X$, we obtain (3.2.9) and carry on arguments from there.

Case 4. $Z(X) = 3$. Here $t = 33$ and $b(t,a) < 210$. We may assume that each of the first three columns of $X$ contains one zero

Then as before we may write

$$C = \begin{bmatrix}
5 & * \\
5 & a_2 \\
a_1 & 5 \\
8 & 3 & 5 \\
| & | & | \\
b_1 & \phantom{b_1} & b_7 \\
b_2 & \phantom{b_2} & b_8 \\
b_3 & \phantom{b_3} & b_9 \\
\end{bmatrix},$$

where $|b_i| \geq 1$ and $V$ is (3.2.4) with $n = 3$. Thus there are at least two $v_{ij}$'s with $i \neq j$, $|v_{ij}| = 2$. Therefore

$$\text{tr } C^2 \geq 3 \times 5^2 + 3 \times 6^2 + 2 \times 9 + 2 \times 2^2 = 209.$$  

By Theorem 3.2.2, we may assume $\text{tr } C^2 = 209$. In this case we may write
The matrix $C$ is given by:

$$
C = \begin{bmatrix}
5 & 0 & 0 & b_1 & b_2 & b_3 \\
0 & 5 & 0 & b_4 & b_5 & b_6 \\
0 & 0 & 5 & b_7 & b_8 & b_9 \\
b_1 & b_4 & b_7 & 6 & 2 & 0 \\
b_2 & b_5 & b_8 & 2 & 6 & 0 \\
b_3 & b_6 & b_9 & 0 & 6 & 0
\end{bmatrix}, \quad |b_1| = 1.
$$

Let

$$
P = \begin{bmatrix}
A_1 & B \\
B^T & A_2
\end{bmatrix}, \quad Q = [6],
$$

where

$$
A_1 = \begin{bmatrix}
5 & 0 & 0 \\
0 & 5 & 0 \\
0 & 0 & 5
\end{bmatrix}, \quad B = \begin{bmatrix}
b_1 & b_2 \\
b_4 & b_5 \\
b_7 & b_8
\end{bmatrix}, \quad A_2 = \begin{bmatrix}
6 & 2 \\
2 & 0
\end{bmatrix}.
$$

By (3.2.3)

$$
\text{tr } P^{-1} = \frac{3}{5} + \frac{2(b_1^2 + a^2 - 10a)}{5(629+20a-a^2)^2} + \frac{270}{629 + 20a - a^2},
$$

where $a = b_1 b_2 + b_4 b_5 + b_7 b_8$.

Since $|a| = 1$, we have

$$
\text{tr } P^{-1} = \frac{3}{5} + \frac{2(b_1^2 - 10a)}{5(628+20a)} + \frac{270}{628 + 20a}
\geq \frac{3}{5} + \frac{2(72)}{5(648)} + \frac{270}{648}.
$$

By Ky Fan's majorization theorem,

$$
\text{tr } C^{-1} \geq \text{tr } P^{-1} + \text{tr } Q^{-1} \geq \frac{3}{5} + \frac{144}{5(648)} + \frac{270}{648} + \frac{1}{6} = 1.2277 > 1.2.
$$

Case 5. $Z(X) = 4$. Here $t = 32$, $b(t, a) < 188$.

We may assume that each of $\bar{x}_1, \bar{x}_2, \bar{x}_3$ and $\bar{x}_4$ contains a zero. So
where \( |c_{ij}| \geq 1 \), \(|c| \geq 0\). Thus
\[
\text{tr } C^2 \geq 4 \times 5^2 + 2 \times 6^2 + 16 \times 1 = 188 > b(t,a) .
\]
By Theorem 3.2.2, \( \text{tr } C^{-1} \geq 1.2 \).

Case 6. \( Z(X) = 5 \). Here \( t = 31 \), \( b(t,a) < 168 \).

We may assume that the first five columns of \( X \) each contain one zero. So
\[
C = \left[ \begin{array}{ccccc}
5 & * & & & \\
5 & * & & & \\
5 & * & & & \\
* & 5 & & & \\
- & - & - & - & - \\
\end{array} \right]
\]
where \( |r_{ij}| \geq 1 \). Thus
\[
\text{tr } C^2 \geq 5 \times 5^2 + 6^2 + 10 \times 1 = 171 > 168 .
\]
By Theorem 3.2.2, \( \text{tr } C^{-1} \geq 1.2 \).

Case 7. \( Z(X) = 6 \). Then by Theorem 3.2.1, \( \text{tr } C^{-1} \geq \frac{36}{30} = 1.2 \).

This completes part A.

Part B: \( N = 10, n < 6 \).

Let \( X \in \mathcal{C}(10,n) \). By Theorem 3.1.1, we may assume \( X \) has \( k \) zero entries \( k \geq 1 \). From table (3.2.1) the cases
\[ n = 3, k \geq 1; n = 4, k \geq 2; n = 5, k \geq 3; n = 6, k \geq 4 \]
follow from Theorem 3.2.1.

Let \( n = 4 \) and \( k = 1 \). Then \( a = 0.41666, b(t, a) < 387 \). By Lemma 2.3.4 of Ehlich we may assume that
\[
X^T X = \begin{bmatrix}
9 & a_1 & a_2 & a_3 \\
10 & c & \\
& 10 & \\
\end{bmatrix}, \quad |a_i| \geq 1, |c| > 2. \]
Thus \( \text{tr}(X^T X)^2 \geq 9^2 + 3 \times 10^2 + 6 \times 1^2 + 2 \times 2^2 = 395 > b(t, a) \).
Therefore, by Theorem 3.2.2, \( \text{tr}(X^T X)^{-1} \geq a \).

Let \( n = 5 \) and \( k = 1 \). Then \( a = 0.52976, b(t, a) < 504 \).
Again by Ehlich's result we may assume that
\[
X^T X = \begin{bmatrix}
9 & a_1 & a_2 & a_3 & a_4 \\
10 & c_1 & \\
10 & c_2 & \\
10 & c_3 & \\
\end{bmatrix}, \quad |a_i| \geq 1; |c_i| \geq 2, \text{ for at least two values of } i. \]
So \( \text{tr}(X^T X) > 9^2 + 4 \times 10^2 + 8 \times 1^2 + 4 \times 2^2 = 505 > b(t, a) \). Theorem 3.2.2 then applies.

Let \( n = 5 \) and \( k = 2 \). Then \( b(t, a) < 471 \). By Lemma 2.3.4, we may assume
\[
X^T X = \begin{bmatrix}
9 & \cdots & a_{ij} & \\
10 & c & \\
10 & c & \\
& 10 & \\
\end{bmatrix}, \quad |a_{ij}| \geq 1, |c| \geq 2 \]
or

\[
X^TX = \begin{bmatrix}
8 & a_j & \\
10 & c_1 & \\
10 & c_2 & \\
10 & c_3 & \\
10 & & \\
\end{bmatrix}, \quad |a_j| > 1; \quad |c_i| > 2,
\]

for at least two values of \( i \).

In either case, \( \text{tr}(X^TX)^2 \geq 480 > b(t,a) \). Hence by Theorem 3.2.2, \( \text{tr}(X^TX)^{-1} \geq a \).

Let \( n = 6 \). We may assume that the zero entries of \( X \) appear in distinct columns. Indeed, suppose that the first column of \( X \) has two or more zero entries. Then we may write

\[
X^TX = \begin{bmatrix}
m & * \\
* & C
\end{bmatrix}, \quad m \leq 8,
\]

therefore, by Ky Fan's majorization theorem and the result for the case \( n = 5 \), we have

\[
\text{tr}(X^TX)^{-1} \geq \text{tr}(m)^{-1} + \text{tr}(C)^{-1} \geq \frac{1}{8} + 0.52976 > 0.64286 = a.
\]

Let \( k = 1 \). Then \( b(t,a) < 625 \). Thus we may assume

\[
\text{tr}(X^TX)^2 \leq 624.
\]

Therefore by Ehlich's Lemma we may assume

\[
X^TX = \begin{bmatrix}
9 & a_1 & a_2 & a_3 & a_4 & a_5 \\
10 & c_1 & \\
10 & & \\
10 & c_2 & c_3 & \\
10 & c_4 & \\
\end{bmatrix}, \quad |a_1| = 1, \quad |c_i| = 2.
\]

Up to similarity we may assume \( a_1 = a_2 = 1, \quad c_2 = c_3 = 2 \). Then by
Ky Fan's theorem we have
\[
\text{tr}(X^TX)^{-1} \geq \text{tr}
\begin{bmatrix}
9 & 1 & 1 \\
1 & 10 & c_1 \\
1 & c_1 & 10
\end{bmatrix}^{-1} + \text{tr}
\begin{bmatrix}
10 & 2 & 2 \\
2 & 10 & c_4 \\
2 & c_4 & 10
\end{bmatrix}^{-1}
\]
\[
= \frac{137}{422+c_1} + \frac{36}{110+c_2} \geq \frac{137}{424} + \frac{36}{112} = .64453 > a.
\]

Let \( k = 2 \). Then \( b(t,a) < 588 \). By Ehlich's result we assume
\[
X^TX =
\begin{bmatrix}
9 & a_{1j} & \cdots & \cdots \\
\vdots & \ddots & \ddots & \cdots \\
\vdots & \cdots & \ddots & \cdots \\
\vdots & \cdots & \cdots & 10
\end{bmatrix}
\]
\[|a_{ij}| \geq 1; |c_i| \geq 2, \]
for at least two values of \( i \).

So \( \text{tr}(X^TX)^2 \geq 2 \times 9^2 + 4 \times 10^2 + 16 \times 1^2 + 4 \times 2^2 = 594 > b(t,a) \).

Let \( k = 3 \). Then \( b(t,a) < 554 \). As above we may assume
\[
X^TX =
\begin{bmatrix}
9 & a_{1j} & \cdots & \cdots \\
\vdots & \ddots & \ddots & \cdots \\
\vdots & \cdots & \ddots & \cdots \\
\vdots & \cdots & \cdots & 9
\end{bmatrix}
\]
\[|a_{ij}| \geq 1; |c| \geq 2, \]

So \( \text{tr}(X^TX)^2 \geq 3 \times 9^2 + 3 \times 10^2 + 18 \times 1^2 + 2 \times 2^2 = 569 > b(t,a) \).

This completes Part B.

Part C: \( N > 10 \) (\( N \equiv 2 \pmod{4} \)), \( n \leq 6 \).

For \( 14 \leq N \leq 42 \), one can proceed as in the case \( N = 10 \).

The proofs are similar and easier. The cases \( N \geq 46 \) and \( n \leq 6 \)
follow from the following lemma and Theorems 3.2.1 and 3.1.1.

Lemma 3.2.1. Let $N \geq 46$, $n \leq 6$, $X \in \mathcal{D}(N,n)$, $\text{tr}(X^TX) \leq nN - 1$.

Then $\text{tr}(X_2^T X_2)^{-1} \leq \frac{n}{n^2} \frac{N}{\text{tr}(X^TX)}$.

Proof. Let $a = \text{tr}(X_2^T X_2)^{-1}$ and $t = \text{tr}(X^TX)$. Suppose first that $n$ is even. Then $a = \frac{n - 2}{N - 2} + \frac{2}{N + n - 2}$. Now at $\leq n^2$ provided

$$
\left[\frac{n - 2}{N - 2} + \frac{2}{N + n - 2}\right] (nN - 1) \leq n^2.
$$

On simplifying the latter inequality we obtain that at $\leq n^2$: if $2n^2 - 5n + 4 \leq N$. Since

$$
\max_{0 \leq n \leq 6} (2n^2 - 5n + 4) = 46,
$$

the result is proven for $n$ even.

Suppose now that $n$ is odd. Then $a = \frac{n-2}{N-2} + \frac{1}{N+n-1} + \frac{1}{N+n-3}$.

On taking $n = 1, 3, 5$ one can easily show that at $\leq n^2$ for $N \geq 46$.

This completes the proof of Theorem 3.2.3.

The above proof suggests that the desired result for $\mathcal{D}(N,n)$ can be proved with the help of the results for $\mathcal{D}(N, n-1)$.

By the above proof of Theorem 3.2.3 (and Theorem 3.2.2), up to similarity of $X^TX$ there are two $A$-optimal designs in $\mathcal{D}(6,6)$.

