# OPTIMAL HIERARCHIAL FACTORIAL DESIGNS: THE MULTIPLE DESIGN MULTIRESPONSE CASE WITH COST CONSTRAINT

by

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# CHAPTER I

## INTRODUCTION

This investigation is concerned with the design of multiresponse experiments. Until recently, the selection of a multiresponse design has been made with little consideration given to the fact that more than one response is of interest. One response was generally chosen as the response of primary concern and a design was formulated where this response was considered to be the only response, with the hope that this design would be reasonably efficient for the other responses. Then on each experimental unit, all responses were measured.

Also, too much work in statistics has completely ignored designing experiments with regard to the amount of money available. Economic considerations are especially applicable to a multivariate situation. Practical considerations and acquaintance with experimental situations indicate that in many situations it is neither necessary nor feasible to study each unit on all characteristics. It is therefore necessary, when designing a multiresponse experiment, that the experimenter be aware of two considerations: i) relative to treatment or factor level combinations, i.e., what type of experimental design should be used, ii) if it is decided that the design will be response-wise incomplete (incomplete meaning that on some observational units not all responses will be measured), which responses should not be measured and on which units this should occur. Response-wise incomplete multiresponse experiments are needed when it is either physically impossible, uneconomical, or otherwise inadvisable to study all responses or characteristics on each experimental unit.

In Chapter II various types of linear models that will be used in this investigation are defined. The most universally used model is the Standard Multiresponse (SM) model, which is applicable when all responses have the same univariate design and are measured on each experimental unit. Elimination of the restriction of measuring all responses on each unit gave rise to the General Incomplete Multiresponse (GIM) model (see Trawinski (1961) and Srivastava (1964)) and a special case of the GIM model, the Hierarchial Multiresponse (HM) model (see Srivastava (1966) and Roy and Srivastava (1965)).

To cover the situation where the uniresponse design matrices may be different, the Multiple Design Multiresponse (MDM) model was introduced (Srivastava (1966), Roy and Srivastava (1965)). This model is response-wise complete and therefore, as for the SM design, two models which are response-wise incomplete are derived from the MDM model: The More General Linear Multiresponse (MGLM) model (Kleinbalm (1968)), and the Hierarchial More General Linear Multiresponse (HMGLM) model.

McDonald (1970) investigated the optimal multiresponse randomized block designs for designs fitting the SM, GIM, and

HM linear models. These designs were optimal with respect to minimizing the trace or determinant of the variance-covariance matrix when the size of the design was restricted by a total cost constraint. For these designs (all blocks being the same size), the optimum numbers of blocks on which each response should be measured were determined.

An interesting extension of this work concerns the use of randomized blocks for factorial experiments. Rather than having to replicate entire blocks of units, possibly portions of blocks, being fractional factorials, could be replicated. In many multiresponse factorial experiments, some factor that is applied to all experimental units may be known not to affect some response while affecting the others. The removal of this factor from the model for this response requires the use of the MDM model. Since it will often be neither practical nor necessary to use a response-wise complete experiment, we will therefore be concerned with MGLM models. In Chapter III for a $2^v$ factorial experiment, under a MGLM model with p responses, the design is found which minimizes the trace of a variance-covariance matrix of estimable functions when the total number of observations is restricted by a cost constraint. Theorems are proven which will allow the experimenter to determine the number of times each response should be measured to give the optimal design. After finding these results for the $2^v$ factorial, we then consider the $p^v$ factorial experiment.

Theorems analogous to those proven for the $2^v$ factorials are proven allowing the determination of the optimal design with respect to the trace criterion and a cost constraint.

In Chapters IV, V, and VI, a different criterion is used for optimization. Rather than the trace criterion, minimization of the determinant of the variance-covariance matrix will be used as the condition for optimality, where once again the design will be restricted by a cost constraint. In these chapters only $2^v$ factorial experiments are considered. Chapter IV concerns the determination of the optimal design for the general p response case. Due to the difficulty in obtaining a general form of the determinant in the p-variate case, optimal designs are found for only certain specific situations.

In Chapters V and VI only the 2-variate cases are considered in an attempt to find more general results for the MGLM design than were found for the p-variate case. This will be possible for the 2 responses where it was not possible for p responses because the determinant can now be evaluated in general. In Chapter V a restricted set of MGLM designs, which includes HMGLM designs is investigated to determine the optimal design from this subclass with respect to the determinant criterion.

It is very difficult to give the determinant of the variance-covariance matrix for a general MGLM design, even for the two variable case, because the exact form of the matrices depends upon so many factors. In Chapter VI, the complement of the subclass of designs used in Chapter V is considered. The designs are found whose determinants are lower bounds for this complement subclass. The optimum design from this set of lower bound designs is found, and when compared to the optimum design from Chapter V, the optimal MGLM design is determined.

Chapter VII suggests some implications and ramifications of further research into economic consideration of multivariate design of experiments.

## CHAPTER II

## DEFINITIONS OF MODELS AND DESIGNS

### 2.1 Introduction

In this chapter, various multivariate linear models are defined, illustrated, and compared in the following context. Consider an experiment in which there is a set S containing s' experimental units which are identical to the observational units and will therefore be referred to simply as units. There are p responses under study denoted by $V_1,\ldots,V_p$; and on each unit, any or all of the p responses can be measured. Denote by $y_{ij}$ the measurement of the $j^{th}$ response on the $i^{th}$ unit ($i = 1,\ldots,s'$ and $j = 1,\ldots,p$). It will be assumed that the unit error structures are independent. The type of model that has been most widely used for describing the measurements is the Standard Multiresponse (SM) model. Extensions in the general area where SM models are applicable have led to the definition of the General Incomplete Multiresponse (GIM) model and the Hierarchial Multiresponse (HM) model.

The awareness of situations where the design matrices differ from response to response led to the Multiple Design Multiresponse (MDM) model. Extensions of the MDM model are the More General Linear Multivariate (MGLM) model and the Hierarchial More General Linear Multiresponse (HMGLM) model. These models will be discussed in detail in the following sections and are then illustrated through examples.

## 2.2 The Standard Multiresponse Model

The standard multiresponse model is defined for the general situation where all p responses are measured on s' units.

Definition 2.2.1 A Standard Multiresponse (SM) model is a model which satisfies the following conditions:

$$E(Y) = A\xi \tag{2.2.1a}$$

$$\begin{aligned} Var(Y) &= E\{(Y-E(Y))(Y-E(Y))'\} \\ &= I_{s'} \otimes \Sigma \end{aligned} \tag{2.2.1b}$$

where

Y is the $(s' \times p)$ observation matrix,

$$Y = \begin{bmatrix} y_{11} & \cdots & y_{1p} \\ y_{21} & \cdots & y_{2p} \\ \vdots & & \vdots \\ y_{s'1} & \cdots & y_{s'p} \end{bmatrix}$$

A is the known $(s' \times m)$ design matrix,

$\xi$ is the $(m \times p)$ matrix of unknown parameters,

$\Sigma$ is the $(p \times p)$ positive definite variance-covariance matrix for the elements of any row of Y, $\Sigma = \{\sigma_{jj'}\}$ $(j,j' = 1,\ldots,p)$. The variance of $y_{ij}$, will equivalently be denoted by $\sigma_{jj}$.

$\otimes$ is a matrix operation called a Kronecker product defined in the following manner: if A is an $n_1 \times m_1$ real matrix and B is an $n_2 \times m_2$ real matrix, then $A \otimes B$ is an $n_1 n_2 \times m_1 m_2$ real matrix where $A \otimes B = \{a_{ij}B\}$. For example

$$I_{s'} \otimes \Sigma = \begin{bmatrix} \Sigma & 0 & \cdots & 0 \\ 0 & \Sigma & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdot & \cdot & \Sigma \end{bmatrix}_{s'p \times s'p} .$$

The measurements on the s' different units are statistically independent, while this is not necessarily the case between p responses on any of the specific units.

Another way of looking at the SM model is by a response-wise representation of the model. The observation matrix Y can be expressed as $Y = [\underline{y}_1, \underline{y}_2, \ldots, \underline{y}_p]$ where $\underline{y}_r$ is an $(s' \times 1)$ vector denoting all measurements on response r for $r = 1,\ldots,p$. In a similar manner, partition the parameter matrix $\xi$ into $\xi = [\underline{\xi}_1, \underline{\xi}_2, \ldots, \underline{\xi}_p]$ where $\underline{\xi}_r$ is an $m \times 1$ vector containing the parameters associated with response r for $r = 1,\ldots,p$. The response-wise model gives the p separate univariate models for each of the responses and the representation of the SM model is then written as follows:

$$E(\underline{y}_r) = A\underline{\xi}_r \tag{2.2.2a}$$

$$\begin{aligned} \mathrm{Cov}(\underline{y}_r,\underline{y}_t) &= E\{(\underline{y}_r-E(\underline{y}_r))(\underline{y}_t-E(\underline{y}_t))'\} \\ &= \sigma_{rt}\, I_s, \qquad (r,t = 1,\ldots,p). \end{aligned} \tag{2.2.2b}$$

## 2.3 The General Incomplete Multiresponse Model

It is often uneconomical, physically impossible, or otherwise inadvisable to design an experiment so that all responses are studied on each experimental unit. This situation calls for the General Incomplete Multiresponse (GIM) design.

Trawinski (1961) and Srivastava (1968) give several examples where it is not possible or not feasible to measure each response on each unit.

An example given by Srivastava (1968) concerns a biologist who is growing similar organisms. He would like to observe p responses, but the measurement process is slow, and it is not possible to take the p measurements before the experimental conditions change. He will thus have to use a design that allows for fewer than p responses on each unit.

Trawinski (1961) gives an example where groups of students are given one of three treatments, there being four variables or responses that are of interest. Measurement of these variables requires that the students take a series of tests. A problem that arises is that the students may be too fatigued after several tests to accurately respond to the last tests. It is also possible that the effect of the treatment has lessened or has possibly worn off. These are situations that require response-wise incomplete designs.

Another occasion where this type of design is applicable is an experimental situation in which some responses are more meaningful than others. The more important responses could be measured on more units than those of lesser importance. This type of design becomes even more appropriate when the size of the experiment is restricted by a total cost criterion.

To obtain a GIM design, partition the set S of experimental units into u disjoint sets $S_1, S_2, \ldots, S_u$, with the set $S_i$ having $s_i'$ units ($\sum_{i=1}^{u} s_i' = s'$). It is assumed that on some units of $S_i$ ($i = 1,\ldots,u$) only responses $V_{\ell_{i,1}}, V_{\ell_{i,2}}, \ldots, V_{\ell_{i,q_i}}$ are measured, where $1 \leq q_i \leq p$ and $1 \leq \ell_{i,k} \leq p$ such that $\ell_{i,k} < \ell_{i,k'}$ if $k < k'$ ($i = 1,\ldots,u$ and $k,k' = 1,\ldots,q_i$). On each of the u sets $S_i$, a different subset of the p responses is measured. For example in $S_i$ and $S_j$ ($i,j = 1,\ldots,u$) if $q_i = q_j = q$ then $\ell_{i,\alpha} = \ell_{j,\alpha}$ ($\alpha = 1,\ldots,q$) can only be true when $i = j$.

<u>Definition 2.3.1</u> A multiresponse model is called a General Incomplete Multiresponse (GIM) model if it satisfies the

following conditions:

$$E(Y_i) = A_i \xi B_i \tag{2.3.1a}$$

$$Var(Y_i) = I_{s_i'} \otimes (B_i' \Sigma B_i) \tag{2.3.1b}$$

for $i = 1,\ldots,u$ where:

$\xi(m\times p)$ and $\Sigma(p\times p)$ are as defined for the SM model (see Definition 2.2.1),

$Y_i(s_i'\times q_i)$ is the observation matrix for the set $S_i$,

$$Y_i = [\underline{y}_{i\ell_{i,1}}, \underline{y}_{i\ell_{i,2}}, \ldots, \underline{y}_{i\ell_{i,q_i}}] ,$$

$A_i(s_i'\times m)$ is the design matrix for $S_i$, and

$B_i(p\times q_i)$ is an incidence matrix with ones in the cells $(\ell_{ij},j)$ for $j = 1,\ldots,q_i$ and zeros elsewhere.

Assume that response $V_r$ $(r = 1,\ldots,p)$ is measured on the $d_r$ sets $S_{k_{r,1}},\ldots,S_{k_{r,d_r}}$ on a total of $n_r = \sum_{t=1}^{d_r} s'_{k_{rt}}$ units where $k_{rt} \leq u$ $(t = 1,\ldots,d_r)$ and $1 \leq d_r \leq u$. Then the response-wise representation of the GIM model is given by

$$E(\underline{y}_r) = \begin{bmatrix} E(\underline{y}_{rk_{r,1}}) \\ \vdots \\ E(\underline{y}_{rk_{r,d_r}}) \end{bmatrix}_{n_r\times 1} = \begin{bmatrix} A_{k_{r,1}} \\ \vdots \\ A_{k_{r,d_r}} \end{bmatrix} \underline{\xi}_r \tag{2.3.2a}$$

$$\mathrm{Cov}(\underline{y}_r,\underline{y}_t) = \sigma_{rt}\ \gamma^{(rt)} \qquad (r,t = 1,\ldots,p), \qquad (2.3.2b)$$

where $\gamma^{(rt)}(n_r \times n_t)$ is of the following form:

$$\gamma^{(rt)} = \begin{bmatrix} \gamma^{(rt)}_{1,1} & \gamma^{(rt)}_{1,2} & \cdots & \gamma^{(rt)}_{1,d_t} \\ \vdots & \vdots & & \vdots \\ \gamma^{(rt)}_{d_r,1} & \gamma^{(rt)}_{d_r,2} & \cdots & \gamma^{(rt)}_{d_r,d_t} \end{bmatrix}$$

with

$$\gamma^{(rt)}_{ij} = I_{s'_{k_{ri}}} \quad \text{if } k_{ri} = k_{tj}$$

and

$$\gamma^{(rt)}_{ij} = 0_{s'_{k_{ri}} \times s'_{k_{tj}}} \quad \text{otherwise}$$

for $i = 1,\ldots,d_r$ and $j = 1,\ldots,d_t$ .

## 2.4 The Hierarchial Multiresponse Model

This design is a subclass of GIM designs. In a GIM design define $U_r = \{S_i \mid \text{the response } V_r \text{ is measured on all units of } S_i \text{ for } i = 1,\ldots,u\}$ for $r = 1,\ldots,p$. Assume that there exists a permutation of the integers $(1,\ldots,p)$, say $r_1,\ldots,r_p$ in a GIM design such that $U_{r_1} \supseteq U_{r_2} \supseteq \cdots \supseteq U_{r_p}$.

Since there is a form of hierarchy here because the response $V_{r_{i+1}}$ can be measured only on units where $V_{r_i}$ is measured ($i = 1,\ldots,p-1$), this design is called a Hierarchial Multiresponse (HM) design. Therefore in the HM design $n_{r_1} \geq n_{r_2} \geq \ldots \geq n_{r_p}$. For simplicity, assume without loss of generality that $r_1 = 1$, $r_2 = 2,\ldots,$ $r_p = p$.

Definition 2.4.1 A multiresponse model is called a Hierarchial Multiresponse (HM) model if it satisfies the following conditions:

$$E(Y_i) = A_i(\underline{\xi}_1,\ldots,\underline{\xi}_i) \qquad (2.4.1a)$$

$$\mathrm{Var}(Y_i) = I_{s_i'} \otimes \Sigma_{ii} \quad (i = 1,\ldots,p), \qquad (2.4.1b)$$

where

$Y_i$, $A_i$, and $\underline{\xi}_i$ are as previously defined

and

$\Sigma_{ii}$ is the $i \times i$ positive definite matrix whose elements are found in the first $i$ rows and $i$ columns of $\Sigma$, i.e., the principal minor of rows $1, 2,\ldots,i$ for $1 \leq i \leq p$.

The class of HM designs is a subclass of the class of GIM designs. For the HM design, $u = p$, there are $i$ responses measured on $S_i$, $\ell_{i,1} = 1,\ldots,\ell_{i,q_i} = i$ (thus $i = q_i$), and

$$B_i = \begin{bmatrix} I_i \\ \hline 0_{(p-i),i} \end{bmatrix}.$$

Response $V_r$ is measured on $n_r = \sum_{i=r}^{p} s_i^!$ units. Denoting the $n_r$ observations on $V_r$ by $y_r$, the response-wise representation of the HM model is given as follows:

$$E(\underline{y}_r) = \begin{bmatrix} A_r \\ \vdots \\ A_p \end{bmatrix} \underline{\xi}_r \quad , \qquad (2.4.2a)$$

$$\mathrm{Var}(\underline{y}_r) = \sigma_{rr}\, I_{n_r} \quad , \qquad (2.4.2b)$$

$$\mathrm{Cov}(\underline{y}_r, \underline{y}_t) = \sigma_{rt} \begin{bmatrix} 0_{n_r-n_t,n_t} \\ \hline I_{n_t} \end{bmatrix} \quad \text{for } r < t \ ,$$

$$\mathrm{Cov}(\underline{y}_r, \underline{y}_t) = \sigma_{rt}[0_{n_r,(n_t-n_r)}, I_{n_r}] \quad \text{for } r > t \ ,$$

where $r,t = 1,\ldots,p$, $r \neq t$.

## 2.5 Example

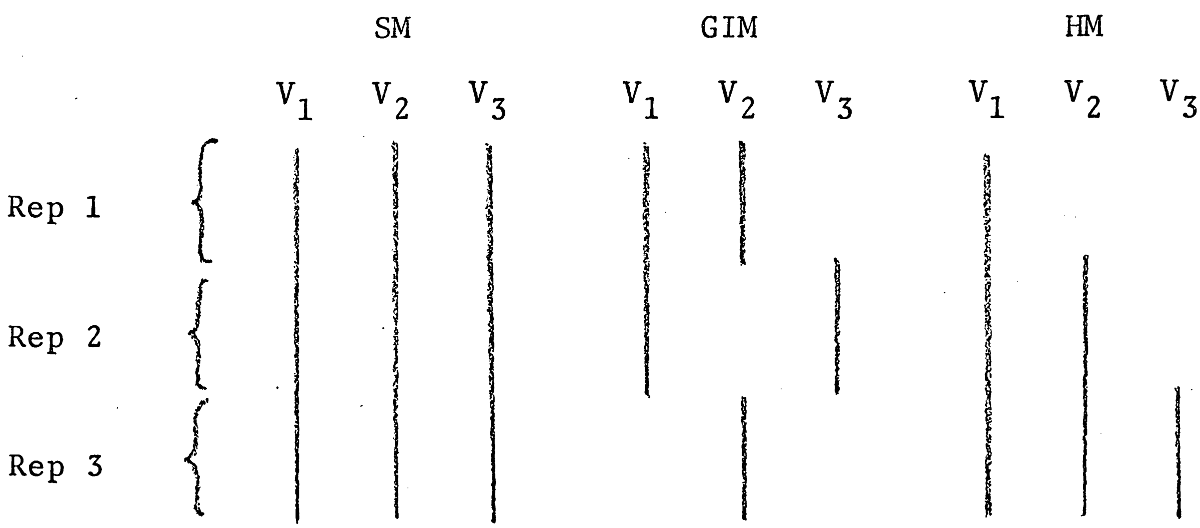
The different models can be illustrated in terms of an experiment performed by the American Meat Institute Foundation (see Harshbarger (1957)). Due to the size and number of factors used in the actual experiment, only certain of these factors will be used in this example in order to simplify it. There were three responses of interest ($p = 3$); shear strength ($V_1$), protein nitrogen ($V_2$), and intra-muscular fat ($V_3$). Four factors were considered in this study: weight of animals (light ($W_0$) or heavy ($W_1$)), days of aging (short term ($A_0$) or long term ($A_1$)), month obtained (January ($M_0$) or June ($M_1$)), and grade of meat (choice ($G_0$) or commercial ($G_1$)). The design was a randomized complete block design of a $2^4$ factorial experiment with 3 blocks (replications). Suppose that all 3 responses are measured on each of the 48 experimental units. This type of arrangement would be an SM design.

Suppose however that $V_1$ was measured in replications 1 and 2, that $V_2$ was measured in replications 1 and 3, and that $V_3$ was measured only in replications 2. Thus with $S_1$ consisting of the 16 units of replication 1, $S_2$ of those of replication 3, it follows that $s_1' = s_2' = s_3' = 16$ and $n_1 = 32$, $n_2 = 32$, and $n_3 = 16$. This is a GIM design.

For another design, suppose that shear strength is measured in all 3 replications; protein nitrogen in replications 2 and 3; and intra-muscular fat only in replication 3. Again

$S_i$ consists of the units in the $i^{th}$ replication $(i = 1,2,3)$, and therefore $U_1 = \{S_1,S_2,S_3\}$, $U_2 = \{S_2,S_3\}$, and $U_3 = \{S_3\}$. Obviously $U_1 \supseteq U_2 \supseteq U_3$ and the design is therefore a HM design.

In the following diagram the vertical lines show where each response was measured for each particular design, illustrating the three preceding designs:




The model for the factorial experiment which will be used throughout this work will employ the general notation used by Kempthorne (1952). The parameter matrix $\xi$ for the SM design will be $\xi = [\underline{\xi}_1,\underline{\xi}_2,\underline{\xi}_3]$ where for $j = 1,2,3$,

$$\underline{\xi}_j' = [\mu_j,\beta_{1,j},\beta_{2,j},\beta_{3,j},W_{0,j},W_{1,j},A_{0,j},A_{1,j},M_{0,j},M_{1,j},$$
$$G_{0,j},G_{1,j},(WA)_{0,j},(WA)_{1,j},(WM)_{0,j},\ldots] \quad (2.5.1)$$

with

$\mu$ being a mean effect,

$\beta$ being a block (replication) effect,

W being the weight effect,

A being the aging effect,

M being the month effect,

G being the grade effect,

WA being the weight × aging interaction effect,

etc.

For a main effect E, the parameter $E_{i,j}$ denotes the deviation of the mean yield of all treatment combinations containing factor E at the $i^{th}$ level on $V_j$ from the mean yield of all treatment combinations on $V_j$ ($i = 0,1$ and $j = 1,2,3$). $E_{0,j}$ will be said to represent the main effect E at the low level and $E_{1,j}$ will represent E at the high level. For an interaction EF of factors E and F, denote by $x_E$ the level of factor E (either 0 or 1) on some treatment combination, and denote by $x_F$ the level of factor F on that same treatment combination. The parameter $(EF)_{ij}$ denotes the deviation of the mean yield of treatment combinations on $V_j$ for which $x_E + X_F = i \pmod 2$ from the mean of all treatment combinations on $V_j$ ($i = 0,1$ and $j = 1,2,3$). It does not make a great deal of sense to talk about the levels of an interaction since it has no real physical interpretation comparable to the levels of a main effect. However, it will be very convenient to let the high and the low level of the interaction EF for the $j^{th}$ response refer to $(EF)_{1,j}$ and $(EF)_{0,j}$ respectively, and for this reason the convention will be employed. (Note that the interaction EF for response $V_j$ is defined as $(EF)_{1,j} - (EF)_{0,j}$.)

The general form of the design matrix will then be the following:

$$A = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & \ldots \\ 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & \ldots \\ \vdots & \vdots & \vdots & & & & & & & & & & & & & & \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & \ldots \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & \ldots \\ 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & \ldots \\ \vdots & \vdots & \vdots & & & & & & & & & & & & & & \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & \ldots \\ 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & \ldots \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & \ldots \\ \vdots & \vdots & \vdots & & & & & & & & & & & & & & \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & \ldots \end{bmatrix} \tag{2.5.2}$$

The parameter matrix for the GIM and the HM designs will be the same as equation (2.5.1). For the GIM and HM designs, $A_1$ consists of the first 16 rows of A; $A_2$ of the second 16 rows; and $A_3$ of the last 16 rows.

For the GIM design

$$B_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad B_2 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad B_3 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix},$$

and for the HM design

$$B_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad B_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad B_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

## 2.6 The Multiple Design Multiresponse Model

The Multiple Design Multiresponse (MDM) linear model arises from the physical situations where, although each response is measured on each experimental unit, the design-model matrices for the p responses are not necessarily the same, i.e., the uniresponse designs may differ from response to response. Different uniresponse design matrices arise due to any of the following situations:

1.) different blocking systems are applicable to different response variates,

2.) some of the response variates are known to be insensitive to certain treatments, or

3.) some response variate is known not to be affected by some treatment interaction or possibly some order of treatment interactions.

Instances where different uniresponse designs arise have been given by Roy and Srivastava (1964) and by Daniel (1960). Roy and Srivastava give an example where different designs are needed due to different amounts of heterogeneity among the units with respect to the different responses. Suppose it is desirable to experiment on different varieties of wheat when interested in the yield ($V_1$) and the susceptibility to pests ($V_2$). Due to differing fertility in the field a randomized block design should be used to decrease the error variation for yield ($V_1$). However the field fertility does not affect the pest susceptibility, and it would be advisable to use a completely randomized experiment with regard to $V_2$.

Daniel's (1960) example concerns 3 factors affecting the flavor ($V_1$) and texture ($V_2$) of a new food. An essential oil affects $V_1$ but not $V_2$. A wheat product affects both $V_1$ and $V_2$. A bran-like substance that is added affects $V_2$ but not $V_1$. As a consequence, the univariate design matrices will be different.

The MDM design has also been investigated under the general title of "Seemingly Unrelated Regressions" by Zellner (1962), (1963), Zellner and Huang (1962), and Kmenta and Gilbert (1967). The MDM designs are similar to the SM designs in that all responses are measured on every unit, but in the MDM design the univariate design matrices are not the same.

<u>Definition 2.6.1</u> A multiple design multiresponse model is called a Multiple Design Multiresponse (MDM) model if it satisfies the following conditions:

$$E(Y) = [A_1\underline{\xi}_1, A_2\underline{\xi}_2, \ldots, A_p\underline{\xi}_p] \qquad (2.6.1a)$$

$$\mathrm{Var}(Y) = I_{s'} \otimes \Sigma \qquad (2.6.1b)$$

where $A_i(s' \times m_i)$ is the univariate design matrix for the $i^{th}$ response $(i = 1, \ldots, p)$,

$\underline{\xi}_i(m_i \times 1)$ is the parameter vector for $V_i$,

$m_i$ is the number of parameters affecting $V_i$.

All other terms have been defined previously.

The response-wise representation of the MDM design is given by the following:

$$E(\underline{y}_r) = A_r\,\underline{\xi}_r\ , \qquad (2.6.2a)$$

$$\mathrm{Cov}(\underline{y}_r, \underline{y}_t) = \sigma_{rt}\, I_{s'} \quad (r,t = 1, \ldots, p)\ . \qquad (2.6.2b)$$

## 2.7 <u>The More General Linear Multivariate Model</u>

The MDM designs consist only of those designs that are response-wise complete. Suppose that the design matrices are not identical for all p responses and that either by design or at random, certain responses are not measured on certain experimental units. For the response-wise incomplete, multi-design situation, Kleinbalm (1968) developed a model called the More General Linear Multivariate (MGLM) model.

This model can be described by using an introduction similar to that used for the GIM model. Divide the set S of s' units into u disjoint sets $S_1,\ldots,S_u$ with $s_1',\ldots,s_u'$ units, respectively. Assume that on the $i^{th}$ subset $S_i$, $q_i$ ($\leq p$) responses are measured, those responses being $V_{\ell_{i,1}},\ldots,V_{\ell_{i,q_i}}$.

<u>Definition 2.7.1</u> A multiple design multiresponse model is called a More General Linear Multivariate (MGLM) model if it satisfies the following conditions:

$$E(Y_i) = [A_{i,\ell_{i,1}}\underline{\xi}_{\ell_{i,1}},\ldots,A_{i,\ell_{i,q_i}}\underline{\xi}_{\ell_{i,q_i}}] \quad , \qquad (2.7.1a)$$

$$\mathrm{Var}(Y_i) = I_{s_i'} \otimes B_i' \, \Sigma \, B_i \quad , \qquad (2.7.1b)$$

where

$A_{i,\ell_{i,j}}$ is the $(s_i' \times m_{\ell_{i,j}})$ design matrix for the response $V_{\ell_{i,j}}$ on the set $S_i$ of units ($i = 1,\ldots,u$ and $j = 1,\ldots,q_i$),

and all other terms have been defined previously.

Assume that response $V_r$ is measured in the $d_r$ sets

$S_{k_{r,1}},\ldots,S_{k_{r,d_r}}$ $(d_r \leq u)$ and let $n_r$ be the number of units on which $V_r$ is measured $(n_r = \sum_{j=1}^{d_r} s'_{k_{r,j}})$. The response-wise representation of the MGLM model is then given by

$$E(\underline{y}_r) = \begin{bmatrix} A_{r,k_{r,1}} \\ \cdot \\ \cdot \\ \cdot \\ A_{r,k_{r,d_r}} \end{bmatrix}_{(n_r \times m_r)} \underline{\xi}_{r\,(m_r \times 1)} \quad , \tag{2.7.2a}$$

$$\mathrm{Cov}(\underline{y}_r,\underline{y}_t) = \sigma_{rt}\ \gamma^{(rt)} \tag{2.7.2b}$$

where $r,t = 1,\ldots,p$ and all other terms have been defined previously.

## 2.8 The Hierarchial More General Linear Multiresponse Model

Just as HM designs were defined as a special subclass of the GIM designs, a special subclass of MGLM designs can also be defined for the case where different design matrices correspond to different responses. For any MGLM design, define the set $U_r$ as follows:

$$U_r = \{S_j \mid \text{the response } V_r \text{ is measured on all units of } S_j \ (j = 1,\ldots,u \text{ and } r = 1,\ldots,p)\}$$

and further let $V_r$ be measured on $d_r$ of the sets $S_j$ $0 < d_r \leq u$. Assume that $U_r = \{S_{k_{r,1}},\ldots,S_{k_{r,d_r}}\}$. Suppose that for a MGLM design there is a permutation of the numbers $1,2,\ldots,p$, say $r_1,r_2,\ldots,r_p$, such that $U_{r_1} \supseteq U_{r_2} \supseteq \cdots \supseteq U_{r_p}$. Subclasses of the MGLM design that possess this property will be called Hierarchiel More General Linear Multiresponse (HMGLM) designs. Without loss of generality, assume that $r_1 = 1,\ldots,r_p = p$.

<u>Definition 2.8.1</u> A multiple design multiresponse model is called a Hierarchial More General Linear Multiresponse (HMGLM) model if it satisfies the following conditions:

$$E(Y_r) = [A_{r,1}\underline{\xi}_1,\ldots,A_{r,r}\underline{\xi}_r] \ , \tag{2.8.1a}$$

$$\mathrm{Var}(Y_r) = I_{s_r'} \otimes \Sigma_{rr} \qquad (r = 1,\ldots,p) \tag{2.8.1b}$$

where all terms have been previously defined.

The response-wise representation is given as follows:

$$E(\underline{y}_r) = \begin{bmatrix} A_{r,r} \\ \cdot \\ \cdot \\ \cdot \\ A_{r,p} \end{bmatrix} \underline{\xi}_r \ , \tag{2.8.2a}$$

$$\mathrm{Var}(\underline{y}_r) = \sigma_{rr}\, I_{n_r}, \tag{2.8.2b}$$

$$\mathrm{Cov}(\underline{y}_r,\underline{y}_t) = \sigma_{rt}\begin{bmatrix} 0_{(n_r-n_t),n_t} \\ - \quad - \quad - \\ I_{n_t} \end{bmatrix} \text{ for } r < t \tag{2.8.2c}$$

and

$$\mathrm{Cov}(\underline{y}_r,\underline{y}_t) = \sigma_{rt}[0_{n_r,(n_t-n_r)}, I_{n_r}] \text{ for } r > t\ , \tag{2.8.2d}$$

where $r,t = 1,\ldots,p$, and all other terms have been previously defined.

## 2.9 Example

Using again the example (see Harshbarger (1957)) given in Section 2.5, the MDM, MGLM, and HMGLM designs can be illustrated. When the actual experiment was conducted, it was found that the factor, days of aging, did not affect the response shear strength, $V_1$. Assuming that this experiment or one similar to it is run at some later date, the experimenter may decide to leave this factor out of his model for $V_1$, but to leave it in the models for the other responses. Of course it is realized that this factor may have appeared insignificant in this particular experiment due to random error, but it will be assumed that the experimenter has possibly run similar tests previous to this one or has other information which leads him to disregard this factor.

Leaving this factor out of the model for $V_1$ of course changes the design matrix. Assuming that no other factors were left out for $V_2$ and $V_3$, their design matrices would be identical to those given in Section 2.5.

The MDM design would be similar to the SM design in Section 2.5 except that the design matrix $A_1$ and the parameter vector $\underline{\xi}_1$ would be different. The MGLM design would be like the GIM design except for the differing design matrix and parameter vector. For the HMGLM design, the observational units would be measured as in the HM design with the difference again being in the differing design matrix and parameter vector for $V_1$.

For these multiple design situations

$$\underline{\xi}_1 = [\mu_1, \beta_{1,1}, \beta_{2,1}, \beta_{3,1}, W_{0,1}, M_{0,1}, M_{1,1}, G_{0,1}, G_{1,1}, (WM)_{0,1}, \text{ etc.}] \ . \qquad (2.9.1)$$

This parameter vector differs from equation (2.5.1) in that there are no aging effects included. The corresponding columns of the design matrix $A_1$ would be obtained from the design matrix A in equation (2.5.2) by omitting the columns corresponding to $A_{0,1}$, $A_{1,1}$ and the appropriate interactions.

# CHAPTER III

# OPTIMIZATION WITH RESPECT TO THE TRACE CRITERION

## 3.1 Introduction

When considering a multiresponse experiment, there is good reason to question whether using a response-wise complete experiment is practical or necessary. A viewpoint frequently not considered in great detail is the monetary aspect of experimentation. This facet becomes especially important when working in a multivariate situation, and can be a very influential element in deciding whether all responses should necessarily be measured on each unit.

Suppose there is a total amount of money $\psi'$ available for conducting the experiment. Assume also that there are known costs $\psi_0, \psi_1, \ldots, \psi_p$, where $\psi_0$ is the cost associated with preparation of a unit for experimentation (a set-up cost) and $\psi_i$ $(i = 1, \ldots, p)$ is the cost of measuring the $i^{th}$ response on an observational unit. It is assumed that these costs are constant throughout the experiment and that there are no relationships between these costs, such as the cost of measuring $V_i$ being less when $V_j$ is measured than when $V_j$ is not measured. One is thus dealing with an additive cost function of the following form:

$$\psi' = \psi_0 n_0 + \psi_1 n_1 + \ldots + \psi_p n_p \qquad (3.1.1)$$

where

$n_0$ is the total number of experimental units made ready for observation, and

$n_i$ is the number of units on which the $i^{th}$ response is measured $(i = 1,...,p)$.

It is therefore obvious that with this type of cost function there will be certain situations where response-wise complete designs may not be in the experimenter's best interest. When only a fixed amount of money is available, (rather than measuring every response on each of say n units $(n \leq n_0)$) it may be better to measure some responses that are not of great interest on fewer than n units so that other important responses can be observed on more than n units. Some criterion must be adopted to help decide which responses if any at all are more important than others. By letting V denote the variance-covariance matrix of estimable functions of the parameters, the trace of V will be used along with the cost constraint in an attempt to order the responses with respect to importance. Also theorems will be proven indicating which responses should be measured on how many and on which units. It is assumed that a multiple design model must be used due possibly to a situation where the responses require different blocking structures; or due to some knowledge of the experimental situation or from results of prior experiments, the experimenter knows that certain factors do not affect certain responses and should thus not be included in the univariate model for these responses. We thus consider a general $2^v$ factorial experiment with a multiple design model, where the applicable models are the MDM and MGLM linear models.

Srivastava and McDonald (1970) derived the formulas for determining the number of observations to be measured on each response for completely randomized and randomized block designs that fall under the classification of the SM or GIM linear models. Their designs are optimal with respect to either the trace or determinant criterion when contrasts on all main effects are studied. This thesis is an extension of the work done by Srivastava and McDonald to the more general case where there can be a multiple design scheme and where the comparisons studied are not necessarily restricted to main effects.

In this chapter we must first determine the form of the variance-covariance matrix V so that a general equation can be formulated for the trace of V. The optimum MGLM design can then be shown to be in the subclass of HMGLM designs and thus only this subclass need be considered in the search for the optimum design. When this equation for the trace is used, the sample sizes can be found that will minimize the trace while not exceeding the amount of money that has been allotted for experimentation. The optimum design will in this way be defined.

## 3.2 The Trace Criterion

For a $2^v$ multiresponse experiment with p responses, although v factors are applied to each experimental unit, assume that the $i^{th}$ response is affected by $v_i$ of these v factors ($v_i \leq v$, for $i = 1,\ldots,p$), thus giving a situation described by a multiple design model. The following notation will be used for a $2^{v_i}$ factorial experiment showing the yield on $V_i$ of the treatment combination of the $\alpha^{th}$ block with the first treatment affecting $V_i$ at level $j_1$, the second treatment affecting $V_i$ at the level $j_2$, etc.

$$E(y_{i\alpha j_1,\ldots,j_{v_i}}) = \mu_i+\beta_{i\alpha}+\tau_{i\ell_{i1}j_1}+\tau_{i\ell_{i2}j_2}+(\tau_{\ell_{i1}}\tau_{\ell_{i2}})_{i,j_1+j_2}$$

$$+\tau_{i\ell_{i3}j_3}+(\tau_{\ell_{i1}}\tau_{\ell_{i3}})_{i,j_1+j_3}+\ldots+ \text{(other main and interaction effects)} \qquad (3.2.1)$$

where: y is an observation whose first subscript i indicates which response is being measured ($i = 1,\ldots,p$), whose second subscript $\alpha$ indicates in which block y is being measured and whose following $v_i$ subscripts $j_m$ indicate the level at which factor $\ell_{im}$ occurs ($m = 1,\ldots,v_i$).

$j_m = 0$ indicates that factor $\ell_{i,m}$ occurs at the low level,

$= 1$ indicates that factor $\ell_{i,m}$ occurs at the high level,

$\mu_i$ is the effect of the mean on $V_i$,

$\beta_{i\alpha}$ is the block effect of the $\alpha^{th}$ block on $V_i$ for $\alpha = 1,\ldots,s_i$, where there are a total of $s_i$ blocks,

$\tau_{i\ell_{im,jm}}$ is the treatment effect of the $\ell_{i,m}^{\;th}$ factor on $V_i$ where this factor is at the level $j_m$ ($\ell_{i,m} = 1,\ldots,v$; $m = 1,\ldots,v_i$),

$(\tau_{\ell_{i,1}}\tau_{\ell_{i,2}}\tau_{\ell_{i,3}}\ldots)_{i,j_1+j_2+j_3+\ldots}$ is the interaction effect of factors $\ell_{i,1},\ell_{i,2},\ldots$ whose first subscript i denotes response $V_i$. The other subscript $j_1+j_2+\ldots$ is to be reduced mod 2; and when 0 this interaction is said to be at the low level, and when 1 it is said to be at the high level. Referring to the high and low level of an interaction employs the convention adopted in Section 2.5.

This form of notation is an extension to a multiresponse situation of the notation used by Kempthorne (1952).