Let

$$
X_2 = \begin{bmatrix}
1 & 1 & -1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 & -1 & 1 \\
1 & 1 & 1 & 1 & -1 & -1 \\
1 & 1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & -1 & -1 & 1 \\
1 & -1 & 1 & 1 & 1 & -1
\end{bmatrix},

Z_2 = \begin{bmatrix}
0 & 1 & 1 & -1 & 1 & -1 \\
1 & 0 & -1 & 1 & 1 & -1 \\
1 & -1 & 0 & -1 & -1 & -1 \\
1 & -1 & 1 & 0 & 1 & 1 \\
1 & 1 & -1 & 1 & 0 & 1 \\
1 & 1 & 1 & 1 & -1 & 0
\end{bmatrix}.
$$
Then \( X_2^T X_2 = \begin{bmatrix} 4I_3 + 2I_3 & 0 \\ 0 & 4I_3 + 2I_3 \end{bmatrix} \) and \( Z_2^T Z_2 = 5I_6 \).

So \( \text{tr}(X_2^T X_2)^{-1} = \text{tr}(Z_2^T Z_2)^{-1} = 1.2 \). Thus both \( X_2 \) and \( Z_2 \) are A-optimal in \( \mathcal{D}(6,6) \). Therefore, A-optimal designs in \( \mathcal{D}(6,6) \), are not unique. Statisticians may prefer the design \( Z_2 \) over \( X_2 \) because \( Z_2 \) is, by Theorem 2.7 of Jacroux, Wong and Masaro [18], E-optimal.

With Theorem 3.2.3, we can prove the E-optimality of \( Z_2 \) in an obvious way: Let \( W \in \mathcal{D}(6,6) \) and let \( \{ \mu_i \} \) be the eigenvalues of \( W^T W \), where \( \mu_1 \leq \mu_2 \leq \ldots \leq \mu_6 \). Then

\[
(3.2.14) \quad 1.2 \leq \text{tr}(W^T W)^{-1} = \sum_{i=1}^{6} \frac{1}{\mu_i} \leq \frac{6}{\mu_1} .
\]

So \( \mu_1 \leq 5 \). \( Z_2 \) shows that it is possible that \( \mu_1 = 5 \). Hence \( Z_2 \)

is E-optimal. In weighing designs, using \( Z_2 \) means that every object can take a single break (i.e. not to be weighed) at different weighings. If \( 3 \leq n < 6 \) and \( Y \in \mathcal{D}(6,n) \) is formed from any \( n \) columns of \( Z_2 \), then from Theorem 2.7 of Jacroux, Wong and Masaro [18], \( Y \) is uniquely E-optimal. Further any \( X_2 \in \mathcal{D}(6,n) \) satisfying (3.1.1) is uniquely A-optimal. This shows that A-optimality does not, in general, imply E-optimality and vice-versa. Also, Theorem 3.2.3 and therefore conjecture (C1) is not an obvious statement to make. To see this, we note that Cheng [5] proved that \( X_2 \) in (3.1.1) is E-optimal over \( \mathcal{D}^+(N,n) \) (\( N \equiv 2 \pmod{4} \)). But it turns out that this, \( X_2 \) is not E-optimal over \( \mathcal{D}(N,n) \). So, it is not automatic that an optimal \( X \) over \( \mathcal{D}^+(N,n) \) will be optimal over \( \mathcal{D}(N,n) \). However, D-optimal \( X \) over \( \mathcal{D}^+(N,n) \) is automatically D-optimal over \( \mathcal{D}(N,n) \).

Galil and Kiefer [13] remark that \( X_2 \) in (3.1.1) is D-optimal and ask
if it has any other optimality properties. Our conjecture says that 
X_2 is also A-optimal in D(N,n).

We will see in Section 3.3 that for each n there exists an 
N_0(n) such that X_2 is A-optimal in D(N,n) if N \geq N_0(n).

3.3. \( \Phi \)-optimal Designs in D(N,n).

Let X_2 and Z_2 be as in Section 1.3 (p.10) Cheng (private 
communication) noted that when N=n X_2 and Z_2 have the same 
performance under A-criterion and that X_2 is \( \Phi_p \)-better than Z_2 for 
0 \leq p < 1 and Z_2 is \( \Phi_p \)-better than X_2 for p > 1. When N > n 
evidence suggests that X_2 is \( \Phi_p \)-optimal for 0 \leq p \leq 1. However, 
X_2 is not \( \Phi_p \)-optimal for all p > 1 since it is not E-optimal. In 
fact for N=6, n=4, \( \Phi_3(X_2^T X_2) = .206 > .2 = \Phi_3(Z_2^T Z_2) \). Further Z_2 
may not be \( \Phi_p \)-optimal for p > 1 since, for example, if N=6, n=4, 
\( \Phi_2(X_2^T X_2) = .197 < .2 = \Phi_2(Z_2^T Z_2) \). The above discussion suggests the 
following conjecture

(C2) For any N \geq n, N \equiv 2(mod 4) there exists a number 
\( \alpha(N,n) \geq 1 \) such that \( \alpha(N,N) = 1 \) and X_2 is \( \Phi_p \)-optimal 
for 0 \leq p \leq \alpha(N,n) and Z_2 is \( \Phi_p \)-optimal for 
p \geq \alpha(N,n).

The following theorem shows that X_2 is \( \Phi_p \)-optimal for 
0 \leq p \leq 1 if N is sufficiently larger than n and hence supports 
conjecture (C2). The case p = 1 was found independently by Cheng, 
and Wong and Masaro; the extension to the case 0 \leq p \leq 1 is due to 
Cheng (see Cheng, Masaro and Wong [7]).
Theorem 3.3.1. For any \( n \), there exists \( N_0(n) \) such that if
\[
N \geq N_0(n),
\]
then \( X_2 \) is \( \Phi_p \)-optimal over \( \mathcal{S}(N,n) \) for all \( 0 \leq p \leq 1 \).

Proof. In Theorem 3.1.1 it was shown that \( X_2 \) is optimal over \( \mathcal{S}(N,n) \)
with respect to all the type 1 criteria \( \Phi_p \), such that \( f(0^+) = +\infty \);
in particular it is \( \Phi_p \)-optimal for all \( p \geq 0 \). So it suffices to
consider matrices \( C \in C(N,n) \setminus C'(N,n) \). We have to show that there
exists an integer \( N_0 \) such that if \( N \geq N_0 \), then for any
\( C \in C(N,n) \setminus C'(N,n) \), \( \Phi_p(C) > \Phi_p(X_2^T X_2) \) for all \( 0 \leq p \leq 1 \).

Now if \( C \in C(N,n) \setminus C'(N,n) \), then \( \text{trace} C \leq Nn - 1 \). Since
\[
\text{trace}(n^{-1}(Nn - 1)I_n) = Nn - 1 \quad \text{by Proposition 1' of Kiefer [24]},
\]
we have
\[
(3.3.1) \quad \Phi_p(C) \geq \Phi_p(n^{-1}(Nn - 1)I_n) \quad \text{for all } p \geq 0.
\]

By a direct comparison of \( \text{trace}(n^{-1}(Nn - 1)I_n)^{-1} = n^2/(Nn - 1) \) with
\[
\text{trace}(X_2^T X_2)^{-1} = \begin{cases}
(n-2)/(N-2) + 2/(N+n-2) & \text{if } n \text{ is even}, \\
(n-2)/(N-2) + 1/(N+n-1) + 1/(N+n-3) & \text{if } n \text{ is odd},
\end{cases}
\]
one can easily show that there exists an integer \( N_0 \) such that
\[
(3.3.2) \quad N \geq N_0 \Rightarrow \Phi_1(n^{-1}(Nn - 1)I_n) > \Phi_1(X_2^T X_2).
\]

Now let \( \mu_1^*, \mu_2^*, \ldots, \mu_n^* \) be the eigenvalues of \( X_2^T X_2 \). Then
\[
\Phi_p(X_2^T X_2) = \left\{ n^{-1} \sum_{i=1}^{n} (\mu_i^*)^{-p} \right\}^{1/p}
\]
is an increasing function of \( p > 0 \).

Since all the eigenvalues of \( n^{-1}(Nn - 1)I_n \) are equal, we have
\[
\Phi_p(n^{-1}(Nn - 1)I_n) = n/(Nn - 1) \quad \text{for all } p > 0.
\]
By (3.3.2), if \( N \geq N_0 \) and \( 0 < p \leq 1 \), then
\[
\Phi_p(X_2^T X_2) \leq \Phi_1(X_2^T X_2) \leq \Phi_p(n^{-1}(Nn - 1)I_n) = \Phi_p(n^{-1}(Nn - 1)I_n).
\]
Combining this with (3.3.1), we conclude that if \( N \geq N_0 \), then \( X_2 \) is \( \Phi_p \)-optimal over \( \mathcal{O}(N,n) \) for all \( 0 < p \leq 1 \). The D-optimality (\( p = 0 \)) is obtained by passing to the limit.

We remark that if \( N_0^*(n) \) is the smallest integer such that \( N \geq N_0^*(n) \) implies \( X_2 \) is \( \Phi_p \)-optimal over \( \mathcal{O}(N,n) \) for \( 0 \leq p \leq 1 \), then, by the above proof, an upper bound for \( N_0^*(n) \) can be obtained by comparing \( \text{tr}(X_2^T X_2)^{-1} \) with \( \text{tr}[(Nn - 1)^{-1}I_n] \). This upper bound is usually quite large. For example if \( n = 6 \), Lemma 3.2.1 shows that \( N_0^*(n) \leq 46 \). So by Theorem 3.3.1, \( X_2 \) is \( \Phi_p \)-optimal over \( \mathcal{O}(N,6) \) for \( 0 \leq p \leq 1 \) and \( N \geq 46 \).

Note that, in general, we cannot conclude that if \( X_2 \) is \( A \)-optimal over \( \mathcal{O}(N,n) \) then it is \( \Phi_p \)-optimal, \( 0 \leq p \leq 1 \). Indeed, the above proof only shows this to be the case if \( \text{tr}(X_2^T X_2)^{-1} \leq \text{tr}[(Nn - 1)^{-1}I_n] \). Hence if \( N_0(n) \) is the smallest integer \( n \) such that \( N \geq N_0(n) \) implies \( X_2 \) is \( A \)-optimal over \( \mathcal{O}(N,n) \), then \( N_0(n) \leq N_0^*(n) \). It is open as to whether \( N_0(n) = N_0^*(n) \). Clearly an upper bound for \( N_0^*(n) \) is also an upper bound for \( N_0(n) \). As mentioned above this bound is usually very large. A much better upper bound for \( N_0(n) \) can be obtained by the following method due to Cheng (see Cheng, Masaro and Wong [7]).

For any \( X \in \mathcal{O}(N,n) \), suppose there are \( k \) columns which contain zero entries. Without loss of generality, we may assume that \( X = (Y_1, Y_2) \) where \( Y_1 \) is \( N \times k \) and consists of all the columns which contain zero entries. By a result of Fan (Theorem 2.1.2) the eigen-
values of $X^T X$ majorize those of \[
\begin{bmatrix}
Y_{11}^T & 0 \\
0 & Y_{22}^T
\end{bmatrix}^{-1}
\]. Since all the diagonal elements of $Y_{11}^T$ are $\leq N - 1$, by Proposition 1' of Kiefer [23], we have
\[
\text{tr}(X^T X)^{-1} \geq \text{tr}
\begin{bmatrix}
Y_{11}^T & 0 \\
0 & Y_{22}^T
\end{bmatrix}^{-1} \geq \text{tr}
\begin{bmatrix}
(N-1)I_k & 0 \\
0 & Y_{22}^T
\end{bmatrix}^{-1}
\]

Now all the entries of $Y_{22}$ are $\pm 1$, i.e., $Y_{22}^T Y_{22} \in C'(N,n - k)$. By an argument similar to that employed in the proof of Theorem 3.1.1, we conclude that
\[
\text{tr}(X^T X)^{-1} \geq \text{tr}
\begin{bmatrix}
(N-1)I_k & 0 \\
0 & (N-2)I_{n-k} + 2J_{n-k}
\end{bmatrix}
\]

where $\lambda = [(n-k)/2]$. Thus an upper bound of $N_0(n)$ is the smallest $N$ such that
\[
\text{tr}
\begin{bmatrix}
(N-2)I_{\lambda} + 2J_{\lambda} & 0 \\
0 & (N-2)I_{n-\lambda} + 2J_{n-\lambda}
\end{bmatrix}
\]

\[
\leq \text{tr}
\begin{bmatrix}
(N-1)I_k & 0 \\
0 & (N-2)I_{\lambda} + 2J_{\lambda}
\end{bmatrix}
\]

for all $k$ such that $1 \leq k \leq n$, where $\lambda = [n/2]$ and $\lambda = [(n-k)/2]$.

The following are some upper bounds of $N_0(n)$ obtained by the above method.
These bounds certainly are not sharp. In fact, it has been shown in Theorem 3.2.3 that $X_2$ is A-optimal over $\mathcal{O}(N,n)$ for all $n \geq 6$ and all $N \geq n$. Thus $N_0(4) = N_0(5) = N_0(6) = 6$. A counter example has not been found such that $X_2$ is not A-optimal in $\mathcal{O}(N,n)$! But the above table is useful for eliminating a lot of cases that have to be considered in proving the A-optimality of $X_2$. 

<table>
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<th>4</th>
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<td>14</td>
<td>14</td>
<td>18</td>
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<td>22</td>
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CHAPTER IV

OPTIMAL N x n WEIGHING DESIGN MATRICES

WITH N ≡ 3(mod 4).

4.1. General Results on A-optimality in \( \mathcal{S}(N,n) \) and \( \mathcal{S}^I(N,n) \).

Throughout this chapter we assume \( N ≡ 3(mod 4) \). Let \( X_3 ∈ \mathcal{S}(N,n) \) be such that \( X_3^T X_3 = (N+1)I_n - J_n \). In this section we will show that if \( N \) is sufficiently larger than \( n \), \( X_3 \) is A-optimal in \( \mathcal{S}(N,n) \) (and in \( \mathcal{S}^I(N,n) \)). The following lemmas are useful in proving this result and in establishing the A-optimality of \( X_3 \) in certain cases. Recall that \( C(N,n) \) (\( C^I(N,n) \)) is the family of all matrices of the form \( X^T X \) where \( X ∈ \mathcal{S}(N,n) \) (\( \mathcal{S}^I(N,n) \)).

Lemma 4.1.1. Let \( C ∈ C^I(N,n) \) be such that \( |c_{ij}| = c \) for all \( i ≠ j \).

Then \( C \) is similar to \( (N+c)I_n - cJ_n \) or \( (N-c)I_n + cJ_n \).

Proof. Let \( C ∈ C^I(N,n) \) be such that \( |c_{ij}| = c \) for \( i ≠ j \). By Lemma 3.1 of Ehlich [9], we may rearrange the columns of \( C \) and multiply appropriate columns by \( -1 \) to obtain a new matrix \( Y \) such that all the off-diagonal elements of \( Y^TY \) are congruents to \( 3(mod 4) \). Then since the absolute value of each off-diagonal element of \( Y^TY \) is also equal to \( c \), we have \( Y^TY = (N+c)I_n - cJ_n \) or \( (N-c)I_n + cJ_n \).

Lemma 4.1.2. Let \( C ∈ C^I(N,n) \). Then \( C \) is similar to a matrix \( D ∈ C^I(N,n) \) such that if \( |d_{ij}| = 1, 3, \) or \( 5 \), then \( d_{ij} = -1, 3 \) or \( -5 \), respectively.

Proof. Again by Lemma 3.1 of Ehlich [9] \( C \) is similar to a matrix \( D \) with all \( d_{ij} ≡ 3(mod 4) \). Then \( D \) has the desired properties.
Lemma 4.1.3. Let $C \in C'(N,n)$. If $\sum_{i,j} c_{ij}^2 \geq n(n-1)N^2/(N-n+2)^2$, then $\text{tr}(B)I_n - J_n)^{-1} \leq \text{tr}C^{-1}$, where $\text{tr}C^{-1}$ is defined to be $+\infty$ if $C$ has no inverse.

Proof. For any $C \in C'(N,n)$, we have $\text{tr}C = nN$ and $nN^2 \leq \text{tr}^2C \leq n^2N^2$. For any $B$ such that $nN^2 \leq B \leq n^2N^2$, let $\mathcal{R}(B,N,n)$ be the set of all the symmetric nonnegative definite $n \times n$ matrices $M$ such that $\text{tr}M = nN$ and $\text{tr}^2M = B$. Let $Z = ((nB - n^2N^2)/(n-1))^{1/2}$. Then from Lemmas A2, A3 and A6 of Cheng [4], $\text{tr}C^{-1} \geq (n-1)/\mu + 1/\lambda$, where $\mu = (nN - Z)/n$ and $\lambda = (nN + (n-1)Z)/n$. It suffices to show $\text{tr}((B+1)I_n - J_n)^{-1} \leq (n-1)/\mu + 1/\lambda$. On substituting the expressions for $\mu$ and $\lambda$, this reduces to

$$(4.1.1) \quad (N-n+2)Z^2 - n(n-2)Z - n^2N \geq 0.$$ 

Since $nN/(N-n+2)$ is the positive root of the equation 

$$(N-n+2)x^2 - n(n-2)x - n^2N = 0,$$ 

(4.1.1) holds provided $Z \geq nN/(N-n+2)$. 

This is equivalent to $B - nN^2 \geq n(n-1)N^2/(N-n+2)^2$. Since for $C \in C'(N,n)$, $\sum_{i,j} c_{ij}^2 = \text{tr}C^2 - nN^2$, the result follows.

Now we are ready to prove

Theorem 4.1.1. For each $n$, there exists a positive integer $N_0(n)$ such that for all $N \geq N_0(n)$, $X_3$ is $A$-optimal in $\mathcal{U}(N,n)$. In particular one can take $N_0(n) = [b_n] + 1$ where $b_n = \max\{(n-2)[n^2 - n + 16 + \sqrt{n(n-1)(n^2-n+16)}/16, n^2 - 2}\}$ or, for simplicity, $b_n = \max\{(n-2)(n^2-n+16)/8, n^2 - 2}\).
Proof. Let $C \in C(N,n)$. If $\sum_{i \neq j} c_{ij}^2 = n(n-1)$, then by Lemma 4.1.1, $C$ is similar to $(N+1)I_n - J_n$. Thus we may assume $\sum_{i \neq j} c_{ij}^2 \geq (n-1)+16$. It is straightforward to see that if
\[ N \geq (n-2)(n^2 - n + 16 + \sqrt{n(n-1)(n^2-n+16)})^{1/2}/16, \]
then
\[ n(n-1) + 16 > n(n-1)N^2/(N-n+2)^2; \text{ therefore } \sum_{i \neq j} c_{ij}^2 > n(n-1)N^2/(N-n+2)^2 \]
and by Lemma 4.1.3, $\text{tr}C^{-1} > \text{tr}(X_3^TX_3)^{-1}$.

For $C \in C(N,n) \setminus C'(N,n)$, we have $\text{tr}C \leq n(n-1)$. Thus $\text{tr}C^{-1} \geq n^2/\text{tr}C \geq n^2/(N(n-1))$. Comparing the last term with $\text{tr}(X_3^TX_3)^{-1} = (n-1)/(N+1) + 1/(N-n+1)$, we conclude that if $N \geq n^2 - 2$, then $\text{tr}C^{-1} \geq \text{tr}(X_3^TX_3)^{-1}$.

The proof is completed by taking $N_0(n) = \lfloor b_n \rfloor + 1$ where $b_n$ is as in the statement of the theorem.

Corollary 4.1.1. $X_3$ is A-optimal in $\mathcal{G}'(N,n)$ if
\[ N \geq (n-2)(n^2-n+16 + \sqrt{n(n-1)(n^2-n+16)})/16 \text{ or } N \geq (n-2)(n^2-n+16)/8. \]

To illustrate the above theorem, let
\[ X = \begin{bmatrix} 1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & -1 \\ 1 & 1 & -1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \end{bmatrix}. \]
Then $X \in \mathcal{G}(7,3)$ and $X^TX = \begin{bmatrix} 7 & -1 & -1 \\ -1 & 7 & -1 \\ -1 & -1 & 7 \end{bmatrix}$. Since $N = 7 = N_0(n)$, by

Theorem 4.1.1, $X$ is A-optimal over $\mathcal{G}(7,3)$. Galil and Kiefer [13]
show that \( X_3 \) in Theorem 4.1.1 is D-optimal over \( \mathcal{D}(N,n) \) provided \( N \geq 2n - 5 \). There is no such nice lower bound for A-optimality. In fact, the lower bound \( N_0(n) \) in Theorem 4.1.1 is sharp in the sense that \( X_3 \) \((X_3^T X_3 = 8I_4 - J_4)\) is not A-optimal over \( \mathcal{D}(7,4) \). Indeed let

\[
Z = \begin{bmatrix}
1 & -1 & 1 & 1 \\
-1 & -1 & 1 & 1 \\
1 & -1 & -1 & 1 \\
1 & -1 & -1 & 1 \\
-1 & 1 & -1 & 1 \\
0 & 1 & 1 & 1
\end{bmatrix}
\]

Then

\[
Z^T Z = \begin{bmatrix}
6 & 0 & 0 & 0 \\
0 & 7 & -1 & -1 \\
0 & -1 & 7 & -1 \\
0 & -1 & -1 & 7
\end{bmatrix}
\]

\[
\text{tr}(X_3^T X_3)^{-1} = \frac{3}{8} + \frac{1}{4} = \frac{5}{8} = .625,
\]

\[
\text{tr}(Z^T Z)^{-1} = \frac{1}{6} + \frac{2}{8} + \frac{1}{5} = \frac{37}{60} < .625.
\]

So \( Z \) is A-better than \( X_3 \). We will see in Section 4.2 that \( Z \) is A-optimal over \( \mathcal{D}(7,4) \).

We now prove:

**Theorem 4.1.2.** \( X_3 \) is A-optimal in \( \mathcal{D}'(N,n) \) for \( N \geq 7, n \leq 5 \) and \( N \geq 15, n \leq 7 \).

**Proof.** We consider only the cases \( n \leq 7, N = 15 \) the rest being similar.

Let \( N = 15, n = 6 \). In this case \( n(n-1)N^2/(N-n+2)^2 \approx 55.8 \).

It is easy to see that all matrices in \( C'(15,6) \) with \( \sum_{i \neq j} c_{ij}^2 \leq 55 \).
must have \(|c_{ij}| = 1\) for all \(i \neq j\) except for at most a pair of off-diagonal elements with \(|c_{ij}| = 3\). By Lemmas 4.1.2 and 4.1.3, the only competitor in \(C'(15,6)\), up to equivalence, is the matrix

\[
C = \begin{bmatrix}
15 & 3 & -1 & -1 & -1 & -1 \\
3 & 15 & -1 & -1 & -1 & -1 \\
-1 & -1 & 15 & -1 & -1 & -1 \\
-1 & -1 & -1 & 15 & -1 & -1 \\
-1 & -1 & -1 & -1 & 15 & -1 \\
-1 & -1 & -1 & -1 & -1 & 15 \\
\end{bmatrix}
\]

Computer calculation gives \(\text{tr}C^{-1} = 0.4151\), while \(\text{tr}(16I_6 - J_6)^{-1} = 0.4125\). Thus \(C_3\) is A-optimal in \(B'(15,6)\).

Since \(N \geq (n-2)(n^2-n+16)/8\) for \(N = 15\) and \(n = 2, 3, 4, 5\), it follows from Corollary 4.1.1 that \(X_3\) is also A-optimal in \(B'(15,n)\) for \(n = 2, 3, 4, 5\).