Consider the situation where the experimenter is interested in making comparisons on $k_i$ main and/or interaction effects for the $i^{th}$ response ($k_i \leq 2^{v_i} - 1$, $i = 1,\ldots,p$). Denote the corresponding $2k_i$ parameters by

$$\underline{\tau}_i' = (\tau_{i\ell_{i,1},0},\tau_{i\ell_{i,1},1},\tau_{i\ell_{i,2},0},\ldots) . \qquad (3.2.2)$$

Thus let $\underline{\xi}_i' = [\underline{\beta}_i',\underline{\tau}_i']$, where $\underline{\beta}_i$ denotes the $((m_i-2k_i)\times 1)$ vector of all parameters in the model not included in $\underline{\tau}_i$. This vector

$\underline{\beta}_i$ includes the mean $\mu_i$, the block effects $\beta_{i,1},\ldots,\beta_{i,s_i}$, and any treatment or interaction parameters not under study.

For the parameters of interest, $\underline{\tau}_1,\ldots,\underline{\tau}_p$, assume that the experimenter is interested in linear sets of these parameters (i.e., a set of linear functions of these parameters). This linear set, of say $\eta$ functions, is expressed in the form

$$\underline{\theta} = C\underline{\tau} = \sum_{i=1}^{p} C_i \, \underline{\tau}_i \tag{3.2.3}$$

where for i = 1,...,p:

$\underline{\tau}_i$ is the $(2k_i \times 1)$ parameter vector for $V_i$,
$C_i$ is a given $(\eta \times 2k_i)$ matrix of coefficients,
$C = [C_1,\ldots,C_p]$, dimension $(\eta \times 2k_p^*)$,
$\underline{\tau}' = [\underline{\tau}_1',\ldots,\underline{\tau}_p']$, dimension $(1 \times 2k_p^*)$,
$\theta$ is a $(\eta \times 1)$ vector of linear functions, and
$k_p^* = \sum_{i=1}^{p} k_i$ .

Naturally, the set $\theta$ should be estimable in some sense. This leads to the following definition and lemma.

Definition 3.2.1  For the MGLM model, a linear set of the form of $\theta$ equation (3.2.3) is said to be a piecewise estimable set if each element of each component vector $C_i\underline{\tau}_i$ $(i = 1,\ldots,p)$ has a BLU estimator under the univariate model for $V_i$.

Thus piecewise estimability is equivalent to requiring that each row of $C_i$ belong to the row space of the portion of the design matrix for $V_i$ that corresponds to the $2k_i$ parameters of interest.

Lemma 3.2.1 (Kleinbalm (1968)) For a MGLM design $\theta$ (equation (3.2.3)) is estimable if and only if it is a piecewise estimable set.

To find a piecewise estimable set, the univariate BLU estimators must be found. These BLU estimators can be obtained by solving the reduced normal equations for each of the p separate univariate models. Denote the design matrix of the $i^{th}$ response by $X_i^*$ and partition $X_i^* = [Z_i, X_i]$ so that

$$X_i^* \underline{\xi}_i = [Z_{i\,(n_i\times(m_i-2k_i))}, X_{i\,(n_i\times 2k_i)}] \begin{bmatrix} \underline{\beta}_{i\,((m_i-2k_i)\times 1)} \\ \hline \underline{\tau}_{i\,(2k_i\times 1)} \end{bmatrix} .$$

$X_i$ is that portion of the design matrix corresponding to the parameters of interest which are the elements of $\underline{\tau}_i$. For a contrast $\underline{c}_i'\underline{\tau}_i$, the BLU estimator for each univariate design is given by $\underline{c}_i\hat{\underline{\tau}}_i$ where $\hat{\underline{\tau}}_i$ is a solution of the reduced normal equations for $\underline{\tau}_i$, adjusted for the parameters in $\underline{\beta}_i$, which are not of interest. The reduced normal equations can be expressed as

$$D_i \underline{\tau}_i = \underline{q}_i \tag{3.2.4}$$

with

$$D_i = X_i'X_i - X_i'Z_i(Z_i'Z_i)^- Z_i'X_i \tag{3.2.5a}$$

and

$$\underline{q}_i = X_i(I - Z_i(Z_i'Z_i)^- Z_i') \underline{y} \quad , \tag{3.2.5b}$$

and $(Z_i'Z_i)^-$ being a generalized inverse of $(Z_i'Z_i)$, where a generalized inverse $A^-$ of a matrix A is a matrix $A^-$ such that $AA^-A = A$. In the present situation (a $2^{V_i}$ factorial experiment), $D_i$ will be a $(2k_i \times 2k_i)$ symmetric, positive semi-definite matrix of rank $k_i$.

Consider now a piecewise estimable set $\theta = P\,\underline{\tau}$ of normalized orthogonal contrasts in the parameters of interest $\underline{\tau}_1, \ldots, \underline{\tau}_p$ such that

$$P\underline{\tau} = \begin{bmatrix} P_1 & 0 & \cdots & 0 \\ 0 & P_2 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & P_p \end{bmatrix} \begin{bmatrix} \underline{\tau}_1 \\ \underline{\tau}_2 \\ \vdots \\ \underline{\tau}_p \end{bmatrix} \tag{3.2.6}$$

where

$P_i$ is a $(k_i \times 2k_i)$ matrix with normalized orthogonal rows

P is a known $(k_p^* \times 2k_p^*)$ matrix,

$\underline{\tau}_i$ is a $(2k_i \times 1)$ vector of parameters of interest for $V_i$ $(i = 1, \ldots, p)$,

$\underline{\tau}$ is a $(2k_p^* \times 1)$ vector of $\underline{\tau}_i$'s, and

$$k_p^* = \sum_{i=1}^{p} k_i \, .$$

Relating this equation to equation (3.2.3), it is seen that $\eta = k_p^*$ and that

$$C_1 = \begin{bmatrix} P_1 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix} , \quad C_2 = \begin{bmatrix} 0 \\ P_2 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix} , \ldots , \quad C_p = \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ P_p \end{bmatrix} .$$

For a $2^v$ factorial experiment, the contrasts to be used are the comparisons between an effect's high level and low level. When the extension is made to the $m^v$ factorial experiment, a set of linearly independent contrasts among the m levels of an effect will be studied. With this type of comparison, the matrix $P_i$ can be expressed as

$$P_i = \begin{bmatrix} P_{i,1} & 0 & \cdots & 0 \\ 0 & P_{i,2} & & 0 \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ 0 & 0 & \cdots & P_{i,k_i} \end{bmatrix} \qquad (3.2.7)$$

where

$P_{ij}$ is the set of coefficients for contrasts on the $j^{th}$ factor or interaction of interest to the experimenter

($i = 1,\ldots,p$ and $j = 1,\ldots,k_i$).

For a $2^v$ factorial experiment $P_{ij}$ will be a $(1\times 2)$ matrix since there are only 2 levels to compare and only 1 degree of freedom for each effect. For an $m^v$ factorial experiment $P_{ij}$ will be a $((m-1)\times m)$ matrix since there are $(m-1)$ linearly independent orthogonal contrasts among the m levels, i.e., m parameters and m-1 degrees of freedom.

By solving the reduced normal equations (3.2.4) for the univariate design of each response, the set of linear estimators $P\hat{\underline{\tau}}$ for $P\underline{\tau}$ as given by equation (3.2.6) can be found. Denote by V the variance-covariance matrix of the estimable functions of interest, thus

$$V = \mathrm{Var}(P\hat{\underline{\tau}}) \tag{3.2.8}$$

and denote by Q, the trace of V,

$$Q = \mathrm{tr}(V) \ . \tag{3.2.9}$$

For each design D there will be a corresponding value of Q, say Q(D). For different designs their Q-values will be compared in order to obtain efficient designs. This criterion will be referred to as the trace criterion.

Next it will be shown that Q is independent of the set of normalized orthogonal contrasts that are used. Although this chapter is concerned primarily with $2^V$ factorial experiments, the fact that Q is not a function of P will be proven for a general $m^V$ factorial experiment so that these results can also be used in Section 3.7.

Consider a $m^V$ factorial experiment and suppose that $k_i$ factors are under study for $V_i$, then $P_i$ is a matrix of dimension $((m-1)k_i \times mk_i)$. Since $P_i$ is a set of normalized orthogonal row vectors $P_{ij}P'_{ij} = I_{m-1}$ and $P_{ij}\underline{j}_m = \underline{0}_{m-1}$ ($i = 1,\ldots,p$ and $j = 1,\ldots,k_i$), where $\underline{j}_z$ denotes a $(z\times 1)$ vectors of ones and $\underline{0}_z$ is a $(z\times 1)$ vector of zeros. The rows of $P_{ij}$ form a basis for a vector space of dimension $(m-1)$. If a $(1\times m)$ vector can be found that is linearly independent of the rows of $P_{ij}$, then this vector along with the rows of $P_{ij}$, will span a vector space of dimension m. Because of the definition of $P_{ij}$ the vector $\underline{j}'_m$ is linearly independent of the rows of $P_{ij}$. Augmenting $P_{ij}$ by the normalized row vector $m^{-\frac{1}{2}}\underline{j}'_m$ yields the following matrix:

$$P^*_{ij} = \begin{bmatrix} & P_{ij} & \\ \hline \frac{1}{\sqrt{m}} & \cdots & \frac{1}{\sqrt{m}} \end{bmatrix}$$

with rank $(P^*_{ij}) = m$ and

$$P^*_{ij}\ P^{*\prime}_{ij} = I_m \quad .$$

Since $P^*_{ij}$ is an orthogonal matrix then

$$I_m = P^{*\prime}_{ij}\ P^*_{ij}$$

$$= [P'_{ij},\ \frac{1}{\sqrt{m}}\ \underset{\sim}{j}_m] \begin{bmatrix} P_{ij} \\ - \quad - \quad - \\ \frac{1}{\sqrt{m}}\ \underset{\sim}{j}'_m \end{bmatrix}$$

or

$$I_m = P'_{ij}\ P_{ij} + \frac{1}{m}\ J_m.$$

Thus
$$P'_{ij}\ P_{ij} = I_m - \frac{1}{m}\ J_m\ .$$

$P'_iP_i$ can therefore be expressed as

$$P'_i\ P_i = \frac{1}{m}\ I_{k_i} \otimes (mI_m - J_m) \tag{3.2.10}$$

and

$$P'P = \begin{bmatrix} P'_1P_1 & 0 & \cdots & 0 \\ 0 & P'_2P_2 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & P'_pP_p \end{bmatrix}$$

It follows then that

$$Q = \text{tr}(\text{Var}(P\hat{\underline{\tau}}))$$

$$= \text{tr}(\text{Var}(\hat{\underline{\tau}})P'P)$$

$$= \text{tr}\left\{\text{Var}(\hat{\underline{\tau}})\begin{bmatrix} P_1'P_1 & 0 & \cdots & 0 \\ 0 & P_2'P_2 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & P_p'P_p \end{bmatrix}\right\}. \quad (3.2.11)$$

Substituting into equation (3.2.11) the expression for $P_i'P_i$ given in equation (3.2.10), Q is seen to be invariant with respect to the choice of P as long as P is normalized. This shows that the trace of the variance-covariance matrix of these estimable functions depends only upon the design, not upon the specific set of contrasts chosen. It would also depend upon the number of factors the experimenter wants studied on each response ($k_i$); but these will have been decided upon by the experimenter, and although variable from one experiment to another, they will be considered constant for any particular experiment.

## 3.3 Reduced Normal Equations for a $2^v$ Factorial Experiment

In this section we will determine if the trace criterion is dependent upon whether a design is made up of full $2^{v_i}$

factorial experiments or of $1/2^{f_i}$ fractions of $2^{v_i}$ factorial experiments. This is of interest because we will eventually be determining the optimal size design to be conducted. Determination of the optimal size design implies finding the number of experimental units for each response. If it can be shown that fractional factorials have the same trace criterion as do full factorials, then it will be to our advantage to work with the fractional factorial. We would like to show that the trace of the variance-covariance matrix is dependent upon the number of observations on each response and not the factorial sizes (assuming that the sizes are large enough to prohibit aliasing of important effects). This will be explained in greater detail later, but for now we will be concerned with the comparison of the two trace criteria.

For two univariate designs, the reduced normal equations will first be determined to find the BLU estimators for the parameters of interest. These univariate solutions are then easily extended to the multivariate case where we can find the piecewise estimators by just combining the separate BLU estimators for each response. The variance-covariance matrix of these estimable functions that are of interest can be determined and the general form of the trace of this matrix is found. The traces of the two designs can then be compared for the case where each design has each response measured the same number of times.

Case 1 concerns the full $2^v$ factorial experiment replicated r times in a randomized block design. The following model is assumed where the block effects are denoted by $\beta_1,\ldots,\beta_r$:

$$y_{ijk\ell\ldots} = \mu+\beta_i+A_j+B_k+(AB)_{j+k}+C_\ell+(AC)_{j+\ell}+\ldots+\varepsilon_{ijk\ell\ldots} \tag{3.3.1}$$

where the model contains v main effects: A,B,C,... (v terms) and $i = 1,\ldots,r$

$j,k,\ell,\ldots = 0$ if the factor appears in the treatment combination at the low level,

$= 1$ if it appears at the high level.

The interaction subscripts are reduced mod 2, and the same interaction convention will be used as introduced in Section 2.5.

The general form of the reduced normal equations adjusted for the mean $\mu$ and the block effects will be developed in an abbreviated form. The main steps are included for ease of understanding. It is assumed that the experimenter is interested in all main effects and interactions. In matrix notation this univariate model is

$$E(\underline{y}) = X^*\underline{\xi}$$

where

$\underline{\xi}' = [\underline{\beta}', \underline{\tau}']$,

$\underline{\beta}$ is a $((r+1)\times 1)$ vector $\underline{\beta}' = [\beta_1, \ldots, \beta_r, \mu]$, (this ordering of the variables is used to ease calculation of the generalized inverse),

$\underline{\tau}$ is a $(2(2^v-1)\times 1)$ vector,

$\underline{\tau}' = [A_0, A_1, B_0, B_1, (AB)_0, (AB)_1, C_0, \ldots]$,

$X^* = [Z, X]$,

$Z$ is an $(r2^v\times(r+1))$ matrix which is that portion of the design matrix associated with the effects for which the effects of interest will be adjusted,

$X$ is the $(r2^v\times 2(2^v-1))$ design matrix associated with the effects under study.

The form of the matrix $X^{*\prime}X^*$ is then

$$X^{*\prime}X^* = \left[\begin{array}{c|c} Z'Z & Z'X \\ \hline X'Z & X'X \end{array}\right] \tag{3.3.2}$$

where

$$X'X = r2^{v-2}J_{2(2^v-1)} + r2^{v-2}I_{(2^v-1)} \otimes (2I_2 - J_2), \tag{3.3.3a}$$

$$Z'X = 2^{v-1}\left[\begin{array}{c} J_{r\ 2(2^v-1)} \\ \hline r\,\underline{j}_{2(2^v-1)}' \end{array}\right] = (X'Z)', \tag{3.3.3b}$$

$$Z'Z = 2^v \left[\begin{array}{c|c} I_r & \underline{j}_r \\ \hline \underline{j}_r' & r \end{array}\right] . \qquad (3.3.3c)$$

For equation (3.2.5) the matrix D of the reduced normal equations is $D = X'X - X'Z(Z'Z)^{-}Z'X$. To find a generalized inverse of $Z'Z$, the following theorem will be used by partitioning a matrix $W'W$ into

$$W'W = \left[\begin{array}{c|c} W_1'W_1 & W_1'W_2 \\ \hline W_2'W_1 & W_2'W_2 \end{array}\right]$$

with the partition of $W'W$ corresponding to that of $Z'Z$ in equation (3.3.3c).

<u>Theorem 3.3.1</u> (Rohde (1964)) A generalized inverse of $W'W$ is given by

$$(W'W)^{-} = \left[\begin{array}{c|c} (W_1'W_1)^{-} + (W_1'W_1)^{-}(W_1'W_2)L^{-}(W_2'W_1)(W_1'W_1)^{-} & -(W_1'W_1)^{-}(W_1'W_2)L^{-} \\ \hline -L^{-}(W_2'W_1)(W_1'W_1)^{-} & L^{-} \end{array}\right]$$

where

$$L = W_2'W_2 - (W_2'W_1)(W_1'W_1)^-(W_1'W_2) \ .$$

In finding $(Z'Z)^-$ using Theorem 3.3.1 and equation (3.3.3c), L is found to be 0 and thus a generalized inverse of Z'Z is given by

$$(Z'Z)^- = 2^{-v} \left[ \begin{array}{c|c} I_r & \underline{0} \\ \hline \underline{0}' & 0 \end{array} \right] . \qquad (3.3.4)$$

Using equations (3.3.3) and (3.3.4) gives

$$X'Z(Z'Z)^-Z'X = r \ 2^{v-2} \ J_{2(2^v-1)} \ ,$$

thus giving $D_{(1)}$, the matrix of the reduced normal equations for case 1, to be

$$D_{(1)} = r \ 2^{v-2} \ I_{2^v-1} \otimes (2I_2 - J_2) \ . \qquad (3.3.5)$$

The form of the matrix of the reduced normal equations was worked out for this case but should actually follow from equation (3.3.2) due to the orthogonality of the design.

This is the general form of the matrix of the reduced normal equations for the general $2^v$ factorial experiment replicated r times. If the experimenter had been interested in contrasts involving only k effects rather than all $(2^v-1)$

effects as was given in equation (3.3.5), then the matrix $D_{(2)}$ of the reduced normal equations adjusted for the mean, for the block effects, and for the $(2^v-1-k)$ effects not of interest, would be

$$D_{(2)} = r\ 2^{v-2}\ I_k \otimes (2I_2 - J_2)\ . \qquad (3.3.6)$$

This follows directly by virtue of the orthogonality between main effects and interactions.

In the second univariate case, instead of repeating full factorial experiments, fractional factorials will be repeated. Assume that there are k effects of interest to the experimenter. Thus the smallest fraction of the $2^v$ factorial experiment can be found that allows all of the k effects of interest to be unaliased with each other and with other effects that are thought to be non-zero. Suppose that this smallest fraction is a $\frac{1}{2}f$ fraction of the $2^v$ factorial experiment $(0 \leq f < v)$.

Let $d = v-f$ and consider a randomized block design with s blocks of $2^d$ experimental units each. Once the value of s is decided upon, the experimenter would not want to repeat the same set of $2^d$ treatment combinations (as specified by the defining contrast) but would attempt to balance the design as much as possible (i.e., use other sets of treatment combinations). This matter will be discussed in greater detail later; the point to be focussed upon now is the general form of the matrix of the reduced normal equations. The model for this fractional replicate, in addition to containing the mean and block effects, will include $2^d$-1 other effects. Among these effects will be those to be studied (generally main effects) with the remaining terms being other terms in the model that will be aliased neither with the main effects nor among themselves. The univariate model is given by

$$E(\underline{y}) = X^* \underline{\xi} = [Z,X] \begin{bmatrix} \underline{\beta} \\ \\ \underline{\tau} \end{bmatrix}$$

where

$X$ is the $(s2^d \times 2(2^d-1)$ design matrix associated with the treatment and interaction parameters,

$Z$ is the $(s2^d \times (s+1))$ design matrix for the mean block effects (the effects for which the effects of interest will be adjusted),

$\underline{\beta}' = [\beta_1,\ldots,\beta_s,\mu]$, $(1\times(s+1))$, and

$\underline{\tau}' = [A_0,A_1,B_0,B_1,\ldots]$, $(1\times 2(2^d-1))$ .

Further

$$[X^{*\prime}X^*] = \left[\begin{array}{c|c} Z'Z & Z'X \\ \hline X'Z & X'X \end{array}\right] ,$$

where

$$Z'Z = 2^d \left[\begin{array}{c|c} I_s & \underline{j}_s \\ \hline \underline{j}'_s & s \end{array}\right]$$

$$Z'X = 2^{d-1} \left[\begin{array}{c} J_{s,2(2^d-1)} \\ \hline s\underline{j}'_{2(2^d-1)} \end{array}\right] = (X'Z)' \ , \quad \text{and}$$

$$X'X = s\ 2^{d-2}\ J_{2(2^d-1)} + s\ 2^{d-2}\ I_{2^d-1} \otimes (2I_2 - J_2)\ .$$

Again Theorem 3.3.1 is used to find the generalized inverse of Z'Z and the matrix $D_{(3)}$ of the reduced normal equations (3.2.4) for this case is

$$D_{(3)} = s\ 2^{d-2}\ I_{2^d-1} \otimes (2I_2 - J_2)\ . \tag{3.3.7}$$

If the experimenter is interested in contrasts involving only k sets of the parameters rather than $2^d$-1 as is assumed in obtaining equation (3.3.7), it is again a simple matter due to the orthogonality of the design to adjust for these $2(2^d$-1-k) parameters. The matrix of the reduced normal equations, $D_{(4)}$, reduced for the mean, for the block effects, and for these $2(2^d$-1-k) parameters not of interest is

$$D_{(4)} = s\ 2^{d-2}\ I_k \otimes (2I_2 - J_2)\ . \tag{3.3.8}$$

In the preceding derivations the assumption of a randomized block situation was not really a restriction. Had we assumed that the units were homogeneous and thus used a completely randomized design, the derivations would have been easier but the reduced normal equations, adjusting now for only the mean and parameters not of interest, would have been equivalent to equations (3.3.6) and (3.3.8). Also, the reduced normal equations for a design containing blocks nested in replications would be equivalent to equations (3.3.6) or (3.3.8). This situation can occur in the second case where $s > 2^f$, thus giving enough units to allow more than one complete factorial experiment.

Having found the general forms of the matrix of the reduced normal equations, it is now of interest to look at the variance-covariance matrix of the estimators for the estimable functions of the treatment parameters. This must be determined so that the traces of these matrices can be found and the designs for the two cases can be compared. With interest still in the univariate case, denote by $P_*$ the matrix whose rows are the contrast coefficients associated with the parameters of interest, the set of contrasts being $P_*\underline{\tau}$. Thus

$$\mathrm{Var}(P_*\hat{\underline{\tau}}) = P_*\ \mathrm{Var}(\hat{\underline{\tau}})P_*' \tag{3.3.9}$$

with $\hat{\underline{\tau}}$ being a solution to the reduced normal equations, i.e., $\hat{\underline{\tau}} = D^{-}\underline{q}$ where $\underline{q}$ is defined in equation (3.2.5b). If $\text{Var}(\underline{y}) = \sigma^2 I$ then

$$\text{Var}(P_*\hat{\underline{\tau}}) = \sigma^2 P_* D^{-} D D^{-} P_*' \ . \tag{3.3.10}$$

For case 1, where the full $2^v$ experiment is repeated r times with the interest being in only k sets of treatment parameters, the matrix $D_{(2)}$ of the reduced normal equations was found in equation (3.3.6). To find $D_{(2)}^{-}$, Theorem 2 (Appendix) and also the fact that a generalized inverse of $(2I_2 - J_2)$ is $\frac{1}{2} I_2$ (Theorem 3, Appendix) given

$$D_{(2)}^{-} = \frac{1}{r2^{v-1}} I_{2k}$$

and therefore

$$D_{(2)}^{-} D_{(2)} D_{(2)}^{-} = \frac{1}{r2^{v}} I_k \otimes (2I_2 - J_2) \ . \tag{3.3.11}$$

For case 2, the matrix $D_{(4)}$ of the reduced normal equations which was found in equation (3.3.8) has a generalized inverse

$$D_{(4)}^{-} = \frac{1}{s2^{d-1}} I_{2k} \tag{3.3.12}$$

and thus

$$D^-_{(4)}D_{(4)}D^-_{(4)} = \frac{1}{s2^d} I_k \otimes (2I_2 - J_2) . \qquad (3.3.13)$$

The reduced normal equations above have been determined for the univariate case with their solutions giving the univariate BLU estimators. To estimate functions of parameters in the multivariate case, the piecewise estimators must be found, i.e., the univariate BLU estimators for each response separately. To return to the multivariate case, the univariate notation is extended to include multivariate situations where for $i = 1,\ldots,p$,

$$\mathrm{Var}(P_i\hat{\underline{\tau}}_i) = \sigma_{ii}(P_iD_i^-D_iD_i^-P_i') \qquad (3.3.14)$$

with $D_i$ representing the matrix of the reduced normal equations for response $V_i$. For the first case considered, a full $2^{v_i}$ factorial experiment replicated $r_i$ times,

$$D^-_{(2)i}D_{(2)i}D^-_{(2)i} = \frac{1}{r_i2^{v_i}} I_{k_i} \otimes (2I_2-J_2) . \qquad (3.3.15)$$

For the second case, a $\frac{1}{2}f_i$ fraction of a $2^{v_i}$ factorial experiment replicated $s_i$ times,

$$D^-_{(4)i}D_{(4)i}D^-_{(4)i} = \frac{1}{s_i2^{d_i}} I_{k_i} \otimes (2I_2-J_2) . \qquad (3.3.16)$$

Q as defined in (3.2.9) can be expressed as

$$Q = \sum_{i=1}^{p} tr(Var(P_i\hat{\underline{\tau}}_i)) \ . \tag{3.3.17}$$

For case 1,

$$Q_{(2)} = \sum_{i=1}^{p} \sigma_{ii} tr(P_i D^-_{(2)i} D_{(2)i} D^-_{(2)i} P_i')$$

or

$$Q_{(2)} = \sum_{i=1}^{p} \sigma_{ii} tr(D^-_{(2)i} D_{(2)i} D^-_{(2)i} P_i' P_i) \ . \tag{3.3.18}$$

Equation (3.2.10) for m = 2 yields

$$P_i' P_i = \frac{1}{2} I_{k_i} \otimes (2I_2 - J_2) \tag{3.3.19}$$

which along with equation (3.3.15) and Theorem 1 (Appendix) gives the following:

$$D^-_{(2)i} D_{(2)i} D^-_{(2)i} P_i' P_i = \frac{1}{r_i 2^{v_i}} I_{k_i} \otimes (2I_2 - J_2). \tag{3.3.20}$$

Using equations (3.3.20) and (3.3.18),

$$Q_{(2)} = \sum_{i=1}^{p} \sigma_{ii} \frac{2k_i}{r_i 2^{v_i}} \ . \tag{3.3.21}$$

For case 2, $D^-_{(4)i} D_{(4)i} D^-_{(4)i}$ is given in equation (3.3.16) and $P_i'P_i$ is the same as equation (3.3.19) and therefore

$$Q_{(4)} = \sum_{i=1}^{p} \sigma_{ii} \frac{2k_i}{s_i 2^{d_i}} . \qquad (3.3.22)$$

Having found the general forms of the trace of the variance-covariance matrix of estimable functions, comparison of the two factorial experiments can now be made. Suppose that a MGLM design is conducted with $n_i$ observational units on the $i^{th}$ response ($i = 1,\ldots,p$). If full factorial experiments are conducted (case 1), then $r_i = n_i 2^{-v_i}$; and if fractional factorials are conducted (case 2), then $s_i = n_i 2^{-d_i}$. As long as the fractions $\frac{1}{2} f_i$ are large enough that the $k_i$ effects under study are not aliased with other non-zero terms, then the precision in estimation will be the same for case 1 or case 2. The value of the trace $Q_{(2)}$ (equation (3.3.21)) equals the trace $Q_{(4)}$ (equation (3.3.22)) since $r_i 2^{v_i} = s_i 2^{d_i}$.

Suppose that for $V_i$, a $\frac{1}{2} f_i$ fraction of a $2^{v_i}$ factorial experiment is the smallest allowable experiment size without aliasing important terms. When determining the optimum size design, it is better to determine how many times we could replicate a group of $2^{d_i}$ units rather than replicating a group of $2^{v_i}$ units because it will be possible to stay closer to the optimum solution. For example, suppose that $v_i = 5$ and $f_i = 2$. Assuming that a fraction this small does not alias important effects, it is better to work with replications of groups of 8 units than to work with replications of 32 units. If the optimum design allocates 48 units to this $i^{th}$ response, then for case 1: $r_i = 1.5$, and for case 2: $s_i = 6$. In case 1 we have the problem of rounding either to 64 units so that two replicates are used, or to 32 units where there is only one replicate. Either rounding up or off we are moving 16 units away from the optimal size; the more the change in units, the further you move from the true optimal design. With case 2 there is no round-off needed. This example illustrates that the smaller the group of units that is being replicated, the closer you can stay to the true optimum. Therefore we will use fractional factorial experiments for the remainder of this work ($0 \leq f_i < v_i$) whenever it is possible not to alias important terms.

### 3.4 General Definitions and Preliminaries

The trace Q of the variance-covariance matrix $Var(P\hat{\underline{\tau}})$ contains only the variances of the normalized contrasts the experimenter desires to study. Minimizing Q, the sum of the variances, has the effect of minimizing the average variance of all contrasts. From equations (3.3.21) or (3.3.22), it is obvious that to make Q smaller and smaller one need only increase the number of observations taken for each response.

It is common knowledge that increasing the sample size increases the precision; however, in a real world situation, the number of observations will be restricted by some amount of money allocated for the experiment. In a multiple design situation it is often the case that there is a total of n experimental units with each response measured on all n units, thus giving a MDM design. The n is chosen so that the total amount of money available is not exceeded. Using a MGLM design the experimenter is not restricted to having $n_1 = n_2 = \ldots = n_p$. If the $i^{th}$ response has a relatively large variance as compared to the other variances, then possibly it should be measured on more units than the other responses. This will decrease the sum of the variances, Q, if the increase in precision on the $i^{th}$ response more than offsets the possible decrease in precision on the other responses. The same situation could occur when one response is easier or cheaper to measure than the other responses.

A total cost function will be defined next, and thus the cost and trace can be determined for any design. When a limited amount of money is available for experimentation, then by use of the cost function, all designs can be considered that do not surpass the allotted resources. Considering only these designs, the design can be found that is the optimal design with respect to minimizing the trace.

Let $\psi_0$ be the cost of preparing an experimental unit for observation (a set-up cost), where any or all of the p responses could be measured on this unit. Define $\psi_i$

($i = 1,\ldots,p$) to be the cost of measuring the response $V_i$ on any observational unit. Use the notation $D(n_0,n_1,\ldots,n_p)$ to denote a design which consists of $n_0$ observational units on which at least one response is measured, and on $n_i$ of these $n_0$ units $V_i$ is measured, $n_0 \geq n_i$. (Recall that in a MDM design $n_0 = n_i$ ($i = 1,\ldots,p$) and in a HMGLM design $n_0 = \max(n_1,\ldots,n_p)$.) Therefore for a design $D(n_0,n_1,\ldots,n_p)$ the total cost function is given by

$$\psi(D) = n_o\psi_o + n_1\psi_1 + \ldots + n_p\psi_p \tag{3.4.1}$$

where $\psi(D)$ will be called the cost of the design D. Assume that there is a total amount of money allocated for experimentation $\psi'$ ($\psi' > 0$). Define $\{\psi'\}$ to be the class of MGLM designs whose costs do not exceed $\psi'$, i.e., for any $D \in \{\psi'\}$, $\psi(D) \leq \psi'$. Denote the subclass of HMGLM designs contained in $\{\psi'\}$ by $[\psi']$.

Definition 3.4.1 A design $D^* \in \{\psi'\}$ will be said to be as good as a design $D \in \{\psi'\}$ relative to the trace criterion if:

$$\psi(D^*) \leq \psi(D) \text{ and } Q(D^*) \leq Q(D) . \tag{3.4.2}$$

$D^*$ is said to be better than D if either inequality is a strict inequality.

Definition 3.4.2  A subclass of designs $[\psi']$ is said to be complete with respect to $\{\psi'\}$ if for any design $D \varepsilon \{\psi'\}$ there is a design $D^* \varepsilon [\psi']$ that is at least as good as D.

Lemma 3.4.1  If for every $D(n_0,n_1,\ldots,n_p) \varepsilon \{\psi'\}$, Q(D) is a function of only $n_1,\ldots,n_p$ then $[\psi']$ is complete with respect to $\{\psi'\}$.

Proof: (The general proof of this theorem (McDonald (1970)) is repeated for completeness.)

For a design $D(n_0,n_1,\ldots,n_p) \varepsilon \{\psi'\}$, the elements $(n_1,\ldots,n_p)$ are ordered such that $n_{i_1} \geq n_{i_2} \geq \ldots \geq n_{i_p}$ and without loss of generality assume that $i_1 = 1$, $i_2 = 2,\ldots,$ $i_p = p$. A design $D^*(n_0^*,n_1^*,\ldots,n_p^*)$ with $n_1^* = n_1,\ldots,n_p^* = n_p$ is constructed in the following manner: From the $n_0$ elements in D, a subset $U_1^*$ of $n_1^*$ elements is chosen and on this subset the response $V_1$ is measured. Notice that $n_1^* \leq n_0$. Select any subset $U_2^*$ of $U_1^*$ containing $n_2^*$ elements and on these $n_2^*$ units measure $V_2$. Continuing in this manner, finally select any subset $U_p^*$ of $U_{p-1}^*$ containing $n_p^*$ elements and on these units measure response $V_p$. (Notice $U_1^* \supseteq U_2^* \supseteq\ldots\supseteq U_p^*$, $n_0^* = n_1^*$, and a hierarchial design has been constructed.) $D^* \varepsilon [\psi']$ and $Q(D^*) = Q(D)$ since $n_i^* = n_i$ $(i = 1,\ldots,p)$ and as the theorem assumes, the trace is a function of only $n_1,n_2,\ldots,n_p$. Further, since $n_0^* = n_1^* \leq n_0$ then $\psi(D^*) \leq \psi(D)$. $[\psi']$ is thus complete with respect to $\{\psi\}$. This completes the proof.

## 3.5 Determination of the Optimum Design

In this section conditions are found that enable the experimenter to determine whether the optimum design is a MDM or HMGLM design. Once the appropriate design is found, the values of $s_i$ $(i = 1,\ldots,p)$ can be determined that make the design optimum with respect to the trace criterion and a cost constraint.

Suppose an experimenter is faced with the multiple design situation described in Section 3.2, such that out of v factors, each at two levels, only $v_i$ affect the $i^{th}$ response $(v_i \leq v$, $i = 1,\ldots,p)$. Contrasts of interest are the differences between the two levels of the $k_i$ effects on $V_i$. Given that there is a restriction on the amount of money that can be spent, say $\psi'$, and that the costs $\psi_0,\psi_1,\ldots,\psi_p$ are known, it is desirable to find the design that minimizes the trace of the variance-covariance matrix subject to the total cost restriction. In order to obtain the optimum design, it must be assumed that the variances $\sigma_{11},\ldots,\sigma_{pp}$ are known (or the variances apart from a common multiplicative constant), although in a real problem 'a priori' estimates will be used. These estimates could be obtained from a pilot study or from other past experience.

It is assumed that the experimenter, knowing the $k_i$ effects of importance for each response, can determine what is the smallest fraction $\frac{1}{2^{f_i}}$ of the $2^{v_i}$ univariate factorial experiment that can be used on each response without aliasing important effects with each other or with blocks. Then for the optimal design, it will be determined how many times each $\frac{1}{2^{f_i}}$ fraction of the $2^{v_i}$ factorial can be repeated. This corresponds to case 2 in section 3.3 and as seen in equations (3.3.21) and (3.3.22), gives the same trace value as does case 1. The notation MGLM(F) and HMGLM(F) will be used in referring to the design using these factorial experiments.

The problem in finding the optimum design D* is to find the values, $n_0^*, s_1^* 2^{d_1}, \ldots, s_p^* 2^{d_p}$ that minimize the non-linear function

$$Q(D) = \sum_{i=1}^{p} 2\sigma_{ii} k_i (s_i 2^{d_i})^{-1} \tag{3.5.1}$$

subject to the linear constraints:

$$\begin{aligned} \psi' &= n_0 \psi_0 + \sum_{i=1}^{p} \psi_i s_i 2^{d_i} , \\ n_0 &\geq s_i 2^{d_i} > 0, \ (i = 1, \ldots, p \text{ and } d_i = v_i - f_i) . \end{aligned} \tag{3.5.2}$$

The $s_i^*$ values in the optimum design D* must be positive integers. The $s_i$ values that minimize equation (3.5.1) subject to equation (3.5.2) need not be integers, but the integers $s_i^*$ will be obtained by rounding off the $s_i$ values.

Theorem 3.5.1  The optimum MGLM(F) design subject to the trace criterion (3.5.1) and the cost constraint (3.5.2) is a member of the subclass of HMGLM(F) designs.

Proof. By virtue of the fact that $\sigma_{ii}$ and $k_i$ are constants, Q(D) is a function of only the number of observations. Thus Lemma 3.4.1 is satisfied and the class of HMGLM(F) designs is complete with respect to the MGLM(F) designs. This means that the subclass of HMGLM(F) designs are the only designs that need be considered.

Since from Theorem 3.5.1, the optimal design $D^*(n_0^*, s_1^* 2^{d_1}, \ldots, s_p^* 2^{d_p})$ is a HMGLM(F) design, then $n_0^* = \max(s_1^* 2^{d_1}, \ldots, s_p^* 2^{d_p})$.

Theorem 3.5.2  If $\frac{k_i \sigma_{ii}}{\psi_i} \geq \frac{k_j \sigma_{jj}}{\psi_j}$ then in D* the $i^{th}$ response will be measured at least as often as the $j^{th}$ response, i.e., $s_i^* 2^{d_i} \geq s_j^* 2^{d_j}$ $(i,j = 1,\ldots,p)$.