In the case \(n = 7\), due to our theory, the only competitors up to similarity are the following matrices:

\[
C_1 = \begin{bmatrix}
15 & 3 & -1 & -1 & -1 & -1 & -1 \\
3 & 15 & -1 & -1 & -1 & -1 & -1 \\
-1 & -1 & 15 & -1 & -1 & -1 & -1 \\
-1 & -1 & -1 & 15 & -1 & -1 & -1 \\
-1 & -1 & -1 & -1 & 15 & -1 & -1 \\
-1 & -1 & -1 & -1 & -1 & 15 & -1 \\
\end{bmatrix}, \quad \text{tr}C_1^{-1} = .4876
\]

\[
C_2 = \begin{bmatrix}
15 & 3 & 3 & -1 & -1 & -1 \\
3 & 15 & -1 & -1 & -1 & -1 \\
3 & -1 & 15 & -1 & -1 & -1 \\
-1 & -1 & -1 & 15 & -1 & -1 \\
-1 & -1 & -1 & -1 & 15 & -1 \\
-1 & -1 & -1 & -1 & -1 & 15 \\
\end{bmatrix}, \quad \text{tr}C_2^{-1} = .4926
\]
\[
C_3 = \begin{bmatrix}
15 & 3 & -1 & -1 & -1 & -1 & -1 \\
3 & 15 & -1 & -1 & -1 & -1 & -1 \\
-1 & -1 & 15 & 3 & -1 & -1 & -1 \\
-1 & -1 & 3 & 15 & -1 & -1 & -1 \\
-1 & -1 & -1 & -1 & 15 & -1 & -1 \\
-1 & -1 & -1 & -1 & -1 & 15 & -1 \\
-1 & -1 & -1 & -1 & -1 & -1 & 15 \\
\end{bmatrix}, \quad \text{tr}C_3^{-1} = 0.4896
\]

\[
C_4 = \begin{bmatrix}
15 & 3 & 3 & -1 & -1 & -1 \\
3 & 15 & -1 & -1 & -1 & -1 \\
3 & -1 & 15 & -1 & -1 & -1 \\
3 & -1 & -1 & 15 & -1 & -1 \\
-1 & -1 & -1 & -1 & 15 & -1 \\
-1 & -1 & -1 & -1 & -1 & 15 \\
-1 & -1 & -1 & -1 & -1 & -1 \\
\end{bmatrix}, \quad \text{tr}C_4^{-1} = 0.5019
\]

\[
C_5 = \begin{bmatrix}
15 & 3 & 3 & -1 & -1 & -1 \\
3 & 15 & -1 & -1 & -1 & -1 \\
3 & -1 & 15 & -1 & -1 & -1 \\
3 & -1 & 15 & -1 & -1 & -1 \\
-1 & -1 & -1 & 15 & -1 & -1 \\
-1 & -1 & -1 & -1 & 15 & -1 \\
-1 & -1 & -1 & -1 & -1 & 15 \\
\end{bmatrix}, \quad \text{tr}C_5^{-1} = 0.4917
\]

\[
C_6 = \begin{bmatrix}
15 & 3 & 3 & -1 & -1 & -1 \\
3 & 15 & -1 & -1 & -1 & -1 \\
3 & -1 & 15 & -1 & -1 & -1 \\
3 & -1 & -1 & 15 & -1 & -1 \\
-1 & -1 & -1 & -1 & 15 & -1 \\
-1 & -1 & -1 & -1 & -1 & 15 \\
-1 & -1 & -1 & -1 & -1 & -1 \\
\end{bmatrix}, \quad \text{tr}C_6^{-1} = 0.4974
\]
\[
C_7 = \begin{bmatrix}
15 & 3 & 3 & -1 & -1 & -1 & -1 \\
3 & 15 & -1 & -1 & -1 & -1 & -1 \\
3 & -1 & 15 & -1 & -1 & -1 & -1 \\
-1 & -1 & -1 & 15 & 3 & -1 & -1 \\
-1 & -1 & -1 & 3 & 15 & -1 & -1 \\
-1 & -1 & -1 & -1 & -1 & 15 & -1 \\
-1 & -1 & -1 & -1 & -1 & -1 & 15 \\
\end{bmatrix}, \quad \text{tr}C_7^{-1} = 0.4951
\]

\[
C_8 = \begin{bmatrix}
15 & 3 & -1 & -1 & -1 & -1 & -1 \\
3 & 15 & -1 & -1 & -1 & -1 & -1 \\
-1 & -1 & 15 & 3 & -1 & -1 & -1 \\
-1 & -1 & -1 & 15 & 3 & -1 & -1 \\
-1 & -1 & -1 & -1 & 15 & 3 & -1 \\
-1 & -1 & -1 & -1 & -1 & 15 & -1 \\
-1 & -1 & -1 & -1 & -1 & -1 & 15 \\
\end{bmatrix}, \quad \text{tr}C_8^{-1} = 0.4922
\]

\[
C_9 = \begin{bmatrix}
15 & -5 & -1 & -1 & -1 & -1 & -1 \\
-5 & 15 & -1 & -1 & -1 & -1 & -1 \\
-1 & -1 & 15 & -1 & -1 & -1 & -1 \\
-1 & -1 & -1 & 15 & -1 & -1 & -1 \\
-1 & -1 & -1 & -1 & 15 & -1 & -1 \\
-1 & -1 & -1 & -1 & -1 & 15 & -1 \\
-1 & -1 & -1 & -1 & -1 & -1 & 15 \\
\end{bmatrix}, \quad \text{tr}C_9^{-1} = 0.5100
\]

Now \(\text{tr}(16I_7 - J_7)^{-1} = 0.486110\). Comparing this with \(\text{tr}C_i^{-1}\), \(i = 1, 2, \ldots, 9\); we see that \(X_3\) is optimal in \(C'(15,7)\). Thus we have shown that \(X_3\) is A-optimal in \(C'(15,n)\) for all \(n \leq 7\).

To show the strength of our results, we conclude by giving an example which shows that in general \((N+1)I_n - J_n\) is not A-optimal in \(C'(N,n)\). This example points out that a matrix that is A-optimal in \(C'(N,n)\) need not be D-optimal in \(C'(N,n)\).

Let \(N = 11, \ n = 7\). From a theorem of Calil and Kiefer[13],
page 1299), the matrix $12I_7 - J_7$ is the unique D-optimal matrix in $C'(11,7)$. It should be noted that $12I_7 - J_7$ can be realized as $X^TX$ where $X$ is an $11 \times 7$ matrix with $x_{ij} = \pm 1$. Indeed, any $X$ such that

$$H = \begin{bmatrix} 1 & 1 & \ldots & 1 \\ 1 \\ \vdots \\ 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{bmatrix}$$

is a Hadamard matrix of order 12 will do.

Such $H$ can be found in Hedayat and Wallis [16]. However, let

$$Z = \begin{bmatrix} 1 & 1 & -1 & -1 & -1 & -1 & -1 \\ -1 & 1 & -1 & 1 & -1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & -1 & -1 \\ -1 & 1 & 1 & 1 & -1 & -1 \\ -1 & 1 & 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & -1 & -1 & 1 \end{bmatrix};$$

then

It is well known that if \( M = \begin{bmatrix} P & Q \\ Q^T & R \end{bmatrix} \) is a nonsingular matrix then
\[
M^{-1} = \begin{bmatrix} S & T \\ Q^T & U \end{bmatrix}
\]
where \( S = P^{-1} + P^{-1} Q (R - Q P^{-1} Q)^{-1} Q^P^{-1} \),

\( U = (R - Q P^{-1} Q)^{-1} \) and \( T = -P^{-1} Q (R - Q P^{-1} Q)^{-1} \). Applying this result to \( Z^T \) we obtain

\[
(X'X)^{-1} = \begin{bmatrix}
\frac{441}{4312} & -\frac{98}{4312} & T \\
-\frac{98}{4312} & \frac{441}{4312} & \\
T^T & (1/12)I_5 + (1/66)(J_5)
\end{bmatrix}
\]

Then \( tr(Z^T Z)^{-1} = 441/2156 + 65/132 = .69696 \). But \( tr[12I_7 - J_7]^{-1} \) is .7.

Thus \( 12I_7 - J_7 \) is not A-optimal in \( C'(11,7) \). Also the A-optimal matrix in \( C'(11,7) \) cannot be D-optimal since \( 12I_7 - J_7 \) is the unique D-optimal matrix in \( C'(11,7) \).

In conclusion we remark that the above example includes a general procedure for constructing \( X_3 \) with \( X_3^T X_3 = (N+1)I_n - J_n \). Using Proposition 2.4.1 or otherwise choose \( X_0 \) in \( \mathcal{E}(N+1,n) \) such that

\( X_0^T X_0 = (N+1)I_n \) and the first row of \( X_0 \) consists entirely of 1's.

The appropriate \( X_3 \) is obtained by removing the first row from \( X_0 \).

4.2. A-optimal Designs in \( \mathcal{E}(N,n) \).

In this section we classify all A-optimal designs in \( \mathcal{E}(N,n) \) for \( n \leq 6 \) and \( N \) arbitrary, \( N \equiv 3(mod 4) \). In this case, the A-optimal matrix will be one of the following three types:

Type I: \( X_3^T X_3 = (N+1)I_n - J_n \).

Type II: \( Y_3^T Y_3 = \begin{bmatrix} N-1 & 0 \\
0 & (N+1)I_{n-1} - J_{n-1} \end{bmatrix} \)
Type III: \[ Z_3^T = \begin{bmatrix} (N-3)I_2 + 2J_2 & 0 \\ 0 & (N+1)I_{n-2} - J_{n-2} \end{bmatrix} \]

Table 4.2.1 below, is a complete list of the A-optimal design matrices in \( \mathcal{O}(N,n) \) for \( N \geq 7 \), \( N \equiv 3 \pmod{4} \), \( n \leq 6 \).

Table 4.2.1. Some A-optimal Designs in \( \mathcal{O}(N,n) \), \( N \equiv 3 \pmod{4} \).

<table>
<thead>
<tr>
<th>N</th>
<th>n</th>
<th>Type of A-optimal Design</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>\leq 3</td>
<td>I</td>
</tr>
<tr>
<td>4,5</td>
<td></td>
<td>II</td>
</tr>
<tr>
<td>6</td>
<td></td>
<td>III</td>
</tr>
<tr>
<td>11</td>
<td>\leq 4</td>
<td>I</td>
</tr>
<tr>
<td>5,6</td>
<td></td>
<td>II</td>
</tr>
<tr>
<td>15</td>
<td>\leq 5</td>
<td>I</td>
</tr>
<tr>
<td>6</td>
<td></td>
<td>II</td>
</tr>
<tr>
<td>\geq 19</td>
<td>\leq 6</td>
<td>I</td>
</tr>
</tbody>
</table>

For \( N \geq 35 \), \( n \leq 6 \) the A-optimality of \( X_3 \) follows from Theorem 4.1.1. Since the cases \( 7 < N < 31 \), \( n \leq 6 \) are similar and easier than the cases \( N = 7 \), \( n \leq 6 \) we only discuss the latter cases. Thus, let \( N = 7 \), \( n \leq 6 \).

Case A: \( n \leq 3 \). An application of Theorem 4.1.1 shows that \( X_3 \) is A-optimal in \( \mathcal{O}(7,n) \). The construction of such \( X_3 \) has already been discussed in Section 4.1.

Case B: \( n = 4 \). In this case the A-optimal design in \( \mathcal{O}(7,4) \) is of Type II. Let
\[ Y_3 = \begin{bmatrix}
0 & -1 & -1 & -1 \\
-1 & 1 & 1 & -1 \\
1 & 1 & -1 & 1 \\
1 & -1 & 1 & -1 \\
-1 & -1 & 1 & 1 \\
-1 & -1 & -1 & 1 \\
-1 & 1 & -1 & -1 \\
\end{bmatrix} \]

then

\[ Y_3^T \begin{bmatrix}
6 & 0 \\
0 & 8I_3 - J_3 \\
\end{bmatrix} \text{ and } \text{tr}(Y_3^T Y_3)^{-1} = \frac{37}{60} = .61666. \]

Let \( X \in \mathcal{G}(7,4) \). We must show that \( \text{tr}(X^T X)^{-1} \geq .61666 \).

If \( X \in \mathcal{G}(7,4) \), the result follows from Theorem 4.1.2.

Let \( X \) have one zero entry. Then,

\[ X^T X = \begin{bmatrix}
6 & * \\
* & c \\
\end{bmatrix} \]

Thus by Ky Fan's theorem and the result for \( n = 3 \),

\[ \text{tr}(X^T X)^{-1} \geq \text{tr}(6)^{-1} + \text{tr}(c)^{-1} \geq \frac{1}{6} + \text{tr}(8I_3 - J_3)^{-1} = .61666. \]

Let \( X \) have two zero entries. Then

\[ X^T X = \begin{bmatrix}
A & * \\
* & .7 \\
\end{bmatrix}, \quad |c| \geq 1, \quad \text{tr}A = 12. \]

By Ky Fan's theorem and Theorem 3.2.1,

\[ \text{tr}(X^T X)^{-1} \geq \text{tr}A^{-1} + \text{tr} \left[ \begin{bmatrix}
.7 & c \\
c & 7 \\
\end{bmatrix} \right]^{-1} \geq \frac{4}{12} + \text{tr} \left[ \begin{bmatrix}
.7 & -1 \\
-1 & 7 \\
\end{bmatrix} \right]^{-1} = .625 > .61666. \]

Let \( X \) have three or more zero entries. Then by Theorem 3.2.1,

\[ \text{tr}(X^T X)^{-1} \geq \frac{n^2}{\text{tr}(X^T X)} \geq \frac{16}{25} = .64 > .61666. \]

Case C: \( n = 5 \). The A-optimal design in \( \mathcal{G}(7,5) \) is of type II.
Let
\[ Y_3 = \begin{bmatrix}
0 & -1 & -1 & -1 & -1 \\
-1 & 1 & 1 & -1 & -1 \\
1 & 1 & -1 & 1 & -1 \\
1 & -1 & 1 & -1 & 1 \\
-1 & -1 & 1 & 1 & -1 \\
-1 & -1 & -1 & 1 & 1 \\
-1 & 1 & -1 & -1 & 1
\end{bmatrix} \]
then
\[ Y_3^T Y_3 = \begin{bmatrix}
6 & 0 \\
0 & 8I_4 - J_4
\end{bmatrix} \quad \text{and} \quad \text{tr}(Y_3^T Y_3)^{-1} = \frac{19}{24} = .79166. \]

Let \( X \in G(7,5) \). We must prove \( \text{tr}(X^T X)^{-1} \geq .79166 \).