Proof. Assume that $s_j^* 2^{d_j} > s_i^* 2^{d_i}$. There are two cases to be considered: i) $n_0^* > s_j^* 2^{d_j}$, ii) $n_0^* = s_j^* 2^{d_j}$. i) Select a value m* such that

$$\frac{2k_i \sigma_{ii}}{s_i^* \, 2^{d_i}} + \frac{2k_j \sigma_{jj}}{s_j^* \, 2^{d_j}} = \frac{1}{m^*} (2k_i \sigma_{ii} + 2k_j \sigma_{jj}) \; , \qquad (3.5.3)$$

or

$$m^* = \frac{(k_i\sigma_{ii}+k_j\sigma_{jj})s_i^*2^{d_i}s_j^*2^{d_j}}{k_i\sigma_{ii}s_j^*2^{d_j}+k_j\sigma_{jj}s_i^*2^{d_i}} \;. \tag{3.5.4}$$

A new design $D'(n_0^*, s_1^*2^{d_1}, \ldots, s_{i-1}^*2^{d_{i-1}}, m^*, \ldots, s_{j-1}^*2^{d_{j-1}}, m^*, \ldots, s_p^*2^{d_p})$ can be constructed. $D'$ has the same s values as does $D^*$ except that in $D'$ $s_i' = m^*2^{-d_i}$ and $s_j' = m^*2^{-d_j}$. From equation (3.5.1) and (3.5.3) it follows then that $Q(D^*) = Q(D')$. Compare now the costs of these two designs:

$$\psi(D^*) - \psi(D') = s_i^*2^{d_i}\psi_i + s_j^*2^{d_j}\psi_j - m^*(\psi_i+\psi_j) \;.$$

This difference in costs will be positive if and only if

$$s_i^*2^{d_i}\psi_i + s_j^*2^{d_j}\psi_j > m^*(\psi_i + \psi_j) \;. \tag{3.5.5}$$

By use of equation (3.5.4)

$$(s_i^*2^{d_i}\psi_i+s_j^*2^{d_j}\psi_j)(k_i\sigma_{ii}s_j^*2^{d_j}+k_j\sigma_{jj}s_i^*2^{d_i}) >$$

$$(k_i\sigma_{ii}+k_j\sigma_{jj})(\psi_i+\psi_j)s_i^*2^{d_i}s_j^*2^{d_j} \;.$$

Multiplying out both sides and cancelling terms gives

$$(s_i^* 2^{d_i})^2 \psi_i k_j \sigma_{jj} + (s_j^* 2^{d_j})^2 \psi_j k_i \sigma_{ii} >$$

$$s_i^* 2^{d_i} s_j^* 2^{d_j} (\psi_i k_j \sigma_{jj} + \psi_j k_i \sigma_{ii}) .$$

Thus

$$s_j^* 2^{d_j} \psi_j k_i \sigma_{ii} (s_j^* 2^{d_j} - s_i^* 2^{d_i}) > s_i^* 2^{d_i} \psi_i k_j \sigma_{jj} (s_j^* 2^{d_j} - s_i^* 2^{d_i}) . \tag{3.5.6}$$

Since $(s_j^* 2^{d_j} - s_i^* 2^{d_i}) > 0$, this term will be divided from both sides of equation (3.5.6) without changing the sign. Dividing through also by $s_i^* 2^{d_i} \psi_j k_i \sigma_{ii}$ yields

$$\frac{s_j^* 2^{d_j}}{s_i^* 2^{d_i}} > \frac{\psi_i k_j \sigma_{jj}}{\psi_j k_i \sigma_{ii}} . \tag{3.5.7}$$

The left hand side (lhs) of (3.5.7) is greater than 1, the right hand side (rhs) is less than 1 since $\frac{k_i \sigma_{ii}}{\psi_i} \geq \frac{k_j \sigma_{jj}}{\psi_j}$ . Thus inequality (3.5.7) is found true and the cost of D* is greater than the cost of D'. This result shows that D' is a better design than D*, which is a contradiction since D* was assumed to be the optimum design. It must therefore be true that

$$s_i^* 2^{d_i} \geq s_j^* 2^{d_j} . \tag{3.5.8}$$

ii) Select m* as in equation (3.5.3) and again construct the new design $D'(m_0', s_1^* 2^{d_1}, \ldots, s_{i-1}^* 2^{d_{i-1}}, m^*, \ldots, s_{j-1}^* 2^{d_{j-1}}, m^*, \ldots, s_p^* 2^{d_p})$ where $m_0' = \max(s_1^* 2^{d_1}, \ldots, s_{i-1}^* 2^{d_{i-1}}, m^*, \ldots, s_{j-1}^* 2^{d_{j-1}}, m^*, \ldots, s_p^* 2^{d_p})$. Comparing D* with D', $Q(D^*) = Q(D')$ and

$$\psi(D^*) - \psi(D') = s_j^* 2^{d_j} \psi_0 + s_i^* 2^{d_i} \psi_i + s_j^* 2^{d_j} \psi_j - m_0' \psi_0 - m^*(\psi_i + \psi_j) \ . \tag{3.5.9}$$

Note that since $m_0' \leq n_0^* = s_j^* 2^{d_j}$ then the difference (3.5.9) is positive if

$$s_i 2^{d_i} \psi_i + s_i 2^{d_j} \psi_j > m^*(\psi_i + \psi_j) \ . \tag{3.5.10}$$

This inequality is the same as (3.5.5) which has shown to be true when $s_j^* 2^{d_j} > s_i^* 2^{d_i}$. This once again leads to a contradiction due to the fact that D* was assumed to be the optimum design, and therefore $s_i^* 2^{d_i} \geq s_j^* 2^{d_j}$. This completes the proof.

This theorem is used to determine the order of the responses with respect to the number of times they are measured. Notice how the conditions of this theorem intuitively make sense with respect to the ordering of the responses. The value $\frac{k_i \sigma_{ii}}{\psi_i}$ reflects basically the ratio of the variance to the cost for the $i^{th}$ response. The theorem states that when a response has a large variance and a small cost, it should be measured at least as often as a response with a smaller variance-to-cost ratio. Since increasing the number of observations decreases the variance of the estimates, then, when attempting to minimize the trace, a greater decrease can be effected by reducing the larger variances, especially when these responses have small costs.

Suppose the order of the responses is found to be such that

$$s_{\ell_1} 2^{d_{\ell_1}} \geq s_{\ell_2} 2^{d_{\ell_2}} \geq \ldots \geq s_{\ell_p} 2^{d_{\ell_p}}$$

where $(\ell_1,\ldots,\ell_p)$ is some permutation of the numbers $(1,\ldots,p)$. Without loss of generality, assume that $\ell_1 = 1,\ldots,\ell_p = p$ and therefore that

$$n_0^* = s_1 2^{d_1} \geq s_2 2^{d_2} \geq \ldots \geq s_p 2^{d_p} .$$

<u>Theorem 3.5.3</u> With the responses ordered so that $s_i 2^{d_i} \geq s_j 2^{d_j}$ if $i < j$, let b be the smallest integer in the set $2,3,\ldots,p$ such that

$$\frac{\sigma^*_{b-1}}{\psi^*_{b-1}} > \frac{2k_b \sigma_{b,b}}{\psi_b} \tag{3.5.11a}$$

and

$$\frac{\sigma^*_{b-2}}{\psi^*_{b-2}} \leq \frac{2k_{b-1}\sigma_{b-1,b-1}}{\psi_{b-1}} \qquad (3.5.11b)$$

where $\sigma^*_i = 2k_1\sigma_{11} + 2k_2\sigma_{22} + \ldots + 2k_i\sigma_{ii}$,

and $\psi^*_i = \psi_0 + \psi_1 + \ldots + \psi_i$ . Then

$$s_1 2^{d_1} = \ldots = s_{b-1} 2^{d_{b-1}} > s_b 2^{d_b} \geq \ldots \geq s_p 2^{d_p}. \qquad (3.5.12)$$

For b = 2 ignore equation (3.5.11b) and if equation (3.5.11b) is satisfied for b = p then

$$s_1 2^{d_1} = s_2 2^{d_2} = \ldots = s_p 2^{d_p} .$$

Proof: From Theorem 3.5.2 and the ordering of the responses, it is known that

$$s_{b-2} 2^{d_{b-2}} \geq s_{b-1} 2^{d_{b-1}}$$

and

$$\frac{k_{b-2}\sigma_{b-2,b-2}}{\psi_{b-2}} \geq \frac{k_{b-1}\sigma_{b-1,b-1}}{\psi_{b-1}}$$

which implies

$$\frac{2k_{b-1}\sigma_{b-1,b-1}}{2k_{b-2}\sigma_{b-2,b-2}} \leq \frac{\psi_{b-1}}{\psi_{b-2}} \; . \tag{3.5.13}$$

Inequality (3.5.11b) can be restated as $\dfrac{\sigma^*_{b-2}}{2k_{b-1}\sigma_{b-1,b-1}} \leq \dfrac{\psi^*_{b-1}}{\psi_{b-1}}$, which used together with inequality (3.5.13) gives

$$\frac{\sigma^*_{b-3}+2k_{b-2}\sigma_{b-2,b-2}}{2k_{b-1}\sigma_{b-1,b-1}} \cdot \frac{2k_{b-1}\sigma_{b-1,b-1}}{2k_{b-2}\sigma_{b-2,b-2}} \leq \frac{\psi^*_{b-3}+\psi_{b-2}}{\psi_{b-1}} \cdot \frac{\psi_{b-1}}{\psi_{b-2}} \; .$$

Thus

$$\frac{\sigma^*_{b-3}}{2k_{b-2}\sigma_{b-2,b-2}} \leq \frac{\psi^*_{b-3}}{\psi_{b-2}} \; ,$$

or

$$\frac{\sigma^*_{b-3}}{\psi^*_{b-3}} \leq \frac{2k_{b-2}\sigma_{b-2,b-2}}{\psi_{b-2}} \; .$$

Continuing in this manner the following can be found:

$$\frac{\sigma^*_1}{\psi^*_1} \leq \frac{2k_2\sigma_{22}}{\psi_2} \; ; \; \frac{\sigma^*_2}{\psi^*_2} \leq \frac{2k_3\sigma_{33}}{\psi_3} \; ; \ldots ; \; \frac{\sigma^*_{b-2}}{\psi^*_{b-2}} \leq \frac{2k_{b-1}\sigma_{b-1,b-1}}{\psi_{b-1}} \; . \tag{3.5.14}$$

Assuming that for the optimum design D* $s_1 2^{d_1} > s_2 2^{d_2}$, then

$$\psi(D^*) = \psi^*_1 s_1 2^{d_1} + \sum_{i=2}^{p} \psi_i s_i 2^{d_i} \; , \tag{3.5.15}$$

and

$$Q(D^*) = \frac{\sigma_1^*}{s_1 2^{d_1}} + \sum_{i=1}^{p} \frac{2k_i\sigma_{ii}}{s_i\ 2^{d_i}} \quad . \tag{3.5.16}$$

Express the product $\psi(D^*)Q(D^*)$, from equations (3.5.15) and (3.5.16) as follows:

$$\psi(D^*)Q(D^*) = [(\sqrt{\psi_1 s_1 2^{d_1}})^2 + \sum_{i=2}^{p} (\sqrt{\psi_i 2^{d_1}})^2]\cdot[(\sqrt{\frac{\sigma_1^*}{s_1 2^{d_1}}})^2 +$$

$$\sum_{i=2}^{p} (\sqrt{\frac{2k_i\sigma_{ii}}{s_i\ 2^{d_i}}})^2] \ .$$

It follows from Cauchy's inequality (see Appendix) that

$$\psi(D^*)Q(D^*) \geq [\sqrt{\psi_1^*\sigma_1^*} + \sum_{i=2}^{p} \sqrt{2\psi_i k_i \sigma_{ii}}\ ]^2 \quad .$$

Equality is attained when

$$\sqrt{\psi_1^* s_1 2^{d_1}} = \alpha\sqrt{\frac{\sigma_1^*}{s_1 2^{d_1}}} \quad \text{and} \quad \sqrt{\psi_i s_i 2^{d_i}} = \alpha\sqrt{\frac{2k_i\sigma_{ii}}{s_i\ 2^{d_i}}}$$

or

$$s_1 = \alpha\ 2^{-d_1}\sqrt{\frac{\sigma_1^*}{\psi_1^*}} \quad \text{and} \quad s_i = \alpha\ 2^{-d_i}\sqrt{\frac{2k_i\sigma_{ii}}{\psi_i}}$$

for any constant $\alpha$ where $i = 2,\ldots,p$. The value of $\alpha$ must be determined so that the cost equation is satisfied, but for now suffice it to say that $\alpha$ is positive. The assumption that $s_1 2^{d_1} > s_2 2^{d_2}$ implies that

$$\alpha\sqrt{\frac{\sigma_1^*}{\psi_1^*}} > \alpha\sqrt{\frac{2k_2\sigma_{22}}{\psi_2}} \ ,$$

which implies that

$$\frac{\sigma_1^*}{\psi_1^*} > \frac{2k_2\sigma_{22}}{\psi_2} \ . \tag{3.5.17}$$

This conclusion contradicts inequality (3.5.14) and thus $s_1 2^{d_1} \leq s_2 2^{d_2}$. But from Theorem 3.5.2 it follows that $s_1 2^{d_1} \geq s_2 2^{d_2}$, hence $s_1 2^{d_1} = s_2 2^{d_2}$.

Assume next that $s_2 2^{d_2} > s_3 2^{d_3}$ giving

$$\psi(D^*) = s_2 2^{d_2}\psi_2^* + \sum_{i=3}^{p} \psi_i s_i 2^{d_i} \ ,$$

and

$$Q(D^*) = \frac{\sigma_2^*}{s_2 2^{d_2}} + \sum_{i=3}^{p} \frac{2k_i\sigma_{ii}}{s_i\ 2^{d_i}} \ .$$

By Cauchy's inequality

$$\psi(D^*)Q(D^*) \geq (\sqrt{\psi_2^*\sigma_2^*} + \sum_{i=3}^{p} \sqrt{2\psi_i k_i\sigma_{ii}})^2 \ .$$

Equality is attained when

$$s_2 = \alpha\, 2^{-d_2}\sqrt{\frac{\sigma_2^*}{\psi_2^*}} \quad \text{and} \quad s_i = \alpha\, 2^{-d_i}\sqrt{\frac{2k_i\sigma_{ii}}{\psi_i}} \ ,$$

for $i = 3,\ldots,p$. Again an $\alpha$ will be selected as a positive constant. The assumption $s_2 2^{d_2} > s_3 2^{d_3}$ implies

$$\alpha\sqrt{\frac{\sigma_2^*}{\psi_2^*}} > \alpha\sqrt{\frac{2k_3\sigma_{33}}{\psi_3}} \ ,$$

or

$$\frac{\sigma_2^*}{\psi_2^*} > \frac{2k_3\sigma_{33}}{\psi_3} \ ,$$

which contradicts inequality (3.5.14) and thus $s_2 2^{d_2} = s_3 2^{d_3}$.

Continuing this line of reasoning it is concluded that $s_1 2^{d_1} = \ldots = s_{b-2} 2^{d_{b-2}}$. Assume now that for the optimum design D*, $s_{b-1} 2^{d_{b-1}} > s_b 2^{d_b}$ giving

$$\psi(D^*) = \psi_{b-1}^* s_{b-1} 2^{d_{b-1}} + \sum_{i=b}^{p} \psi_i s_i 2^{d_i} \ , \qquad (3.5.18)$$

and

$$Q(D^*) = \frac{\sigma_{b-1}^*}{s_{b-1} 2^{d_{b-1}}} + \sum_{i=b}^{p} \frac{2k_i\sigma_{ii}}{s_i\, 2^{d_i}} \ .$$

Using Cauchy's inequality as before, equality is attained when

$$\sqrt{\psi^*_{b-1} s_{b-1} 2^{d_{b-1}}} = \alpha \sqrt{\frac{\sigma^*_{b-1}}{s_{b-1} 2^{d_{b-1}}}} \text{ and } \sqrt{\psi_i s_i 2^{d_i}} = \alpha \sqrt{\frac{2k_i\sigma_i}{s_i\, 2^{d_i}}} ,$$

or

$$s_{b-1} = \alpha 2^{-d_{b-1}} \sqrt{\frac{\sigma^*_{b-1}}{\psi^*_{b-1}}} \text{ and } s_i = \alpha 2^{-d_i} \sqrt{\frac{2k_i\sigma_{ii}}{\psi_i}} , \qquad (3.5.19)$$

for $i = b,\ldots,p$.

In order that $s_{b-1}2^{d_{b-1}} > s_b 2^{d_b}$ it must be true that

$$\sqrt{\frac{\sigma^*_{b-1}}{\psi^*_{b-1}}} > \sqrt{\frac{2k_b\sigma_{bb}}{\psi_b}}$$

which is true by virtue of the manner in which b was chosen, inequality (3.5.11a). These results along with Theorem 3.5.2 show that

$$s_1 2^{d_1} = \ldots = s_{b-1} 2^{d_{b-1}} > s_b 2^{d_b} \geq \ldots \geq s_p 2^{d_p} .$$

This completes the proof.

<u>Corollary 3.5.4</u> If the p responses are numbered so that

$$\frac{k_i\sigma_{ii}}{\psi_i} \geq \frac{k_j\sigma_{jj}}{\psi_j} \quad (i < j,\ i,j = 1,\ldots,p) ,$$

and b is defined as in Theorem 3.5.3, then the optimum values

$n_0^*, s_1, \ldots, s_p$ are given by:

$$s_i = \frac{\psi'}{\delta} 2^{-d_i} \sqrt{\frac{\sigma_{b-1}^*}{\psi_{b-1}^*}} \quad (i = 1,2,\ldots,b-1), \qquad (3.5.20a)$$

and

$$s_j = \frac{\psi'}{\delta} 2^{-d_j} \sqrt{\frac{2k_j\sigma_{jj}}{\psi_j}} \quad (j = b,b+1,\ldots,p), \qquad (3.5.20b)$$

and

$$n_0^* = s_1 2^{d_1} ,$$

where:

$\psi'$ = the total amount of money available for experimentation,

$\delta = \sqrt{\psi_{b-1}^* \sigma_{b-1}^*} + \sum_{i=b}^{p} \sqrt{2\psi_i k_i \sigma_{ii}}$ ,

$\sigma_i^* = 2k_1\sigma_{11} + \ldots + 2k_i\sigma_{ii}$ ,

and

$\psi_i^* = \psi_0 + \psi_1 + \ldots + \psi_i$ .

Proof: The result follows from the proof of Theorem 3.4.3: From equation (3.5.19)

$$s_i = \alpha 2^{-d_i} \sqrt{\frac{\sigma_{b-1}^*}{\psi_{b-1}^*}} \text{ for } i = 1,\ldots,b-1, \qquad (3.5.21a)$$

and

$$s_j = \alpha 2^{-d_j} \sqrt{\frac{2k_j\sigma_{jj}}{\psi_j}} \text{ for } j = b,\ldots,p, \qquad (3.5.21b)$$

where $\alpha$ is a positive constant. This $\alpha$ must be chosen so that the cost equation (3.5.18) is satisfied for the amount of money available $\psi'$. Thus to satisfy equation (3.5.18)

$$\psi' = \psi^*_{b-1}\alpha\sqrt{\frac{\sigma^*_{b-1}}{\psi^*_{b-1}}} + \sum_{i=b}^{p} \psi_i\alpha\sqrt{\frac{2k_i\sigma_{ii}}{\psi_i}} ,$$

or

$$\psi' = \alpha[\sqrt{\sigma^*_{b-1}\psi^*_{b-1}} + \sum_{i=b}^{p} \sqrt{2\psi_i k_i \sigma_{ii}}] . \qquad (3.5.22)$$

Solving for $\alpha$ yields $\alpha = \psi'/\delta$, where $\delta$ is the term in brackets on the rhs of equation (3.5.22). Substituting $\alpha$ into equations (3.5.21) gives (3.5.20). This completes the proof.

The preceding theorems and corollary make it clear that under a trace criterion and a cost constraint the optimum design is not always the MDM(F) design (all responses measured on each unit); but instead the HMGLM(F) design is often better when there is some prior knowledge of the experimental situation. There will still of course be situations where the optimal HMGLM(F) design is in fact the MDM(F) design.

Knowing which factors, if any, should be omitted from the univariate model, through an understanding of the experimental situation is essential in finding the best optimal design. (The term 'best optimal' seems to be redundant but really is not. For each experimental situation an optimal design exists. A misunderstanding of this situation gives a design that, although optimal for this misunderstood case, is not necessarily the same design that would be obtained if the situation were more fully understood.) The number of effects $k_i$ that are of interest to the experimenter is generally influenced by $v_i$, the number of the v factors that effect the $i^{th}$ response. Therefore, knowledge of the experimental situation may cause a decrease in $k_i$. This change in $k_i$ can affect the $s_i$ values $(i = 1,\ldots,p)$ and may also alter the order of the responses. Take for example a case where the experimenter is interested only in the main effects $(k_i = v_i)$. If he is not aware that one factor does not affect the $i^{th}$ response and so uses $v_i = v = k_i$, this design will have a larger trace value than the optimal design using $v_i = v-1 = k_i$. The purpose of this example is not necessarily to reduce the number of effects of interest. However, if some of the $k_i$ effects are effects that do not influence the $i^{th}$ response and should have been left out of the univariate model, then the supposedly optimum design will have the $i^{th}$ response measured on too many units at the expense of the other responses that should be measured on more units.

It is interesting to note how the initial cost $\psi_0$ influences whether the design should be an MDM or HMGLM. From a practical point of view, if the initial cost of preparing a unit to be sampled, $\psi_0$, is very large in relation to the cost of measuring the individual responses, $\psi_i$, then one should use as few individual units as possible and try to get as much information as possible from these few units. This would be done by measuring all responses on each unit, a procedure which implies the use of the MDM design. On the other hand if $\psi_0$ is small, then introducing more units into the design scheme will not present a large additional cost. This additional cost can be offset by the increased precision obtained by measuring responses with comparatively large variances on these additional units. This situation calls for a HMGLM design.

In comparing this to the theorems already proven, first recall that the responses $V_i$ were numbered so that $\frac{2k_i\sigma_{ii}}{\psi_i} \geq \frac{2k_j\sigma_{jj}}{\psi_j}$ for $i < j$ $(i,j = 1,\ldots,p)$. Thus

$$\frac{2k_1\sigma_{11}}{\psi_1} \geq \frac{2k_2\sigma_{22}}{\psi_2} \geq \cdots \geq \frac{2k_p\sigma_{pp}}{\psi_p} . \qquad (3.5.23)$$

In Theorem 3.5.3, the integer b is determined so that

$$s_1 2^{d_1} = \cdots = s_{b-1} 2^{d_{b-1}} > s_b 2^{d_b} \geq \cdots \geq s_p 2^{d_p} .$$

Therefore in order that a MDM design is the optimal design, $p = b-1$. From equation (3.5.11b) this can only occur if

$$\frac{2k_p\sigma_{pp}}{\psi_p} \geq \frac{2(k_1\sigma_{11}+\ldots+k_{p-1}\sigma_{p-1,p-1})}{\psi_0 + (\psi_1+\ldots+\psi_{p-1})} \ . \tag{3.5.24}$$

Due to the manner in which the responses were ordered, inequalities (3.5.23) and (3.5.24) will be true for large values of $\psi_0$, a fact which implies a MDM design. For small $\psi_0$, inequality (3.5.23) is less likely to be true implying the MDM will not be the optimum design. When $\psi_0 = 0$, the lhs of inequality (3.5.23) can never be greater than the rhs, and equality is attained only when

$$\frac{2k_1\sigma_{11}}{\psi_1} = \ldots = \frac{2k_p\sigma_{pp}}{\psi_p} \ .$$

The theorems therefore certainly parallel what seems intuitively correct.

## 3.6 Interpretation of Results

The optimum values $s_1,s_2,\ldots,s_p$ obtained in Theorem 3.5.4 will not necessarily be integers. They thus must be rounded off to the nearest integer. This round-off design would still give a trace very close to the optimum value. The problem here is that the round-off does not imply the difference of one observational unit but rather the difference of a group of $2^{d_i}$ units on each response. This much change could substantially alter the total cost of the design, and it is therefore advisable to check $\psi(D^*)$ after the round-off and if necessary change $D^*$ appropriately. Sometimes $\psi'$ is a negotiable figure and therefore a design costing slightly more would present no problem.

A way to obtain the best possible integer solution in the area of the real numbered optimum would be to consider two values around each $s_i$, one attained by rounding each $s_i$ up to the next larger integer $s_i^+$ and the other by rounding off to the next smaller integer $s_i^-$. Then looking at all possible combinations of the $(s_i^+)$ and $(s_i^-)$'s, find the combination that gives the smallest trace criterion while still giving an 'acceptable' cost ('acceptable' meaning either $\leq \psi'$ or not too much more than $\psi'$ as deemed necessary for the particular situation.) This would entail checking $2^p$ designs, finding their costs and traces. A computer program has been written (Appendix 2) that will search the integer values around the optimum real solution $s_1,\ldots,s_p$. This program gives the experimenter a chance to find the best design rather than just hoping that rounding off the $s_i$ values will not affect the optimality of the design.

One important point that has only been mentioned briefly concerns the fractional replication used. It has been assumed that the smallest size fraction was used without aliasing important effects with other non-zero effects. This assumption is made so that when $s_i$ is rounded to an integer value, the total number of observations on the $i^{th}$ response will be changed only slightly, leaving the design close to optimum.

Once the $s_i$ values are determined, effort should be made to reduce the alias structure. For example, suppose that on one response, i', the optimum design required 4 replications of a $\frac{1}{8}$ fraction ($s_{i'} = 4$, $f_{i'} = 3$). If the same block of treatment combinations were repeated 4 times, then each effect in the model would still be aliased with 7 other possibly non-zero terms. If there is no trouble with homogeneity of experimental units, then a $\frac{1}{2}$ fraction should be conducted. This would substantially reduce the number of terms with which each effect is aliased and thus reduce the chance of aliasing an important effect with another effect that may be significant. For a situation where the units are only homogeneous enough to conduct $\frac{1}{8}$ fractions, then there should be confounding within the $\frac{1}{2}$ fraction. This confounds some terms with block effects, but terms of lesser importance can be sacrificed for this.

It must be remembered that a parameter E in the model may also include the influence of other aliased non-zero effects, in addition to the effect of factor E. As long as this is realized, the orthogonal model that has been used is appropriate.

It will generally be true that the experimenter would like to obtain an estimate of $\sigma_{ii}$ that could be compared with the 'a priori' estimate used or possibly be used as the estimate of $\sigma_{ii}$ if the experiment will be conducted again. Situations can occur where the optimum design assigns very few observational units to some responses, so few that the experimenter does not feel that this arrangement will give a reliable variance estimate. Suppose it is decided that the $i^{th}$ response $(i = 1,\ldots,p)$ should be measured on at least $s_{ix}2^{d_i}$ units. After the optimum design is determined, if it is found that say z $(<p)$ responses are to be measured on too few units (assume for simplicity that these are the last z responses, i.e., $s_{p-z+1} < s_{p-z+1,x},\ldots,s_p < s_{px}$), then the following procedure is recommended: Set $s_{p-z-1} = s_{p-z-1,x},\ldots$ $s_p = s_{px}$ and define $\psi^{**} = \psi' - \sum_{i=p-z+1}^{p} \psi_i s_{ix} 2^{d_i}$. Then drop these z responses from the model and find the optimum design for the p-z remaining responses when the amount of money $\psi^{**}$ is available. This, in effect, adds z constraints to the problem. When the optimum values $s_1^{**},\ldots,s_{p-z}^{**}$ are found for this reduced case they should again be checked to insure that $s_i^{**} \geq s_{ix}$ $(i = 1,\ldots,p-z)$. If $s_\alpha^{**} < s_{\alpha x}$, then this response should be constrained and the process repeated on the remaining p-z-1 responses. These $s_i$ values must be checked after each iteration until an admissible design is found (an admissible design being a design whose $s_i$ values satisfy the restrictions imposed by the experimenter and whose cost does not exceed $\psi'$). These lower size bounds, $s_{ix}$, must be checked originally to make sure that they were not set too high for the amount of money available.

This same procedure can also be used to constrain the size of the design in the other direction. Suppose now that there is a fixed number of units n* that could be used in this experiment. If the optimum design has some response to be measured on too many units, then this response should be restricted to the maximum number of units, and a new total cost $\psi^* = \psi' - n^*(\psi_0 + \psi_1)$ must be defined. Dropping this response from the model, the optimum design with a total cost $\psi^*$ should be found for the remaining p-1 responses where $\psi_0$ should now be considered zero since this set-up cost was accounted for when $\psi'$ was adjusted to $\psi^*$. This procedure may have to be repeated several times until an admissible design is found. Repetition may be necessary because $s_2$ will now be larger than it was originally found to be, because not as much money will be spent on $V_1$. It is therefore possible that $s_2 2^{d_2} > n^*$, thus requiring the procedure to be repeated, this time leaving out the first two responses and using $\psi^* = \psi' - n^*(\psi_0 + \psi_1 + \psi_2)$.

There is another interesting way that money can be saved when using a HMGLM design. It is not accounted for in the cost constraint and is applicable only to certain types of MGLM designs. It can best be explained through an example. Suppose there are 2 responses, 5 factors (A,B,C,D,E), each at two levels, with $V_1$ being affected only by factors A, B, C, D, and $V_2$ being affected by only B, C, D, E. It is decided that $\frac{1}{2}$ fractions of each of the $2^4$ factorial experiments are the smallest allowable fractions. The optimum design is found to have $s_1=2$ and $s_2=1$. The treatment combinations applied to each experimental unit will involve the different levels of the 5 factors, even though $V_1$ and $V_2$ are each affected by only 4 of these factors. Thus the replication of $\frac{1}{2}$ fractions (8 units) on each response (4 factors) corresponds to the replication of $\frac{1}{4}$ fractions (8 units) on the entire experiment (5 factors). If the defining contrast $I \equiv ABCD \equiv BCDE$ ($\equiv AE$) is used on the entire design, then $V_1$ has the defining contrast $I_1 \equiv ABCD$, and $V_2$ has $I_2 = BCDE$. The following treatment levels will be used for the design:

| Entire Design $I \equiv ABCD \equiv BCDE$ | Response 1 $I_1 \equiv ABCD$ | Response 2 $I_2 \equiv BCDE$ |
|---|---|---|
| '1' | '1' | '1' |
| bc | bc | bc |
| bd | bd | bd |
| cd | cd | cd |
| abe | ab | be |
| ace | ac | ce |
| ade | ad | de |
| abcde | abcd | bcde |
| ae | a | |
| abce | abc | |
| abde | abd | |
| acde | acd | |
| b | b | |
| c | c | |
| d | d | |
| bcd | bcd | |

On the second set of 8 treatment combinations only the first response is measured. Therefore, on these 8 units, the experiment could have been designed so that the factor E appeared at the low level in all 8 treatment combinations or at the high level in these treatment combinations. If factor E costs less to apply at the low level than at the high level, money could be saved by having E at the low level on these experimental units. Considering the cost of factor E at either level, money could be saved if rather than using 5 factors on these 8 units, one used only factors A, B, C, D, completely omitting factor E. This is possible since E does not affect $V_1$ anyway, and would result in using treatment combinations a, abc, abd, acd, b, c, d, bcd on these 8 experimental units where only $V_1$ will be measured. For an experiment with 2 responses, it will often be advisable to alias, on the entire experiment, the two factors that affect one response but not the other. Suppose, as in the example, that A affects only $V_1$ and that E affects only $V_2$. Let X and Y be effects or interactions that contain respectively A and E and whose generalized interaction is AE. Then, if in the defining contrast for the entire experiment X and Y are confounded, i.e., $I \equiv X \equiv Y$ ($\equiv AE$), then the defining contrast for $V_1$ will be $I_1 = X$ and for $V_2$, $I_2 = Y$.

A difficulty in using designs that are optimum with respect to the trace criterion is that the responses under study should be measured in the same or at least similar units of measurement. Changing the unit of scale on a group of responses causes a multiplicative change in their variances. Since the optimum design is very dependent upon the relative variance sizes, changing the variance on some of the responses causes an alteration in a number of factors that help determine the optimum design. The values of $n_0, s_1, \ldots, s_p$ change and not to a number proportional to its original value. The order of the responses and the size of the integer b from Theorem 3.4.3 could also possibly change. Changing the unit of measurement on only a subset of responses causes the values of $s_i$ to change due to the change of $\delta$ (Corollary 3.5.4) and possibly due also to a change of $\sigma^*_{b-1}$ or the new variances on this subset of responses.

If, however, the measurement units on all p responses are changed by some constant factor $\gamma$, the $s_i$ values remain the same and Q(D) changes by a factor of $\gamma$. Using a design that is optimum with respect to the trace criterion is most appropriate for an experiment where all responses are measured in the same unit of scale. This design will therefore be invariant with respect to change of scale due to the fact that the change in variance on all responses will be by a constant factor.

## 3.7 Example

An example of a multiresponse design where each response is measured in the same units of measurement is found in tobacco experimentation. Edmondson (1972) gives an example where it is of interest to study how several factors affect the percentage of carbohydrates in four different places of a tobacco plant. These four responses or places in the plant (p=4) are these: $V_1$, the $5^{th}$ leaf, $V_2$, the $10^{th}$ leaf, $V_3$, the $15^{th}$ leaf, and $V_4$, the root. There are five factors (v=5) each at two levels and it is of interest to the experimenter to determine whether there is any difference in the effect of the two levels of each of these factors. These 5 factors and their levels are as follows:

N, Nitrogen fertilizer, $N_0$: 45 lbs./acre, $N_1$: 90 lbs./acre,

T, Varieties of Tobacco, $T_0$: Coker 139, $T_1$: Hicks,

P, Potassium Oxide fertilizer, $P_0$: 80 lbs./acre, $P_1$: 160 lbs./acre,

V, Viruses, $V_0$: Potato Virus Y, $V_1$: Tobacco Mosaic Virus,

C, Time of innoculation, $C_0$: 4 weeks, $C_1$: 6 weeks.

One of two types of viruses, both common diseases affecting tobacco crops, is being applied to each of the plants for it is desirable to study the effects of these viruses in a controlled experiment. Due to the fact that the $5^{th}$ leaf of the plant is already fully developed before the virus can grow to a strength sufficient to retard the carbohydrate levels in the plant, the virus factor and thus also the factor, time of innoculation, do not affect the percentage of carbohydrates in the $5^{th}$ leaf, $V_1$. Response

$V_1$ is affected by the other 3 factors while the other responses are affected by all 5 factors giving $v_1 = 3$, $v_2 = v_3 = v_4 = 5$.

We are interested in studying only the main effects on each response, but there may possibly be a non-zero interaction between viruses and time of innoculation (VC). We therefore do not want to allow our fraction size to be so small that 1.) main effects are aliased with each other, or that 2.) the (VC) interaction is aliased with a main effect. By using $\frac{1}{2}$ fractions of $2^5$ experiments on $V_2$, $V_3$, and $V_4$, the defining contrasts can be chosen to avoid these difficulties. For example use I = NTP for response 1 and for the other responses use I $\equiv$ NTV $\equiv$ PCT ($\equiv$ VPCN). For $V_1$, the main effects are not aliased with each other, and for $V_2$, $V_3$, and $V_4$ the main effects though aliased with some two factor interactions are not aliased with the one thought to be non-zero.

Therefore in this example, $p = 4$, $v = 5$, $v_1 = 3$, $v_2 = v_3 = v_4 = 5$, $f_1 = 1$, $f_2 = f_3 = f_4 = 2$, $d_1 = 2$, $d_2 = d_3 = d_4 = 3$. The cost of preparing a plant for measurement is approximately \$2.67 ($= \psi_0$). For the leaves, the cost of picking, drying, grinding, and running the chemical analysis is approximately \$3.40 per leaf ($= \psi_1 = \psi_2 = \psi_3$). The cost of measuring $V_4$ is greater than $V_i$ ($i = 1,2,3$) due mostly to the extra care that must be taken in digging up the roots and is approximately \$4.67 (= $\psi_4$). Five thousand dollars is allotted for experimentation ($\psi' = 5000$), and from similar experiments, the variances were estimated to be $\sigma_{11} = 1.71$, $\sigma_{22} = 3.10$, $\sigma_{33} = 1.98$, and $\sigma_{44} = 2.23$. Having this information enables one to find the optimum design.

From Theorem 3.5.1, the optimal design will be a HMGLM design and therefore Theorem 3.5.2 will first be used to order the responses so that we can determine which responses should be measured more frequently. For this experiment $\frac{k_1\sigma_{11}}{\psi_1} \equiv 1.51$, $\frac{k_2\sigma_{22}}{\psi_2} \equiv 4.56$, $\frac{k_3\sigma_{33}}{\psi_3} \equiv 2.91$, $\frac{k_4\sigma_{44}}{\psi_4} \equiv 2.39$. Thus in the optimal design $s_2 2^{d_2} \geq s_3 2^{d_3} \geq s_4 2^{d_4} \geq s_1 2^{d_1}$. Denoting the reordered responses by $V_i'$, renumeration of the responses gives $V_1' = V_2$, $V_2' = V_3$, $V_3' = V_4$, $V_4' = V_1$.

In order to use Theorem 3.5.3 the following table is devised giving an easier and more orderly way to find b. Let j denote the subscript of $V_j$ for the original ordering of the responses and let i denote the subscript of the reordered response $V_i'$.

| $j$ | $i$ | $\frac{2k_i\sigma_{ii}}{\psi_i}$ | $\frac{\sigma_i^*}{\psi_i^*}$ | $\sigma_i^*$ | $\psi_i^*$ |
|---|---|---|---|---|---|
| 2 | 1 | 9.12 | 5.11 | 31.0 | 6.07 |
| 3 | 2 | 5.82 | 5.36 | 50.8 | 9.47 |
| 4 | 3 | 4.78 | 5.17 | 73.1 | 14.14 |
| 1 | 4 | 3.02 | | 83.4 | 17.54 |

Since $\frac{2k_2\sigma_{22}}{\psi_2} \geq \frac{\sigma_1^*}{\psi_1^*}$ (5.82 > 5.11) and $\frac{2k_3\sigma_{33}}{\psi_3} < \frac{\sigma_2^*}{\psi_2^*}$ (4.78 < 5.36), $b = 3$, and therefore $V_1'$ and $V_2'$, are measured on the same number of units, and $V_1'$ (or $V_2$) is the response most frequently observed.

Corollary 3.5.4 is used to determine exactly how many units in the optimal design each response should be measured. With $b = 3$, $\delta = 38.045$ and the optimum values for the design (given in their original numberation) are found to be these:

$$s_2 = s_3 = 38.05;\ s_4 = 35.90;\ s_1 = 57.08.$$

Use of the computer program (Appendix 2) to find the best integer design gives the following

$$s_1 = 57,\ s_2 = s_3 = 38,\ s_4 = 36 \text{ with } \psi(D) = \$4999.04.$$

It is interesting to notice how the design would change if $\psi_0$ had been different. The order of the responses with respect to the number of units measured does not change, as $\psi_0$ does not enter in Theorem 3.5.2. The value of b however can change (depending upon how much $\psi_0$ is changed) and the optimal numbers of units also change. Notice how the optimal design for the preceding situation would change for different $\psi_0$ values: Had $\psi_0 = 1$, then $b = 2$, $\delta = 35.995$, and $s_2 = 46.088$, $s_3 = 41.626$, $s_4 = 37.943$, and $s_1 = 60.325$. Increasing $\psi_0$ to 4 would give $b = 4$, $\delta = 39.534$, and $s_2 = s_3 = s_4 = 33.227$, $s_1 = 54.925$. When $\psi_0 = 13$, then $b > 4$ and a MDM design is optimal with

$$s_2 = s_3 = s_4 = 22.4255, \; s_1 = 44.8510. \tag{3.7.1}$$

For the case where $\psi_0 = 13$, an unusual but interesting point is illustrated. The design that minimizes the trace while costing less than \$5000, given in equation (3.7.1), is a MDM design. To keep a MDM design, the real valued $s_i^!$s must be rounded off to integer values. They cannot be rounded up for this would give a design whose cost exceeds $\psi'$. We must therefore round off to $s_1 = 44$, $s_2 = s_3 = s_4 = 22$, giving a design whose cost is \$4905.12 and whose trace is .4736. Normally we try to make use of the remaining \$94.88 by measuring some response or responses in several more units, thus lowering the trace but still keeping the cost under $\psi'$, a method which would result in a HMGLM design rather than a MDM design. For a MDM design this response is normally the most frequently observed response, $V_1'$, since it is basically the response that will give the greatest decrease in the trace for the least amount of money (this was the basic consideration in the ordering of the responses by Theorem 3.5.2). However increasing $s_2$ to 23 ($V_2 = V_1'$) brings an additional $(\psi_0 + \psi_2)2^{d_2} = (13 + 3.4) \times 8 = \$131.20$, thus giving a HMGLM design whose cost exceeds \$5000, with the same thing happening had $V_3$ or $V_4$ been measured on an extra group of units. Measurement of $V_1$ however, on an additional group of units adds $(\psi_0 + \psi_1)2^{d_1} = (13 + 3.4)4 = \$65.60$, a smaller amount since $V_1$ is measured on a smaller fractional factorial. Thus the best admissible design is a HMGLM design with $s_1 = 45$, $s_2 = s_3 = s_4 = 22$, a design whose cost is \$4970.72 and whose trace is .4723. If $\psi'$ had been \$4950, then the addition of one more group of 4 units on $V_1$ would also have exceeded the total amount of money and the best design would then have been the MDM design with $s_1 = 44$, $s_2 = s_3 = s_4 = 22$.

The preceding illustrates how the theorems of Section 3.5 give the region of the optimal design. The computer program then will find the best integer design.