If \( X \in G^*(7,5) \), this follows from Theorem 4.1.2.

Let \( X \) have one zero entry. Then, by using Ky Fan's theorem and Theorem 4.1.2 we can proceed in the case \( n = 4 \).

Let \( X \) have two zero entries. We may assume the zeros appear in distinct columns or proceed as in the case \( n = 4 \). Thus,
\[ X^T X = \begin{bmatrix}
6 & c \\
-6 & -a_{ij} \\
\vdots & \vdots \\
7 & b_{ij} \\
7 & \vdots
\end{bmatrix}, \quad |c| \geq 0, \quad |a_{ij}| \geq 1. \]

If \( |c| \geq 1 \), then by Ky Fan's result and Theorem 4.1.2,
\[ \text{tr}(X^T X)^{-1} \geq \text{tr} \left[ \begin{bmatrix}
6 & 1 \\
1 & 6
\end{bmatrix} \right]^{-1} + \text{tr} \left[ 8I_3 - J_3 \right]^{-1} = \frac{12}{35} + \frac{2}{8} + \frac{1}{5} = .79285 > .79166. \]
Thus we may assume \( c = 0 \). Then the zero entries of \( X \) must lie on the same row. Thus, by Lemma 2.3.2, \( |a_{ij}| \geq 2 \) for at least three pairs \((i,j)\). Hence,
\[ \text{tr}(X^T X)^2 \geq 2 \times 6^2 + 3 \times 7^2 + 6 \times 2^2 + 6 \times 1^2 = 249. \]
Now applying Theorem 3.2.2 with \( t = \text{tr}(X^TX) = 33 \) and \( a = .79166 \) we have
\[
 b(t,a) < 231 < \text{tr}(X^TX)^2 .
\]
Therefore, \( \text{tr}(X^TX)^{-1} \geq a \).

Let \( X \) have three zero entries. Then
\[
X^TX = \begin{bmatrix}
A & * \\
7 & c \\
7 & 7
\end{bmatrix}, \quad |c| \geq 1, \quad \text{tr}A = 18 .
\]

By Ky Fan's theorem and Theorem 3.2.1,
\[
\text{tr}(X^TX)^{-1} \geq \text{tr}A^{-1} + \text{tr} \begin{bmatrix} 7 & 1 \\ 1 & 7 \end{bmatrix}^{-1} \geq \frac{9}{18} + \frac{14}{48} = .79166 .
\]

Let \( X \) have four or more zero entries. Then by Theorem 3.2.1,
\[
\text{tr}(X^TX)^{-1} \geq \frac{25}{31} = .80645 > .79166 .
\]

Case D: \( n = 6 \). Then the A-optimal design in \( \mathcal{S}(7,6) \) is of Type III.

Let
\[
Z_3 = \begin{bmatrix}
0 & 0 & -1 & -1 & -1 & -1 \\
1 & 1 & 1 & 1 & -1 & -1 \\
-1 & -1 & 1 & -1 & 1 & -1 \\
-1 & -1 & -1 & 1 & -1 & 1 \\
-1 & 1 & -1 & 1 & 1 & -1 \\
1 & 1 & -1 & -1 & 1 & 1 \\
-1 & 1 & 1 & -1 & -1 & 1
\end{bmatrix}
\]

then
\[
Z_3^T Z_3 = \begin{bmatrix}
4I_2 + 2J_2 & 0 \\
0 & 8I_4 - J_4
\end{bmatrix}
\]
and \( \text{tr}(Z_3^T Z_3)^{-1} = 1 . \)

Let \( X \in \mathcal{S}(7,6) \). We must show \( \text{tr}(X^TX)^{-1} \geq 1 \).

Let \( X \in \mathcal{S}(7,6) \). Then by Lemma 4.1.2,
\( X^T X = \begin{bmatrix} 7 & a_{ij} \\ 7 & 7 & a_{ij} \\ 7 & 7 & 7 \end{bmatrix}, \ a_{ij} = -1, 3 \text{ or } -5. \)

Suppose all \( a_{ij} = -1 \), then,

\[ \text{tr}(X^T X)^{-1} = \text{tr}(8I_6 - J_6)^{-1} = \frac{9}{8} > 1. \]

Let some \( a_{ij} = -5 \) then by Ky Fan's theorem and Theorem 4.1.2,

\[ \text{tr}(X^T X)^{-1} \geq \text{tr} \begin{bmatrix} 7 & -5 \\ -5 & 7 \end{bmatrix}^{-1} + \text{tr}(8I_4 - J_4)^{-1} = \frac{14}{24} + \frac{5}{8} = \frac{29}{24} > 1. \]

Thus we may assume \( a_{ij} = -1 \) or 3. Let \( t = \text{tr}(X^T X) = 42, a = 1 \).

then \( b(t,a) < 376 \). Therefore, by Theorem 3.2.2, we may assume further that \( \text{tr}(X^T X)^2 < 375 \). Hence six or less of the \( a_{ij} \) satisfy \( a_{ij} = 3 \). If two of the \( a_{ij} \) equal 3, then

\[ \text{tr}(X^T X)^{-1} = \text{tr} \begin{bmatrix} 7 & 3 & 7 \\ 3 & 7 & 7 \\ 7 & 7 & 7 \end{bmatrix}^{-1} = 1.0625 > 1. \]

If four of the \( a_{ij} \) equal 3, then up to similarity of \( X^T X \), either

\[ \text{tr}(X^T X)^{-1} = \text{tr} \begin{bmatrix} 7 & 3 & 7 \\ 3 & 7 & -1 \end{bmatrix}^{-1} + \text{tr}(8I_3 - J_3)^{-1} = 1.11166 > 1 \]

or

\[ \text{tr}(X^T X)^{-1} = \text{tr} \begin{bmatrix} 7 & 3 \\ 3 & 7 \\ -1 & 7 \end{bmatrix}^{-1} = 1.0583 > 1. \]
If six of the $a_{ij}$ equal 3, then the only remaining cases to be covered are

$$
\text{tr}(X^TX)^{-1} = \text{tr} \left[ \begin{array}{ccc}
7 & 3 & 3 \\
3 & 7 & 3 \\
\cdots & \cdots & \cdots \\
3 & 3 & 7 \\
\end{array} \right]^{-1} \geq \text{tr} \left[ \begin{array}{ccc}
7 & 3 & 3 \\
3 & 7 & 3 \\
\cdots & \cdots & \cdots \\
3 & 3 & 7 \\
\end{array} \right]^{-1} + \text{tr} [8I_3 - J_3]^{-1} = 1.026 > 1.
$$

or

$$
\text{tr}(X^TX)^{-1} = \text{tr} \left[ \begin{array}{ccc}
7 & 3 & 3 \\
3 & 7 & 3 \\
\cdots & \cdots & \cdots \\
3 & 3 & 7 \\
\end{array} \right]^{-1} \geq 3 \text{tr} \left[ \begin{array}{ccc}
7 & 3 \\
3 & 7 \\
\cdots & \cdots \\
3 & 7 \\
\end{array} \right]^{-1} = \frac{42}{40} > 1.
$$

This completes the case where $X \in \mathcal{B}^*(7, 6)$.

Let $X$ have one zero entry. Then one can proceed as in the case $n = 4$.

Let $X$ have two zero entries. The usual arguments allow us to assume that the zeros appear in distinct columns. Thus,

$$
X^TX = \begin{bmatrix}
6 & c & a_1 & a_2 & a_3 & a_4 \\
6 & a_5 & a_6 & a_7 & a_8 \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
7 & b_1 & b_2 & b_3 \\
7 & b_4 & b_5 \\
7 & 7
\end{bmatrix}, \quad |c| \geq 0, \quad |b_i| \geq 1.
$$

If $|c| \geq 2$, then

$$
\text{tr}(X^TX)^{-1} \geq \text{tr} \left[ \begin{array}{cc}
6 & 2 \\
2 & 6 \\
\end{array} \right]^{-1} + \text{tr} [8I_4 - J_4]^{-1} = \frac{12}{32} + \frac{5}{8} = 1.
$$

If $c = 0$, then the zero entries of $X$ lie in the same row. So by Lemma 2.3.2, $|a_i| \geq 2$ for at least four of the $a_i$. Thus,
\[
\text{tr}(X^T X)^2 \geq 2 \times 6^2 + 4 \times 7^2 + 8 \times 2^2 + 12 \times 1^2 = 312.
\]

But \( b(40,1) < 314 \). So by Theorem 3.2.2 and Lemma 4.1.2, we may assume that exactly four of the \( a_i \) are \( \pm 2 \), the rest being 0, and that all \( b_i = -1 \). Noting that Lemma 2.3.2 implies that \( a_i = a_{i+4} = 0 \), \( i = 1, 2, 3, 4 \) is not possible, we have, up to similarity of \( X^T X \), the following cases:

<table>
<thead>
<tr>
<th>( a_1 )</th>
<th>( a_2 )</th>
<th>( a_3 )</th>
<th>( a_4 )</th>
<th>( a_5 )</th>
<th>( a_6 )</th>
<th>( a_7 )</th>
<th>( a_8 )</th>
<th>( \text{tr}(X^T X)^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1.7917</td>
</tr>
<tr>
<td>-2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1.2024</td>
</tr>
<tr>
<td>-2</td>
<td>-2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1.1042</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1.3194</td>
</tr>
<tr>
<td>-2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>1.1144</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>2</td>
<td>1.225</td>
</tr>
<tr>
<td>-2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>2</td>
<td>1.1417</td>
</tr>
<tr>
<td>-2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-2</td>
<td>2</td>
<td>1.075</td>
</tr>
</tbody>
</table>

In all cases, \( \text{tr}(X^T X)^{-1} > 1 \).

Now let \( c = 1 \) (or -1). If two of the \( b_i \) satisfy \( |b_i| \geq 3 \) or one \( b_i \) satisfies \( |b_i| \geq 5 \) then

\[
\text{tr}(X^T X)^2 \geq 2 \times 6^2 + 4 \times 7^2 + 10 \times 1^2 + 4 \times 3^2 = 314 > b(40,1).
\]

So, Theorem 3.2.2 applies. If say, \( b_1 = 3, b_i = -1, i = 2,3,\ldots,6 \), then by Ky Fan's theorem

\[
\text{tr}(X^T X)^{-1} \geq \text{tr}
\begin{bmatrix}
6 & 1 \\
1 & 6
\end{bmatrix}^{-1}
+ \text{tr}
\begin{bmatrix}
7 & 3 & -1 & -1 \\
3 & 7 & -1 & -1 \\
-1 & -1 & 7 & -1 \\
-1 & -1 & -1 & 7
\end{bmatrix}^{-1}
= \frac{12}{35} + \frac{1184}{1792}
= 1.00356 > 1.
\]

Thus we may assume that all \( b_i = -1 \). If four or more of the \( a_i \) satisfy \( |a_i| \geq 2 \) or one \( a_i \) satisfies \( |a_i| \geq 4 \), then —
\[ \text{tr}(X^TX)^2 \geq 2 \times 6^2 + 4 \times 7^2 + 8 \times 2^2 + 14 \times 1^2 = 314 > b(40,1). \]

Therefore, we may assume that at most three of the \( a_i \) satisfy \( |a_i| = 2 \). But by Lemma 2.3.2, at least two of the \( a_i \) have absolute value 2. Thus we are left with the following cases:

i) \( a_1 = -a_2 = 2 \)

\[
\text{tr}(X^TX)^{-1} \geq \text{tr} \begin{bmatrix} 6 & 1 & 2 \\ 1 & 6 & -2 \\ -2 & 6 & 7 \end{bmatrix} + \text{tr} \begin{bmatrix} 8I_3 - J_3 \end{bmatrix}^{-1} = \frac{111}{189} + \frac{2}{8} + \frac{1}{5} = 1.037 > 1.
\]

ii) \( a_1 = a_2 = \pm 2 \)

Lemma 2.3.2 implies that \( |a_i| = 2 \) for some \( i \neq 1, 5 \). Without loss of generality, we may assume \( |a_2| = 2 \). Then

\[
\text{tr}(X^TX)^{-1} \geq \text{tr} \begin{bmatrix} 6 & 1 & a_1 \\ 1 & 6 & 0 \\ a_1 & 1 & 7 \end{bmatrix} + \text{tr} \begin{bmatrix} 7 & -1 \\ -1 & 7 \end{bmatrix}^{-1} = \frac{918 - 2a_1 a_2}{1248 - 10a_1 a_2} + \frac{14}{48} = \frac{926 + 14}{1288} > 1.0106 > 1.
\]

(iii) \( a_1 = a_2 = \pm 2 \)

We may assume \( a_5 = a_6 = 0 \) or else proceed as in i) and ii) above.