## 3.8 Extensions to Factorial Experiments With More Than 2 Levels on Each Factor

In this section p' will denote the number of responses under study so that the standard notation p can be used to denote a prime number. Now, rather than being restricted to a $2^v$ factorial experiment, the extension will be made to the case where there are v factors, each factor having p levels. Theorems are proven in this section that enable the experimenter to determine, for a $p^v$ factorial experiment, the design that is optimum with respect to the trace criterion and a cost constraint. It will again be assumed that the experiment can be explained by the general MGLM model and, as done for the $2^v$ experiment, a randomized block design will be used. For a $p^v$ factorial experiment where p is a prime number, the following univariate model will be assumed and the notation of Kempthorne (1952) used

$$\begin{aligned} E(y_{\alpha ijk\ldots}) = {} & \mu+\beta_\alpha+A_i+B_j+AB_{i+j}+AB^2_{i+2j}+\ldots+AB^{p-1}_{i+(p-1)j} \\ & + AC_{i+k}+\ldots+BC_{j+k}+\ldots+ABC_{i+j+k}+\ldots \\ & + AB^2C_{i+2j+k}+\ldots+ \text{ etc.} \end{aligned} \tag{3.8.1}$$

for v factors A, B, C, D,...

where

$\alpha = 1,2,\ldots,s$

$i = 0,1,\ldots,p-1$

$j = 0,1,\ldots,p-1$

$\vdots$

and where $\beta_\alpha$ represents the block effect of the $\alpha^{th}$ block ($\alpha = 1,\ldots,s$).

Associated with each (p-1) degree of freedom main effect E are p parameters $E_0, E_1, \ldots, E_{p-1}$ which are analogous to the parameters used in the $2^v$ experiment except that instead of 2 levels, there are now p levels. The interactions, for example EF, have been partitioned into portions, each having (p-1) degrees of freedom, $EF^1$, $EF^2, \ldots, EF^{p-1}$. Associated with each of these portions are p parameters, for example for $EF^2$: $EF_0^2, EF_1^2, \ldots, EF_{p-1}^2$. These parameters, as in the $2^v$ experiment, will be referred to as the levels of the $EF^2$ portion of the EF interaction.

Analogous to the procedure for the $2^v$ experiment, the smallest fraction $\frac{1}{p^f}$ of the $p^v$ experiment will be considered that will not allow terms of interest to be aliased with other non-zero terms, and the number of times this fraction can be repeated will be determined. Remember that when considering, say the interaction of A with B (AB) that this interaction has been broken down into p-1 terms $AB^1, AB^2, \ldots AB^{p-1}$ and AB is unaliased when all of these terms are unaliased.

For a $1/p^f$ fraction there will be f terms in the defining contrast, leading to a total of $(p^f-1)/(p-1)$ terms confounded with the mean $\mu$. Each term with (p-1) degrees of freedom (d.f.) is aliased with $p^f-1$ other (p-1) d.f. terms. The model will contain $w=(p^d-1)/(p-1)$ terms each with (p-1) d.f. (d = v-f), these terms containing the effect of the denoted term and also effects of aliased terms. The size of the fraction and the defining contrasts are chosen however so that these aliased terms are either non-significant effects or they are aliased with terms not of interest. If the model in equation (3.8.1) is written in matrix notation

$$E(\underline{y}) = X^*\underline{\xi}$$

where

$X^*$ is a design matrix of dimension $(a \times b)$,

$\underline{\xi}$ is the parameter vector, $(b \times 1)$,

$a = sp^d$,

$b = pw + 1 + s$.

Following the argument in 3.2, $X^*$ and $\underline{\xi}$ will be partitioned

$$X^*\underline{\xi} = [Z,X]\begin{bmatrix} \underline{\beta} \\ -- \\ \underline{\tau} \end{bmatrix}$$

where Z is the $(a\times(s+1))$ matrix associated with those terms that will be adjusted for and whose parameters are contained in $\underline{\beta}$, and

X is the $(a\times pw)$ design matrix associated with the main effects and interaction effects of interest which are contained in $\underline{\tau}$.

The incidence matrix $X^{*\prime}X^{*}$ is found to be

$$X^{*\prime}X^{*} = \left[\begin{array}{c|c} Z'Z & Z'X \\ \hline X'Z & X'X \end{array}\right]$$

with

$$Z'Z = \left[\begin{array}{cccc|c} p^d & 0 & \cdots & 0 & p^d \\ & \ddots & & & \vdots \\ \text{sym.} & & & p^d & p^d \\ & & & & sp^d \end{array}\right]_{(s+1)\times(s+1)}$$

and

$$Z'X = \left[\begin{array}{ccc} p^{d-1} & \cdots & p^{d-1} \\ \vdots & & \vdots \\ p^{d-1} & \cdots & p^{d-1} \\ sp^{d-1} & & sp^{d-1} \end{array}\right]_{(s+1)\times pw} = (X'Z)'$$

and

$$X'X = \begin{bmatrix} sp^{d-1}I_p & sp^{d-2}J_p & \cdots & sp^{d-2}J_p \\ & sp^{d-1}I_p & & sp^{d-2}J_p \\ \text{sym.} & & \ddots & \vdots \\ & & & sp^{d-1}I_p \end{bmatrix}$$

$$X'X = sp^{d-2}J_{pw} + sp^{d-2}I_w \otimes (pI_p - J_p)$$

Again Theorem 3.3.1 can be used to obtain

$$(Z'Z)^- = p^{-d} \left[\begin{array}{c|c} I_s & \underline{0} \\ \hline \underline{0}' & 0 \end{array}\right] .$$

The generalized form for the matrix of the reduced normal equations (3.2.4) is thus

$$D = sp^{d-2}I_w \otimes (pI_p - J_p) . \qquad (3.8.2)$$

Reducing the normal equations for additional main effects or interactions not of interest is easy, due to the orthogonality of the design. This will often be necessary because of the fact that often parts of interactions will be unaliased while other parts will be aliased. These parts will therefore often require adjustments. Assuming that the experimenter is interested in k effects, adjusting for the other w-k effects gives

$$D = sp^{d-2} I_k \otimes (pI_p - J_p) \; . \tag{3.8.3}$$

By use of Theorems 2 and 3 (Appendix) the generalized inverse of D is $D^- = \frac{1}{sp^{d-1}} I_{pk}$ . Therefore

$$D^- D D^- = \frac{1}{sp^d} I_k \otimes (pI_p - J_p) \; . \tag{3.8.4}$$

After finding the form of the reduced normal equations for one response, it will now be extended to p' responses to fit the MGLM model. To find an estimable function on all p' responses, the BLU estimators for each univariate response must be found, and for this reason the reduced normal equations were solved. Denote by $v_i$, the number of factors affecting the $i^{th}$ response; by $f_i$ the size of the fraction $1/p^{f_i}$ used on the $p^{v_i}$ experiment for the $i^{th}$ response; by $s_i$ the number of times the $1/p^{f_i}$ fraction will be repeated; and by $k_i$, the number of factors to be studied on the $i^{th}$ response $(i = 1,\ldots,p')$. Thus for each response

$$D_i = s_i p^{d_i - 2} I_{k_i} \otimes (pI_p - J_p) \tag{3.8.5}$$

and

$$D_i^- D_i D_i^- = \frac{1}{s_i p^{d_i}} I_{k_i} \otimes (pI_p - J_p) \ . \qquad (3.8.6)$$

The trace of the variance-covariance matrix of estimable functions from (3.3.16) is

$$Q = \sum_{i=1}^{p'} \operatorname{tr}(\operatorname{Var}(P_i \hat{\underline{\tau}}_i))$$

which from (3.3.13) and (3.3.17) is

$$Q = \sum_{i=1}^{p'} \sigma_{ii} \operatorname{tr}(D_i^- D_i D_i^- P_i' P_i) \ . \qquad (3.8.7)$$

For $P_i$ the matrix of normalized orthogonal contrasts $P_i'P_i$ was found for a $p^v$ experiment in (3.2.10) to be

$$P_i'P_i = \frac{1}{p} I_k \otimes (pI_p - J_p) \ .$$

Using this equation along with (3.8.6) and (3.8.7)

$$Q = \Sigma\, \sigma_{ii} \frac{p(p-1)k_i}{s_i\, 2^{d_i}} \ .$$

The MGLM(F) design $D(n_0^*, s_1^* p^{d_1}, \ldots, s_{p'} p^{d_{p'}})$ will be determined that minimizes

$$Q = \sum_{i=1}^{p'} p(p-1) \frac{k_i \sigma_{ii}}{s_i p^{d_i}} \qquad (3.8.8a)$$

subject to the cost constraint:

$$\psi' = n_0 \psi_0 + \sum_i s_i p^{d_i} \psi_i \qquad (3.8.8b)$$

and

$$s_i \geq 1 \quad (i = 1, \ldots, p') .$$

For the $p^v$ factorial experiment the proof of Lemma 3.4.1 remains the same, and due to the fact that Q (3.8.8a) is a function of only $s_i$, Theorem 3.5.1 is also true, i.e., the optimal MGLM(F) design subject to (3.8.8) is a member of the subclass of HMGLM(F) designs.

<u>Theorem 3.8.2</u> (The theorems will be numbered to coincide with the equivalent theorems in Section 3.5.)

If

$$\frac{k_i \sigma_{ii}}{\psi_i} \geq \frac{k_j \sigma_{jj}}{\psi_j}$$

then in the optimal design

$$s_i p^{d_i} \geq s_j p^{d_j} .$$

Proof: The proof follows that of Theorem 3.5.2.

Without loss of generality, assume that the responses are ordered so that

$$n_0 = s_1 p^{d_1} \geq s_2 p^{d_2} \geq \ldots \geq s_{p'} p^{d_{p'}} . \qquad (3.8.9)$$

Theorem 3.8.3 With the responses ordered as in (3.8.9), let b be the smallest integer in the set 2,3,...,p' such that

$$\frac{\sigma^*_{b-1}}{\psi^*_{b-1}} > \frac{p(p-1)k_b \sigma_{b,b}}{\psi_b} \qquad (3.8.10a)$$

and

$$\frac{\sigma^*_{b-2}}{\psi^*_{b-2}} \leq \frac{p(p-1)k_{b-1}\sigma_{b-1,b-1}}{\psi_{b-1}} \qquad (3.8.10b)$$

where

$$\sigma^*_i = p(p-1)\sigma_{11} + \ldots + p(p-1)\sigma_{ii}$$

and

$$\psi^*_i = \psi_0 + \psi_1 + \ldots + \psi_i \quad (i = 1,\ldots,p') .$$

Then

$$s_1 p^{d_1} = \ldots = s_{b-1} p^{d_{b-1}} > s_b 2^{d_b} \geq \ldots \geq s_{p'} 2^{d_{p'}} . \qquad (3.8.11)$$

For b = 2 ignore equation (3.7.10b) and if equation (3.7.10b) is satisfied at b = p' then:

$$s_1 p^{d_1} = \ldots = s_{p'} p^{d_{p'}} .$$

Proof: The proof follows that of Theorem 3.5.3.

Corollary 3.8.4 If the p' responses are numbered so that $\frac{k_i \sigma_{ii}}{\psi_i} \geq \frac{k_j \sigma_{jj}}{\psi_j}$ $(i < j,\ i,j = 1,\ldots,p')$ and b is defined as in Theorem 3.8.3, then the optimum values $n_0^*, s_1^*, \ldots, s_p^*$ are given by

$$s_i = \frac{\psi'}{\delta} p^{-d_i} \sqrt{\frac{\sigma_{b-1}^*}{\psi_{b-1}^*}} \quad \text{for } i = 1,\ldots,b-1 \qquad (3.8.12a)$$

and

$$s_j = \frac{\psi'}{\delta} p^{-d_j} \sqrt{\frac{p(p-1)k_j \sigma_{j,j}}{\psi_j}} \quad \text{for } j = b,\ldots,p' \qquad (3.8.12b)$$

and

$$n_0 = s_1 p^{d_1}$$

where

$\psi'$ is the total amount of money available for experimentation,

$$\delta = \sqrt{\psi_{b-1}^* \sigma_{b-1}^*} + \sum_{i=b}^{p'} \sqrt{p(p-1)\psi_i k_i \sigma_{i,i}}$$

$$\sigma_i^* = p(p-1)k_1\sigma_{1,1} + \ldots + p(p-1)k_i\sigma_{i,i}$$

and

$$\psi_i^* = \psi_0 + \psi_1 + \ldots + \psi_i \quad (i = 1,\ldots,p') .$$

Proof: The proof follows that of Corollary 3.5.4.

It is apparent that in many situations when using a $p^v$ factorial experiment, the HMGLM(F) design will be better than the MDM(F) design (the HMGLM(F) design is always better than the MGLM(F) design because of completeness). The comments on philosophy and interpretation of these designs are the same as those that were made about the $2^v$ factorial experiment. The round-off of $s_i$ values to an integer is even more important than it was previously due to the larger group of units being repeated. The program (Appendix 2) can be used for $p^v$ factorials as well as $2^v$ factorial experiments to find the best design.

## CHAPTER IV

## OPTIMIZATION WITH RESPECT TO THE DETERMINANT CRITERION; RESULTS FOR SOME SPECIFIC p-RESPONSE SITUATIONS

### 4.1 Introduction

Minimization of the determinant of the variance-covariance matrix V of estimable functions can also be used as a criterion for choice of a design from the class of MGLM designs, using the same cost constraint as in Chapter 3. Minimization of the variance-covariance determinant was first introduced by Isaacson (1951) under the heading of D-optimal designs. D-optimal regression designs have been investigated by Hoel (1958) and good reference lists are given in Kiefer (1959) and in Stigler (1971).

As previously noted, the use of the trace of V as a criterion gives a design which minimizes the average variance of the BLU estimators of the normalized linear contrasts in the parameters of interest, however as also noted, these designs are not invariant, with a simple change in scale, changing the optimum design. The criterion of minimizing the determinant of V or minimizing the generalized variance of the BLU estimators has the desirable property of invariance under change of scale. The optimal design D* under the determinant criterion also has another attractive property in that the volume of the confidence region for $P\underline{\tau}$ is minimized under Gaussian error structure.

D*, the optimal design, is also important when testing hypotheses. Under a normality assumption for a fixed size locally unbiased test, the power function of D* has maximum Gaussian curvature at the null hypothesis (Kiefer (1959)). (The reciprocal of the Gaussian curvature of a surface can be geometrically explained by considering a cross-section of a surface an infinitesimal distance above the minimum point, see Isaacson (1951).)

In this chapter the determinant of the variance-covariance matrix, $\mathrm{Var}(P\underline{\tau})$ will be used as a criterion for optimality. The general form of $\mathrm{Var}(P\underline{\tau})$ must first be found so that $\det(\mathrm{Var}(P\underline{\tau}))$ can be determined. The values of $s_1, s_2, \ldots, s_p$ can then be found that minimize $\det(\mathrm{Var}(P\underline{\tau}))$ subject to the cost constraint and therefore the optimal design can be defined.

The problem that we encounter is that for a general p-variate case, the matrix $\mathrm{Var}(P\underline{\tau})$ can be found, but the determinant is very hard to acquire except for some very specific cases. These cases are considered and the optimal designs are determined.

In the following chapters the $p=2$ response case is considered where, because the determinant can be found, the optimal design can be determined.

## 4.2 The General Form for $\mathrm{Var}(P\hat{\underline{\tau}})$

In this chapter the determinant of an MGLM design D will be used as a criterion for optimality. It will be denoted by $|D|$ and will be defined by

$$|D| = \det(\mathrm{Var}(P\hat{\underline{\tau}})). \tag{4.2.1}$$

When using the trace criterion, we were concerned with only the univariate variance-covariance matrices for the parameters of each response and even then only the diagonal elements need be found. However with the determinant criterion, the concern is with not only the p univariate variance-covariance matrices, but also with the off-diagonal covariance matrices whose elements are the covariances between the different responses. It is these covariance matrices that add greater difficulty to the problem. The covariance matrix between the $i^{th}$ and $j^{th}$ response (for $i \neq j$, $i,j = 1,\ldots,p$) depends on

1. How many observational units the $i^{th}$ and $j^{th}$ responses have in common,
2. Which treatment combinations have been applied to these common units,
3. Which of the v factors affect each response and which of these factors affects both $V_i$ and $V_j$, and

4. What alias structure is used in the entire experiment.

Some of these problems are eased by the fact that we will be trying to determine how many times we can replicate (possibly in different blocks) a group of experimental units where these groups of units are the smallest fraction that can be used without aliasing main effects.

In a univariate situation, recall that when "estimating" a vector $\underline{\tau}$ adjusted for a vector of nuisance parameters $\underline{\beta}$, it was found that

$$D\underline{\tau} = \underline{q}$$

where:

$$D = X'X - X'Z(Z'Z)^{-}Z'X$$

$$\underline{q} = M\underline{y}$$

$$M = X'(I - Z(Z'Z)^{-}Z').$$

With $\mathrm{Var}(\underline{y}) = \sigma^2 I$, then

$$\mathrm{Var}(\underline{q}) = \sigma^2 D \ ,$$

and

$$\mathrm{Var}(\hat{\underline{\tau}}) = \sigma^2 D^{-} D D^{-} \ .$$

Because $\hat{\underline{\tau}}$ is not estimable, $\mathrm{Var}(\hat{\underline{\tau}})$ depends upon which generalized inverse of D is used and therefore is not a unique matrix. We will however work with $\mathrm{Var}(\hat{\underline{\tau}})$ for upon finding its general form we can easily determine the general form of the unique matrix $\mathrm{Var}(P\hat{\underline{\tau}})$, the variance-covariance matrix of the estimable functions of the parameters of $\hat{\underline{\tau}}$.

Considering now the $i^{th}$ response in a p-response MGLM model for a $2^v$ factorial experiment, the experimental units on $V_i$ are composed of $s_i$ $1/2^{f_i}$ fractions of a $2^{v_i}$ factorial experiment $(d_i = v_i - f_i)$, and the experimenter is interested in making $k_i$ comparisons $(i = 1,\ldots,p)$. For this situation

$$D_i = s_i 2^{d_i - 2} I_{k_i} \otimes (2I_2 - J_2) ,$$

$$D_i^- = \frac{1}{s_i 2^{d_i - 1}} I_{2k_i} ,$$

$$\mathrm{Var}(\hat{\underline{\tau}}_i) = \frac{\sigma_{ii}}{s_i 2^{d_i}} I_{k_i} \otimes (2I_2 - J_2) . \qquad (4.2.2)$$

The covariance between $\hat{\underline{\tau}}_i$ and $\hat{\underline{\tau}}_j$ is

$$\begin{aligned} \mathrm{Cov}(\hat{\underline{\tau}}_i,\hat{\underline{\tau}}_j) &= D_i^- \,\mathrm{Cov}(\underline{q}_i,\underline{q}_j) D_j^- \\ &= D_i^- M_i \,\mathrm{Cov}(\underline{y}_i,\underline{y}_j) M_j' D_j^- \qquad (4.2.3) \end{aligned}$$

with

$$\mathrm{Cov}(\underline{y}_i,\underline{y}_j) = \sigma_{ij} Q_{ij} ,$$

where $Q_{ij}$ is a $(s_i 2^{d_i} \times s_j 2^{d_j})$ matrix whose (r,s) element $q_{rs}$ is given by

$q_{rs} = 1$ if the $r^{th}$ element of $\underset{\sim}{y}_i$ and the $s^{th}$ element of $\underset{\sim}{y}_j$ are observed on the same experimental unit, and

$q_{rs} = 0$ otherwise.

The rank of $Q_{ij}$ will be denoted by $n_{ij}$ where $n_{ij}$ is the number of observational units on which both the $i^{th}$ and $j^{th}$ response are measured $(n_{ij} \leq \min(s_i 2^{d_i}, s_j 2^{d_j}))$.

The matrix $Q_{ij}$ simply performs the task of lining up the observations that were measured on the same observational units and eliminating the other measurements because the covariance is computed only from those measurements coming from the same observational units. For example, in a HMGLM design suppose $s_i 2^{d_i} > s_j 2^{d_j}$ and the $j^{th}$ response is measured on the first $s_j 2^{d_j}$ units of the $s_i 2^{d_i}$ observational units where the $i^{th}$ response is measured. Then $Q_{ij}$ is a $(s_i 2^{d_i} \times s_j 2^{d_j})$ matrix of rank $r = s_j 2^{d_j}$ and $Q_{ij} = \begin{bmatrix} I_r \\ 0 \end{bmatrix}$. Thus only the first r units on response i are used in calculating the covariance.

A univariate case will be looked at first and then the extension will be made to the multivariate case. Attention is given to the case where all $2^d$-1 main effects and interactions are of interest and the $1/2^f$ fraction is repeated s times. The portion of the design matrix associated with the s+1 parameters to be adjusted for is

$$Z = [I_s \otimes \underline{j}_{2^d}, \underline{j}_{s2^d}]_{(s2^d \times (s+1))}$$

giving

$$Z'Z = \left[\begin{array}{c|c} 2^d\ I_s & 2^d \underline{j}_s \\ \hline 2^d\ \underline{j}_s' & s2^d \end{array}\right]_{((s+1)\times(s+1))}$$

A generalized inverse of Z'Z is

$$(Z'Z)^- = 2^{-d} \left[\begin{array}{c|c} I_s & \underline{0} \\ \hline \underline{0}' & 0 \end{array}\right]$$

and thus

$$Z(Z'Z)^- Z' = 2^{-d} I_s \otimes J_{2^d} .$$

Premultiplying this by X' yields

$$X'Z(Z'Z)^- Z' = \frac{1}{2} J_{(2^d-1)\times s2^d} .$$

Suppose that rather than being interested in all $2^d$-1 effects in the model, the experimenter is interested in only k effects. Due to the orthogonality of the model, it is easily found that

$$X'Z(Z'Z)^{-}Z' = \frac{1}{2} J_{2k\times s2^d} . \qquad (4.2.4)$$

The extension will now be made to the p-variate case, where i and j are used to denote any two of the responses ($i \neq j$, $i,j = 1,\ldots,p$). The following two assumptions are made in general and arise as a result of the restrictions made on the size of the fraction used.

1. For each response, there is no aliasing among the $k_i$ effects of interest and other effects that influence $V_i$. This assumption arises through our previous assumption that the fraction size chosen will not create aliasing of non-zero effects.

2. If X is an effect influencing $V_i$ but not $V_j$ and Y is an effect influencing $V_j$, then X and Y are not confounded. This confounding can be avoided through the choice of block sizes, defining contrasts, and also through the choice of treatment combinations used on the overall experiment. In a univariate experiment, the experimenter has no choice in treatment combinations in that they are determined when the defining contrasts are chosen. In some multivariate cases, however, there can be more leeway. Consider the following example: $p = 2$, $v = 4$, $v_1 = v_2 = 3$, $f_1 = 0$, $f_2 = 1$, $s_1 = s_2 = 1$. Of the 4 factors A, B, C, D let $V_1$ be affected by A, B, C and $V_2$ by B, C, D. Suppose that for $V_2$ the defining contrast

$I_2$ = BCD is used and the treatment combinations to be used are '1', bc, bd, cd. In the following table, column 1 gives the actual treatment combination (t.c.) of 4 factors applied to each experimental unit, and column 2 gives the effective treatment combination on $V_1$ considering only those factors affecting $V_1$. The effective treatment combinations on $V_2$ are given in columns 3, 4, and 5 in three different assignments of the four treatment combinations for $V_2$. Only the units in which both $V_1$ and $V_2$ are measured change; the defining contrast remains the same.

Table 4.2.1

| Actual tc | $V_1$ tc | $V_2$ tc | $V_2$ tc | $V_2$ tc |
|---|---|---|---|---|
| '1' | '1' | '1' | '1' | '1' |
| a | a | | | |
| bd | b | | | |
| abd | ab | bd | bd | bd |
| cd | c | cd | | |
| acd | ac | | cd | cd |
| bc | bc | | | bc |
| abc | abc | bc | bc | |

If the allignment in column 3 is used, A and D are not confounded; if that of column 4 is used, A and D are partially confounded; and if that of column 5 is used, A and D are completely confounded.

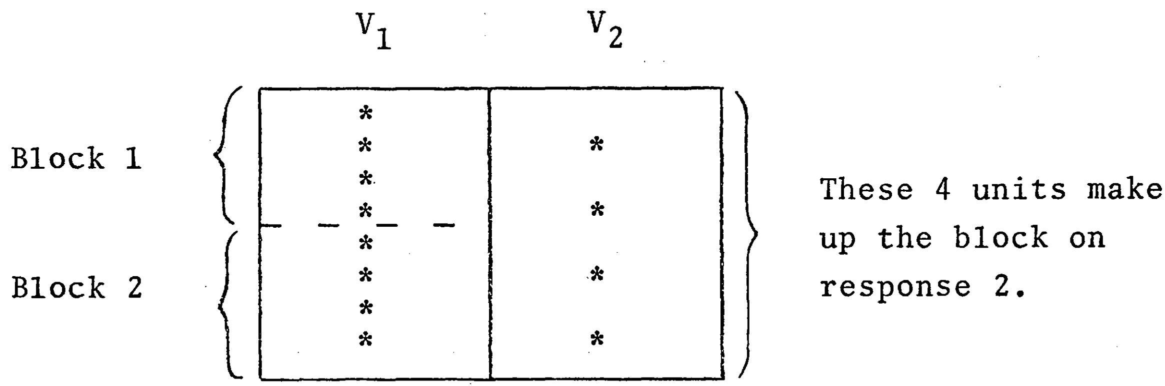
This second assumption in some instances makes the selection of block sizes a tricky problem. Unfortunately in some cases more must be done than simply using fractions big enough to prevent aliasing of effects on this response. The alias structure between $V_i$ and $V_j$ must also be considered. Determine first the fraction size for each response, $V_i$, based only on the effects influencing $V_i$. Then using one fraction for each response, check to make sure effects are not aliased between responses. If this occurs it may be necessary to enlarge some fraction sizes. Once the smallest admissible fraction sizes are determined (admissible meaning that the assumptions are satisfied), the optimum design can be found by determining how many times each fraction should be replicated on each response.

This assumption may be necessary at times when $2^{d_i} \geq 2^{d_j}$ because some of the $(k_i - k_{ij})$ effects that influence $V_i$ but not $V_j$ may be partially confounded with effects on $V_j$. It may not even be necessary that these effects on $V_i$ be confounded with effects on $V_j$ that do not affect $V_i$. It is possible (when $2^{d_i} > 2^{d_j}$) that some effect on $V_i$ be unaliased with another effect on $V_i$ while being aliased with that same effect on $V_j$. Consider the following very simple illustration:

$$X_1 = \begin{array}{cc} \quad A & \quad B \\ \multicolumn{2}{c}{\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}} \end{array} \qquad X_2 = \begin{array}{c} A \\ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \end{array}$$

In $V_1$ effects A and B are unaliased but when only the $n_{12} = 2$ units that $V_1$ and $V_2$ have in common are considered then B of $V_1$ and A of $V_2$ are completely confounded.

Another assumption that will be used only in the following derivations is that the blocks (groups) of fractional replicates coincide. This assumption is not truly necessary and later it will be shown that it is not needed; but for now it is made because it makes the following discussion easier to comprehend. This assumption requires neither that the fractions are the same size nor that $2^{d_i} = 2^{d_j}$, but assumes the units for a fraction on $V_j$ come from either several complete fractions on $V_i$ (when $2^{d_j} > 2^{d_i}$) or that they come entirely from one fraction on $V_i$ (when $2^{d_j} \leq 2^{d_i}$). This assumes that there will not be cases like the following: $2^{d_1} = 4 = 2^{d_2}$, $s_1 = 2$, $s_2 = 1$, where the symbol * in the diagram below represents that a response is measured on this observational unit




The assumption requires that the 4 units for $V_2$ come entirely from either block 1 or block 2 for $V_1$.

To find the determinant of $\mathrm{Var}(P\hat{\underline{\tau}})$, the general form of $\mathrm{Var}(\hat{\underline{\tau}}_i)$ and $\mathrm{Cov}(\hat{\underline{\tau}}_i,\hat{\underline{\tau}}_j)$ $(i,j = 1,\ldots,p)$ must first be found. In equation (4.2.2) the general form of $\mathrm{Var}(\hat{\underline{\tau}}_i)$ was given; next the covariance matrix for the two responses $V_i$ and $V_j$ will be found in a more general form than was given in equation (4.2.3). Recall that

$$
\begin{aligned}
\mathrm{Cov}(\underline{q}_i,\underline{q}_j) &= \sigma_{ij}M_iQ_{ij}M_j' \\
&= \sigma_{ij}\{X_i'Q_{ij}X_j - X_i'Q_{ij}Z_j(Z_j'Z_j)^{-}Z_j'X_j \\
&\quad + X_i'Z_i(Z_i'Z_i)^{-}Z_i'Q_iX_j \\
&\quad + X_i'Z_i(Z_i'Z_i)^{-}Z_i'Q_{ij}Z_j(Z_j'Z_j)^{-}Z_j'X_j\} .
\end{aligned}
$$

For any i and j $(i,j = 1,\ldots,p)$ either case (1.)

$$2^{d_i} \geq 2^{d_j} , \qquad \text{or}$$

case (2.) $\qquad 2^{d_i} < 2^{d_j}$ .

If case (1.) is true and $s_i 2^{d_i} \geq s_j 2^{d_j}$ then

$$X_i' Z_i (Z_i' Z_i)^- Z_i' Q_{ij} = \frac{1}{2} J_{2k_i \times s_j 2^{d_j}} , \tag{4.2.5}$$

and

$$X_i' Z_i (Z_i' Z_i)^- Z_i' Q_{ij} X_j = s_j 2^{d_j - 2} J_{2k_i \times 2k_j} . \tag{4.2.6}$$

If however $s_i 2^{d_i} < s_j 2^{d_j}$ then

$$X_i' Z_i (Z_i' Z_i)^- Z_i' Q_{ij} = \frac{1}{2} [J_{2k_i \times s_i 2^{d_i}}, 0]_{2k_i \times s_j 2^{d_j}} , \tag{4.2.7}$$

and

$$X_i' Z_i (Z_i' Z_i)^- Z_i' Q_{ij} X_j = s_i 2^{d_i - 2} J_{2k_i \times 2k_j} . \tag{4.2.8}$$

Also

$$X_i' Z_i (Z_i' Z_i)^- Z_i' Q_{ij} Z_j (Z_j' Z_j)^- Z_j' X_j = a J_{2k_i \times 2k_j} \tag{4.2.9}$$

where

$$a = s_j 2^{d_j - 2} \qquad \text{when} \qquad s_i 2^{d_i} \geq s_j 2^{d_j}$$

and

$$a = s_i 2^{d_i - 2} \qquad \text{when} \qquad s_i 2^{d_i} < s_j 2^{d_j} .$$

Thus for case (1) when $s_i 2^{d_i}$ is either $\geq$ or $<$ $s_j 2^{d_j}$:

$$X_i' Z_i (Z_i' Z_i)^{-} Z_i' Q_{ij} (I - Z_j (Z_j' Z_j)^{-} Z_j') X_j = 0,$$

or

$$X_i' Z_i (Z_i' Z_i)^{-} Z_i' Q_{ij} M_j' = 0 . \qquad (4.2.10)$$

Similarly, if case (2.) is true, it is found that

$$M_i Q_{ij} Z_j (Z_j' Z_j)^{-} Z_j' X_j = 0 . \qquad (4.2.11)$$

Therefore to find Cov($\underline{q}_i$,$\underline{q}_j$) when case (1) is true:

$$M_i Q_{ij} M_j' = X_i' Q_{ij} M_j' \qquad (4.2.12)$$

and when case (2) is true

$$M_i Q_{ij} M_j' = M_i Q_{ij} X_j . \qquad (4.2.13)$$

In an attempt to give more justification for equations (4.2.10) and (4.2.11), we look first at the situation where case (1.) is true and there will thus exist a non-negative integer c such that $2^{d_i} = 2^c 2^{d_j}$. Suppose that $s_j 2^{d_j} > s_i 2^{d_i}$ and thus equation (4.2.7) is applicable. (Equation (4.2.7) as was (4.2.5) was obtained from the definition of $Q_{ij}$ along with the extension of equation (4.2.4) to the multivariate case.) With $s_i 2^{d_i} = (s_i 2^c) 2^{d_j}$, then $s_i 2^c$ groups of $2^{d_j}$ units will enter in the calculation of $\mathrm{Cov}(\underline{y}_i, \underline{y}_j)$. The matrix in equation (4.2.7) is a $(2k_i \times s_j 2^{d_j})$ matrix with 1's in the first $n_{ij}$ columns where $n_{ij}$ is the number of observational units response i and response j have in common, which for this hierarchial design is $n_{ij} = s_i 2^{d_i}$. Equation (4.2.8) is the product of this matrix (4.2.7) post multiplied by X; and it is thus a type of incidence matrix. Associated with each column of $X_j$ is either the high or low level of some main effect or interaction affecting $V_j$. Each element of a column of matrix (4.2.8) indicates the total number of times the level of the effect associated with this column of $X_j$ occurred at this level over all $n_{ij}$ treatment combinations in common with $V_i$. Due to the orthogonality in each univariate model, each effect for response $V_j$ appears $2^{d_j - 1}$ times at both the high level and at the low level, in each fraction of $2^{d_j}$ units in the matrix $X_j$. This along with the fact that $n_{ij}$ is $s_i 2^c$ complete fractions of $2^{d_j}$ units means that each effect will have occurred an equal number of times at the high and low levels, i.e., in each column of $S_j$ there are $\frac{1}{2} n_{ij}$ ones in the first $n_{ij}$ rows, the remaining

$\frac{1}{2} n_{ij}$ elements are zeros. Thus pre-multiplying $X_j$ by a matrix of constants (say $a \cdot J$) gives a resulting matrix of constants $\frac{1}{2} an_{ij}$, i.e., $aJX_j = \frac{1}{2} an_{ij}J$. In this manner equation (4.2.8) was determined.

If $s_i 2^{d_i} > s_j 2^{d_j}$ then all $s_j$ fractions are used to determine the covariance. Since all factors appear the same number of times in each fraction, then equation (4.2.6) follows obviously from equation (4.2.5) for the same reasons equation (4.2.8) followed from (4.2.7). Equation (4.2.9) is found directly from the fact that

$$X_i Z_i (Z_i' Z_i)^- Z_i' = \frac{1}{2} J_{2k_i \times s_i 2^{d_i}}$$

along with the definition of $Q_{ij}$, thus giving equation (4.2.10).

If case (2) is true, then the same argument holds after simply switching the subscripts i and j, thus giving equation (4.2.11)...

<u>Example 4.2.1</u> As an example, consider the HMGLM situation with $p = 2$, $v = 4$, $v_1 = 4$, $v_2 = 3$, $f_1 = 1$, $f_2 = 1$, $s_1 = 1$, $s_2 = 1$ and with factor B not affecting response 2. The defining contrasts I = ABCD and I = -ACD will be used for the individual responses. The treatment combinations applied to response 1 are '1', ac, ad, cd, ab, bc, bd, abcd and for

response 2 only the first 4 observational units '1', ac, ad, cd. To simplify the example, only main effects will be considered to be of interest and will be included in the model; all other interactions are assumed negligible, thus $k_1 = 4$ and $k_2 = 3$.

$$X_1 = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix}. \qquad X_2 = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 \end{bmatrix} \qquad Z_1 = \underline{j}_8 \qquad Z_2 = \underline{j}_4 \tag{4.2.14}$$

$$Z_1(Z_1'Z_1)^- Z_1' = \frac{1}{8} I_8 ,$$

$$Z_2(Z_2'Z_2)^- Z_2' = \frac{1}{4} I_4 , \qquad Q_{12} = \begin{bmatrix} I_4 \\ --- \\ 0_4 \end{bmatrix} ,$$

$$X_1'Z_1(Z_1'Z_1)^- Z_1' = \frac{1}{2} J_8 ,$$

$$Z_2(Z_2'Z_2)^- Z_2'X_2 = \frac{1}{2} J_{4\times 6} ,$$

$$X_1'Q_{12}X_2 = \begin{bmatrix} 2 & 0 & 1 & 1 & 1 & 1 \\ 0 & 2 & 1 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 2 & 0 & 1 & 1 \\ 1 & 1 & 0 & 2 & 1 & 1 \\ 1 & 1 & 1 & 1 & 2 & 0 \\ 1 & 1 & 1 & 1 & 0 & 2 \end{bmatrix}, \quad (4.2.15)$$

$$X_1'Z_1(Z_1'Z_1)^- Z_1'Q_{12}X_2 = J_{8\times 6} \;, \quad (4.2.16)$$

$$X_1'Q_{12}Z_2(Z_2'Z_2)^- Z_2'X_2 = \frac{1}{2}\begin{bmatrix} 2 & 2 & 2 & 2 & 2 & 2 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 4 & 4 & 4 & 4 & 4 & 4 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 2 & 2 & 2 & 2 & 2 & 2 \end{bmatrix}, \quad (4.2.17)$$

$$X_1'Z_1(Z_1'Z_1)^- Z_1'Q_{12}Z_2(Z_2'Z_2)^- Z_2'X_2 = J_{8\times 6} \;. \quad (4.2.18)$$

Since $2^{d_1} > 2^{d_2}$, case (1) is true and from equations (4.2.16) and (4.2.18) it is obvious that $X_1'Z_1(Z_1'Z_1)^- Z_1'Q_{12}M_2 = 0$ illustrating equation (4.2.10).

Having simplified a portion of $\text{Cov}(\hat{\underline{\tau}}_i, \hat{\underline{\tau}}_j)$, we now consider finding a more general expression for the right hand side of equation (4.2.12) or (4.2.13). Equation (4.2.12) is applicable when $2^{d_i} \geq 2^{d_j}$, equation (4.2.13) when $2^{d_i} < 2^{d_j}$.

When effects associated with response $V_i$ but not with $V_j$ are not confounded with those effects that are associated with $V_j$, then the matrix $X_i'Q_{ij}X_j$ will be of the general form

$$X_iQ_{ij}X_j = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1,k_j} \\ A_{21} & A_{22} & \cdots & A_{2,k_j} \\ \vdots & \vdots & & \\ A_{k_i,1} & A_{k_i,2} & \cdots & A_{k_ik_j} \end{bmatrix} \qquad (4.2.19)$$

where the submatrices $A_{xw} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$ are 2×2 matrices.

(If these submatrices were to be used throughout this work, a more extensive notation identifying each matrix uniquely would be defined, such as using $A_{ijxw}$ and $a_{ijxw11}$. We will however leave the notation in a simplified form as these matrices are used here for illustration and will not be used later.) These submatrices have the following properties:

(i) $a_{11} + a_{12} + a_{21} + a_{22} = n_{ij}$

(ii) $a_{11} + a_{21} = \frac{1}{2} n_{ij} = a_{12} + a_{22}$ for case 1 $(2^{d_i} > 2^{d_j})$, $\qquad (4.2.20)$

$$a_{11} + a_{12} = \frac{1}{2} n_{ij} = a_{21} + a_{22}$$
$$\text{for case 2 } (2^{d_i} < 2^{d_j}) \text{ .} \qquad (4.2.21)$$

When the $x^{th}$ effect on $V_i$ is the same treatment effect as the $w^{th}$ effect on $V_j$, $A_{xw}$ has

$$a_{11} = a_{22} = \frac{1}{2} n_{ij} \text{ ,} \qquad (4.2.22a)$$

$$a_{12} = a_{21} = 0 \text{ .} \qquad (4.2.22b)$$

These matrices $A_{xw}$ are indications of the alias structure between the two effects compared, x and w. If for case 1

$$a_{11} = a_{12} \quad \text{and} \quad a_{21} = a_{22}$$

then the effects are not confounded. If for case 2

$$a_{11} = a_{21} \quad \text{and} \quad a_{12} = a_{22} \text{ ,}$$

then the effects are not confounded. When these equations are not satisfied then there is some degree of confounding. Equation (4.2.22) illustrates a case where the two effects are completely confounded (since the two effects are the same).