Thus

\[
\text{tr}(X^TX)^{-1} \geq \text{tr} \begin{bmatrix} 6 & 1 & a_2 \\ 1 & 6 & 0 \\ a_2 & 0 & 7 \end{bmatrix} + \text{tr} \begin{bmatrix} 7 & -1 \\ -1 & 7 \end{bmatrix}^{-1} = \frac{954}{1296} + \frac{14}{48} = 1.0277 > 1.
\]

iv) \( a_1 = -a_2 = \pm 2 \)

As above we may assume \( a_5 = a_6 = 0 \). If \( |a_i| = 2 \) for \( i = 3 \) or \( i = 4 \) then one of the above cases apply. Thus we may assume...
\[
X^T X = C_r = \begin{bmatrix}
6 & 1 & 2 & -2 & 0 & 0 \\
6 & 0 & 0 & -r & 0 \\
7 & -1 & -1 & -1 \\
7 & -1 & -1 \\
\ast & \end{bmatrix}, \quad |r| = 0 \text{ or } 2.
\]

Now, \( C_r \) is similar to \( C_{-r} \) since \( C_{-r} \) can be obtained from \( C_r \) by multiplying rows one and two by \(-1\), columns one and two by \(-1\), then interchanging rows three and four and columns three and four. Therefore,

\[
\text{tr}(X^T X)^{-1} = \frac{4}{2} \text{tr}C_r^{-1} + \frac{1}{2} \text{tr}C_{-r}^{-1}
\]

\[
\geq \text{tr}\left[\frac{1}{2} C_r + \frac{1}{2} C_{-r}\right]^{-1}
\]

\[
= \text{tr} \begin{bmatrix}
6 & 1 & 2 & -2 & 0 & 0 \\
6 & 0 & 0 & 0 & 0 \\
7 & -1 & -1 & -1 \\
7 & -1 & -1 \\
7 & \end{bmatrix}^{-1}
\]

\[
= 1.0302 \quad > 1.
\]

This completes the case where \( X \) has two zero entries.

Let \( X \) have three zero entries.

If the three zero entries appear in the first column of \( X \), then we can apply the usual arguments using Ky Fan's theorem and Theorem 4.1.2.

Suppose \( X \) has two zeros in the first column and one in the second column. Then,
\[ X^TX = \begin{bmatrix}
5 & c & a_1 & a_2 & a_3 & a_4 \\
6 & b_1 & b_2 & b_3 & b_4 \\
7 & c_1 & c_2 & c_3 \\
7 & c_4 & c_5 \\
\star & \star & 7 & c_6 \\
\end{bmatrix} \]

where \( |a_i| = 1, 3, 5 \), \( |b_i| = 0, 2, 4, 6 \), \( |c_i| = 1, 3, 5 \). If \( |c| \geq 1 \), then

\[ \text{tr}(X^TX)^{-1} \geq \text{tr}\left[\begin{bmatrix} 5 & 1 \\ 1 & 6 \end{bmatrix}\right]^{-1} + \text{tr}[8I_4 - J_4]^{-1} = \frac{233}{232} > 1. \]

Thus assume \( c = 0 \). Now,

\[ \text{tr}(X^TX)^2 = 5^2 + 6^2 + 4 \times 7^2 + 2 \sum a_i^2 + 2 \sum b_i^2 + 2 \sum c_i^2 \]
\[ = 257 + 2 \sum a_i^2 + 2 \sum b_i^2 + 2 \sum c_i^2, \]

and

\[ b(39, 1) < 286. \]

Therefore if one \( |a_i| \geq 3 \) or two \( |b_i| \geq 2 \) or one \( |c_i| \geq 3 \) then \( \text{tr}(X^TX)^2 > b(39, 1) \) and Theorem 3.2.2 applies. Thus we may assume that \( |a_i| = 1 \), \( |b_i| = 2 \) or \( 0 \), \( b_i = 0 \), \( i = 2, 3, 4 \) and \( c_i = -1 \). Hence, up to similarity

\[ X^TX = C_s \equiv \begin{bmatrix}
5 & 0 & 1 & a_2 & a_3 & a_4 \\
6 & s & 0 & 0 & 0 \\
7 & -1 & -1 & -1 \\
7 & -1 & -1 \\
\star & 7 & -1 \\
\end{bmatrix}, \quad |s| = 0 \text{ or } 2. \]
Since $C_s$ is similar to $C_{-s}$,

$$\text{tr}(X^TX)^{-1} = \frac{1}{2} \text{tr}C_s^{-1} + \frac{1}{2} \text{tr}C_{-s}^{-1}$$

$$\geq \text{tr} \left[ \frac{1}{2} C_s + \frac{1}{2} C_{-s} \right]^{-1}$$

$$= \text{tr} \begin{bmatrix}
5 & 0 & 1 & a_2 & a_3 & a_4 \\
6 & 0 & 0 & 0 & 0 & 0 \\
7 & -1 & -1 & -1 \\
7 & -1 & -1 \\
7 & -1 \\
7
\end{bmatrix}^{-1}$$

$$= \begin{cases} 
1.1042 & \text{if } a_2 = a_3 = a_4 = 1 \\
1.0452 & \text{if } a_2 = a_3 = 1, a_4 = -1 \\
1.0278 & \text{if } a_2 = 1, a_3 = a_4 = -1.
\end{cases}$$

This completes the case where two zeros occur in the first column and one zero in the second column of $X$.

Now assume the three zeros occur in distinct columns. Then

$$X^TX = \begin{bmatrix}
6 & a_1 & a_2 & b_1 & b_2 & b_3 \\
6 & a_3 & b_4 & b_5 & b_6 \\
6 & b_7 & b_8 & b_9 \\
7 & c_1 & c_2 \\
7 & c_3 \\
7
\end{bmatrix}$$

where $|b_1| = 0, 2, 4, 6, |c_1| = 1, 3, 5$.

Now, by Lemma 2.3.1, $|a_i| \geq 1$ for some $i$. Assume $|a_1| \geq 1$.

If $|a_i| \geq 2$ for some $i$, then

$$\text{tr}(X^TX)^{-1} \geq \text{tr} \begin{bmatrix} 6 & 2 \\ 2 & 6 \end{bmatrix}^{-1} + \text{tr}[8I_4 - J_4]^{-1} = \frac{12}{32} + \frac{3}{8} + \frac{1}{4} = 1.$$
Thus we may assume \( a_1 = 1 \). Therefore,
\[
\text{tr}(X^TX)^2 = 3 \times 6^2 + 3 \times 7^2 + 2 \times 1^2 + 2 \sum 2 a_i^2 + 2 \sum 9 b_i^2 + 2 \sum 3 c_i^2
\]
\[
= 257 + 2 \sum 3 a_i^2 + 2 \sum 1 \cdot b_i^2 + 2 \sum 3 c_i^2.
\]
If \(|c_i| \geq 3\) for two or more values of \( i \) or \(|c_i| \geq 5\) for one \( i \), then
\[
\text{tr}(X^TX)^2 \geq 286 \geq b(39, 1).
\]
So Theorem 3.2.2 applies. If \( c_i = 3 \), \( c_i = -1 \) for \( i \neq 1 \), then
\[
\text{tr}(X^TX)^{-1} \geq \text{tr}\left[ \begin{bmatrix} 6 & 1 \\ 1 & 6 \end{bmatrix}^{-1} + \text{tr}[6]^{-1} + \text{tr}\left[ \begin{bmatrix} 7 & 3 \\ -1 & 1 \end{bmatrix}^{-1} \right] \right] = \frac{12}{35} + \frac{1}{6} + \frac{1}{2} = 1.0095 \geq 1.
\]
Thus we may assume \( c_i = -1 \), \( i = 1, 2, 3 \). Further if \( a_2 = 0 \) or \( a_3 = 0 \) then by Lemma 2.3.2, \(|b_i| \geq 2\) for at least three values of \( i \), whence \( \text{tr}(X^TX)^2 > b(39, 1) \). The same holds if \(|b_i| \geq 4\) for at least one \( i \). Thus we may assume that \( a_1 = 1 \), \(|a_i| = 1\), \( i = 2, 3 \) and (by Lemma 2.3.3) that exactly two of the \( b_i \) satisfy \(|b_i| = 2\), the rest being zero. Thus up to similarity of \( X^TX \) we have
\[
X^TX = \begin{bmatrix}
6 & 1 & a_2 & b_1 & b_2 & b_3 \\
6 & 1 & b_4 & b_5 & b_6 \\
6 & 2 & b_8 & b_9 & \\
7 & -1 & -1 & \\
7 & -1 & & \\
7 & & & &
\end{bmatrix},
\]
where \( a_2 = \pm 1 \), and exactly one \( b_i = \pm 2 \), the rest being zero. If \(|b_8| = 2\) or \(|b_9| = 2\), then by Lemma 2.3.3 \(|b_i| = 2\) for some \( i = 1, 2, \ldots, 6 \), whence \( \text{tr}(X^TX)^2 > b(39, 1) \). Thus we may further
assume $b_8 = b_9 = 0$. The remaining cases up to similarity of $X^T X$
are computed below.

\[
\begin{array}{ccc}
\text{tr}(X^T X)^{-1} \\
a_3 = 1 & b_1 = 2 & 1.0445 \\
b_1 = -2 & & 1.0882 \\
b_2 = 2 & & 1.0511 \\
b_2 = -2 & & 1.0602 \\
a_3 = -1 & b_1 = 2 & 1.1188 \\
b_1 = -2 & & 1.0480 \\
b_2 = 2 & & 1.0784 \\
b_2 = -2 & & 1.0640 \\
\end{array}
\]

This completes the case where $X$ has three zero entries.

Now suppose $X$ has four zero entries.

If the four zeros appear in the first two columns of $X$, then

\[
X^T X = \begin{bmatrix}
A & \ast & \ast & \ast \\
7 & 7 & \ast & \ast \\
7 & 7 & 7 & \\
\end{bmatrix}, \quad \text{tr} \ A = 10.
\]

Thus by Ky Fan's theorem, Theorems 3.2.1 and 4.1.2

\[
\text{tr}(X^T X)^{-1} \geq \text{tr} \ A^{-1} + \text{tr} \left( 8I_4 - J_4 \right)^{-1} \geq \frac{4}{10} + \frac{5}{8} = 1.025 > 1.
\]

Now assume two zeros appear in the first column and one zero in
the second and third columns of $X$. Then,
\[ X^T X = \begin{bmatrix}
5 & a_1 & a_2 & b_1 & b_2 & b_3 \\
6 & a_3 & c_1 & c_2 & c_3 \\
6 & c_4 & c_5 & c_6 \\
7 & d_1 & d_2 \\
7 & d_3 \\
7 & 6
\end{bmatrix}, \quad |b_1| \geq 1, \quad |d_i| \geq 1, \quad |c_i| \geq 0.
\]

Therefore,
\[
\text{tr}(X^T X)^2 = 5^2 + 2 \times 6^2 + 3 \times 7^2 + 3 \sum_{i=1}^{3} a_i^2 + 3 \sum_{i=1}^{3} b_i^2 + 3 \sum_{i=1}^{6} c_i^2 + 3 \sum_{i=1}^{3} d_i^2
\]
\[
= 244 + \sum_{i=1}^{3} a_i^2 + \sum_{i=1}^{3} b_i^2 + \sum_{i=1}^{6} c_i^2 + \sum_{i=1}^{3} d_i^2.
\]

Also,
\[ b(38,1) < 260. \]

If \(|a_3| \geq 2\) or \(|d_i| \geq 3\) for some \(i\), then \(\text{tr}(X^T X)^2 \geq 260 > b(38,1)\). Thus we may assume \(|a_3| \leq 1\) and \(d_i = -1\) for all \(i\). Further if \(|a_3| = 1\), Lemma 2.3.3 implies \(|c_i| \geq 2\) for some \(i\) and hence \(\text{tr}(X^T X)^2 > b(38,1)\). Finally, if \(a_3 = 0\), then by Lemma 2.3.2, at least three of the \(c_i\) satisfy \(|c_i| \geq 2\) whence \(\text{tr}(X^T X)^2 > b(38,1)\).

Now suppose the four zeros of \(X\) lie in distinct columns. Then
\[
X^T X = \begin{bmatrix}
6 & a_1 & a_2 & a_3 & b_1 & b_2 \\
6 & a_4 & a_5 & b_3 & b_4 \\
6 & a_6 & b_5 & b_6 \\
6 & b_7 & b_8 \\
7 & c_1 \\
7
\end{bmatrix}, \quad |c_1| \geq 1
\]

Thus,
\[
\text{tr}(X^T X)^2 \geq 4 \times 6^2 + 2 \times 7^2 + 2 \times 1^2 + 2 \sum a_i^2 + 8 \sum b_i^2
\]
\[
= 244 + 2 \sum a_i^2 + 2 \sum b_i^2
\]

If two of the zeros of \( X \) occur in the same row then by Lemma 2.3.2,
\[|b_i| \geq 2 \quad \text{for at least two } b_i.\]

Therefore
\[
\text{tr}(X^T X)^2 \geq 260 > b(38,1).
\]

Thus assume the zeros lie in distinct rows. Then \[|a_i| \geq 1, \ i=1,2,\ldots,6.\]

Since we may assume \( \text{tr}(X^T X)^2 \leq 259 \), the only remaining cases up to similarity of \( X^T X \) are \( a_1 = a_2 = a_3 = 1 \), \( |a_i| = 1, \ i=4,5,6 \), \( b_i = 0 \), \( i=1,2,\ldots,8 \). Then,
\[
\text{tr}(X^T X)^{-1} = \text{tr} \begin{bmatrix}
6 & 1 & 1 & 1 \\
6 & a_4 & a_5 \\
* & 6 & a_6 \\
& & 6
\end{bmatrix}^{-1} + \text{tr} \begin{bmatrix}
7 & 1 \\
1 & 7
\end{bmatrix}^{-1}
\]
\[
= \frac{792 + 2(a_4 + a_5 + a_6) + 2a_4a_5a_6}{1083 - 2(a_4 + a_5 + a_6)^2 + 12(a_4 + a_5 + a_6) + 12a_4a_5a_6 + 14} + \frac{14}{48}
\]
\[
> \frac{800}{1125} + \frac{14}{48}
\]
\[
= 1.0027
\]
\[
> 1.
\]
This completes the case where $X$ has four zero entries.

Now let $X$ have five zero entries.

If the five zero entries occur in the first three columns, then

$$X^TX = \begin{bmatrix}
A & - & - & - & - \\
- & 1 & - & - & - \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
7 & * & * & 7 & 7
\end{bmatrix}, \quad \text{tr}A = 16.
$$

Therefore, as in previous cases,

$$\text{tr}(X^TX)^{-1} \geq \text{tr}A^{-1} + \text{tr}\left[8I_3-J_3\right]^{-1} \geq \frac{9}{16} + \frac{2}{8} + \frac{1}{5} = 1.0125 > 1.
$$

Now suppose two zeros lie in the first column of $X$ and one in each of the next three columns. Then

$$X^TX = \begin{bmatrix}
5 & * & a_1 & a_2 \\
6 & * & 6 & * \\
\vdots & \vdots & \vdots & \vdots \\
7 & c & 7 & 7
\end{bmatrix}, \quad |a_1| \geq 1, |c| \geq 1.
$$

Thus

$$\text{tr}(X^TX)^2 \geq 5^2 + 3 \times 6^2 + 2 \times 7^2 + 6 \times 1^2
$$

$$= 237
$$

$$> b(37,1).
$$

So Theorem 3.2.2 applies.

Finally, assume there is a zero entry in each of the first five columns of $X$. Then,
\[
X^T X = \begin{bmatrix}
6 & a_1 & a_2 & a_3 & a_4 & b_1 \\
6 & a_5 & a_6 & a_7 & b_2 \\
6 & a_8 & a_9 & b_3 \\
6 & a_{10} & b_4 \\
6 & b_5 \\
7
\end{bmatrix}
\]

Therefore,
\[
\text{tr}(X^T X)^2 \geq 5 \times 6^2 + 7^2 + 5 \sum_{i=1}^{10} a_i^2 + 2 \sum_{i=1}^{5} b_i^2
\]
\[
= 229 + 2 \sum_{i=1}^{5} b_i^2
\]

If \( |a_i| = 0 \) for some \( i \) then by Lemma 2.3.2, \( |b_i| \geq 2 \), for some \( i \), hence \( \text{tr}(X^T X)^2 \geq 237 > b(37,1) \). Thus assume \( |a_i| \geq 1 \) for all \( i \). Then again \( \text{tr}(X^T X)^2 > b(37,1) \).

Finally if \( X \) has six or more zero entries, then
\[
\text{tr}(X^T X)^{-1} \geq \frac{\text{tr}(X^T X)}{6^2} = \frac{36}{36} = 1
\]

This completes the case \( N = 7, n = 6 \).

As mentioned previously the rest of Table 4.2.1 can be proved in a similar but easier manner.

It has already been discussed how Type I designs can be constructed and it is clear that such designs exist for \( n \leq 6 \) and all \( N \geq 7 \), \( N \equiv 3 \mod 4 \). To construct a Type II design for \( N = 11, n = 6 \), choose a \( 12 \times 12 \) Hadamard matrix \( H \) such that
\[
H = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
\end{bmatrix}
\]
Let X be the matrix obtained from H by removing the first row, the
first five columns, and the last column of H. Then a Type II matrix
is obtained by replacing $x_{11}$ by 0. Similarly Type II designs can
be constructed for $N = 11, n = 5$ and $N = 15, n = 6$. Thus all
designs in Table 4.2.1 have been constructed.

Finally, we mention that in the saturated cases, $N = n = 7$
and $N = n = 11$ the above techniques are not very useful since they
fail to reduce the number of competitors in any substantial manner.

4.3 $\phi_p$-optimality in $\mathcal{B}(N,n)$ and $\mathcal{B}'(N,n)$

In this section, we shall extend Theorem 4.1.1 to other criteria.
A technique is developed to show that if a certain design is $\phi_p$-optimal,
then it is also optimal with respect to a large class of other criteria.
A result of this kind is interesting and important in its own right.
The method used is a modification of the result of Cheng [4].

Lemma 4.3.1. For any positive numbers $A, S$ and $r$ such that

$S > n^2/A$, $0 \leq r \leq n$, the system of equations $(n-r)\mu + r\lambda = A$ and $(n-r)/\mu + r/\lambda = S$, $\mu \leq \lambda$, has exactly one solution

$\lambda(r;A,S) > \mu(r;A,S) > 0$. Further, if $S = n^2/A$ there is only one
solution $\lambda(r;A,S) = \mu(r;A,S) > 0$.

Proof. By solving for $\mu$ in the first equation and substituting into
the second, we obtain the equation $Sr\lambda^2 + (n^2 - 2nr - SA)\lambda + rA = 0$. The
discriminant of the quadratic is $h(S) = (n^2 - 2nr - SA)^2 - 4ASr^2$. The
result now follows by noting that $h(n^2/A) = 0$ and

$h'(S) = 2A(SA - n^2) + 4A(nr - r^2) > 0$ if $S > n^2/A$.

Lemma 4.3.2. Let $\mu(r;A,S)$ and $\lambda(r;A,S)$ be as in Lemma 4.3.1 with
$A \leq a_0$ and $S > n^2/A$. Let $f$ be a real-valued function defined on $[0,a_0]$ such that

(i) $f$ is continuous on $(0,a_0)$ (we allow $\lim_{x \to 0^+} f(x) = f(0) = \infty$),

(ii) $g'' < 0$ on $(1/a_0, \infty)$, where $g(x) = f(1/x)$,

(4.3.1)

(iii) $f'' > 0$ on $(0,a_0)$,

(iv) For $a < b \in (0,a_0)$, $\{f(b) - f(a)\}/(b-a) < \{af'(a) + bf'(b)\}/(a+b)$,

and $F(r;A,S) = (n-r)f\{\mu(r;A,S)\} + rf\{\lambda(r;A,S)\}$. Then $F$ is a strictly decreasing function of $r$, strictly increasing function of $S$, and strictly decreasing function of $A$.

Proof. By differentiating the equations $(n-r)\mu + r\lambda = A$ and $(n-r)/\mu + r/\lambda = S$ with respect to $r$ and $S$, then by solving the remaining equations for $\partial\mu/\partial r$, $\partial\lambda/\partial r$, $\partial\mu/\partial S$, and $\partial\lambda/\partial S$, we obtain

$$\partial\mu/\partial r = -(\lambda - \mu)/(n-r)(\lambda + \mu), \quad \partial\lambda/\partial r = -(\lambda - \mu)/r(\lambda + \mu),$$

$$\partial\mu/\partial S = -\lambda^2\mu^2/(n-r)(\lambda^2 - \mu^2), \quad \partial\lambda/\partial S = \lambda^2\mu^2/r(\lambda^2 - \mu^2).$$

Thus

$$\partial F/\partial r = -f(\mu) + (n-r)f'(\mu)\partial\mu/\partial r + f(\lambda) + rf'(\lambda)\partial\lambda/\partial r$$

$$= f(\lambda) - f(\mu) - (\lambda - \mu)\{\mu f'(\mu) + \lambda f'(\lambda)\}/(\lambda + \mu)$$

$$< 0, \text{ by (iv).}$$

Similarly it follows from (iii) that $\partial F/\partial S > 0$. We remark that if $f'' < 0$ on $(0,a_0)$, then $F$ is a decreasing function of $S$. This fact will be used below in the proof of the decreasing monotonicity of $F$ in $A$.

To show that $F$ is a decreasing function of $A$, we write

$$F = (n-r)g(\mu') + rg(\lambda'),$$

where $\mu' = \mu^{-1}$, $\lambda' = \lambda^{-1}$ and $g(x) = f(x^{-1})$. Then $(n-r)\mu' + r\lambda' = S$ and $(n-r)/\mu' + r/\lambda' = A$. By
(ii) and the remark in the last paragraph, we conclude that \( F \) is a strictly decreasing function of \( A \). This completes the proof.

Lemma 4.3.3. Let \( H = \{ (x_1, x_2, \ldots, x_n) : x_i > 0, \sum_{i=1}^{n} x_i = A, \sum_{i=1}^{n} x_i^{-1} = S \} \),

where \( A \leq a_0 \) and \( S \geq n^2/A \). Also let \( F_f : H \to \mathbb{R} \) be defined by

\[
F_f(x_1, x_2, \ldots, x_n) = \sum_{i=1}^{n} f(x_i),
\]

where \( f \) is a real-valued function defined on \([0, a_0]\) which satisfies (4.3.1) and the following condition:

(4.3.2) The equation \( x^2 f'(x) + \alpha x^2 - \beta = 0 \) has at most two solutions in \((0, a_0)\) for all real numbers \( \alpha \) and \( \beta \).

Then the minimum of \( F_f(x_1, x_2, \ldots, x_n) \) on \( H \) occurs at the point \((u(n-1; A, S), \lambda(n-1; A, S), \ldots, \lambda(n-1; A, S))\), where \( u(r; A, S) \) and \( \lambda(r; A, S) \) are as in Lemma 4.3.1.