Define $k_{ij}$ to be the number of effects that $V_i$ and $V_j$ have in common. Thus there are $k_{ij}$ matrices as described by (4.2.22). The remaining $k_i k_j - k_{ij}$ matrices will be described by (4.2.20) or (4.2.21) depending upon which case is applicable.

In the matrix $X_i$, each column consists of zeros and ones, the number of ones being the number of times this effect appeared at this level. There are $n_{ij}$ experimental units in common between the $i^{th}$ and $j^{th}$ responses. Denote by $n_{ijxh}$ the number of times the effect x occurs at the high level on the $n_{ij}$ units and denote by $n_{ijx\ell}$ the number of times effect x occurs at the low level thus giving $n_{ijxh}$ + $n_{ijx\ell} = n_{ij}$. Due to the orthogonality in the design and the way the fractional replicates were chosen, each effect appears the same number of times at each level in each fraction of $2^{d_i}$ units, and this will also be true when considering all measurements on $V_i$ due to the fact that complete fractions are repeated $s_i$ times.

Assume that for a hierarchial design $s_i 2^{d_i} \geq s_j 2^{d_j}$, thus $n_{ij} = s_j 2^{d_j}$, and assume for ease of discussion that these $n_{ij}$ units are the first $n_{ij}$ units of the $s_i 2^{d_i}$ units on which $V_i$ is measured. The matrix $Q_{ij}$ when pre-multiplied by $X_i'$ has the effect of 'reducing' the matrix $X_i'$. This 'reducing' of $X_i$ eliminated all but the first $n_{ij}$ rows (those rows corresponding to those units where $V_i$ and $V_j$ were both measured), dropping the remaining $(s_i 2^{d_i} - n_{ij})$ rows, and thus making $X_i'Q_{ij}$ conformable for post-multiplication by $X_j$. If $2^{d_i} \leq 2^{d_j}$, then an integer $c_1$ can be found such that $n_{ij} = c_1 2^{d_i}$, and each effect in $X_i$ will occur $c_1 2^{d_i - 1}$ times at both high and low levels. Each effect in $X_j$ will also occur $c_1 2^{d_i - 1}$ or $\frac{1}{2} n_{ij}$ times at each level. Thus if two column vectors are neither identical nor exactly opposite (i.e., the effects compared are not the same or different levels of the same effect or the effects are not aliased), then their dot product will be

$$c_1 2^{d_i - 2} = \frac{1}{4} n_{ij} = s_j 2^{d_j - 2} \quad .$$

This is obviously true because effect B at the low level on $V_i$ will occur with effect C on $V_j$, $c_1 2^{d_i - 1}$ times, half the time with $C_0$ and half the time with $C_1$, the same being true for B at the high level. For example consider the 2×2 submatrix $A_{BC}$ of the matrix $X_i'Q_{ij}X_j$ results from the dot products of the vectors corresponding to the two levels of effect B for $V_i$, denoted by $[\underline{B}_{0,i}, \underline{B}_{1,i}]$, with those of effect C on $V_j$, $[\underline{C}_{0,j}, \underline{C}_{1,j}]$. $\underline{B}_{0,i}$ is defined to be the $(n_{ij} \times 1)$ vector of zeros and ones from $X_i'Q_{ij}$ that corresponds to the effect B at the low (0) level for $V_i$ and the other vectors $\underline{B}_{1,i}$, $\underline{C}_{0,i}$, $\underline{C}_{1,i}$ are defined in a similar fashion. Then

$$\begin{bmatrix} \underline{B}'_{0,i} \\ -- \\ \underline{B}'_{1,i} \end{bmatrix} [\underline{C}_{0,j}, \underline{C}_{1,j}] = \left[\begin{array}{c|c} \underline{B}'_{0,i}\underline{C}_{0,j} & \underline{B}'_{0,i}\underline{C}_{1,j} \\ \hline \underline{B}'_{1,i}\underline{C}_{0,j} & \underline{B}_{1,i}\underline{C}_{1,j} \end{array}\right] = s_j 2^{d_j - 2} J_2 \ . \qquad (4.2.23)$$

The product of B for $V_i$ with B for $V_j$ gives

$$\begin{bmatrix} \underline{B}'_{0,i}\underline{B}_{0,j} & \underline{B}'_{0,i}\underline{B}_{1,j} \\ \underline{B}'_{1,i}\underline{B}_{0,j} & \underline{B}'_{1,i}\underline{B}_{1,j} \end{bmatrix} = s_j 2^{d_j - 1} I_2 \ .$$

Consider now the possibly more complicated case where $2^{d_i} > 2^{d_j}$. When this happens it is still true that $n_{ij} = s_j 2^{d_j}$, but there will not necessarily exist an integer $c_2$ such that

$$n_{ij} = c_2 2^{d_i}, \quad \text{(see Example (4.2.14))}. \qquad (4.2.24)$$

The problem that can arise is that for some of the effects of the $i^{th}$ response $n_{ijxh} \neq n_{ijx\ell}$. Suppose that for effect B of the $i^{th}$ response $n_{ijBh} \neq n_{ijB\ell}$. Effect C on $V_j$ has $n_{jiCh} = n_{jiC\ell}$ due to the fact that only complete fractions on this response have been considered, whereas on the $i^{th}$ response the last fraction is not complete since $c_2$ is not an integer. Thus

$$\begin{bmatrix} \underline{B}'_{0,i} \\ --- \\ \underline{B}'_{1,i} \end{bmatrix} [\underline{C}_{0,j}, \underline{C}_{1,j}] = \frac{1}{2} \begin{bmatrix} n_{ijB\ell} & n_{ijB\ell} \\ & \\ n_{ijBh} & n_{ijBh} \end{bmatrix} .$$

Notice that this can only occur where B is an effect that affects only $V_i$ and not $V_j$. If B also affected $V_j$, then B would necessarily have $n_{jiBh} = n_{jiB\ell}$ necessitating $n_{ijBh} = n_{ijB\ell}$. When effect B on $V_i$ does occur at the high level as often as at the low level then the 2×2 matrix portion of $X_i'Q_{ij}X_j$ associated with B of $V_i$ and C of $V_j$ is $s_j 2^{d_j-2} J_2$, the same matrix as given in equation (4.2.23).

In the previous discussion, it has been assumed that $s_i 2^{d_i} \geq s_j 2^{d_j}$. If response $V_j$ is to be measured more than $V_i$, then, since no restriction was placed on i and j, the subscripts can be reversed and the same derivation is still applicable.

Therefore the matrix $X_i'Q_{ij}X_j$ is a $2k_i \times 2k_j$ matrix partitioned into $k_i \cdot k_j$ submatrices of dimension 2×2. Of these $k_i \cdot k_j$ matrices, $k_{ij}$ are of the form $\frac{1}{2} n_{ij} I_2$, and there are a' rows of $k_j$ matrices that are of the form

$$\frac{1}{2} \begin{bmatrix} n_{ijx\ell} & n_{ijx\ell} \\ & \\ n_{ijxh} & n_{ijxh} \end{bmatrix}$$ where a' is an integer such that

$$0 \leq a' \leq k_i - k_{ij} , \tag{4.2.25}$$

the value of a' is dependent upon the size of the design, the size of the fractions used, and the number of factors affecting $V_i$ but not $V_j$. The remaining matrices are of the form $\frac{1}{4} n_{ij} J_2$.

When $c_1$ is an integer then a' = 0. There can be no more than $k_i - k_{ij}$ effects that influence $V_i$ but not $V_j$. Of these effects denote by a' the number that have $n_{ijxh} \neq n_{ijx\ell}$, with these a' effects generating rows of matrices

$$\frac{1}{2} \begin{bmatrix} n_{ijx\ell} & n_{ijx\ell} \\ n_{ijxh} & n_{ijxh} \end{bmatrix} .$$

In this section we have been trying to determine the general form of $\mathrm{Cov}(\hat{\underline{\tau}}_i, \hat{\underline{\tau}}_j)$ or more basically of $M_i Q_{ij} M_j'$. This was simplified in equation (4.2.12) and (4.2.13) with

$$X_i' Q_{ij} M_j' = X_i' Q_{ij} X_j - X_i' Q_{ij} Z_j (Z_j' Z_j)^- Z_j' X_j$$

and

$$M_i Q_{ij} X_j = X_i' Q_{ij} X_j - X_i' Z_i (Z_i' Z_i)^- Z_i' Q_{ij} X_j .$$

Having just determined the general form of $X_i'Q_{ij}X_j$, we now consider $X_i'Q_{ij}Z_j(Z_j'Z_j)^-Z_j'X_j$ so that for the situation where $2^{d_i} \geq 2^{d_j}$, the general form of $M_iQ_{ij}M_j'$ can be determined. From equation (4.2.4) $Z_j(Z_j'Z_j)^-Z_j'X_j = \frac{1}{2} J_{s_j 2^{d_j} \times 2k_j}$.

Consider first the case where $2^{d_i} \leq 2^{d_j}$; it was previously concluded that for any effect on response i, $n_{ijxh} = n_{ijx\ell}$. Thus each row of $X_i'Q_{ij}$ has $n_{ijxh}$ ones and $n_{ijxh}$ zeros. Therefore

$$X_i'Q_{ij}Z_j(Z_j'Z_j)^-Z_j'X_j = \frac{1}{2} n_{ijxh}J_{2k_i \times 2k_j} = \frac{1}{4} n_{ij}J_{2k_i \times 2k_j} .$$

This will be used in equation (4.2.12) along with equation (4.2.23), to find the partitioned matrix $M_iQ_{ij}M_j'$. Of the $2\times2$ submatrices of $M_iQ_{ij}M_j'$, $k_{ij}$ are of the form $s_j2^{d_j-1}I_2 - s_j2^{d_j-2}J_2$ and all remaining submatrices are $0_{2\times2}$. The rank of $M_iQ_{ij}M_j'$ is $k_{ij}$.

Turning attention now to the situation where $2^{d_i} > 2^{d_j}$, when either $c_2$, as defined in (4.2.24), is an integer or a' in (4.2.25) is equal to zero, then $M_iQ_{ij}M_j'$ is identical to the result found in the preceding paragraph. When however $a' \neq 0$, then the form of $X_iQ_{ij}Z_j(Z_j'Z_j)^-Z_j'X_j$ is different. Suppose now that the $\alpha^{th}$ of the $k_i$ effects on $V_i$ has $n_{ij\alpha h} \neq n_{ij\alpha\ell}$. Then speaking in terms of rows of $2\times2$ matrices, the $\alpha^{th}$ row of $X_i'Q_{ij}Z_j(Z_j'Z_j)^-Z_j'X_j$ will be composed of $k_j$

matrices $\frac{1}{2}\begin{bmatrix} n_{ij\alpha\ell} & n_{ij\alpha\ell} \\ n_{ij\alpha h} & n_{ij\alpha h} \end{bmatrix}$. The same is true for a'-1 other rows. Each remaining row of matrices however will consist of $k_j$ matrices of the form $\frac{1}{4} n_{ij}J_2$. These a' rows of matrices correspond to the same a' rows of matrices in $X_i'Q_{ij}X_j$ and therefore $M_iQ_{ij}M_j'$ will be identical with the situation where $2^{d_i} \leq 2^{d_j}$.

In the preceding discussion it was assumed that $s_i2^{d_i} > s_j2^{d_j}$. If $s_i2^{d_i} \leq s_j2^{d_j}$, a change of subscripts reduces this to the same general case just studied.

This discussion leads to the generalization of the form of $M_iQ_{ij}M_j'$ which will be expressed as

$$M_iQ_{ij}M_j' = \frac{1}{2} n_{ij}D_{ij} \otimes (2I_2 - J_2). \qquad (4.2.26)$$

The $(k_i \times k_j)$ matrix $D_{ij}$ is dependent upon which effects influence $V_i$ and $V_j$. Denote the $k_i$ effects on $V_i$ by $A_1, A_2, \ldots, A_{k_i}$ and denote by $B_1, B_2, \ldots, B_{k_j}$ the $k_j$ effects on $V_j$. Then

$$D_{ij} = \begin{bmatrix} \delta_{A_1B_1} & \cdots & \delta_{A_1B_{k_j}} \\ \vdots & & \\ \delta_{A_{k_i}B_1} & \cdots & \delta_{A_{k_i}B_{k_j}} \end{bmatrix} \qquad (4.2.27)$$

where

$\delta_{A_\alpha B_\gamma}$ is the Kronecker delta defined by

$$\delta_{A_\alpha B_\gamma} = 1 \text{ if the } \alpha^{th} \text{ effect influencing } V_i \text{ is the same as the } \gamma^{th} \text{ effect influencing } V_j,$$

$$\delta_{A_\alpha B_\gamma} = 0 \text{ otherwise,}$$

for $\alpha = 1,\ldots,k_i$ and $\gamma = 1,\ldots,k_j$. Notice that there will be $k_{ij}$ unity elements with the remaining elements being zero such that there will never be more than one unity element in any row or column. Therefore the rank of $D_{ij}$ is $k_{ij}$.

As an example, suppose that $k_1 = 4$; $k_2 = 3$; $V_1$ is influenced only by main effects A, B, D, E; and $V_2$ is affected only by main effects B, C, E. Thus $k_{12} = 2$ and

$$D_{12} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} .$$

As a further example, we refer back to example (4.2.14). In this example $2^{d_1} > 2^{d_2}$ and on the 4 observational units where both responses were measured, the effect B for $V_1$ occurs only at the low level and therefore $n_{12B\ell} = 4$ and $n_{12Bh} = 0$. In this example $a' = 1$, $n_{12} = 4$, $k_1 = 4$, $k_2 = 3$, and $k_{12} = 3$. The third row of $X_1'Q_{12}X_2$, in equation (4.2.15), is therefore $2\underline{j}_6'$ and the fourth row is $\underline{0}_6'$, as are the third and fourth rows of $X_1'Q_{12}Z_2(Z_2'Z_2)^-Z_2'X_2$ in equation (4.2.18).

Thus

$$M_1Q_{12}M_2' = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix} = \frac{1}{4} n_{12} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \otimes (2I_2 - J_2).$$

The covariance between $\hat{\underline{\tau}}_i$ and $\hat{\underline{\tau}}_j$ is

$$\mathrm{Cov}(\hat{\underline{\tau}}_i, \hat{\underline{\tau}}_j) = \sigma_{ij} D_i^- M_i Q_{ij} M_j' D_j^-$$

where $D_\alpha^-$ was found in equation (3.3.12) to be

$$D_\alpha^- = \frac{1}{s_\alpha 2^{d_\alpha - 1}} I_{2k_\alpha} .$$

Thus

$$\mathrm{Cov}(\hat{\underline{\tau}}_i, \hat{\underline{\tau}}_j) = \frac{\sigma_{ij}\, n_{ij}}{s_i 2^{d_i} s_j 2^{d_j}} D_{ij} \otimes (2I_2 - J_2) \qquad (4.2.28)$$

The preceding has been the proof of the following theorem, applicable to a HMGLM $2^v$ factorial experiment with p responses where a $\frac{1}{2}\, f_i$ fraction of a $2^{v_i}$ factorial experiment is repeated $s_i$ times for $V_i$ $(i = 1,\ldots,p)$. Considering each response separately the reduced normal equations $D_i\underline{\tau}_i = \underline{q}_i$ can be solved for $\hat{\underline{\tau}}_i$ adjusted for the mean, block effects, and any main effects or interactions not of interest.

<u>Theorem 4.2.1</u> For the above HMGLM(F) designs

$$\mathrm{Var}(\hat{\underline{\tau}}_i) = \frac{\sigma_{ii}}{s_i 2^{d_i}} I_{k_i} \otimes (2I_2 - J_2)$$

and

$$\mathrm{Cov}(\hat{\underline{\tau}}_i, \hat{\underline{\tau}}_j) = \frac{\sigma_{ij} n_{ij}}{s_i 2^{d_i} s_j 2^{d_j}} D_{ij} \otimes (2I_2 - J_2) \; ,$$

where $D_{ij}$ is defined in equation (4.2.27) $(i,j = 1,\ldots,p)$.

In equation (4.2.1) the determinant criterion was defined to be $\det(\mathrm{Var}(P\hat{\underline{\tau}}))$ where P was a matrix of normalized orthogonal contrast coefficients given by equation (3.2.6) and $\hat{\underline{\tau}}$ was a vector of univariate BLU parameter estimates given in (3.2.4). Using these definitions

$$\mathrm{Var}(P\hat{\underline{\tau}}) = \begin{bmatrix} P_1 \mathrm{Var}(\hat{\underline{\tau}}_1) P_1' & P_1 \mathrm{Cov}(\hat{\underline{\tau}}_1, \hat{\underline{\tau}}_2) P_2' & \cdots & P_1 \mathrm{Cov}(\hat{\underline{\tau}}_1, \hat{\underline{\tau}}_p) P_p' \\ \vdots & \vdots & & \vdots \\ P_p \mathrm{Cov}(\hat{\underline{\tau}}_p, \hat{\underline{\tau}}_1) P_1' & P_p \mathrm{Cov}(\hat{\underline{\tau}}_p, \hat{\underline{\tau}}_2) P_2' & \cdots & P_p \mathrm{Var}(\hat{\underline{\tau}}_p) P_p' \end{bmatrix} \qquad (4.2.29)$$

For the case under study, with each factor occurring at two levels, we have

$$P_i = I_{k_i} \otimes \frac{\sqrt{2}}{2} [1 \quad -1], \quad i = 1,\ldots,p.$$

$$P_i \operatorname{Var}(\hat{\underline{\tau}}_i) P_i' = \frac{2\sigma_{ii}}{s_i 2^{d_i}} I_{k_i} \tag{4.2.30}$$

$$P_i \operatorname{Cov}(\underline{\tau}_i, \underline{\tau}_j) P_j' = \frac{2\sigma_{ij} n_{ij}}{s_i 2^{d_i} s_j 2^{d_j}} D_{ij} \quad . \tag{4.2.31}$$

Therefore

$$\operatorname{Var}(P\hat{\underline{\tau}}) = 2 \begin{bmatrix} \frac{\sigma_{11}}{s_1 2^{d_1}} I_{k_1} & \frac{\sigma_{12} n_{12}}{s_1 2^{d_1} s_2 2^{d_2}} D_{12} & \cdots & \frac{\sigma_{1p} n_{1p}}{s_1 2^{d_1} s_p 2^{d_p}} D_{1p} \\ & \frac{\sigma_{22}}{s_2 2^{d_2}} I_{k_2} & & \frac{\sigma_{2p} n_{2p}}{s_2 2^{d_2} s_p 2^{d_p}} D_{2p} \\ \text{(sym.)} & & \ddots & \vdots \\ & & & \frac{\sigma_{pp}}{s_p 2^{d_p}} I_{k_p} \end{bmatrix}$$

(4.2.32)

The reason for assuming that blocks coincided was so that the discussion of $\mathrm{Cov}(\hat{\underline{\tau}}_i, \hat{\underline{\tau}}_j)$ would be easier to understand. By requiring the blocks to 'line up', the comparative fraction sizes of the two responses can be used to determine the different situations that can occur when finding the general form of $M_i Q_{ij} M_j'$. Even without the assumption, the general form of $M_i Q_{ij} M_j'$ is the same as was found before, equation (4.2.26), as long as the design is kept 'balanced'. Let E denote some effect influencing $V_i$ but not $V_j$. The design will be 'balanced' as long as both levels on each effect of $V_j$ appear with the low level of E an equal number of times, even if $n_{ijEh} \neq n_{ijE\ell}$. (This implies that both levels of each effect of $V_j$ will also appear at the high level of E an equal number of times.) Thus as long as care is taken to make sure that the treatment combinations are chosen so that terms occurring in one response but not the other are not aliased, then the assumption about blocks coinciding is not needed.

## 4.3 Optimal Designs for p Responses

In this section some theorems will be proven giving conditions under which optimal experimental designs can be found. We consider the general p-variate multiresponse $2^v$ factorial experiment, and show that under certain limitations the design can be found that is optimal, subject to the determinant criterion and a cost constraint. In Chapter 5, some general results are obtained for the situation where there are only two responses (p=2).

Suppose we have v factors, each at two levels, and p responses possibly having different design matrices. Assume the $i^{th}$ response ($i = 1,\dots,p$) is affected by $v_i$ factors ($v_i \le v$) and that on $V_i$ the experimenter is interested in studying contrasts for $k_i$ effects. The optimal design will consist of $s_i$ blocks of a $1/2^{f_i}$ fraction of a $2^{v_i}$ factorial experiment.

Because the general form of the determinant of a HMGLM design is usually difficult to attain, we will consider a different function, f, of the values $s_i 2^{d_i}$. Some theorems will be proven that will allow us to solve for the design that is optimum with respect to maximizing f subject to a cost constraint. For some specific p-variate situations the reciprocal of $\det(\mathrm{Var}(P\hat{\underline{\tau}}))$ can be shown to be a function of f. Therefore in these situations maximization of f corresponds to minimization of $\det(\mathrm{Var}(P\hat{\underline{\tau}}))$ and the optimum MGLM design can thus be determined.

Consider finding a design, subject to a cost constraint, that maximizes the function

$$f = (s_1 2^{d_1})^{k_1} (s_2 2^{d_2})^{k_2} \dots (s_p 2^{d_p})^{k_p} ,$$

with respect to $s_1, s_2, \ldots, s_p$. Because f is a function of only $s_1 2^{d_1}, \ldots, s_p 2^{d_p}$ then by use of Lemma 3.4.1, the subclass of HMGLM(F) designs is complete with respect to the class of MGLM(F) designs when one is considering finding the design that maximizes f. Therefore the search for an optimal design can be restricted to the subclass of HMGLM(F) designs.

Definition 4.3.1 The response $V_\gamma$ is called the Most Frequently Observed Response (MFOR) if $\gamma$ is the smallest integer, $1 \leq \gamma \leq p$, for which

$$s_\gamma 2^{d_\gamma} = \max(s_1 2^{d_1}, \ldots, s_p 2^{d_p}) .$$

Suppose the responses are ordered as follows

$$\psi_1/k_1 \leq \psi_2/k_2 \leq \cdots \leq \psi_p/k_p \tag{4.3.1}$$

where $\psi_i$ is the cost of measuring the $i^{th}$ response on any experimental unit.

Lemma 4.3.1 If $m_1, m_2, \ldots, m_p$ denotes the values $s_1, \ldots, s_p$ which minimize

$$f = (s_1 2^{d_1})^{k_1} \cdots (s_p 2^{d_p})^{k_p} \tag{4.3.2}$$

subject to the cost constraint

$$\psi' = \psi_0 m_0 + \psi_1 m_1 2^{d_1} + \ldots + \psi_p 2^{d_p} \qquad (4.3.3)$$

where $m_0 = \max(m_1 2^{d_1}, \ldots, m_p 2^{d_p})$, then

$$m_1 2^{d_1} \geq m_2 2^{d_2} \geq \ldots \geq m_p 2^{d_p} .$$

Proof: Due to the completeness of the subclass of HMGLM(F) designs, only these designs will be considered and therefore $m_0 = m_\gamma 2^{d_\gamma}$ where $V_\gamma$ is the MFOR. Define

$$Y_i = \psi_0 + \psi_i \quad \text{if } i = \gamma,$$

$$Y_i = \psi_i \qquad \text{otherwise } (i = 1, \ldots, p).$$

The cost constraint can now be written

$$\psi' = Y_1 m_1 2^{d_1} + \ldots + Y_p m_p 2^{d_p} . \qquad (4.3.4)$$

The method of La Grange is used to find the maximum of

$$L = (m_1 2^{d_1})^{k_1} \ldots (m_p 2^{d_p})^{k_p} + \lambda (Y_1 m_1 2^{d_1} + \ldots + Y_p m_p 2^{d_p} - \psi')$$

with respect to the $m_i$, i.e., the maximum of f subject to (4.3.4). For $V_i$ and $V_{i+1}$, $\frac{\partial L}{\partial m_i}$ and $\frac{\partial L}{\partial m_{i+1}}$ are found to be

$$\frac{\partial L}{\partial m_i} = k_i 2^{d_i}(m_1 2^{d_1})^{k_1} \cdots (m_i 2^{d_i})^{k_i - 1} \cdots (m_p 2^{d_p})^{k_p} + 2^{d_i} Y_i \lambda$$

(4.3.5a)

$$\frac{\partial L}{\partial m_{i+1}} = k_{i+1} 2^{d_{i+1}}(m_1 2^{d_1})^{k_1} \cdots (m_i 2^{d_i})^{k_i} (m_{i+1} 2^{d_{i+1}})^{k_{i+1} - 1} \cdots$$

$$(m_p 2^{d_p})^{k_p} + 2^{d_{i+1}} Y_{i+1} \lambda \qquad (4.3.5b)$$

for $i = 1,2,\ldots,p-1$. Setting both equations equal to zero, solving for $\lambda$ in (4.3.5a), substituting this $\lambda$ into (4.3.5b), and finally solving for $m_i$ yields

$$m_i = \frac{Y_{i+1}/k_{i+1}}{Y_i/k_i} 2^{d_{i+1} - d_i} m_{i+1} \quad . \qquad (4.3.6)$$

Assume that

$$m_{i+1} 2^{d_{i+1}} > m_i 2^{d_i} \quad . \qquad (4.3.7)$$

For equation (4.3.6) this would imply that

$$c = \frac{Y_{i+1}/k_{i+1}}{Y_i/k_i} \qquad (4.3.8)$$

is less than 1. If $V_{i+1}$ is not the MFOR then $c = \dfrac{\psi_{i+1}/k_{i+1}}{\psi_i/k_i}$ and it is not possible that $c < 1$ from the way the responses were originally numbered in equation (4.3.1). For the case where $V_{i+1}$ is the MFOR then

$$c = \frac{\psi_0/k_{i+1} + \psi_{i+1}/k_{i+1}}{\psi_i/k_i} \quad .$$

Since $\psi_0 \geq 0$, it is again impossible that $c < 1$. This is a contradiction to equation (4.3.7), and thus $m_i 2^{d_i} \geq m_{i+1} 2^{d_{i+1}}$. Since this holds for every i, it follows then that

$$m_1 2^{d_1} \geq m_2 2^{d_2} \geq \ldots \geq m_p 2^{d_p} \; .$$

This completes the proof.

Lemma 4.3.2 For the responses ordered as in equation (4.3.1), let b denote the first integer such that

$$\psi_{b-1}/k_{b-1} \leq \psi^*_{b-2}/k^*_{b-2} \; , \tag{4.3.9a}$$

and

$$\psi_b/k_b > \psi^*_{b-1}/k^*_{b-1} \; , \tag{4.3.9b}$$

where

$2 \leq b \leq p+1$,

$\psi^*_i = \psi_0 + \psi_1 + \ldots + \psi_i$ , and

$k^*_i = k_1 + k_2 + \ldots + k_i \quad (i = 1,\ldots,p)$ .

Then the values of $m_1 2^{d_1}, \ldots, m_p 2^{d_p}$ that maximize $f = (m_1 2^{d_1})^{k_1} \ldots (m_p 2^{d_p})^{k_p}$ subject to the cost constraint (4.3.3) have the following property:

$$m_1 2^{d_1} = \ldots = m_{b-1} 2^{d_{b-1}} > m_b 2^{d_b} \geq \ldots \geq m_p 2^{d_p} .$$

When b = 2, ignore inequality (4.3.9a) and when inequality (4.3.9a) is still satisfied at b = p+1 then

$$m_1 2^{d_1} = m_2 2^{d_2} = \ldots = m_p 2^{d_p} .$$

Proof: Inequality (4.3.9a) is equivalent to

$$\psi^*_{b-2} \geq k^*_{b-2} \left(\frac{\psi_{b-1}}{k_{b-1}}\right)$$

or

$$\psi^*_{b-3} + \psi_{b-2} \geq k^*_{b-3} \left(\frac{\psi_{b-1}}{k_{b-1}}\right) + k_{b-2} \left(\frac{\psi_{b-1}}{k_{b-1}}\right) . \qquad (4.3.10)$$

From equation (4.3.1) $k_{b-2} \frac{\psi_{b-1}}{k_{b-1}} \geq \psi_{b-2}$. Applying this to inequality (4.3.10) gives

$$\frac{\psi^*_{b-3}}{k^*_{b-3}} \geq \frac{\psi_{b-2}}{k_{b-2}} .$$

Following this same line of reasoning, the following is determined:

$$\frac{\psi_i^*}{k_i^*} \geq \frac{\psi_{i+1}}{k_{i+1}} \text{ , for } i = 1,\ldots,b-2 \text{ .} \tag{4.3.11}$$

Assume that

$$m_1 2^{d_1} > m_2 2^{d_2} \tag{4.3.12}$$

and thus equations (4.3.7) and (4.3.8) imply that

$$c = \frac{\psi_2/k_2}{\psi_0/k_1 + \psi_1/k_1} > 1 \text{ ,}$$

since $V_1$ is the MFOR. The fact that $c > 1$ implies that $\psi_2/k_2 > \psi_1^*/k_1$; however this cannot be true by virtue of inequality (4.3.11). Therefore by contradiction of (4.3.12)

$$m_1 2^{d_1} = m_2 2^{d_2} \text{ .}$$

Since $m_1 2^{d_1} = m_2 2^{d_2}$ then assume that

$$m_1 2^{d_1} > m_3 2^{d_3} \text{ .} \tag{4.3.13}$$

LaGrangian multipliers are again used, giving

$$L = (m_1 2^{d_1})^{k_1+k_2}(m_3 2^{d_3})^{k_3} \ldots (m_p 2^{d_p})^{k_p}$$

$$+ \lambda(m_1 2^{d_1}\psi_2^* + m_3 2^{d_3}\psi_3 + \ldots + m_p 2^{d_p}\psi_p - \psi')$$

to be maximized with respect to $m_1, m_3, m_4, \ldots, m_p$.

$$\frac{\partial L}{\partial m_1} = (k_1+k_2)2^{d_1}(m_1 2^{d_1})^{k_1+k_2-1}(m_3 2^{d_3})^{k_3} \ldots (m_p 2^{d_p})^{k_p} + \lambda 2^{d_1}\psi_2^* \tag{4.3.14a}$$

$$\frac{\partial L}{\partial m_3} = k_3 2^{d_3}(m_1 2^{d_1})^{k_1+k_2}(m_3 2^{d_3})^{k_3-1} \ldots (m_p 2^{d_p})^{k_p} + \lambda 2^{d_3}\psi_3 . \tag{4.3.14b}$$

Setting these equations equal to zero, solving for $\lambda$ in (4.3.14a), and substituting this $\lambda$ into (4.3.14b), give the following:

$$m_1 = \frac{\psi_3/k_3}{\psi_2^*/k_2^*} 2^{d_3-d_1} m_3 .$$

For inequality (4.3.13) to be satisfied, then $\psi_3/k_3 > \psi_2^*/k_2^*$ which cannot be true because of inequality (4.3.11). Thus by contradiction, it is concluded that $m_1 2^{d_1} = m_3 2^{d_3}$.

This line of reasoning can be continued until it is found that $m_1 2^{d_1} = m_{b-1} 2^{d_{b-1}}$. When the relationship between $m_1 2^{d_1}$ and $m_b 2^{d_b}$ is considered, because of inequality (4.3.9b), we determine $m_1 2^{d_1} > m_b 2^{d_b}$. Therefore

$$m_1 2^{d_1} = \ldots = m_{b-1} 2^{d_{b-1}} > m_b 2^{d_b} \geq \ldots \geq m_p 2^{d_p} .$$

This completes the proof.

Lemma 4.3.1 and 4.3.2 allow the experimenter to find the HMGLM(F) design that maximizes the function f subject to the cost constraint (4.3.3). They are helpful in finding the optimal design for certain situations when the determinant can be expressed as a function of f. These cases will be considered next.

Consider the case where the responses are uncorrelated, i.e., $\sigma_{ij} = 0$ $(i \neq j,\ i,j = 1,\ldots,p)$. Then from equation (4.2.32)

$$\mathrm{Var}(\hat{P\underline{\tau}}) = 2 \begin{bmatrix} \frac{\sigma_{11}}{s_1 2^{d_1}} I_{k_1} & 0 & \cdots & 0 \\ 0 & \frac{\sigma_{22}}{s_2 2^{d_2}} I_{k_2} & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & 0 \cdots & \frac{\sigma_{pp}}{s_p 2^{d_p}} I_{k_p} \end{bmatrix}_{k_p^* \times k_p^*} .$$

For this MGLM(F) design D(M), the determinant is given by

$$|D(M)| = |\mathrm{Var}(\hat{P\underline{\tau}})| = 2^{k_p^*} \sigma_{11}^{k_1} \cdots \sigma_{pp}^{k_p} \frac{1}{(s_1 2^{d_1})^{k_1} \cdots (s_p 2^{d_p})^{k_p}} \tag{4.3.15}$$

Theorem 4.3.3 If the responses $V_1,\ldots,V_p$ are uncorrelated, then the subclass of HMGLM(F) designs is complete (in reference to the determinant criterion) with respect to the class of MGLM(F) designs.

Proof: For an MGLM(F) design D', if $\sigma_{ij} = 0$ $(i \neq j,\ i,j = 1,\ldots,p)$ then $|D(M)|$ is given by equation (4.3.15). $|D(M)|$ is minimized when $(s_1 2^{d_1})^{k_1} \ldots (s_p 2^{d_p})^{k_p}$ is maximized. From Lemmas 3.3.1 and 4.3.1 $|D(M)|$ is minimized when using a HMGLM(F) design. This completes the proof.

Consequently in the search for an optimal design, when the responses are uncorrelated, only the HMGLM(F) designs should be considered. Denote by $m_1,\ldots,m_p$, the values $s_1,\ldots,s_p$ for the optimal HMGLM(F) design.

Lemma 4.3.4 If the responses are uncorrelated and ordered as in inequality (4.3.1), and b denotes the first integer $(2 \leq b \leq p+1)$ such that

$$\frac{\psi_{b-1}}{k_{b-1}} \leq \frac{\psi^*_{b-2}}{k^*_{b-2}} \tag{4.3.16a}$$

and

$$\frac{\psi_b}{k_b} > \frac{\psi^*_{b-1}}{k^*_{b-1}} \tag{4.3.16b}$$

then

$$m_1 2^{d_1} = \ldots = m_{b-1} 2^{d_{b-1}} > m_b 2^{d_b} \geq \ldots \geq m_p 2^{d_p} \; . \qquad (4.3.17)$$

When b = 2 ignore inequality (4.3.16a) and when inequality (4.3.16a) is still satisfied when b = p+1 then

$$m_1 2^{d_1} = \ldots = m_p 2^{d_p} \; .$$

Proof: Since maximizing f in equation (4.3.15) minimizes $|D(M)|$, then Lemma 4.3.2 can be applied giving equation (4.3.17). This completes the proof.

<u>Theorem 4.3.5</u> If Lemma 4.3.4 is satisfied with b being the smallest integer that satisfies inequalities (4.3.16a) and (4.3.16b) then the $m_i$ values for the optimum HMGLM(F) design are given by

$$m_i = \left(\frac{\psi'}{k_p^*}\right)\left(\frac{\psi_{b-1}^*}{k_{b-1}^*}\right)^{-1} 2^{-d_i} \; , \text{ for } i = 1,\ldots,b-1 \; , \qquad (4.3.18)$$

and

$$m_j = \frac{\psi'}{\psi_j}\, \frac{k_j}{k_p^*}\, 2^{-d_j} \; , \text{ for } j = b,\ldots,p \; , \qquad (4.3.19)$$

and

$$m_0 = m_1 2^{d_1} \; .$$

Proof: From Lemma 4.3.4, $m_1 2^{d_1} = \ldots = m_{b-1} 2^{d_{b-1}}$. Minimization of $|D(M)|$ is equivalent to maximizing $f = (m_1 2^{d_1})^{k^*_{b-1}} (m_b 2^{d_b})^{k_b} \ldots (m_p 2^{d_p})^{k_p}$. Use of the method of LaGrangian multipliers to maximize f subject to the cost constraint

$$\psi' = \psi^*_{b-1} m_1 2^{d_1} + \sum_{i=b}^{p} \psi_i m_i 2^{d_i}$$

gives

$$L = (m_1 2^{d_1})^{k^*_{b-1}} (m_b 2^{d_b})^{k_b} \ldots (m_p 2^{d_p})^{k_p}$$
$$+ \lambda (\psi^*_{b-1} m_1 2^{d_1} + \sum_{i=b}^{p} \psi_i m_i 2^{d_i} - \psi') .$$

The partial derivatives of L are

$$\frac{\partial L}{\partial m_1} = k^*_{b-1} 2^{d_1} (m_1 2^{d_1})^{k^*_{b-1}-1} (m_b 2^{d_b})^{k_b} \ldots (m_p 2^{d_p})^{k_p} + \lambda \psi^*_{b-1} 2^{d_1} \tag{4.3.20a}$$

$$\frac{\partial L}{\partial m_i} = k_i 2^{d_i} (m_1 2^{d_1})^{k^*_{b-1}} (m_b 2^{d_b})^{k_b} \ldots (m_i 2^{d_i})^{k_i - 1} \ldots$$
$$(m_p 2^{d_p})^{k_p} + \lambda \psi_i 2^{d_i} \quad \text{for } i = b, \ldots, p , \tag{4.3.20b}$$

$$\frac{\partial L}{\partial \lambda} = \psi^*_{b-1} m_1 2^{d_1} + \sum_{i=b}^{p} \psi_i m_i 2^{d_i} - \psi' . \tag{4.3.20c}$$

Setting these equations equal to zero, solving for in equation (4.3.20a) and substituting into (4.3.20b) yields

$$m_i = \frac{\psi^*_{b-1}/k^*_{b-1}}{\psi_i/k_i}\, m_1 2^{d_1-d_i} \; . \qquad (4.3.21)$$

Using this in equation (4.3.20c) gives

$$\psi' = \psi^*_{b-1} m_1 2^{d_1} + \sum_{i=b}^{p} \psi_i \frac{\psi^*_{b-1}}{k^*_{b-1}} \frac{k_i}{\psi_i}\, m_1 2^{d_1}$$

$$\psi' = m_1 2^{d_1} \frac{\psi^*_{b-1}}{k^*_{b-1}} [k^*_{b-1} + \sum_{i=b}^{p} k_i] \; .$$

Therefore

$$m_1 = \frac{\psi'}{k^*_p} \left(\frac{\psi^*_{b-1}}{k^*_{b-1}}\right)^{-1} 2^{-d_1} \; , \qquad (4.3.22)$$

or since $m_1 2^{d_1} = \ldots = m_{b-1} 2^{d_{b-1}}$

$$m_j = \frac{\psi'}{k^*_p} \left(\frac{\psi^*_{b-1}}{k^*_{b-1}}\right)^{-1} 2^{-d_j} \text{ for } j = 1,\ldots,b-1 \; .$$

From Theorem 4.3.3, the optimum design will be a HMGLM(F) design, therefore $m_0 = m_1 2^{d_1}$. Substituting equation (4.3.22) into equation (4.3.21) gives equation (4.3.19). This completes the proof.

We now consider an example to illustrate how the optimum design is found under the determinant criterion for a situation with uncorrelated responses.

Example 4.3.1 Assume that a situation with uncorrelated responses is determined by the following parameters: $p = 3$, $v = 4$, $v_1 = 4$, $v_2 = 3$, $v_3 = 4$, $f_1 = f_2 = f_3 = 1$, $k_1 = 4$, $k_2 = 3$, $k_3 = 4$, $\sigma_{11} = 25$, $\sigma_{22} = 25$, $\sigma_{33} = 20$, $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0$, $\psi' = 1100$, $\psi_0 = 3$, $\psi_1 = 2$, $\psi_2 = 3$, $\psi_3 = 12$. The responses have been numbered so that inequality (4.3.1) is satisfied and therefore Lemma 4.3.1 is satisfied, i.e., $s_1 2^3 \geq s_2 2^2 \geq s_3 2^3$. From Lemma 4.3.4, $b = 3$ since

$$\psi_3/k_3 > \psi_2^*/k_2^* \quad (3 > \tfrac{8}{7})$$

while

$$\psi_2/k_2 \leq \psi_1^*/k_1^* \quad (\tfrac{3}{3} \leq \tfrac{5}{4})$$

and therefore

$$8s_1 = 4s_2 > 8s_3 \ .$$

From Theorem 4.3.5

$$s_1 = \frac{1100}{8} \left(\frac{7}{11}\right) 2^{-3} = 10.94 \ ,$$

$$s_2 = 21.87 \ ,$$

$$s_3 = \frac{1100}{12} \left(\frac{4}{11}\right) 2^{-3} = 4.17 \ .$$

Using the program in the appendix to calculate the best design after rounding off we find that the best admissible (cost $\leq \psi'$) integer design has $s_1 = 11$, $s_2 = 22$, and $s_3 = 5$.

Thus when the responses are uncorrelated, the exact design can be found that is optimum with respect to the determinant criterion and a cost constraint.

Consider a situation where each response is affected only by factors which do not affect any other response, i.e., all $k_{ij} = 0$ $(i \neq j,\ i,j = 1,\ldots,p)$. Since $D_{ij}$ has $k_{ij}$ unity elements and the rest zeros, then for this case $D_{ij}$ is a matrix of zeros. Thus $\mathrm{Var}(P\hat{\underline{\tau}})$ for this situation is the same as for the case of uncorrelated responses, and $\det(\mathrm{Var}(P\hat{\underline{\tau}}))$ is given by equation (4.3.15). Theorems 4.3.3 and 4.3.5 and Lemma 4.3.4 are therefore applicable.

Another case will next be considered where $\det(\mathrm{Var}(P\hat{\underline{\tau}}))$ is a function of f. Therefore Lemmas 4.3.1 and 4.3.2 are necessary for the proof of a theorem which defines the optimal design. Some preliminaries must be taken care of first, before the theorem is proven. Consider the MDM(F) design with $s_1 2^{d_1} = \ldots = s_p 2^{d_p} = m$ and, because it is an MDM design, $n_{ij} = m$ $(i = 1,\ldots,p)$. For this design, denote by D(MD) the following matrix

$$\mathrm{Var}(P\hat{\underline{\tau}}) = \frac{2}{m}\begin{bmatrix} \sigma_{11}I_{k_2} & \sigma_{12}D_{12} & \cdots & \sigma_{1p}D_{1p} \\ \sigma_{12}D_{21} & \sigma_{22}I_{k_2} & & \sigma_{2p}D_{2p} \\ \vdots & & \ddots & \vdots \\ \sigma_{1p}D_{p1} & \sigma_{2p}D_{p2} & \cdots & \sigma_{pp}I_{k_p} \end{bmatrix} . \tag{4.3.23}$$

The theorem to be proven does not apply to designs as general as the MGLM(F) design, but does apply to a type of designs that are not so restrictive as the HMGLM(F) designs. This type of design is defined as follows:

<u>Definition 4.3.1</u> A Restricted More General Linear Multi-response RMGLM(F) design is a MGLM(F) design with $n_0$ total experimental units and with the $i^{th}$ response measured on $s_i$ groups of $2^{d_i}$ units where for convenience it is assumed (without loss of generality) that the responses are ordered so that

$$s_1 2^{d_1} \geq s_2 2^{d_2} \geq \cdots \geq s_p 2^{d_p} .$$

The RMGLM(F) design also satisfies the following condition: For any two responses $V_i$ and $V_j$ where $i < j$ ($i = 1,\ldots,p-1$ and $j = i+1,\ldots,p$), the number of units on which both $V_i$ and

$V_j$ are measured, $n_{ij}$, is $r_{ij}$ groups of $2^{d_j}$ units where $0 \leq r_{ij} \leq s_j$. The remaining $(s_j - r_{ij})$ groups of $2^{d_j}$ units are measured on experimental units where $V_i$ is not measured.

An illustration might aid in the understanding of a RMGLM(F) design. Suppose $p = 3$, $d_i = 2$ $(i = 1,2,3)$, and $s_1 = 3$, $s_2 = s_3 = 2$. Letting * represent the fact that a response was measured on this experimental unit, consider the following two examples:

```
   RMGLM(F)              MGLM(F)  (but not RMGLM(F))

  V1  V2  V3             V1  V2  V3
  *   *                  *   *
  *   *                  *   *
  *   *                  *   *
  *   *                  *   *
 _   _   _   _          _   _   _   _
  *       *              *       *
  *       *              *       *
  *       *              *       *
  *       *              *       *
 _   _   _   _          _   _   _   _
  *                      *
  *                      *
  *                      *   *
  *                      *   *
 _   _   _   _          _   _   _   _
      *   *                  *   *
      *   *                  *   *
      *   *                      *
      *   *                      *
```

In both examples $n_0 = 16$, with $n_{12} = n_{13} = n_{23} = 4 = (1 \cdot 2^2)$ for the RMGLM(F) design, but for the MGLM(F) design $n_{12} = 6$ and $n_{23} = 2$, neither of which can be expressed in the form $n_{ij} = r\ 2^2$ for an integer r.

The class of RMGLM(F) designs are a subclass of MGLM(F) designs. The restriction on the MGLM(F) design is that the $(s_j - r_{ij})2^{d_j}$ units, where $V_j$ but not $V_i$ is measured, must be $(s_j - r_{ij})$ block (or groups) of fractional factorials of $2^{d_j}$ units and cannot be $(s_j - r_{ij})2^{d_j}$ individual experimental units. Denote by j' the smallest integer $(1 \leq j' \leq p)$ such that $d_{j'} = \min(d_1, \ldots, d_p)$. For a RMGLM(F) design there will exist an integer $s_0$ such that $n_0 = s_0 2^{d_{j'}}$.

HMGLM(F) designs and thus also MDM(F) designs are subclasses of RMGLM(F) designs. For a RMGLM(F) design to be a HMGLM(F) design, $r_{ij} = s_j$ $(i < j)$ and $s_0 = s_1 2^{d_1 - d_{j'}}$.

The following definition will be needed to prove the next theorem.

<u>Definition 4.3.2</u> If A $(\{a_{ij}\})$ and B $(\{b_{ij}\})$ are real $n \times n'$ matrices then the Hadamard product $A*B$ is the $n \times n'$ real matrix whose (i,j) element is $a_{ij} b_{ij}$.

For a RMGLM(F) design with $n_0$ total units and $V_i$ measured on $s_i 2^{d_i}$ units $(i = 1, \ldots, p)$, the matrix $\mathrm{Var}(P\underline{\hat{\tau}})$ will be denoted by D(R), and for a HMGLM(F) design denote the matrix $\mathrm{Var}(P\underline{\hat{\tau}})$ by D(H). The matrices D(H) and D(R) will be very similar in form since both designs are concerned with replicates of complete fractional factorial experiments of $2^{d_i}$ units. The partitioned matrices $\mathrm{Var}(P_i \underline{\hat{\tau}}_i)$ will be the

the same for both designs since $V_i$ is measured on $s_i 2^{d_i}$ units on both designs. The matrices $\mathrm{Cov}(P_i\hat{\underline{\tau}}_i, P_j\hat{\underline{\tau}}_j)$ (for $i < j$) will have the same basic form with possibly different coefficients since $n_{ij} = s_j 2^{d_j}$ for the HMGLM(F) design and in the RMGLM(F) design $n_{ij} = r_{ij} 2^{d_j}$ ($r_{ij} \leq s_{ij}$). For the RMGLM(F) design

$$\mathrm{Cov}(P_i\hat{\underline{\tau}}_i, P_j\hat{\underline{\tau}}_j) = \frac{2n_{ij}}{s_i 2^{d_i} s_j 2^{d_j}} D_{ij} = \frac{2r_{ij} 2^{d_j}}{s_i 2^{d_i} s_j 2^{d_j}} D_{ij} \quad .$$

D(R) can be expressed as the Hadamard product

$$D(R) = 2(N^*\Delta) \qquad (4.3.24)$$

where

$$N = \begin{bmatrix} \frac{1}{s_1 2^{d_1}} J_{k_1} & \frac{n_{12}}{s_1 2^{d_1} s_2 2^{d_2}} J_{k_1,k_2} \cdots & \frac{n_{1p}}{s_1 2^{d_1} s_p 2^{d_p}} J_{k_1,k_p} \\ \vdots & \vdots & \vdots \\ \frac{n_{1p}}{s_1 2^{d_1} s_p 2^{d_p}} J_{k_p,k_1} & \frac{n_{2p}}{s_2 2^{d_2} s_p 2^{d_p}} J_{k_p,k_1} \cdots & \frac{1}{s_p 2^{d_p}} J_{k_p} \end{bmatrix} \qquad (4.3.25)$$

and

$$\Delta = \begin{bmatrix} \sigma_{11}I_{k_1} & \sigma_{12}D_{12} & \cdots & \sigma_{1p}D_{1p} \\ \vdots & \vdots & & \vdots \\ \sigma_{1p}D_{p1} & \sigma_{2p}D_{p2} & \cdots & \sigma_{pp}I_{k_p} \end{bmatrix} . \quad (4.3.26)$$

<u>Theorem 4.3.6</u> If $\frac{\psi_p}{k_p} \leq \frac{\psi^*_{p-1}}{k^*_{p-1}}$, then for the class of RMGLM(F) designs, the optimal design with respect to the determinant criterion and a cost constraint is the MDM(F) design with $s_i = \frac{\psi'}{\psi^*_p} 2^{-d_i}$ $(i = 1,\ldots,p)$.

Proof: For the MDM(F) design, the determinant of $\mathrm{Var}(P\hat{\underline{\tau}})$, equation (4.3.24), is given as follows

$$|D(MD)| = 2^{k^*_p} m^{-k^*_p} |\Delta|$$

where $\Delta$ is given in equation (4.3.26).

For the RMGLM(F) design, the determinant of $\mathrm{Var}(P\hat{\underline{\tau}})$, equation (4.3.24), is given as

$$|D(R)| = 2^{k^*_p} |(N^*\Delta)| .$$

Since N and $\Delta$ are both non-negative symmetric matrices with N being a singular matrix, then by use of Theorem 4 (Appendix) the following inequality holds:

$$|N^*\Delta| \geq (s_1 2^{d_1})^{-k_1} \ldots (s_p 2^{d_p})^{-k_p} |\Delta| \, .$$

Consider now the difference between the determinants of the two designs:

$$|D(R)|-|D(MD)| \geq 2^{k_p^*}|\Delta|\left(\frac{1}{(s_1 2^{d_1})^{k_1}\ldots(s_p 2^{d_p})^{k_p}} - \frac{1}{m^{k_p^*}}\right) .$$

Since $\Delta$ is a positive definite variance-covariance matrix, then the difference $|D(R)| - |D(MD)| \geq 0$ if and only if:

$$\frac{1}{(s_1 2^{d_1})^{k_1}\ldots(s_p 2^{d_p})^{k_p}} - \frac{1}{m^{k_p^*}} \geq 0 \, . \qquad (4.3.27)$$

Because $\frac{\psi_p}{k_p} \leq \frac{\psi_{p-1}^*}{k_{p-1}^*}$ , then from Lemma 4.3.2 the values $s_1^*,\ldots,s_p^*$ that maximize $f = \prod_{i=1}^{p} (s_i 2^{d_i})^{k_i}$ are $s_1 2^{d_1} = \ldots = s_p 2^{d_p} = m$ and therefore $m^{k_p^*} \geq (s_1 2^{d_1})^{k_1}\ldots(s_p 2^{d_p})^{k_p}$. Thus $|D(R)| - |D(MD)| \geq 0$ and the optimal RMGLM(F) design is the MDM(F) design.

The cost function for the MDM(F) design is given by $\psi' = m(\psi_0 + \psi_1 +\ldots+ \psi_p)$ and therefore

$$s_i = \frac{\psi'}{\psi_p^*} 2^{-d_i} \quad (i = 1,\ldots,p) \, .$$

This completes the proof.

This theorem illustrates an intuitive principle that was also true for the trace criterion. When searching for the design that is optimum with respect to the determinant criterion, if the set-up cost, $\psi_0$, is large in relation to the response measurement costs, $\psi_1,\psi_2,\ldots,\psi_p$, then the MDM(F) design is better than a HMGLM(F) design or a RMGLM(F) design.

# CHAPTER V

## OPTIMIZATION WITH RESPECT TO THE DETERMINANT CRITERION: SOME GENERAL RESULTS FOR TWO RESPONSES

### 5.1 Introduction

In Chapter 4, attention centered on trying to find the optimal design with respect to the determinant criterion for a multiple design situation with p responses. Due to the difficulty in attaining the general form of the determinant of $\mathrm{Var}(P\hat{\underline{\tau}})$, it has not yet been possible to justify reducing the search for the optimal design from the class of MGLM designs to the subclass of HMGLM designs. This reduction could be done for the trace criterion in Chapter 3 because it was shown that the class of HMGLM designs was complete with respect to the MGLM designs.

In this chapter the 2-response case will be studied for more general situations than were considered in Chapter 4. The true form of the determinant can be found, and it will therefore be possible to compare different designs to find the optimal designs. It is hoped that this work concerning only two responses will give some insight into the extension to a case for p (> 2) responses. In this chapter the subclass RMGLM(F) designs, of the class of MGLM designs will be considered. In Chapter 6, attention will be given to the more general class of MGLM(F) designs.

The general form of the determinant for the HMGLM(F) designs will first be determined, and then after comparison of this form to the determinant of the RMGLM(F) design, the subclass of HMGLM(F) designs can be shown to be complete with respect to the class of RMGLM(F) designs (Sections 5.2 and 5.3). The optimal RMGLM(F) design will therefore be either a HMGLM or MDM design (the MDM design being a subclass of HMGLM designs).

The general form of the optimal HMGLM design is then determined where the MFOR can be either $V_1$ or $V_2$ (Section 5.4). It is shown in Section 5.5 that as long as the variables are ordered so that $\psi_1/k_1 \leq \psi_2/k_2$ then $V_1$ must be the MFOR. Two critical values are discovered when trying to determine the optimal design. One is shown to give a local maximum, the other a local minimum. Since we wish to minimize the determinant of $\text{Var}(P\hat{\underline{\tau}})$ we need only compare this value to the determinant of the appropriate MDM design with the minimum of these two being the optimum RMGLM(F) design (Sections 5.6, 5.7, 5.8).

Two computer programs that are used in this chapter are reviewed in Section 5.9. One program determines the optimal RMGLM(F) design, while the other program determines the best integer design.

## 5.2 The General Form of the Determinant of RMGLM(F) Designs

In this section for 2 responses the general form of the determinant of $\mathrm{Var}(P\hat{\underline{\tau}})$ will be determined. Consider a RMGLM(F) design which from equation (4.2.32) for p = 2 is given by

$$\mathrm{Var}(P\hat{\underline{\tau}}) = D(R) = 2\begin{bmatrix} \dfrac{\sigma_{11}}{s_1 2^{d_1}} I_{k_1} & \dfrac{\sigma_{12} n_{12}}{s_1 2^{d_1} s_2 2^{d_2}} D_{12} \\ & \\ \dfrac{\sigma_{12} n_{12}}{s_1 2^{d_1} s_2 2^{d_2}} D_{21} & \dfrac{\sigma_{22}}{s_2 2^{d_2}} I_{k_2} \end{bmatrix} . \tag{5.2.1}$$

This matrix holds for the RMGLM(F), HMGLM(F), and MDM(F) designs (with different $s_1$, $s_2$, and $n_{12}$ values), but is not the matrix for a general MGLM(F) design. In order to find and express $|\mathrm{Var}(P\hat{\underline{\tau}})|$ in a suitable form, we make use of the following

Theorem 5.2.1 (Graybill (1969)) Let B be an n×n matrix that is partitioned as follows:

$$B = \left[\begin{array}{c|c} B_{11} & B_{12} \\ \hline B_{21} & B_{22} \end{array}\right]$$

where $B_{ij}$ has dimension $n_i \times n_j$ $(i,j = 1,2)$ and where $n_1 + n_2 = n$.

1.) If $B_{11}$ is a non-singular matrix, then the determinant of B can be written as

$$|B| = |B_{11}| \cdot |B_{22} - B_{21} B_{11}^{-1} B_{12}|. \tag{5.2.2}$$

2.) If $B_{22}$ is a non-singular matrix, then the determinant of B can be written as

$$|B| = |B_{22}| \cdot |B_{11} - B_{12} B_{22}^{-1} B_{21}|. \tag{5.2.3}$$

The matrices in equation (5.2.1) corresponding to $B_{11}$ and $B_{22}$ are both non-singular so either equation (5.2.2) or (5.2.3) could be used to find $|Var(P\hat{\underline{\tau}})|$. Using equation (5.2.2)

$$|Var(P\hat{\underline{\tau}})| = 2^{k_1+k_2} \left(\frac{\sigma_{11}}{s_1 2^{d_1}}\right)^{k_1} |R| \tag{5.2.4}$$

where:

$$R = \frac{\sigma_{22}}{s_2 2^{d_2}} I_{k_2} - \frac{s_1 2^{d_1} \sigma_{12}^2 n_{12}^2}{(s_1 2^{d_1})^2 (s_2 2^{d_2})^2 \sigma_{11}} D_{21} I_{k_1} D_{12}$$

or

$$R = \frac{\sigma_{22}}{s_2 2^{d_2}} [I_{k_2} - \frac{\sigma_{12}^2}{\sigma_{11}\sigma_{22}} \frac{n_{12}^2}{s_1 2^{d_1} s_2 2^{d_2}} D_{21} D_{12}] \cdot \qquad (5.2.5)$$

Matrix $D_{12}$ was defined in equation (4.2.27) and has at most one element equal to 1 in each column and row with the remaining elements being 0's. Thus the $(\alpha,\gamma)^{th}$ element of $D_{21}D_{12}$ is the dot product of the $\alpha^{th}$ and $\gamma^{th}$ columns of $D_{12}$ and will be zero whenever $\alpha \neq \gamma$ $(\alpha,\gamma = 1,\ldots,k_2)$. When $\alpha = \gamma$, this element will be one, only when the $\alpha^{th}$ effect of interest on $V_2$ is also under study on $V_1$, otherwise this element will be zero. It thus follows that

$$D_{21}D_{12} = \begin{bmatrix} \delta_{1,2,1} & 0 & \cdots & 0 \\ 0 & \delta_{1,2,2} & & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & & \delta_{1,2,k_2} \end{bmatrix}_{k_2 \times k_2} , \qquad (5.2.6)$$

where

$\delta_{1,2,\alpha} = 1$ if the $\alpha^{th}$ effect of interest studied on $V_2$ is also an effect of interest on $V_1$,

$= 0$ otherwise,

for $\alpha = 1,2,\ldots,k_2$.

Of these $k_2$ diagonal elements $k_{12}$ will be 1's and $(k_2-k_{12})$ will be 0's, where $k_{12}$ is defined as the number of effects that are being studied on both $V_1$ and $V_2$ $(k_{12} \leq \min(k_1,k_2))$. (Had equation (5.2.3) been used, the $k_1 \times k_1$ matrix $D_{12}D_{21}$ would have $k_{12}$ 1's along the main diagonal and the rest 0's, as did $D_{21}D_{12}$.)

Using equation (5.2.6) in (5.2.5) gives the following:

$$|R| = \left(\frac{\sigma_{22}}{s_2 2^{d_2}}\right)^{k_2} \left(1 - \rho^2 \frac{n_{12}^2}{s_1 2^{d_1} s_2 2^{d_2}}\right)^{k_{12}} ,$$

where $\rho^2 = \frac{\sigma_{12}^2}{\sigma_{11}\sigma_{22}}$. Substitution of this equation into equation (5.2.4) gives

$$|D(R)| = 2^{k_1+k_2} \sigma_{11}^{k_1} \sigma_{22}^{k_2} \frac{1}{(s_1 2^{d_1})^{k_1}} \frac{1}{(s_2 2^{d_2})^{k_2}} \left(\frac{s_1 2^{d_1} s_2 2^{d_2} - \rho^2 n_{12}^2}{s_1 2^{d_1} s_2 2^{d_2}}\right)^{k_{12}} . \tag{5.2.7}$$

This is the general form of $|\mathrm{Var}(P\hat{\underline{\tau}})|$ for a RMGLM(F) design.

For an MDM(F) design (i.e., $s_1 2^{d_1} = s_2 2^{d_2} = n_{12}$),

$$|D(MD)| = 2^{k_1+k_2} \sigma_{11}^{k_1} \sigma_{22}^{k_2} (s_1 2^{d_1})^{-k_1} (s_2 2^{d_2})^{-k_2} (1-\rho^2)^{k_{12}} . \tag{5.2.8}$$

For the HMGLM(F) designs there are two cases,

(i) $s_1 2^{d_1} \geq s_2 2^{d_2}$ $(= n_{12})$, with

$$|D(H)| = 2^{k_1+k_2}\sigma_{11}^{k_1}\sigma_{22}^{k_2}(s_1 2^{d_1})^{-k_1}(s_2 2^{d_2})^{-k_2}\left(\frac{s_1 2^{d_1}-\rho^2 s_2 2^{d_2}}{s_1 2^{d_1}}\right)^{k_{12}}, \tag{5.2.9}$$

(ii) $s_2 2^{d_2} > s_1 2^{d_1}$ $(= n_{12})$, with

$$|D(H)| = 2^{k_1+k_2}\sigma_{11}^{k_1}\sigma_{22}^{k_2}(s_1 2^{d_1})^{-k_1}(s_2 2^{d_2})^{-k_2}\left(\frac{s_2 2^{d_2}-\rho^2 s_1 2^{d_1}}{s_2 2^{d_2}}\right)^{k_{12}}. \tag{5.2.10}$$

## 5.3 Optimality of the HMGLM(F) Design

In this section the subclass of HMGLM(F) designs will be shown to be complete with respect to the RMGLM(F) designs for the two-response case. The importance of showing completeness is that when searching for the optimal RMGLM(F) design only the subclass of HMGLM(F) designs need be considered. The subclass of MDM(F) designs need not be considered since if an MDM(F) design is an optimal design then the optimal HMGLM(F) design will have $s_1 2^{d_1} = s_2 2^{d_2}$, and therefore is an MDM(F) design.

Theorem 5.3.1 For the two-response case, the class of HMGLM(F) designs is complete (in reference to the determinant criterion) with respect to the RMGLM(F) design.

Proof: Assume that $V_1$ is the MFOR and consider a RMGLM(F) design $D(n_0, s_1 2^{d_1}, s_2 2^{d_2})$ with $V_1$ measured on $s_1 2^{d_1}$ experimental units, $V_2$ measured on $s_2 2^{d_2}$ units of which $n_{12} = \alpha 2^{d_2}$ are in common with $V_1$ (for integer values: $s_1$, $s_2$, $d_1$, $d_2$, $\alpha$, $0 \leq \alpha \leq s_2$). Thus $n_0 = s_1 2^{d_1} + (s_2-\alpha)2^{d_2}$. The cost of this RMGLM(F) design, D(R) is

$$\psi[D(R)] = [s_1 2^{d_1} + (s_2-\alpha)2^{d_2}]\psi_0 + s_1 2^{d_1}\psi_1 + s_2 2^{d_2}\psi_2 \ ,$$

and the determinant is given in equation (5.2.7) with $n_{12} = \alpha 2^{d_2}$.

For the same experimental situation, construct a HMGLM(F) design $D(n_0', s_1' 2^{d_1}, s_2' 2^{d_2})$ denoted by D(H), in the following manner: Again with $V_1$ the MFOR, let $s_1' = s_1$, $s_2' = s_2$ and thus $n_{12} = s_2' 2^{d_2}$ and $n_0 = s_1' 2^{d_1}$. The cost of D(H) is

$$\psi(D(H)) = s_1 2^{d_1}\psi_0 + s_1 2^{d_1}\psi_1 + s_2 2^{d_2}\psi_2 \ ,$$

and the determinant is given in equation (5.2.9).

The difference in the costs of the two designs is

$$\psi[D(R)2 - \psi[D(H)] = (s_2-\alpha)2^{d_2}\psi_0 \geq 0 \ .$$

With the cost of the RMGLM(F) design being greater than or equal to that of the HMGLM(F) design, we now consider the difference in determinants for the two designs. If

$|D(H)| \leq |D(R)|$, then the class of HMGLM(F) designs is complete with respect to the RMGLM(F) designs since a HMGLM(F) design can always be found that is at least as good as any RMGLM(F) design. Consider

$$|D(R)|-|D(H)| = 2^{k_1+k_2}\sigma_{11}^{k_1}\sigma_{22}^{k_2}(s_1 2^{d_1})^{-k_1}(s_2 2^{d_2})^{-k_2} \cdot$$

$$\left\{\left[\frac{s_1 2^{d_1} s_2 2^{d_2} - \rho^2 \alpha^2 2^{2d_2}}{s_1 2^{d_1} s_2 2^{d_2}}\right]^{k_{12}} - \left[\frac{s_1 2^{d_1} - \rho^2 s_2 2^{d_2}}{s_1 2^{d_1}}\right]^{k_{12}}\right\} .$$

This will be greater than or equal to zero if the term in brackets is non-negative. Since $\alpha 2^{d_2} \leq s_2 2^{d_2} \leq s_1 2^{d_1}$, the terms in both braces are non-negative. Thus the term in brackets is non-negative if

$$1-\rho^2 \frac{\alpha}{s_2} \frac{\alpha 2^{d_2}}{s_1 2^{d_1}} - 1+\rho^2 \frac{s_2 2^{d_2}}{s_1 2^{d_1}} \geq 0 ,$$

or when

$$\rho^2 \frac{2^{d_2}}{s_1 s_2 2^{d_1}} (s_2^2 - \alpha^2) \geq 0 .$$

Since $\alpha \leq s_2$, this inequality is true and thus the determinant for the HMGLM(F) design is less than or equal to the determinant for the RMGLM(F) design. This completes the proof.

For the remainder of this chapter when discussing optimal designs, this term will refer to the optimal design from the class of RMGLM(F) designs, unless otherwise stated.

## 5.4 A General Form for the Optimal HMGLM(F) Design

In this section the method of LaGrangian multipliers will be used to determine the values of $s_1$ and $s_2$ that minimize the determinant of Var($\hat{P\underline{\tau}}$) subject to the cost constraint for the class of HMGLM(F) designs for the general case where the MFOR could be either $V_1$ or $V_2$. As in Chapter 4, the responses will be ordered, without loss of generality, so that $\psi_1/k_1 \leq \psi_2/k_2$. Equations (5.2.9) and (5.2.10) give the form of the determinant for a HMGLM(F) design. Rather than finding the design which minimizes this determinant, we will maximize the reciprocal of the determinant, an equivalent procedure giving the same result.

Since the form of the determinant depends upon which response, $V_1$ or $V_2$, is the MFOR, consider the following definition of terms:

$$\left.\begin{aligned} x &= s_i 2^{d_i} \\ X &= \psi_0 + \psi_1 \\ m &= k_i + k_{12} \end{aligned}\right\} \quad \text{if } V_i \text{ is the MFOR } (i = 1,2)\ ,$$

$y \quad = s_i 2^{d_i}$

$Y \quad = \psi_i$ if $V_i$ is not the MFOR $(i = 1,2)$ ,

$n \quad = k_i$

$k_{12}$ = the number of effects under study that are common to both $V_1$ and $V_2$,

$\psi'$ = the total amount of money allotted for experimentation,

$$\rho^2 = \frac{\sigma_{12}^2}{\sigma_{11}\sigma_{22}} .$$

Using this notation allows one to rewrite equations (5.2.9) and (5.2.10) in one equation. The reciprocal of the determinant for a HMGLM(F) design can be expressed as follows:

$$|\text{Var}(P\hat{\underline{\tau}})|^{-1} = \frac{1}{2^{k_1+k_2}\sigma_{11}^{k_1}\sigma_{22}^{k_2}} x^m y^n \left(\frac{1}{x-\rho^2 y}\right)^{k_{12}} \qquad (5.4.1)$$

the cost constraint being

$$\psi' = Xx + Yy . \qquad (5.4.2)$$

Equivalently, since $\sigma_{11}$ and $\sigma_{22}$ are constants for any particular experiment, the function of x and y

$$x^m y^n \left(\frac{1}{x-\rho^2 y}\right)^{k_{12}} \qquad (5.4.3)$$

will be maximized subject to the cost constraint.

Using the method of LaGrangian multipliers gives

$$L = x^m y^n \left(\frac{1}{x-\rho^2 y}\right)^{k_{12}} + \lambda(Xx + Yy - \psi') ,$$

as the function to be maximized, with

$$\frac{\partial L}{\partial x} = m x^{m-1} y^n \left(\frac{1}{x-\rho^2 y}\right)^{k_{12}} - k_{12} x^m y^n \left(\frac{1}{x-\rho^2 y}\right)^{k_{12}+1} + \lambda X ,$$

$$\frac{\partial L}{\partial y} = n x^m y^{n-1} \left(\frac{1}{x-\rho^2 y}\right)^{k_{12}} + k_{12} x^m y^n \left(\frac{\rho^2}{x-\rho^2 y}\right)^{k_{12}+1} + \lambda Y .$$

Set $\frac{\partial L}{\partial x} = 0$, divide through by $m-k_{12}$, and define $X_1 = \frac{X}{m-k_{12}}$ . Set $\frac{\partial L}{\partial y} = 0$, divide through by n, and define $Y_1 = \frac{Y'}{n}$. Solving $\frac{\partial L}{\partial y} = 0$ for $\lambda$ and substituting this value into $\frac{\partial L}{\partial x} = 0$ gives

$$\left(\frac{1}{x-\rho^2 y}\right)^{k_{12}+1} x^{m-1} y^{n-1} \left\{\frac{m}{m-k_{12}} y(x-\rho^2 y) - \frac{k_{12}}{m-k_{12}} xy\right\} =$$

$$\left(\frac{1}{x-\rho^2 y}\right)^{k_{12}+1} x^{m-1} y^{n-1} \frac{X_1}{Y_1} \left\{x(x-\rho^2 y) + \frac{k_{12}}{n} xy\rho^2\right\}$$

which after combining terms and defining $W = \frac{X_1}{Y_1}$ gives

$$\left(\frac{1}{x-\rho^2 y}\right)^{k_{12}+1} x^{m-1} y^{n-1} \{Wx^2 + xy[-W\rho^2(1-\frac{k_{12}}{n})-1]$$

$$+ y^2\rho^2(1+\frac{k_{12}}{m-k_{12}})\} = 0 \; . \qquad (5.4.4)$$

The quadratic formula solving $ax^2 + bx + c = 0$ will be used on the bracketed portion of equation (5.4.4) to solve for x in terms of y. For this equation

$$a = W$$

$$b = -W\rho^2 \; (1 - \frac{k_{12}}{n}) - 1 \; ,$$

$$c = \rho^2 \; (1 + \frac{k_{12}}{m-k_{12}}) \; ,$$

and thus the following solution is obtained

$$x = \frac{1+W\rho^2(1-\frac{k_{12}}{n}) \pm \sqrt{\rho^4 W^2 (1-\frac{k_{12}}{n})^2 + 2W\rho^2[(1-\frac{k_{12}}{n}) - 2(1+\frac{k_{12}}{m-k_{12}})] + 1}}{2W} \; y. \qquad (5.4.5)$$

Since x is the number of times the MFOR will be observed, only real solutions to equation (5.4.5) will be studied. There are two cases to be considered: (i) $k_{12} < n$ and (ii) $k_{12} = n$. (Notice that since $k_{12} = m-k_{12}$ does not change equation (5.4.5), as does $k_{12} = n$, it need not be considered as a special case.) We consider first (i): In order that x is real, $b^2 > 4ac$, which is true for $k_{12} < n$ when

$$W^2\rho^4(1-\frac{k_{12}}{n})^2+W\rho^2[2(1-\frac{k_{12}}{n})-4(1+\frac{k_{12}}{m-k_{12}})]+1 \geq 0 . \qquad (5.4.6)$$

Considering the equality, we can solve for W yielding the following solutions:

$$W = \frac{2(1+\frac{k_{12}}{m-k_{12}})-(1-\frac{k_{12}}{n})\pm 2\sqrt{(1+\frac{k_{12}}{m-k_{12}})[(1+\frac{k_{12}}{m-k_{12}})-(1-\frac{k_{12}}{n})]}}{(1-\frac{k_{12}}{n})^2\ \rho^2} \qquad (5.4.7)$$

which always are real solutions. Denoting these two roots by $W^{(+)}$ and $W^{(-)}$ it must next be determined whether values inside or outside the interval $(W^{(-)},W^{(+)})$ satisfy inequality (5.4.6). We do this by studying the critical point of the quadratic in (5.4.6) to see if it is a maximum or a minimum. Since the critical point falls inside the interval, then if it is a maximum, the values between $(W^{(-)},W^{(+)})$ satisfy inequality (5.4.6); if the critical point is a minimum, then the solutions to inequality (5.4.6) will be outside the interval. The second partial of (5.4.6) is $2\rho^4(1-\frac{k_{12}}{n})^2 > 0$ implying that the critical point is a minimum and therefore x will have a real solution when

$$W \leq W^{(-)} \quad \text{or} \quad W \geq W^{(+)} . \tag{5.4.8}$$

We now consider (ii): The bracketed portion of (5.4.3) becomes

$$Wx^2 - xy + y^2(1 + \frac{n}{m-n}) .$$

The solution for x in terms of y, for $n = k_{12}$, is given by

$$x = \frac{1 \pm \sqrt{1-4W\rho^2(1+ \frac{n}{m-n})}}{2W} \; y . \tag{5.4.9}$$

The discriminant is greater than or equal to zero when

$$W < \frac{1}{4\rho^2(1+ \frac{n}{m-n})} \tag{5.4.10}$$

which when satisfied implies a real solution for x in equation (5.4.9).

Now that the form of the optimal hierarchial design for the general case where the MFOR is measured on m units, has been derived, attention will be directed to the two possible specific cases, $m = s_2 2^{d_2}$ (i.e., $s_2 2^{d_2} > s_1 2^{d_1}$) and $m = s_1 2^{d_1}$ (i.e., $s_1 2^{d_1} \geq s_2 2^{d_2}$) .

## 5.5 HMGLM(F) Designs When $V_2$ is the MFOR

In Section 5.4 a general formulation of the optimal HMGLM(F) design was made to minimize $|Var(\hat{P\underline{\tau}})|$. This formulation however is dependent upon knowledge of which response is the MFOR. With only two possible cases (i.e., the MFOR is either $V_1$ or $V_2$), we will look at each case separately. In this section we shall show that for the optimal HMGLM(F) design, $V_2$ cannot be the MFOR.

To show this, we assume that $V_2$ is the MFOR, which will lead to a contradiction. Assume that $s_2 2^{d_2} > s_1 2^{d_1}$ and therefore the following terms are equivalent to the general case derived in Section 5.4:

$$x = s_2 2^{d_2},$$

$$y = s_1 2^{d_1},$$

$$X = \psi_0 + \psi_2 ,$$

$$Y = \psi_1 ,$$

$$m = k_2 + k_{12} ,$$

$$n = k_1 , \quad \text{and}$$

$$W = \frac{(\psi_0+\psi_2)/k_2}{\psi_1/k_1} .$$

When $k_1 > k_{12}$ the value of $s_2$, obtained from equation

(5.4.5) is given by:

$$s_2 = s_1 2^{d_1 - d_2} \cdot \frac{1+W\rho^2(1-\frac{k_{12}}{k_1}) \pm \sqrt{\rho^4 W^2(1-\frac{k_{12}}{k_1})^2 + 2W\rho^2[(1-\frac{k_{12}}{k_1}) - 2(1+\frac{k_{12}}{k_2}) + 1}}{2W} \tag{5.5.1}$$

When the square root of the discriminant is taken positively, the equation will be denoted by $s_2 = c_2^{(+)} s_1 2^{d_1-d_2}$, and when the square root of the discriminant is taken negatively, the equation will be denoted by $s_2 = c_2^{(-)} s_1 2^{d_1-d_2}$.

From inequality (5.4.8), in order that $s_2$ be real, either

$$\frac{(\psi_0+\psi_2)/k_2}{\psi_1/k_1} \geq W_2^{(+)}$$

or

$$\frac{(\psi_0+\psi_2)k_2}{\psi_1/k_1} \leq W_2^{(-)}$$

where $W_2^{(+)}$ and $W_2^{(-)}$ are the two roots of equation (5.4.7) defined by

$$\left.\begin{array}{l} W_2^{(+)} \\ W_2^{(-)} \end{array}\right\} = \frac{2(1+\frac{k_{12}}{k_2}) - (1-\frac{k_{12}}{k_1}) \pm 2\sqrt{(1+\frac{k_{12}}{k_2})[(1+\frac{k_{12}}{k_2}) - (1-\frac{k_{12}}{k_1})]}}{(1-\frac{k_{12}}{k_1})^2\ \rho^2} \ . \tag{5.5.2}$$

Given that the requirements can be met so that $c_2^{(+)}$ and $c_2^{(-)}$ are real, what conditions must hold so that $c_2^{(-)} > 1$ and/or that $c_2^{(+)} > 1$, for this must be the case if it is true that $s_2 2^{d_2} > s_1 2^{d_1}$? Consider first the conditions that allow $c_2^{(+)} > 1$. The inequality $c_2^{(+)} > 1$ will be true if (from equation (5.5.1)) the following holds:

$$\sqrt{W^2\rho^4(1-\frac{k_{12}}{k_1})^2+2W\rho^2[(1-\frac{k_{12}}{k_1})-2(1+\frac{k_{12}}{k_2})]+1} > 2W-1-W\rho^2(1-\frac{k_{12}}{k_1}) \tag{5.5.3}$$

Since it is assumed that the roots are real, a sufficient condition that $c_2^{(+)} > 1$ is that the r.h.s. of inequality (5.5.3) is less than 0, which is true only if

$$W < \frac{1}{2-\rho^2(1-\frac{k_{12}}{k_1})} . \tag{5.5.4}$$

By virtue of the fact that $\psi_2/k_2 \geq \psi_1/k_1$, $W \geq 1$. Since the r.h.s. of inequality (5.5.4) is less than 1, (5.5.4) can never be true; thus both sides of inequality (5.5.3) are greater than zero and can thus be squared without changing the direction of the inequality.

Squaring both sides of inequality (5.5.3) and simplifying yields

$$0 > W[W(1-\rho^2(1-\frac{k_{12}}{k_1}))-(1-\rho^2(1+\frac{k_{12}}{k_1}))] = f_2(W) \quad , \tag{5.5.5}$$

which when solved as an equality yields the two roots

$$W_{2,1} = 0$$

and

$$W_{2,2} = \frac{1-\rho^2(1+\frac{k_{12}}{k_2})}{1-\rho^2(1-\frac{k_{12}}{k_1})} \quad . \tag{5.5.6}$$

Since $\frac{\partial^2 f_2(W)}{\partial W^2} > 0$, inequality (5.5.5) is satisfied when $W_{2,1} < W < W_{2,2}$. Inspection of equation (5.5.6) yields $W_{2,2} \leq 1$. By definition $W > 1$ so that it is not possible that $W < W_{2,2}$; therefore $c_2^{(+)}$ can never be greater than 1. By nature of the way $c_2^{(-)}$ was defined, $c_2^{(-)} \leq c_2^{(+)}$ and therefore $c_2^{(-)} \leq 1$. Thus when $k_{12} < k_1$ it is not possible for $V_2$ to be the MFOR.