Proof. First assume \( S > n^2/A \). Since \( H \) is compact, the minimum of \( F_f \) on \( H \) is attained at some point \((a_1, a_2, \ldots, a_n)\). Clearly not all the \( a_i \)'s are equal (since \( S > n^2/A \)), so by the symmetry of \( F_f \), we may assume \( a_1 < a_2 \). Letting \( g_1(x_1, x_2, \ldots, x_n) = \sum_{i=1}^{n} x_i^{-1} - A \) and \( g_2(x_1, x_2, \ldots, x_n) = \sum_{i=1}^{n} x_i^{-1} - S \); then

\[
\det_{j=1}^{n} g_1(a_1, a_2, \ldots, a_n)_{i,j} = a_1^{-2} - a_2^{-2} \neq 0.
\]

So by Lagrange's theorem (see Apostol, [1], p.381), there exist numbers \( \alpha \) and \( \beta \) such that \( a_1, a_2, \ldots, a_n \) satisfy the following equations:

(4.3.3) \( \beta(F_f(x_1, x_2, \ldots, x_n) + \alpha g_1(x_1, x_2, \ldots, x_n) + \beta g_2(x_1, x_2, \ldots, x_n))/\partial x_i = 0, \)

\( i = 1, 2, \ldots, n \).

Now (4.3.3) simplifies to \( f'(x_i) + \alpha - \beta x_i^{-2} = 0, \) \( i = 1, 2, \ldots, n \). By
(4.3.2), each $x_i$ can take on at most two possible values. So the point $(a_1, a_2, \ldots, a_n)$ must be such that $a_1 = a_1$ or $a_2$. The result now follows from Lemma 4.3.1 and Lemma 4.3.2.

Now suppose $S = \frac{n^2}{A}$. Then the result follows since for $(x_1, \ldots, x_n) \in H^\perp, (\frac{A}{n^2}, \ldots, \frac{A}{n})^T = (x_1, x_2, \ldots, x_n)^T (x_1, \ldots, x_n)^T$ and $f$ is continuous and convex.

Now we are ready to prove the main result of this section.

Theorem 4.3.1. Let $\mathcal{M}$ be a family of $n \times n$ symmetric nonnegative definite matrices. Let $M_0 \in \mathcal{M}$ be such that

(i) $M_0$ is a multiple of $I_n$ or has two distinct eigenvalues $\lambda > \mu$ such that the multiplicity of $\lambda$ is $n - 1$

(ii) $M_0$ maximizes $\text{tr} M$ over $\mathcal{M}$

(iii) $M_0$ minimizes $\text{tr} M^{-1}$ over $\mathcal{M}$.

Then $M_0$ minimizes $\Phi_f(M)$ over $\mathcal{M}$ for all $f$ satisfying (4.3.1) and (4.3.2) (with $a_0 = \text{tr} M_0$).

Proof. Let $M_0 \in \mathcal{M}$ satisfy (i) - (iii) and let $S_0 = \text{tr} M_0^{-1}$, $a_0 = \text{tr} M_0$. Let $M \in \mathcal{M}$ be arbitrary and let $S = \text{tr} M^{-1}$, $a = \text{tr} M$.

Then by assumption $S_0 \leq S$ and $a_0 \geq a$, so by Lemma 4.3.2 and 4.3.3 we have

\[
\sum_{i=1}^{n} f(u_i) \geq (n-1)f(\lambda(n-1;A,S)) + f(\mu(n-1;A,S)) \\
\geq (n-1)f(\lambda(n-1;A,S_0)) + f(\mu(n-1;A,S_0)) \\
\geq (n-1)f(\lambda(n-1;a_0,S_0)) + f(\mu(n-1;a_0,S_0)) \\
= \sum_{i=1}^{n} f(u_i^*)
\]
where \( \mu^*_1, \mu^*_2, \ldots, \mu^*_n \) are the eigenvalues of \( M_0 \). The last equality holds since \( \text{tr} M_0 = a_0, \text{tr} M_0^{-1} = S_0 \) and \( M_0 \) has two distinct eigenvalues with the smaller one being a simple root. This completes the proof.

Combining Theorems 4.1.1 and 4.3.1, we have

**Corollary 4.3.1.** For each \( n \), there exists a positive integer \( N_0(n) \) such that for all \( N \geq N_0(n) \), \( X_j \) is \( \Phi_{f_{-}} \)-optimal over \( L(N,n) \) for all \( f \) satisfying the conditions in (4.3.1) and (4.3.2).

Cheng [7] found the following simple sufficient condition for (4.3.1) and (4.3.2).

**Lemma 4.3.4.** If \( f : [0,a_0] \to \mathbb{R} \) is such that (i), (ii) and (iii) in (4.3.1) hold, and \( x^3f''(x) \) is an increasing function on \( (0, a_0) \), then all the conditions in (4.3.1) and (4.3.2) hold.

**Proof.** We need to verify (4.3.2) and condition (iv) in (4.3.1). Now the latter is equivalent to
\[
\{af'(a)+bf'(b)(b-a)\}+(f(b)-f(a))(a+b) > 0.
\]
For fixed \( a \), let
\[
h(b) = \{af'(a)+bf'(b)(b-a)-(f(b)-f(a))(a+b)\}.
\]
Then since \( h(a) = 0 \), to show \( h(b) > 0 \) for all \( b > a \), it suffices to prove \( h'(b) > 0 \) for all \( b > a \). Now
\[
h'(b) = f'(b)(b-a) + a[f'(a) - f'(b)] + bf''(b)(b-a) - f(b) + f(a).
\]
So it is enough to prove \( h''(b) > 0 \) for all \( b > a \). We have
\[
h''(b) = 3f''(b)(b-a) + 2f''(b)(b-a) + f'(b) + f'(b).
\]
Since \( x^3f''(x) \) is an increasing function, \( d[x^3f''(x)]/dx > 0 \), i.e.,
\[
(4.3.4) \quad xf''(x) + 3f''(x) > 0 \quad \text{for all} \quad x \in (0, a_0)\).
\]
Therefore \( h''(b) = \{bf''(b) + 3f''(b)(b-a) > 0 \quad \text{for all} \quad b > a \). This proves condition (iv) in (4.3.1).
Now we prove (4.3.2). Suppose \( x \) and \( y \) are two distinct solutions of the equation \( \alpha x^2 - \beta = 0 \). Then
\[
x^2 f'(x) + \alpha x^2 - \beta = y^2 f'(y) + \alpha y^2 - \beta \quad \text{and hence}
\]
(4.3.5) \[
\frac{x^2 f'(x) - y^2 f'(y)}{(x^2 - y^2)} = -\alpha .
\]
Let \( g(x) = xf'(\sqrt{x}) \). We shall show that \( g \) is a strictly convex function; then for each fixed \( x \), there is at most one \( y \) satisfying (4.3.5) and therefore (4.3.2) is proved. Now
\[
g''(x) = 4x^{-1/2}\left(f''(\sqrt{x})\sqrt{x} + 3f'(\sqrt{x})\right) \quad \text{which, by (4.3.4), is positive.}
\]
This completes the proof.

It is easy to see that if \( 0 < p < 1 \), then the function \( f(x) = x^{-p} \) satisfies the conditions in Lemma 4.3.4. Therefore Theorem 4.3.1 and Corollary 4.3.1 hold for all the \( \Phi_p \)-criteria with \( 0 < p \leq 1 \). By passing to the limit or taking \( f(x) = -\log x \), D-optimality also follows. We state this in the following:

Corollary 4.3.2. For each \( n \), there exists a positive integer \( N_0(n) \) such that for all \( N \geq N_0(n) \), \( X_3 \) is \( \Phi_p \)-optimal over \( \mathcal{G}(N,n) \) for all \( 0 \leq p \leq 1 \); in particular, it is D-optimal.

As shown in Theorem 4.1.1, one can take
\[
N_0(n) = \max\{(n-2)(n^2-n+16)/8, n^2 - 2\} \quad \text{in Corollaries 4.3.1 and 4.3.2.}
\]
This is by no means the smallest bound. But since our result is much stronger than the D-optimality, the smallest \( N_0(n) \) must be larger than \( 2n - 5 \), the bound found by Galil and Kiefer [13] for the D-criterion.

Also note that, unlike Theorem 3.3.1, one can choose \( N_0(n) \) above to be the smallest integer \( k(n) \) such that for all \( N \geq k(n) \), \( X_3 \) is A-optimal in \( \mathcal{G}(N,n) \). Hence we have:
Corollary 4.3.3. If $X_3$ is $A$-optimal in $\mathcal{C}(N,n)$ ($\mathcal{C}'(N,n)$) then it is $\Phi_p$-optimal for all $0 \leq p \leq 1$.

As an application of Corollary 4.3.3 we obtain:

Corollary 4.3.4. All Type I designs in Table 4.2.1 are $\Phi_p$-optimal, $0 \leq p \leq 1$, over $\mathcal{C}(N,n)$.

Proof. By definition $X_3$ is a Type I design. The result now follows from Corollary 4.3.3 since all designs in Table 4.2.1 are $A$-optimal.

Corollary 4.3.5. $X_3$ is $\Phi_p$-optimal, $0 \leq p \leq 1$, over $\mathcal{C}'(N,n)$ for $n \leq 5$, $N \geq 7$ and $n \leq 7$, $N \geq 15$.

Proof. This follows from Theorem 4.1.2 and Corollary 4.3.3.

Remark. Using a similar method, one could generalize Corollary 4.3.2 to show that for any $n$ and $p > 0$, there exists a positive integer $N(n,p)$ such that for all $N \geq N(n,p)$, $X_3$ is $\Phi_q$-optimal over $\mathcal{C}(N,n)$ for all $0 \leq q \leq p$. However, since $X_3$ is not $E$-optimal (even when $N$ gets large), one has $\lim_{p \to \infty} N(n,p) = \infty$. Such a result is not very useful practically. Furthermore, for $p \neq 1$, there is no simple way to calculate a bound for $N(n,p)$ as we did in Section 4.1 for $p = 1$. 
CHAPTER V
PROPOSALS FOR FURTHER RESEARCH

In this dissertation various techniques were developed for proving designs optimal in $\mathcal{D}(N,n)$ (or $\mathcal{D}'(N,n)$). We now give some proposals for future research toward improving and generalizing these methods.

Asymptotic results such as Theorem 3.3.1 and Corollary 4.3.2 enable one to show that a particular design satisfies certain optimality properties if $N$ is sufficiently larger than some $N_0(n)$. It has been mentioned that the upper bounds given for $N_0(n)$ are by no means the smallest possible bounds. Thus further work on reducing these bounds is clearly needed.

Another technique used in determining $\Phi_f$-optimal designs is to minimize $\sum_{i=1}^{n} f(x_i)$ subject to the constraints $\sum_{i=1}^{n} x_i = \text{constant}$, $\sum_{i=1}^{n} g(x_i) = \text{constant}$, and $x_i \geq 0$. This method was successfully applied in Cheng [4] with $g(x) = x^2$ and in our Theorem 4.3.1 with $g(x) = 1/x$. It is our hope that other fruitful choices of $g(x)$ can be found.

It has been observed that $A$-optimal designs in $\mathcal{D}(N,n)$ may not be $A$-optimal in $\mathcal{D}'(N,n)$ (see for example, Table 4.2.1). Such a phenomena is in fact not uncommon. We need the following geometrical result (which we state without proof).

Theorem 5.1. Let $X \in \mathbb{R}^{n \times n}$ such that $(X^T X)^{-1}$ exists. Let $Z$ be obtained from $X$ by replacing $x_i$ in $X = [x_{ij}] = [X_1, X_2, \ldots, X_n]$ by $Z_i$ where $Z_i^T X_i = 0$, $i \geq 2$. Suppose further that $|X^T X| = |Z^T Z|$. Then
\[ \text{tr}(Z^T Z)^{-1} \leq \text{tr}(X^T X)^{-1} \]

with equality if and only if \( X_i^T X_i = 0 \) for \( i \geq 2 \).

By Theorem 3.2.1, Theorem 5.1 and Ky Fan's majorization theorem we conclude that

\[
X = \begin{bmatrix}
0 & 1 & -1 \\
1 & -1 & -1 \\
1 & 1 & 1
\end{bmatrix}
\]

is A-optimal in \( \mathcal{S}(3,3) \). Unfortunately, aside from trivial cases, Theorem 5.1 is not a very useful tool in proving designs A-optimal. A strengthening of this result would be welcome.

In general, the difficulty of proving designs optimal becomes much more difficult as \( N \) approaches \( n \). Stronger methods are then required for these cases, especially the saturated case \( N = n \). The case \( N = n = 7 \) is an example where our techniques are of little help in finding the A-optimal designs (although this case is statistically less important).

Finally, we hope that improved techniques will result in the proofs of conjecture (C1) of Section 3.2 and conjecture (C2) of Section 3.3.
REFERENCES


[34] Wong, C.S. and Masaro, J.C. (1983). A-optimal design matrices $X = (x_{ij})_{n \times n}$ with $x_{ij} = -1, 0, 1$. (To appear in Linear and Multilinear algebra).


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