Consider now the situation in which $k_{12} = k_1$, where we are still assuming $s_2 2^{d_2} > s_1 2^{d_1}$. From equation (5.4.9) $s_2 = c_2^{(+)} s_1 2^{d_1-d_2}$ and $s_2 = c_2^{(-)} s_1 2^{d_1-d_2}$ can be found, where

$$c_2 = \frac{1 \pm \sqrt{1-4\rho^2(1+\frac{k_1}{k_2})}}{2W} \quad .$$

Since $W > 1$, it is not possible for $c_2^{(+)} > 1$ and thus $c_2^{(-)} < 1$. The same result was found when $k_1 = k_{12}$ or when $k_1 > k_{12}$ and therefore the following conclusion has been proven:

Theorem 5.5.1 Given that the responses are ordered so that

$$\psi_1/k_1 \leq \psi_2/k_2 , \tag{5.5.7}$$

then the optimal HMGLM(F) design has

$$s_1 2^{d_1} \geq s_2 2^{d_2} .$$

## 5.6 Conditions for the Optimal HMGLM(F) Design

In the last section it was shown that for the optimal RMGLM(F) design, the MFOR could not be $V_2$ and must therefore be $V_1$. In this section the general form of this optimal design, found in Section 5.4, is applied to the specific case where $V_1$ is the MFOR. We desire to determine the conditions where the optimal RMGLM(F) design is hierarchial with $s_1 2^{d_1} > s_2 2^{d_2}$. When these conditions are not satisfied, the optimal design is the MDM design.

We consider the situation with $s_1 2^{d_1} \geq s_2 2^{d_2}$, with the following terms equivalent to the terms used in the general derivation in Section 5.4:

$$x = s_1 2^{d_1} ,$$

$$y = s_2 2^{d_2} ,$$

$$X = \psi_0 + \psi_1 = \psi_1^* ,$$

$$Y = \psi_2 ,$$

$$m = k_1 + k_{12} ,$$

$$n = k_2 , \quad \text{and}$$

$$W = (\psi_1^*/k_1)(\psi_2/k_2)^{-1} .$$

From equation (5.4.5), $s_1$ is given by

$$s_1 = s_2 2^{d_2 - d_1} .$$

$$\frac{1+W\rho^2(1-\frac{k_{12}}{k_2}) \pm \sqrt{W^2\rho^4(1-\frac{k_{12}}{k_2})^2+2\rho^2 W[(1-\frac{k_{12}}{k_2})-2(1+\frac{k_{12}}{k_1})]+1}}{2W} .$$

(5.6.1)

Denote the two roots by $s_1 = c_1^{(+)} s_2 2^{d_2-d_1}$ and $s_1 = c_1^{(-)} s_2 2^{d_2-d_1}$. From inequalities (5.4.8) the conditions that $s_1$ is real are that either

$$\frac{\psi_1^*/k_1}{\psi_2/k_2} \geq W_1^{(+)} , \tag{5.6.2}$$

or that

$$\frac{\psi_1^*/k_1}{\psi_2/k_2} \leq W_1^{(-)} \ . \tag{5.6.3}$$

where $W_1^{(+)}$ and $W_1^{(-)}$ are the two roots of equation (5.4.7), defined by

$$\left.\begin{matrix} W_1^{(+)} \\ \\ W_1^{(-)} \end{matrix}\right\} = \frac{2(1+\frac{k_{12}}{k_1})-(1-\frac{k_{12}}{k_2})\underline{+}2\sqrt{(1+\frac{k_{12}}{k_1})[(1+\frac{k_{12}}{k_1})-(1-\frac{k_{12}}{k_2})]}}{(1-\frac{k_{12}}{k_2})^2\ \rho^2} \ . \tag{5.6.4}$$

From Theorem 4.3.6 for p = 2, it was found that the MDM(F) design is the optimal HMGLM(F) design if $\psi_2/k_2 \leq \psi_1^*/k_1$ or, alternatively if

$$W = \frac{\psi_1^*/k_1}{\psi_2/k_2} \geq 1 \ . \tag{5.6.5}$$

If the rhs of (5.6.4) is expressed as $a \underline{+} b$, it is easily shown that $a \geq 1$, $b > 0$, and $a \geq b$, and therefore that $W_1^{(+)} \geq 1$. Thus when inequality (5.6.2) is satisfied, then from inequality (5.6.5) and from Theorem 4.3.6, it is already known that the MDM(F) design is the optimal design.

Inequality (5.6.2) will thus not be considered and attention will be given to the root $W_1^{(-)}$. Since $W > 0$, the concern is with the real values of $s_1$, which occur when

$$0 < W \leq W_1^{(-)} \quad \text{if} \quad W_1^{(-)} < 1 \ , \tag{5.6.6a}$$

and

$$0 < W < 1 \quad \text{if} \quad W_1^{(-)} \geq 1 \ . \tag{5.6.6b}$$

It is of interest to determine when $W_1^{(-)} \geq 1$ for this would greatly simplify finding the HMGLM(F). Manipulation of the inequality $W_1^{(-)} > 1$ gives the following inequality:

$$1 + \rho^2 (1 - \frac{k_{12}}{k_2})^2 > 4\rho^2 \ (1 + \frac{k_{12}}{k_1}) \ . \tag{5.6.7}$$

Inspection of inequality (5.6.7) reveals that it will only be satisfied for small values of $\rho^2$. Inequality (5.6.6a) can only be satisfied if $W_1^{(-)} > 0$. Manipulation of $W_1^{(-)} > 0$ shows that this inequality is true whenever $k_2 > k_{12}$ (the special case $k_2 = k_{12}$ will be considered shortly).

Assuming that the conditions are satisfied so that $c_1^{(+)}$ and $c_1^{(-)}$ are real, the next things to be considered are the conditions where $c_1^{(-)}$ and/or $c_1^{(+)}$ are greater than 1. (When $c_1^{(+)} \leq 1$ then the optimal hierarchial design will be the MDM (F) design.) Recall that it was assumed that $s_1 2^{d_1} \geq s_2 2^{d_2}$ and the form of the determinant for a HMGLM(F) design was used. The conditions will now be determined where the use of this form is justified. It has already been shown that the optimal design cannot have $s_2 2^{d_2} > s_1 2^{d_1}$. Thus the two types of designs to be considered when looking for an optimal design are the MDM(F) design $s_1 2^{d_1} = s_2 2^{d_2}$ and the HMGLM(F) design with $s_1 2^{d_1} > s_2 2^{d_2}$.

From equation (5.6.5) if $W \geq 1$ then the optimal HMGLM(F) design is the MDM(F) design. Thus for the case where $W < 1$, the conditions necessary for the optimal HMGLM(F) design with $s_1 2^{d_1} > s_2 2^{d_2}$ are desired. Attention will first be given to $c_1^{(+)}$, where

$$c_1^{(+)} =$$

$$\frac{1+W\rho^2(1-\frac{k_{12}}{k_2})+\sqrt{W^2\rho^4(1-\frac{k_{12}}{k_2})^2+2W\rho^2[(1-\frac{k_{12}}{k_2})-2(1+\frac{k_{12}}{k_1})]+1}}{2W} . \tag{5.6.8}$$

Thus $c_1^{(+)} > 1$ when

$$\sqrt{W^2\rho^4(1-\frac{k_{12}}{k_2})^2+2W\rho^2[(1-\frac{k_{12}}{k_2})-2(1+\frac{k_{12}}{k_1})]+1} > 2W-1-W\rho^2(1-\frac{k_{12}}{k_2}) . \tag{5.6.9}$$

The lhs of inequality (5.6.9) is greater than or equal to zero because of the assumption that $c_1^{(+)}$ is real. Therefore a sufficient condition that $c_1^{(+)} > 1$ is that the rhs < 0 which happens when

$$W < \frac{1}{2-\rho^2(1-\frac{k_{12}}{k_2})} . \tag{5.6.10}$$

If inequality (5.6.10) is not satisfied, then squaring both sides of inequality (5.6.9) will not change the direction of the inequality. After squaring and simplifying, $c_1^{(+)} > 1$ if

$$0 > W[W(1-\rho^2(1-\frac{k_{12}}{k_2}))-(1-\rho^2(1+\frac{k_{12}}{k_1}))] = f_1(W). \quad (5.6.11)$$

Solving $f_1(W) = 0$ yields two roots, $W_{1,1} = 0$ and

$$W_{1,2} = \frac{1-\rho^2(1+\frac{k_{12}}{k_1})}{1-\rho^2(1-\frac{k_{12}}{k_2})} \quad . \quad (5.6.12)$$

To determine what values of W satisfy inequality (5.6.11) the second partial derivative of $f_1(W)$ is found to be

$$\frac{\partial^2 f_1(W)}{\partial W^2} = 2-2\rho^2(1-\frac{k_{12}}{k_2}) > 0.$$

Thus values of W between $W_{1,1}$ and $W_{1,2}$ satisfy inequality (5.6.11). $W_{1,2}$ is not necessarily greater than 0, and with $W > 0$ inequality (5.6.11) can only be satisfied if $W_{1,2} > 0$. Since the denominator of (5.6.12) is greater than zero, $W_{12} > 0$ when

$$\frac{k_1}{k_1 + k_{12}} > \rho^2 \quad . \quad (5.6.13)$$

Thus if inequality (5.6.10) is not satisfied, then $c_1^{(+)} > 1$

if both inequality (5.6.13) is satisfied and $W < W_{1,2}$ .

Attention will now be given to real roots of $c_1^{(-)}$. With $c_1^{(+)} \geq c_1^{(-)}$, all conditions must be satisfied for $c_1^{(+)} > 1$ before considering $c_1^{(-)} > 1$ where

$$c_1^{(-)} =$$

$$\frac{1+W\rho^2(1-\frac{k_{12}}{k_2})-\sqrt{W^2\rho^4(1-\frac{k_{12}}{k_2})^2+2W\rho^2[(1-\frac{k_{12}}{k_2})-2(1+\frac{k_{12}}{k_1})]+1}}{2W} \quad . \tag{5.6.14}$$

Thus $c_1^{(-)} > 1$ when

$$\sqrt{W^2\rho^4(1-\frac{k_{12}}{k_2})^2+2W\rho^2[(1-\frac{k_{12}}{k_2})^2-2(1+\frac{k_{12}}{k_1})]+1} < (1-2W)+W\rho^2(1-\frac{k_{12}}{k_2}) \tag{5.6.15}$$

With $c_1^{(-)}$ being real, a necessary condition that (5.6.15) be satisfied is that the rhs be greater than zero, which is true whenever

$$W < \frac{1}{2-\rho^2(1-\frac{k_{12}}{k_2})} \quad . \tag{5.6.16}$$

Assuming (5.6.16) to be true, both sides of inequality (5.6.15) are squared and simplified yielding

$$0 < W[W(1-\rho^2(1-\frac{k_{12}}{k_2}))-(1-\rho^2(1+\frac{k_{12}}{k_1}))] = f_3(W) \quad . \tag{5.6.17}$$

Solving $f_3(W) = 0$ gives $W_{2,1} = 0$ and

$$W_{2,2} = \frac{1-\rho^2(1+k_{12}/k_1)}{1-\rho^2(1-k_{12}/k_2)} \quad . \tag{5.6.18}$$

With $\frac{\partial^2 f_3(W)}{\partial W^2} > 0$, inequality (5.6.17) is satisfied implying $c_1^{(-)} > 1$ where W is outside the interval between $W_{2,1}$ and $W_{2,2}$. Since $W > 0$ then whenever $W_{2,2} < 0$, W will be outside the interval $(W_{2,2},0)$. $W_{2,2}$ is less than zero if

$$\rho^2 \geq \frac{k_{12}}{k_1 + k_{12}} \quad . \tag{5.6.19}$$

All of these conditions must be satisfied in order that $c_1^{(-)} > 1$.

The preceding derivations are proof of the following lemmas concerning the two roots $s_1 = c_1^{(+)} s_2 2^{d_2-d_1}$ and $s_1 = c_1^{(-)} s_2 2^{d_2-d_1}$ for the optimal HMGLM(F) design as found in equation (5.6.1).

<u>Lemma 5.6.1</u> A necessary condition that a HMGLM(F) design be optimal with $s_1 2^{d_1} > s_2 2^{d_2}$ for the case where $k_2 > k_{12}$ is that $c_1^{(+)}$ and $c_1^{(-)}$, as given by (5.6.8) and (5.6.14), respectively, are real numbers.

<u>Lemma 5.6.2</u> $c_1^{(+)}$ and $c_1^{(-)}$ of Lemma 5.6.1 are real numbers if

$$W \leq W_1^{(-)} \quad \text{if } W_1^- < 1, \tag{5.6.20a}$$

or

$$W < 1 \quad \text{if } W_1^- \geq 1 , \tag{5.6.20b}$$

where

$$W = \frac{\psi_1^*/k_1}{\psi_2/k_2} \quad ,$$

$$W_1^- = \frac{2(1+\frac{k_{12}}{k_1})-(1-\frac{k_{12}}{k_2})-2\sqrt{(1+\frac{k_{12}}{k_1})[(1+\frac{k_{12}}{k_1})-(1-\frac{k_{12}}{k_2})]}}{(1-\frac{k_{12}}{k_2})^2\ \rho^2}$$

and

$$W_1^{(-)} > 1 \quad \text{if} \quad [1+\rho^2(1-\frac{k_{12}}{k_2})]^2 > 4\rho^2(1+\frac{k_{12}}{k_2})] \ .$$

If inequality (5.6.20) is not satisfied, then the optimum design is a MDM(F) design.

Assuming that the conditions in Lemmas 5.6.1 and 5.6.2 are satisfied, then the following two lemmas indicate when $c_1^{(-)}$ and/or $c_1^{(+)}$ is greater than 1, thus implying $s_1 2^{d_1} > s_2 2^{d_2}$ in the optimal design.

Lemma 5.6.3 If

$$W < \frac{1}{2-\rho^2(1-\frac{k_{12}}{k_2})} \qquad (5.6.21)$$

then $c_1^{(+)} > 1$. If inequality (5.6.21) is not satisfied and if

$$\rho^2 < \frac{k_1}{k_1 + k_{12}}, \qquad (5.6.22)$$

$$0 < W < \frac{1-\rho^2(1+\frac{k_{12}}{k_1})}{1-\rho^2(1-\frac{k_{12}}{k_2})} \qquad (5.6.23)$$

then $c_1^{(+)} > 1$. Otherwise $c_1^{(+)} \leq 1$ and the MDM(F) design will be optimum.

Consider now $c_1^{(-)}$ which can only be greater than one when $c_1^{(+)} > 1$ since $c_1^{(+)} \geq c_1^{(-)}$.

Lemma 5.6.4 If

$$\frac{1-\rho^2(1+\frac{k_{12}}{k_1})}{1-\rho^2(1-\frac{k_{12}}{k_2})} < W < \frac{1}{2-\rho^2(1-\frac{k_{12}}{k_2})} \qquad (5.6.24)$$

then $c_1^{(-)} > 1$. Otherwise $c_1^{(-)} \leq 1$.

The special case with $k_{12} = k_2$ where $V_1$ is still the MFOR will now be considered. From equation (5.4.9), the solution for $s_1$ in terms of $s_2$ is given by

$$s_1 = \frac{1 \pm \sqrt{1-4W\rho^2(1+\frac{k_{12}}{k_1})}}{2W} \quad s_2 2^{d_2-d_1} \tag{5.6.25}$$

or, for short, $s_1 = c_3^{(+)} s_2 2^{d_2-d_1}$ and $s_1 = c_3^{(-)} s_2 2^{d_2-d_1}$. From inequality (5.4.10), real solutions exist for $s_1$ when

$$W < \frac{1}{4\rho^2(1+k_2/k_1)} \quad .$$

The following lemmas are equivalent to Lemmas 5.6.1 and 5.6.2 for the case where $k_2 = k_{12}$ .

<u>Lemma 5.6.5</u> A necessary condition that a HMGLM(F) design be optimum with $s_1 2^{d_1} > s_2 2^{d_2}$ for the case where $k_2 = k_{12}$ is that $c_3^{(+)}$ and $c_3^{(-)}$ are real numbers.

<u>Lemma 5.6.6</u> $c_3^{(+)}$ and $c_3^{(-)}$ are real numbers if

$$W < \frac{1}{4\rho^2(1+k_2/k_1)} \quad . \tag{5.6.26}$$

When (5.6.26) is not satisfied, then the optimal design is a MDM(F) design.

Assuming that the conditions of Lemmas 5.6.5 and 5.6.6 are satisfied, it is important to know when $c_3^{(-)}$ and/or $c_3^{(+)}$ are greater than one. With the equation for $c_3^{(+)}$ and $c_3^{(-)}$

derived for the case where $s_1 2^{d_1} \geq s_2 2^{d_2}$, we must determine when these formulas are valid. When $c_3^{(+)} < 1$, then $s_1 2^{d_1} \not> s_2 2^{d_2}$, and since it has previously been shown that $s_2 2^{d_2} \not> s_1 2^{d_1}$, then the MDM(F) design must be the optimal design.

From equation (5.4.9) $c_3^{(+)} > 1$ when

$$\sqrt{1-4W\rho^2(1+\frac{k_2}{k_1})} > 2W - 1 \ . \tag{5.6.27}$$

Assuming that Lemmas 5.6.5 and 5.6.6 are satisfied then a sufficient condition that $c_3^{(+)} > 1$ is that the rhs of inequality (5.6.27) is less than zero which occurs when

$$W < \frac{1}{2} \ . \tag{5.6.28}$$

When this is not satisfied, then squaring both sides of (5.6.27) and simplifying yields

$$0 > 4W[W-(1-\rho^2(1+\frac{k_2}{k_1}))] = f_4(W) \ . \tag{5.6.29}$$

Solving $f_4(W) = 0$ gives the roots

$$W_{3,1} = 0, \quad \text{and} \quad W_{3,2} = 1-\rho^2(1+\frac{k_2}{k_1}) \ .$$

Since $\frac{\partial^2 f_4(W)}{\partial W^2} > 0$, then inequality (5.6.29) is satisfied when

$$0 < W < 1-\rho^2(1+ \frac{k_2}{k_1}) \ . \tag{5.6.30}$$

This can only be satisfied if $W_{3,2} > 0$ which occurs when

$$\rho^2 < \frac{k_1}{k_1 + k_2} \ . \tag{5.6.31}$$

Therefore $c_1^{(+)} > 1$ if $W < \frac{1}{2}$. If $W \geq \frac{1}{2}$ then if $W < W_{3,2}$ where $W_{3,2} > 0$ if $\rho^2 < k_1/(k_1+k_2)$, then $c_1^{(+)} > 1$. These conditions for $k_{12} = k_2$ are equivalent to those conditions found for $k_2 > k_{12}$ in Lemma 5.6.3 when $k_{12}$ is replaced by $k_2$ and the simplifications made. For this reason the restriction that $k_2 > k_{12}$ was not made in Lemma 5.6.3.

Consider now $c_3^{(-)}$, which from equation (5.4.9) is greater than 1 when

$$\sqrt{1-4W\rho^2(1+ \frac{k_2}{k_1})} < 1 - 2W \ . \tag{5.6.32}$$

A necessary condition that inequality (5.6.32) be satisfied is that the rhs is greater than zero since we are only concerned with real solutions for c. The rhs of (5.6.32) is greater than zero if $W < \frac{1}{2}$. Assuming that this is satisfied, squaring both sides of (5.6.32) and simplifying yields

$$0 < 4W(W-(1-\rho^2(1+\frac{k_2}{k_1}))) = f_5(W) \ .$$

Solution of $f_5(W) = 0$ gives the two roots

$$W_{5,1} = 0 \quad \text{and} \quad W_{5,2} = 1-\rho^2(1+\frac{k_2}{k_1}) \ .$$

Since $\dfrac{\partial^2 f_5(W)}{\partial W^2} > 0$ then inequality (5.6.32) is satisfied when W is outside the interval $(0,W_{5,2})$ or outside the interval $(W_{5,2},0)$ depending upon whether $W_{5,2}$ is greater than or less than zero. When $\rho^2 > k_1/k_1+k_2$, $W_{5,2} < 0$. Because $W > 0$, then for either interval, $c_3^{(-)} > 1$ if

$$W_{5,2} < W < \frac{1}{2}$$

which is equivalent to the conditions found in Lemma 5.6.4, when $k_2$ replaces $k_{12}$ in the formulas.

To summarize the situation $k_2 = k_{12}$: $c_3^{(+)}$ and $c_3^{(-)}$ are real when the conditions of Lemmas 5.6.5 and 5.6.6 are satisfied (conditions different from those given in Lemma 5.6.2 when $k_2 > k_{12}$). The conditions that $c_3^{(+)} > 1$ and $c_3^{(-)} > 1$ are the same for $k_2 = k_{12}$ as were given in Lemmas 5.6.3 and 5.6.4 for $k_2 > k_{12}$.

## 5.7 Investigation of the Critical Values of the Determinant

In order to find the values of $s_1$ and $s_2$ that minimize the determinant of the variance-covariance matrix in equation (5.2.9), we instead maximized the reciprocal of (5.2.9) and by the use of the method of LaGrange, we determined the possible local maxima and minima by solving equation (5.4.4). This equation was expressed in terms of x and y and for the case where $s_1 2^{d_1} \geq s_2 2^{d_2}$ results in

$$(s_1 2^{d_1} - \rho^2 s_2 2^{d_2})^{-k_{12}-1} (s_1 2^{d_1})^{k_1+k_{12}-1} (s_2 2^{d_2})^{k_2-1} \{W(s_1 2^{d_1})^2 + s_1 2^{d_1} s_2 2^{d_2} [-\rho^2 W(1 - \frac{k_{12}}{k_2}) - 1] + (s_2 2^{d_2})^2 \rho^2 (1 + \frac{k_{12}}{k_1})\} = 0 \tag{5.7.1}$$

where $W = ((\psi_0+\psi_1)/k_1)(\psi_2/k_2)^{-1}$. The possible solutions of (5.7.1) are

a.) $(s_1 2^{d_1} - \rho^2 s_2 2^{d_2})^{-1} = 0$ ,

b.) $s_1 = 0$ ,

c.) $s_2 = 0$ ,

d.)

$$W(s_1 2^{d_1})^2 + s_1 2^{d_1} s_2 2^{d_2} [-\rho^2 W(1 - \frac{k_{12}}{k_2}) - 1] + (s_2 2^{d_2})^2 \rho^2 (1 + \frac{k_{12}}{k_1}) = 0. \tag{5.7.2}$$

Since equation (5.7.1) was derived from a formula which was only applicable to the HMGLM(F) design where $s_1 2^{d_1} > s_2 2^{d_2}$, the interval of admissible values that $s_1$ can assume are $(\frac{\psi'}{\psi_2^*} 2^{-d_1}, \frac{\psi'}{\psi_1^*} 2^{d_1})$. The lower bound occurs when a MDM design is applicable $(s_1 2^{d_1} = s_2 2^{d_2})$; the upper bound occurs when $s_2 = 0$ and all resources are allotted to measuring $V_1$. The interval of possible values for $s_2$ is $(0, \frac{\psi'}{\psi_2^*} 2^{-d_2})$.

Consider the solution to equation (5.7.1)

a.) This can only be a solution when $s_1 = \infty$, a case with which we need not be concerned.

b.) The solution $s_1 = 0$ is inadmissible since $s_1 2^{d_1} \geq s_2 2^{d_2}$ and could only be admissible if $s_2$ also equaled zero.

c.) The solution $s_2 = 0$, although admissible, gives a zero value for the reciprocal of the determinant (5.4.3). This is the minimum value of the function and therefore since we are only concerned with maximization of (5.4.3), this solution can also be ignored.

d.) The solution of (5.7.2) was found in Section 5.6 to be $s_1 = c^+ s_2 2^{d_2 - d_1}$ and $s_1 = c^- s_2 2^{d_2 - d_1}$. These two solutions will now be examined to see if, at one of these values, the determinant is a maximum and at the other it is a minimum. We will refer to the first solution as $c^+$ and to the second as $c^-$.

To try to determine whether these points yield relative maxima or minima, we consider the matrix of second partial derivatives:

$$M = \begin{bmatrix} \dfrac{\partial^2 L}{\partial s_1^2} & \dfrac{\partial^2 L}{\partial s_1 \partial s_2} \\ \\ \dfrac{\partial^2 L}{\partial s_2 \partial s_1} & \dfrac{\partial^2 L}{\partial s_2^2} \end{bmatrix} . \tag{5.7.3}$$

After elimination of $\lambda$, a positive definite M, evaluated at a critical initial point (in this case at either $c^+$ or $c^-$) is a sufficient condition that the reciprocal of the determinant of the variance-covariance matrix achieves a local minimum at this critical point. Conversely, negative definiteness is a sufficient condition for a local maximum. If the matrix is indefinite then further investigation around this critical point is necessary to determine what sort of stationary point has been found.

We consider only the case where $s_1 2^{d_1} \geq s_2 2^{d_2}$ and where we are still attempting to maximize the reciprocal of the variance-covariance matrix. $\dfrac{\partial^2 L}{\partial s_1^2}$ is found and after simplification is given by

$$\frac{\partial^2 L}{\partial s_1^2} = 2^{2d_1}(s_1 2^{d_1})^{k_1+k_{12}-2}(s_2 2^{d_2})^{k_2-2}(s_1 2^{d_1} - \rho^2 s_2 2^{d_2})^{-k_{12}-2} A_1$$

where

$$A_1 = (s_2 2^{d_2})^2 [k_1 s_1 2^{d_1} - (k_1+k_{12})\rho^2 s_2 2^{d_2}]$$

$$[(k_1-1)s_1 2^{d_1} - (k_1+k_{12}-1)\rho^2 s_2 2^{d_2}]$$

$$+ k_{12}\,\rho^2\, s_1 2^{d_1}\,(s_2 2^{d_2})^3 .$$

$\frac{\partial^2 L}{\partial s_2^2}$ and $\frac{\partial^2 L}{\partial s_1 \partial s_2}$ can likewise be determined. Attempting to analyse (5.7.3) for definiteness at $c^+$ or $c^-$ is very difficult due to the complicated nature of $\frac{\partial^2 L}{\partial s_1^2}$, $\frac{\partial^2 L}{\partial s_2^2}$, and $\frac{\partial^2 L}{\partial s_1 \partial s_2}$ as witnessed by $\frac{\partial^2 L}{\partial s_1^2}$. In an attempt to determine which points yielded local maxima and minima, many different conditions were considered. By use of a computer program the two critical values were determined for each set of conditions and then the matrix of second partial derivatives was checked at these critical values for positive or negative definiteness. In many cases the matrices were indefinite. Since definiteness was only a sufficient condition, the indefiniteness of the matrices gives no indication of the true nature of this stationary point.

An explanation as to why this method breaks down here is as follows: Express the LaGrangian equation as

$$L = f(s_1,s_2) + \lambda\ g(s_1,s_2)$$

where $f(s_1,s_2)$ is the reciprocal of the determinant of the variance-covariance matrix and $g(s_1,s_2)$ is the restriction imposed on $f(s_1,s_2)$, i.e., the cost constraint.

$$f(s_1,s_2) = (s_1 2^{d_1})^{k_1+k_{12}} (s_2 2^{d_2})^{k_2} (s_1 2^{d_1} - \rho^2 s_2 2^{d_2})^{-k_{12}} \ . \tag{5.7.4}$$

The critical values, say $s_1^*$ and $s_2^*$, of L are not necessarily the critical values for $f(s_1,s_2)$ due to the restriction $g(s_1,s_2)$. However when $g(s_1,s_2)$ is a linear function of $s_1$ and $s_2$, then

$$\frac{\partial^2 L}{\partial s_1^2} = \frac{\partial^2 f}{\partial s_1^2}\ ;\ \frac{\partial^2 L}{\partial s_2^2} = \frac{\partial^2 f}{\partial s_2^2}\ ;\ \frac{\partial^2 L}{\partial s_1 \partial s_2} = \frac{\partial^2 f}{\partial s_1 \partial s_2}\ . \tag{5.7.5}$$

Since the cost constraint is linear in terms of $s_1$ and $s_2$, then matrix (5.7.3) is equal to the matrix of second partials of f with respect to $s_1$ and $s_2$. Since $s_1^*$ and $s_2^*$ are not critical values of $f(s_1,s_2)$, it is not surprising that the matrix (5.7.3) is indefinite. When $g(s_1,s_2)$ is a higher than first order equation, then equations (5.7.5) will not be true and $\lambda$ will appear in at least one of the terms in (5.7.3). The matrices of second partials are now no longer equal, and we could thus expect the matrix (5.7.3) to be definite.

This difficulty can be avoided if the problem is reduced from the two variables $s_1$, $s_2$ to a one variable problem by solving for say $s_2$ in terms of $s_1$ in $g(s_1,s_2)$ and then substituting this equation into $f(s_1,s_2)$. Solving for $s_2$ in $g(s_1,s_2)$ yields

$$s_2 = 2^{-d_2}(\psi' - \psi_1^* s_1 2^{d_1})/\psi_2 \ . \qquad (5.7.6)$$

The substitution of (5.7.6) into $f(s_1,s_2)$ gives $f(s_1)$, the reciprocal of the determinant of the variance-covariance matrix in terms of one variable:

$$f(s_1) = (s_1 2^{d_1})^{k_1+k_{12}}\left(\frac{\psi'-\psi_1^* s_1 2^{d_1}}{\psi_2}\right)^{k_2}\left[s_1 2^{d_1} - \rho^2\left(\frac{\psi'-\psi_1^* s_1 2^{d_1}}{\psi_2}\right)\right]^{-k_{12}}.$$

After taking the first derivative of $f(s_1)$ and evaluating at zero, the critical points can be obtained:

$$f'(s_1) = 2^{d_1}(s_1 2^{d_1})^{k_1+k_{12}-1}\left(\frac{\psi'-\psi_1^* s_1 2^{d_1}}{\psi_2}\right)^{k_2-1}$$

$$\left(s_1 2^{d_1}\left(1+\rho^2 \frac{\psi_1^*}{\psi_2}\right) - \rho^2 \frac{\psi'}{\psi_2}\right)^{-k_{12}-1} A(s_1)$$

where

$$A(s_1) = (k_1+k_{12})\left(\frac{\psi' - \psi_1^* s_1 2^{d_1}}{\psi_2}\right)(s_1 2^{d_1}(1+\rho^2 \frac{\psi_1^*}{\psi_2})$$

$$- k_2 \frac{\psi_1^*}{\psi_2}(s_1 2^{d_1})(s_1 2^{d_1}(1+\rho^2 \frac{\psi_1^*}{\psi_1})$$

$$- k_{12}(1+\rho^2 \frac{\psi_1^*}{\psi_2}) s_1 2^{d_1}\left(\frac{\psi' - \psi_1^* s_1 2^{d_1}}{\psi_2}\right) .$$

The critical points are found to be

a) $s_1 = 0$,

b) $s_1 = \frac{\psi'}{\psi_1^*} 2^{-d_1}$ ,

c) $[s_1 2^{d_1}(1+\rho^2 \frac{\psi_1^*}{\psi_2}) - \rho^2 \frac{\psi'}{\psi_2}]^{-1} = 0$ ,

d) $s_1 = 2^{-d_1}(\frac{\psi'}{\psi_2})$ .

$$\frac{k_1+[(k_1+k_2)+(k_1+k_{12})]\rho^2\frac{\psi_1^*}{\psi_2} \pm \sqrt{[k_1+(k_2-k_{12})\rho^2\frac{\psi_1^*}{\psi_2}]^2 - 4k_2(k_1+k_{12})\rho^2\frac{\psi_1^*}{\psi_2}}}{2(k_1+k_2)\frac{\psi_1^*}{\psi_2}(1+\rho^2 \frac{\psi_1^*}{\psi_2})} .$$

We will not be concerned with the critical point $s_1 = 0$, for due to the ordering of the variable we have proved that the optimal design has $s_1 2^{d_1} \geq s_2 2^{d_2}$. Critical point (c) can be satisfied when $\rho^2 \neq 0$ only if $\psi_2 = 0$, $\psi_0 = \infty$ (thus $\psi_1^* = \infty$), or $\psi' = \infty$. $\psi_2 = 0$ is not realistic because of the fashion in which the responses were numbered or ordered ($\psi_1/k_1 \leq \psi_2/k_2$). (We can assume that both costs do not equal 0 for then the MDM design would obviously be optimum.) We will also ignore critical point (c) by making the sensible assumption that neither $\psi_0 = \infty$ nor $\psi' = \infty$. Critical point (b) has all resources allocated to sampling $V_1$ thus leaving $s_2 = 0$. Because our interest is in maximizing $f(s_1)$ we will ignore this critical value for at this point the function attains a minimum with $f(s_1 = \frac{\psi'}{\psi_1^*} 2^{-d_1}) = 0$.

The two critical points given in (d), denoted by $s_1^+$ and $s_1^-$ are obtained by solving $A(s_1) = 0$. These two values are equivalent to the values $s_1 = c^+ s_2 2^{d_2 - d_1}$ and $s_1 = c^- s_2 2^{d_2 - d_1}$, obtained when using both responses. Evaluation of $f''(s_1)$ and $s_1^+$ and $s_1^-$ allows us to determine whether $f(s_1)$ at these points yield a local maximum or minimum. If it can be shown that at $s_1^+$, $f(s_1)$ has a local maximum and at $s_1^-$, $f(s_1)$ has a local minimum then we can ignore $s_1^-$, since our only concern is in determining the sample size which maximizes $f(s_1)$.

The second partial of $f(s_1)$ is given by

$$f''(s_1)=2^{2d_1}(s_1 2^{d_1})^{k_1+k_2-1}B^{k_{12}-2}C^{-k_{12}-2}\{(k_1+k_{12})(k_1+k_{12}-1)B^2C^2 -$$

$$2s_1 2^{d_1}BC^2\,\frac{\psi_1^*}{\psi_2}\,[k_2(k_1+k_{12})] -$$

$$2s_1 2^{d_1}B^2C(1-\rho^2\,\frac{\psi_1^*}{\psi_2})k_{12}(k_1+k_{12}) +$$

$$(s_1 2^{d_1})^2C^2(\frac{\psi_1^*}{\psi_2})^2k_2(k_2-1) +$$

$$2(s_1 2^{d_1})^2BC(\frac{\psi_1^*}{\psi_2})(1-\rho^2\,\frac{\psi_1^*}{\psi_2})k_2k_{12} +$$

$$(s_1 2^{d_1})^2B^2(1-\rho^2\,\frac{\psi_1^*}{\psi_2})^2k_{12}(k_{12}+1)\} ,$$

where

$$B = (\psi' - \psi_1^*\, s_1 2^{d_1})/\psi_2 ,$$

and

$$C = s_1 2^{d_1}(1 + \rho^2\,\frac{\psi_1^*}{\psi_2}) - \rho^2\,\frac{\psi'}{\psi_2} .$$

When this is analysed at $s_1^+$ or $s_1^-$ the equation remains very complicated, and as we have so far been unable to show in general that at these two points, $f''(s_1)$ is either always positive or always negative. However, in the aforementioned program which calculates the critical values $s_1^+$ and $s_1^-$ for any particular set of parameters, the value of $f''(s_1)$ was evaluated at these two critical points $s_1^+$ and $s_1^-$. In all of the many parameter sets that were analysed, $f''(s_1=s_1^+) < 0$ and $f''(s_1=s_1^-) > 0$. The reciprocal of the determinant of the variance-covariance matrix of estimable functions thus attains a local maximum at $s_1^+$ and a local minimum at $s_1^-$.

In addition to evaluation of the matrix of second partial derivatives for positive or negative definiteness in the two variable case and evaluation of $f''(s_1)$ at $s_1^+$ and $s_1^-$ in the univariate case, the program also examines the value of the reciprocal of the variance-covariance determinant $f(s_1,s_2)$, in the area of $s_1 = c^+ s_2 2^{d_2-d_1}$ and $s_1 = c^- s_2 2^{d_2-d_1}$, for the two variable case. Let us denote these critical points by $s_1(+)$, $s_2(+)$ and $s_1(-)$, $s_2(-)$. It is not appropriate in this problem to hold, say, $s_1(+)$ constant and look at $f(s_1,s_2)$ at values of $s_2$ around $s_2(+)$ nor should we hold $s_2(+)$ constant and vary $s_1(+)$. This method of evaluating the function at the critical points would be correct if $s_1(+)$ and $s_1(-)$ were critical points for $f(s_1,s_2)$, i.e., the case where $s_1$ and $s_2$ are independent. For our problem $s_1$ and $s_2$ are restricted by the cost constraint, and thus an increase of $s_1$ causes a decrease in the corresponding $s_2$ value. Study of the value of $f(s_1,s_2)$ around the critical point $s_1(+)$, $s_2(+)$ subject to the cost constraint is thus tantamunt to considering values of c around $c_1^+$. A value of $s_1$ a little greater than $s_1(+)$ corresponds to a value of c a little greater than $c^+$. We can thus consider the restricted $f(s_1,s_2)$ as a function of c, say $f_1(c)$. In the many different situations considered, $f_1(c)$ was evaluated at values of c sufficiently close to $c^+$ and $c^-$, and when $c_1^+ \neq c_1^-$ $f_1(c^+)$ was always found to be a local maximum and $f_1(c^-)$ was found to be a local minimum. (When $c^+ = c^-$, $f_1(c^+)$ was found to be a horizontal inflexion point.)

To determine whether $f(s_1,s_2)$ attains a global maximum or just a local maximum at the critical value $s_1 = c^+ s_2 2^{d_2-d_1}$, we must compare the value of the function here, to that at the boundary points. The function $f(s_1,s_2)$ is only applicable to those RMGLM(F) designs with $s_1 2^{d_1} \geq s_2 2^{d_2}$ which does not restrict us since it has previously been shown that if (5.5.7) is satisfied then $V_1$ is the MFOR for the optimal RMGLM(F) design. The range of admissible values for $s_1 2^{d_1}$ is therefore $(\frac{\psi'}{\psi_2^*}, \frac{\psi'}{\psi_1^*})$ where $\frac{\psi'}{\psi_1^*}$ is analogous to $s_2 = 0$ or $c = \infty$. We first consider the upper boundary $s_2 = 0$, where $f(s_1, s_2 = 0) = 0$. As long as observations are taken on both $V_1$ and $V_2$ with $s_1 2^{d_1} \geq s_2 2^{d_2}$ then $f(s_1,s_2) > 0$, and thus at the upper boundary, the function has a global minimum for admissable $s_1$, $s_2$ values. Therefore, it is only necessary to compare $f_1(c^+)$ to $f_1(c = 1)$, the larger of the two indicating which design is optimal.

As a heuristic approach to the determination of the local maximum and local minimum, consider the following argument. The constrained function $f_1(c)$ is continuous in the interval $\rho^2 < c \leq \infty$. When we consider the case where $c^- > \rho^2$, the function has only two real critical values in this interval, those being $c^+$ and $c^-$. If $c^+ = c^-$ we have a horizontal point of inflexion otherwise we have a local maximum and a local minimum. We consider the case where $c^+ \neq c^-$. At all points in the interval $f_1(c) \geq 0$, equaling 0 only at $c = \infty$. At the lower boundary $\lim_{c \to \rho^2+} f_1(c) = \infty$.

This can be seen by noting that $\lim f(s_1, s_2) = \infty$ as $s_1 \to \rho^2 s_2 2^{d_2-d_1}$. Since $f_1(c)$ is continuous in the interval with the function ranging between $\infty$ and 0, then considering this graphically as c goes from $\rho^2$ to $\infty$, $f_1(c)$ must first attain a local minimum, at $c^-$, and then attain a local maximum at $c^+$. (This argument is graphically illustrated in the next section.) Restating this argument at c close to $\rho^2+$, $f(c) = \infty$ and as c moves to infinity $f_1(c)$ goes to zero. In this interval, $\rho^2 \leq c \leq \infty$, there are two critical values. Assuming $c^+ \neq c^-$ then the first change of slope at $c^-$ is a change from a negative slope to a positive slope which implies a local minimum at $c^-$. The second change of slope from positive to negative at $c^+$ implies a local maximum.

If we denote $s_1$ in $s_1 = c^+ s_2 2^{d_2-d_1}$ as $s_1^*$ and eliminate

$s_2$ by using equation (5.7.6) we find

$$s_1^* \, 2^{d_1} \psi_2 = c^+(\psi' - \psi_1^* s_1 2^{d_1})$$

or

$$s_1^* = \frac{c^+ \psi'}{(c^+\psi_1^* + \psi_2)} 2^{-d_1} . \tag{5.7.8a}$$

Therefore using $s_1^*$ in (5.7.6) to solve for $s_2$ denoted by $s_2^*$ we obtain

$$s_2^* = \frac{\psi'}{(c^+\psi_1^* + \psi_2)} 2^{-d_2} . \tag{5.7.8b}$$

Based on (i) the results of the many different situations studied in all cases showed the reciprocal of the variance-covariance determinant to exhibit a local maximum at $s_1 = c^+ s_2 2^{d_2 - d_1}$ and a local minimum at $s_1 = c^- s_2 2^{d_2 - d_1}$ and (ii) the heuristic argument just stated, we make the following conjecture:

<u>Conjecture 5.7.1</u> At the value $(s_1^*, s_2^*)$, the determinant of the variance-covariance matrix (equation (5.2.9)), when restricted by the cost constraint

$$\psi' = \psi_1^* \, s_1 2^{d_1} + \psi_2 \, s_2 2^{d_2}$$

attains a local minimum where $s_1^*$ and $s_2^*$ are given in equation (5.7.8) and $c^+$ is defined in equation (5.6.8).

## 5.8 Interpretation of Results

In Section 5.7, the critical value of the reciprocal of the variance-covariance determinant at the point $(s_1(+), s_2(+))$ was shown to be a local maximum where $s_1(+)$ and $s_2(+)$ are obtained from $s_1 = c^+ s_2 2^{d_2 - d_1}$. When we refer to a global maximum, we will restrict our "globe" to those admissible values of $s_1$ and $s_2$, i.e., $s_1 2^{d_1} \geq s_2 2^{d_2}$ and such that the cost constraint is not exceeded. In the last section we found that there are only two values that can possibly give the global maximum. Those points are $(s_1(+), s_2(+))$ and $(s_1(\text{MDM}), s_2(\text{MDM}))$ where $s_1(\text{MDM}) 2^{d_1} = s_2(\text{MDM}) 2^{d_2} = \psi_1/\psi_2^*$. To determine which of these two points gives the true maximum $f(s_1(+), s_2(+))$ must be compared to $f(s_1(\text{MDM}), s_2(\text{MDM}))$.

The values $c^+$ and $c^-$ can be very useful in the determination of the global maximum and thus in the determination of the optimal design. Recall that the design with $c = 1$ corresponds to a MDM design. There are 3 important relationships between the values of c that will be discussed and illustrated graphically:

i) $c^+ < 1$ and thus $c^- < 1$,

ii) $c^+ > 1$ and $c^- < 1$, and

iii) $c^+ > 1$ and $c^- > 1$.

For case (i), the MDM(F) design is the optimal design. Even though $f(s_1(+),s_2(+)) > f(s_1(MDM),s_2(MDM))$, the critical value $(s_1(+),s_2(+))$ is not admissible since $c^+ < 1$ and therefore $s_1 2^{d_1} < s_2 2^{d_2}$.

For case (ii), the HMGLM(F) design is optimum. As long as $c^- < 1$ and $c^+ > 1$, then $c = 1$ falls between these two critical values. Since $f(s_1,s_2)$ is a strictly increasing function between $c^-$ and $c^+$ then

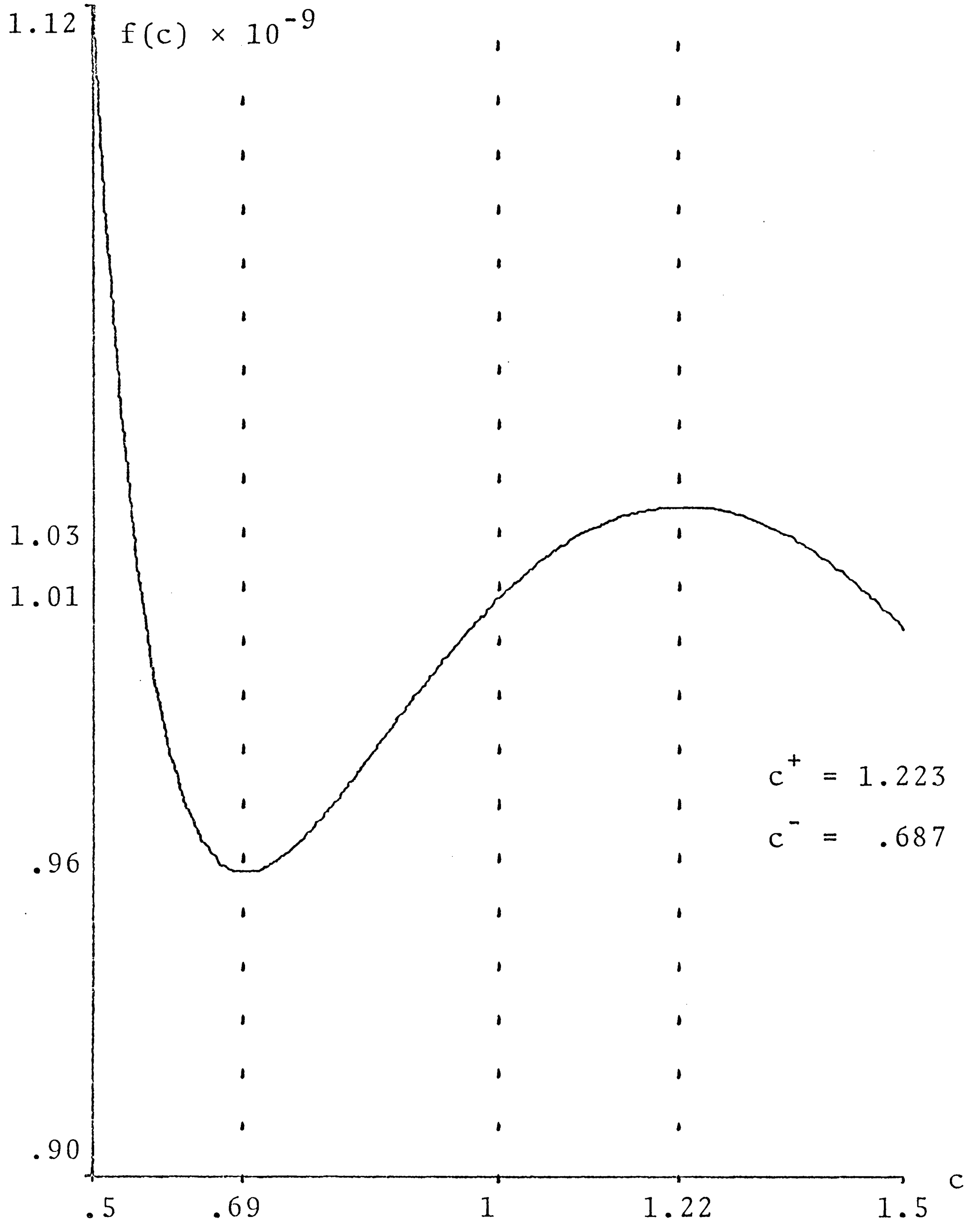
$$f(s_1(-),s_2(-)) < f(s_1(MDM),s_2(MDM)) < f(s_1(+),s_2(+)).$$

This situation is illustrated in Figure 5.8.1.

When $c^- > 1$ (case iii), the optimal design is not so easily determined. The actual values of $f(s_1,s_2)$ evaluated at $(s_1(+),s_2(+))$ and $(s_1(MDM),s_2(MDM))$ must be compared to determine which design is optimal. Figure 5.8.2 illustrates an example where $f(s_1(MDM),s_2(MDM)) > f(s_1(+),s_2(+))$ and therefore the MDM(F) design is optimum. The HMGLM(F) design is optimum in the case illustrated by Figure 5.8.3.

Thus $c^+$ and $c^-$ are more than just intermediate values in the computation of $s_1(+)$ and $s_1(-)$. Apart from allowing an easier understanding of the problem and the relationship between $s_1$ and $s_2$, their importance lies in often allowing

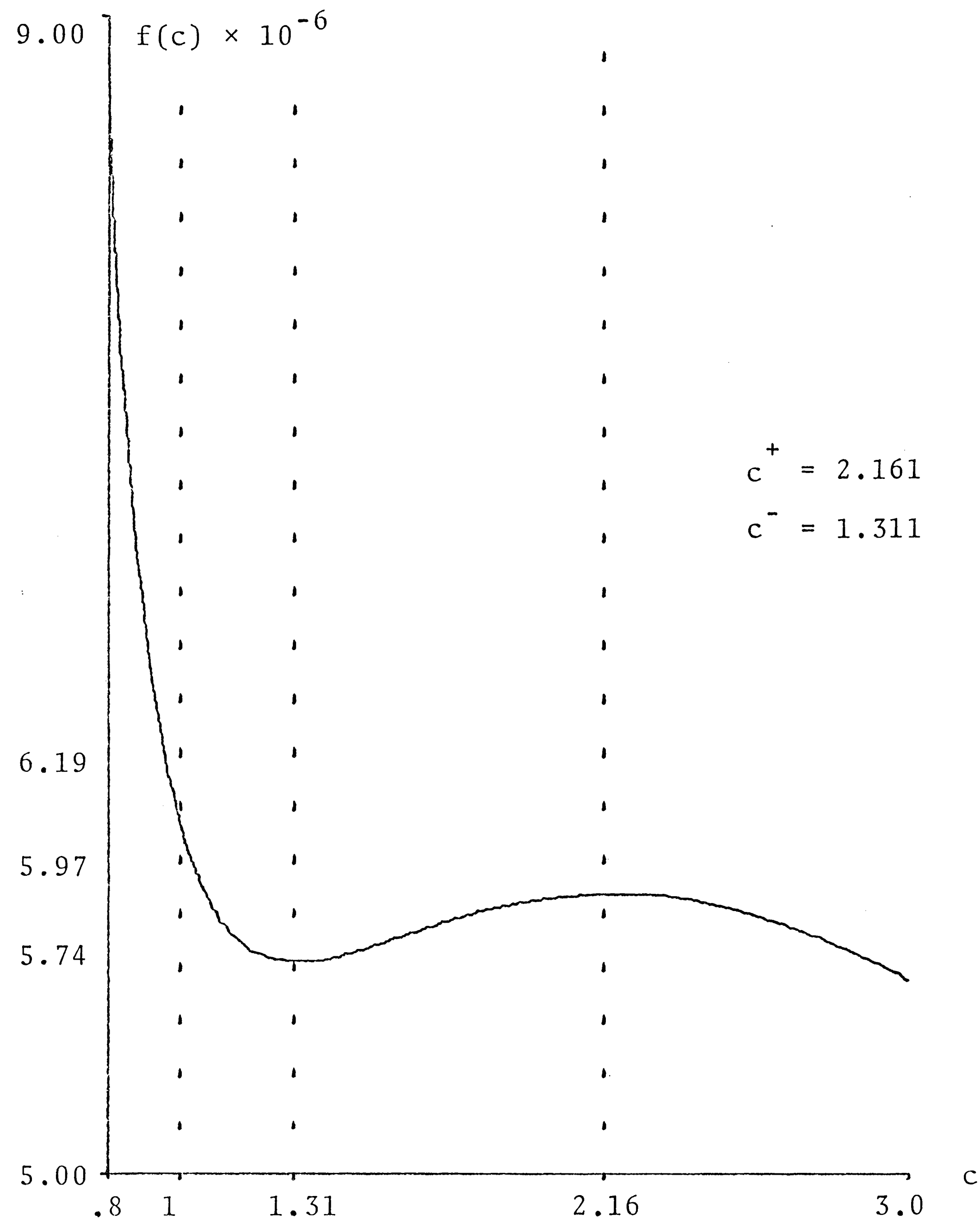
Figure 5.8.1 Reciprocal of $|V|$ for $c^- < 1 < c^+$




$(d_1, d_2, k_1, k_2, k_{12}, \psi_0, \psi_1, \psi_2, \psi', \rho^2) = (4,4,4,4,2,2,2,2,7,100,.32)$

f(c) denotes the reciprocal of the constrained variance-covariance determinant, expressed in terms of c.

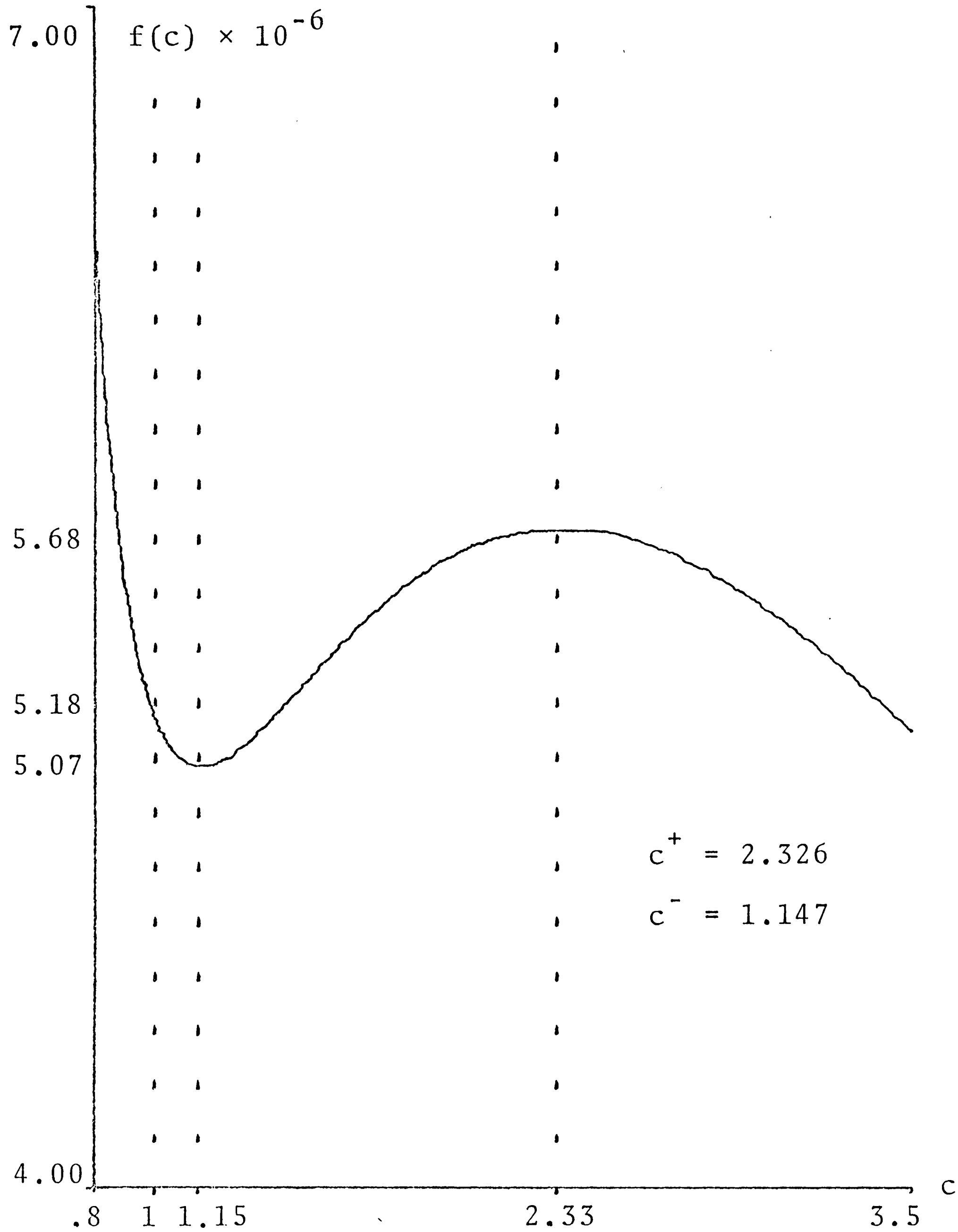
Figure 5.8.2 Reciprocal of $|V|$ for $c^- > 1$, $f(1) > f(c^+)$




$(d_1, d_2, k_1, k_2, k_{12}, \psi_0, \psi_1, \psi_2, \psi', \rho^2) = (5,3,5,3,3,4,8,25,200,.51)$

f(c) denotes the reciprocal of the constrained variance-covariance determinant, expressed in terms of c.

Figure 5.8.3 Reciprocal of $|V|$ for $c^- > 1$, $f(1) < f(c^-)$




$(d_1, d_2, k_1, k_2, k_{12}, \psi_0, \psi_1, \psi_2, \psi', \rho^2) = (5,3,5,3,3,4,8,25,200,.48)$

f(c) denotes the reciprocal of the constrained variance-covariance determinant, expressed in terms of c.

a quick recognition of the optimal design without evaluating the function at several points.

The above discussion along with Theorem 4.3.6 applied to the two-response situation leads to the following theorem.

Theorem 5.8.1 If the responses are ordered so that $\psi_1/k_1 \leq \psi_2/k_2$, then the optimal RMGLM(F) design with respect to the determinant criterion and a cost constraint is found as follows:

a.) If $\psi_2/k_2 \leq (\psi_0+\psi_1)/k_1$ then the MDM(F) design is the optimal RMGLM(F) design.

When this condition is not satisfied then the following conditions should be applied.

b.) If $c^+ < 1$ then the MDM(F) design is optimum.

c.) If $c^+ > 1$ and $c^- < 1$ then the HMGLM(F) design is the optimal RMGLM(F) design.

d.) If $c^- > 1$ then the HMGLM(F) design is optimum when $f(s_1(+),s_2(+)) > f(s_1(\text{MDM}),s_2(\text{MDM}))$. Otherwise the MDM(F) design is optimum.

For the MDM(F) design, $s_1(\text{MDM})2^{d_1} = s_2(\text{MDM})2^{d_2} = \psi'/\psi_2^*$. For the HMGLM(F) design, $s_1(+)$ and $s_2(+)$ are defined by equations (5.7.8) and $c^+$ and $c^-$ are defined by equations (5.6.8) and (5.6.14). The function $f(s_1,s_2)$ is defined by equation (5.7.4).

In order to find the optimal HMGLM design, an 'a priori' estimate of $\rho^2$ is required. If one does not know $\rho^2$ but has a rough idea of its value then the following suggestion is made. Using this rough estimate, say $\hat{\rho}^2$, run the program to determine the optimal HMGLM design. The program outputs a value PLIM, which is not a function of $\hat{\rho}^2$. We can determine the values of $\rho^2$, such that $c^+ > 1$ by using equation (5.6.21) and (5.6.23). When $\rho^2 <$ PLIM then a HMGLM design will be optimum, i.e., $c^+ > 1$, otherwise the MDM design will be the optimal design. If $\hat{\rho}^2$ falls decisively on either side of PLIM then one can determine whether or not the optimal design will be the MDM design. If one feels that $\rho^2 <$ PLIM then some conservative HMGLM design can be used. This design, although probably not optimum will at least be better than the standard MDM design.

## 5.9 Explanation of Computer Programs

Two programs have been written that were necessary and helpful in the basic area of research discussed in this chapter.

The important aspects of one program, that have been eluded to in earlier sections, will be summarized. This program was necessary in our attempt through simulation to show $f(s_1(+),s_2(+))$ to be a local maximum. For any particular set of parameters $d_1, d_2, k_1, k_2, k_{12}, \psi_0, \ldots$ the program calculates and outputs many intermediate steps in determining $c^+$ and $c^-$. These intermediate steps often give an indication as to how a change in certain parameter values effects a change in the design. After calculating $c^+$ and $c^-$, the program determines the critical values $(s_1(+), s_2(+))$ and $(s_1(-), s_2(-))$ and then determines $(s_1(\mathrm{MDM}), s_2(\mathrm{MDM}))$. The main purpose of the program was to determine whether $f(s_1, s_2)$, the reciprocal of the variance-covariance determinant, attained a local maximum or minimum at one of the critical points. Because the equations to be analysed were so involved, we were in general unable to state that at $c^+$, $f(s_1, s_2)$ attained a local maximum and that at $c^-$, it attained a local minimum. Thus a simulation approach was taken, with the thought that if for the many diverse parameter sets considered, $c^+$ always gave a local maximum and $c^-$ always gave a local minimum, then this conclusion would be assumed true. The program also has the capacity to change the $\rho^2$-value holding the other parameters constant to give an even greater number of parameter sets.

The program performs the following operations:

1.) It analyses the matrix of second partial derivatives at $(s_1(+), s_2(+))$ and $(s_1(-), s_2(-))$ for positive or negative definiteness outputting the matrix and the determinants of the principal minors. (As discussed in Section 5.8, this method was not successful.)

2.) The program outputs the second partial derivative of $f(s_1)$ evaluated at $s_1(+)$ and $s_1(-)$, where $f(s_1)$ is the reciprocal of the variance-covariance determinant expressed in terms of only one variable.

3.) The program evaluates $f(s_1,s_2)$ at values $(s_1,s_2)$ close to $(s_1(+),s_2(+))$ that satisfy the cost constraint and then compares these values to $f(s_1(+),s_2(+))$. The same thing is done at values $(s_1,s_2)$ close to $(s_1(-),s_2(-))$.

For all parameter sets, (2.) and (3.) showed $f(s_1(+),s_2(+))$ to be a local maximum and $f(s_1(-),s_2(-))$ to be a local minimum. The program then compares $f(s_1(+),s_2(+))$ to $f(s_1(\text{MDM}),s_2(\text{MDM}))$ to determine the global maximum.

Another output capacity of this program is that it will punch the parameters and the optimal design on cards to be used as input to a program that is necessary in the next chapter.

The second program determines the optimal integer design once the non-integer $(s_1(+),s_2(+))$ values have been found. Therefore this program takes the $(s_1(+),s_2(+))$ and $(s_1(\text{MDM}),s_2(\text{MDM}))$ values and looks at the possible integer solutions close to it so that one can find the best integer design rather than just rounding off the $s_i$ values hoping to obtain the optimal integer design. It is therefore analogous to the program written to round-off the $s_i$ values when we were concerned with minimizing the trace rather than the determinant.

This program is also applicable to finding the integer design which maximizes $f = (s_1 2^{d_1})^{k_1} \ldots (s_p 2^{d_p})^{k_p}$ subject to the cost constraint. It is thus used in those instances covered in Chapter 4 where Theorems 4.3.3 and 4.3.5 and Lemma 4.3.4 are applicable (i.e., when $\sigma_{ij} = 0$ or when $k_{ij} = 0$ for $i \neq j$, $i,j = 1,\ldots,p$).

The necessary control cards as input for these two programs along with their program listings are given in Appendix 2.

# CHAPTER VI

## COMPARISON OF GENERAL MGLM(F) DESIGNS TO OPTIMUM HMGLM(F) DESIGNS FOR TWO RESPONSE SITUATIONS

### 6.1 Introduction

In Chapter 5 for the two response situation, the RMGLM(F) design was found which maximizes the determinant of Var($\hat{\underline{P}}_T$) while not exceeding a fixed total cost. We would like to determine the optimal MGLM(F) design but so far have only determined the optimal design for a subclass of these designs, the RMGLM(F) designs. In this chapter we will attempt to find the optimal MGLM(F) design from the complement subclass of MGLM(F) designs. Upon finding this design, it can be compared to the optimum RMGLM(F) design with the better of these two designs being the optimum MGLM(F) design.

First we shall define this subclass of MGLM designs, and then we will show how these designs are formed.

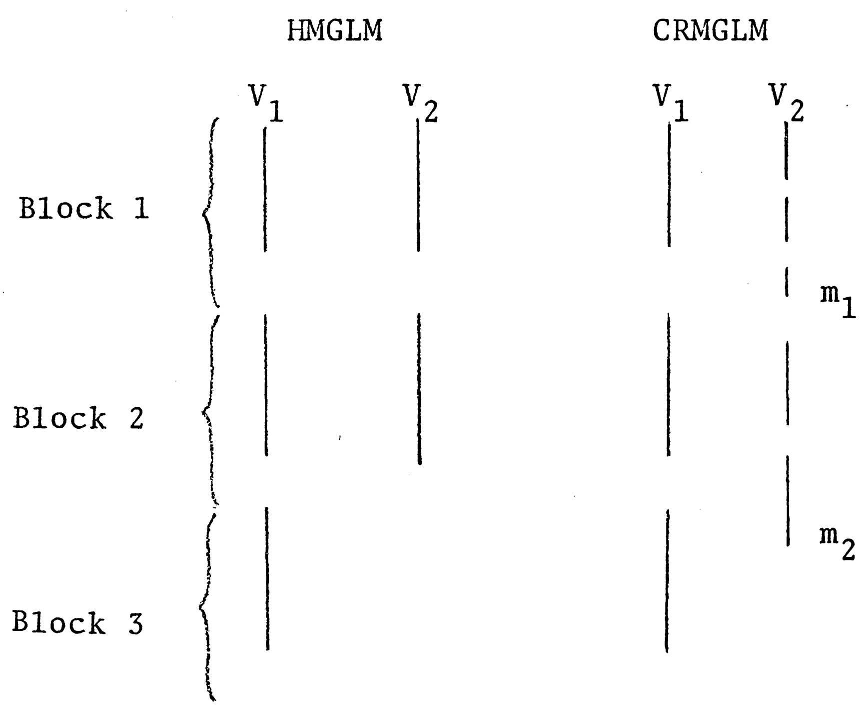
Definition 6.1.1 All members of the class of MGLM(F) designs that are not members of the subclass of RMGLM(F) designs will be said to be elements of the subclass called Complementary Restricted More General Linear Multiresponse (CRMGLM(F)) designs, i.e.,

$$\{CRMGLM(F)\} = \{MGLM(F)\} - \{RMGLM(F)\} .$$

CRMGLM designs will be formed by first considering a HMGLM design and then modifying this design to create a CRMGLM design. This method will be advantageous since we eventually will be comparing the optimal CRMGLM design to the optimal RMGLM design (a HMGLM design).

We will consider CRMGLM designs where the responses are measured on groups of $2^{d_i}$ units as was done for the HMGLM design and RMGLM design. The differences in designs lies of course in the number of common units on which both $V_1$ and $V_2$ are measured ($n_{12}$). For a HMGLM design $n_{12} = s_2 2^{d_2}$. When the RMGLM(F) design was defined, the restriction of common units was eased allowing $n_{12} = (s_2-\alpha)2^{d_2}$ for an integer ($0 \leq \alpha \leq s_2$). Recall that by definition, $V_2$ was measured on $\alpha$ entire fractions of $2^{d_2}$ units where $V_1$ was not measured. The restriction is eased even further in the creation of the CRMGLM design through the assumption: Of the $s_2 2^{d_2}$ units where $V_2$ is observed, any m of the observations can be taken on units where $V_1$ is not measured ($0 < m < s_2 2^{d_2}$). Since the CRMGLM design was defined as the complement of the RMGLM design we will not consider $m = 0$ since this gives a HMGLM design nor will be consider $m = s_2 2^{d_2}$ for this gives a RMGLM design with $\alpha = s_2$. The assumption will be made that block sizes are large enough that if in block $B_j$, $m_j$ experimental units have $V_2$ measured but not $V_1$, then these $m_j$ units can be measured in the same block with the other $2^{d_2}-m_j$ units. When this assumption is made it allows us to make a standard adjustment for blocks without having to adjust one fraction of units for several different blocks, i.e., each fractional factorial is associated with only one block. This assumption is illustrated by the following line graph contrasting a HMGLM(F) design to a CRMGLM(F) design. The lines indicate that an observation has been taken on this unit.

<u>Example 6.1.1</u>




For the $s_1 2^{d_1}$ total units in a HMGLM(F) design we will denote by $tc_k$ the treatment combination applied to the $k^{th}$ unit $(k = 1,\ldots,s_1 2^{d_1})$. Actually $tc_k = (tc_{k,1},tc_{k,2})$ where

$tc_{k,i}$ would be the treatment combination applied to this $k^{th}$ unit if we consider a univariate experiment on only $V_i$ $(i = 1,2)$. Recall that because $V_1$ and $V_2$ may be influenced by different factors, it is not necessary that any of the 3 treatment combinations $tc_k$, $tc_{k,1}$, $tc_{k,2}$ be equal. This same notation will be used for the $(s_1 2^{d_1}+m)$ units of a CRMGLM design.

It is convenient to form CRMGLM designs by first considering a HMGLM(F) design with $s_1 2^{d_1} \geq s_2 2^{d_2}$ and with $V_2$ measured on the first $s_2 2^{d_2}$ of the $s_1 2^{\bar{d}_1}$ units. Take any m of these first $s_2 2^{d_2}$ units, and on these units measure only $V_1$. Then on, say, units $s_1 2^{d_1}+1, \ldots, s_1 2^{d_1}+m$ only $V_2$ is measured. It is important that the observations on these m extra units receive the same treatment combinations as were applied to the m units in the first $s_2 2^{d_2}$ units where only $V_1$ was measured. This precaution insures that each response is measured on $s_i$ groups of complete fractional factorials.

Notice how the cost of a HMGLM design compares with the cost of a similar CRMGLM design. If on both designs $V_1$ and $V_2$ are measured on the same number of units and $\psi_0 > 0$, then for $m > 0$, the CRMGLM design, since it encompasses more experimental units, costs more than the HMGLM design. The search for the optimal design thus concerns the following question: Is the increase in cost using a CRMGLM design justified by a substantial decrease in $\det(\mathrm{Var}(P\hat{\underline{\tau}}))$?

For a fixed amount of money $\psi'$, the larger m becomes, the more money must be used for set-up costs leaving less money to be allocated to sampling $V_1$ and $V_2$. Therefore the question really becomes: Is the fact that the CRMGLM design requires smaller sample sizes compensated for by a reduction in the $\det(\mathrm{Var}(P\hat{\underline{\tau}}))$ when compared to the optimal design? The answer to this question is the major thrust of this chapter.

In order to determine the optimal CRMGLM(F) design, the general form of $\mathrm{Var}(P\hat{\underline{\tau}})$ must be found. Once this matrix is found then $\det(\mathrm{Var}(P\hat{\underline{\tau}}))$ can be found and minimized with respect to $s_1$, $s_2$, and m. A problem encountered here is that $\mathrm{Var}(P\hat{\underline{\tau}})$ depends not only upon $s_1$, $s_2$, and m, but also upon the inter-relations between the tc's applied to these m units. We find the association between the m tc's that gives the $\min(|\mathrm{Var}(P\hat{\tau})|)$ when compared to the determinants given by any other set of m possible tc's. This gives us a type of lower bound determinant, which is a function of $s_1$, $s_2$, and m. This expression can now be used as our function to be minimized with respect to $s_1$, $s_2$, and m.

LaGrangian multipliers are again used to determine the values of $s_1$ and $s_2$ which give the optimum CRMGLM design for a particular m. The solution of the LaGrangian equation in terms of $s_1$ is a $5^{th}$ order polynomial which cannot in general be solved to give a general expression for the optimal values of $s_1$ and thus $s_2$. A computer program has been written to solve this equation for $s_1$ and thus determine the optimal design for a particular value of m. A range of m-values is then considered with the best design over this range of m-values being the optimal CRMGLM design. This design is then compared to the optimal RMGLM design (either a HMGLM or a MDM design) with the better of these two designs being the optimal MGLM design.

In the last section some further thoughts and observations are given which concern finding the optimal MGLM design.

## 6.2 The General Form of $Var(P\hat{\underline{\tau}})$ for a CRMGLM(F) Design

In this section we wish to determine the general form of $Var(P\hat{\underline{\tau}})$ for a CRMGLM(F) design. It is necessary that this general form be specified before an expression for the determinant of $Var(P\hat{\underline{\tau}})$ for this subclass of MGLM(F) designs can be obtained.

Denote the $Var(P\hat{\underline{\tau}})$ matrix for the CRMGLM design by

$$D(CR) = \begin{bmatrix} P_1 Var(\hat{\underline{\tau}}_1)P_1' & P_1 Cov(\hat{\tau}_1, \hat{\tau}_2)P_2' \\ & \\ P_2 Cov(\hat{\underline{\tau}}_2, \hat{\underline{\tau}}_1)P_1' & P_2 Var(\hat{\tau}_2)P_2' \end{bmatrix} . \quad (6.2.1)$$

Since $V_1$ and $V_2$ are still measured on groups of complete fractional factorials, then the main diagonal matrices are identical to their counterparts in D(R) or D(H), i.e.,

$$P_i(Var(\hat{\underline{\tau}}_i))P_i' = 2 \frac{\sigma_{ii}}{s_i 2^{d_i}} I_{k_i} \quad \text{for } i = 1,2. \quad (6.2.2)$$

The off-diagonal covariance matrices are different however from their counterparts in D(R) or D(H) due to the fact that there are no longer complete fractions of elements measured on common units. The general form of these off-diagonal covariance matrices is the topic of basic interest in this section. Since

$$P_1 \; Cov(\hat{\underline{\tau}}_1, \hat{\underline{\tau}}_2)P_2' = [P_2 \; Cov(\hat{\underline{\tau}}_2, \hat{\underline{\tau}}_1)P_1']' \; ,$$

we shall denote these covariance matrices for the CRMGLM(F) design by Cov(CR).

Using the notation of earlier chapters, $V_1$ is influenced by $k_1$ effects, $V_2$ by $k_2$ effects, with $k_{12}$ of the

$k_1$ effects of $V_1$ also influencing $V_2$. If the $i^{th}$ effect on $V_1$ ($i = 1,\ldots,k_1$) is one of the $k_{12}$ effects which also influence $V_2$, and on $V_2$ this effect is the $j^{th}$ effect, then we shall say the $i^{th}$ effect = the $j^{th}$ effect. If the $i^{th}$ effect on $V_1$ and the $j^{th}$ effect on $V_2$ are not the same then we shall say the $i^{th}$ effect $\neq$ the $j^{th}$ effect.

In the process of finding Cov(CR) we shall first determine a general form of $\mathrm{Cov}(\hat{\underline{\tau}}_1,\hat{\underline{\tau}}_2)$. Although this matrix is not of full rank and is not unique since $\hat{\underline{\tau}}_1$ and $\hat{\underline{\tau}}_2$ are not estimable, we can determine a general form from which it will be easy to determine Cov(CR), the unique covariance matrix of estimable functions.

The following equation was determined in Section 4.2

$$\mathrm{Cov}(\hat{\underline{\tau}}_1,\hat{\underline{\tau}}_2) = \sigma_{12}D_1^-M_1Q_{12}M_2'D_2^- \ .$$

The general form of the matrix $M_1Q_{12}M_2'$ will be found first, where

$$M_1Q_{12}M_2' = X_1'Q_{12}X_2-\tfrac{1}{2}X_1'Q_{12}J-\tfrac{1}{2}JQ_{12}X_2+\tfrac{1}{4}JQ_{12}J \ .$$

We now consider each term individually:

$$JQ_{12}J = n_{12}J = (s_2 2^{d_2}-m)J \ ,$$

$$X_1'Q_{12}J = \begin{bmatrix} n_{12,1,0} & n_{12,1,0} & \cdots & n_{12,1,0} \\ n_{12,1,1} & n_{12,1,1} & \cdots & n_{12,1,1} \\ \vdots & \vdots & & \vdots \\ n_{12,k_1,0} & n_{12,k_1,0} & \cdots & n_{12,k_1,0} \\ n_{12,k_1,1} & n_{12,k_1,1} & \cdots & n_{12,k_1,1} \end{bmatrix}$$

$$JQ_{12}X_2 = \begin{bmatrix} n_{21,1,0} & n_{21,1,1} & \cdots & n_{21,k_2,0} & n_{21,k_2,1} \\ n_{21,1,0} & n_{21,1,1} & & n_{21,k_2,0} & n_{21,k_2,1} \\ \vdots & & & & \\ n_{21,1,0} & n_{21,1,1} & \cdots & n_{21,k_2,0} & n_{21,k_2,1} \end{bmatrix}$$

$$X_1'Q_{12}X_2 = \begin{bmatrix} n_{12,1,0,1,0} & n_{12,1,0,1,0} & \cdots & n_{12,1,0,k_2,1} \\ n_{12,1,1,1,0} & n_{12,1,1,1,1} & \cdots & n_{12,1,1,k_2,1} \\ \vdots & \vdots & & \vdots \\ n_{12,k_1,1,1,0} & n_{12,k_1,1,1} & \cdots & n_{12,k_1,1,k_2,1} \end{bmatrix}$$

where

$n_{12}$ = the number of units $V_1$ and $V_2$ have in common

$\quad = s_2 2^{d_2} - m$ ,

$n_{12,ik}$ = the number of times the $i^{th}$ effect on $V_1$ appears at the $k^{th}$ level on the $n_{12}$ common units $(i = 1,\ldots,k_1,\ k = 0,1)$ ,

$n_{21,j\ell}$ = the number of times the $j^{th}$ effect on $V_2$ appears at the $\ell^{th}$ level on the $n_{12}$ units ($j = 1,\ldots,k_2$, $\ell = 0,1$) ,

$n_{12,ikj\ell}$ = the number of units on which the $i^{th}$ effect on $V_1$ appears at the $k^{th}$ level while the $j^{th}$ effect on $V_2$ appears at the $\ell^{th}$ level.

For any effect on either response

$$n_{12,ikj,0} + n_{12,ikj,1} = n_{12,ik} \tag{6.2.3}$$

and

$$n_{12,i,0,j\ell} + n_{12,i,1,j\ell} = n_{21,j\ell} \tag{6.2.4}$$

Obviously if the $i^{th}$ effect = the $j^{th}$ effect and if $k = \ell$, then $n_{12,ijk\ell} = n_{12,ik}$, and if $k \neq \ell$ then $n_{12,ikj\ell} = 0$.

The (1,1) element of $M_1Q_{12}M_2'$ is therefore

$$n_{12,1,0,1,0} - \frac{1}{2}\, n_{12,1,0} - \frac{1}{2}\, n_{21,1,0} + \frac{1}{4}\, n_{12} \;.$$

The $(2i+k-1,\ 2j+\ell-1)$ element of $M_1Q_{12}M_2'$, which is the element associated with the $i^{th}$ effect on $V_1$ at the $k^{th}$ level and the $j^{th}$ effect on $V_2$ at the $\ell^{th}$ level, can be expressed as

$$n_{12,ikj\ell} - \frac{1}{2} n_{12,ik} - \frac{1}{2} n_{21,j\ell} + \frac{1}{4} n_{12} .$$

We shall now consider two relationships between the elements in the matrix $M_1Q_{12}M_2'$. Consider first the elements associated with the high and low levels of any effect on $V_1$ for either level of any effect on $V_2$. The element associated with the low level is given by

$$n_{12,i,0,j\ell} - \frac{1}{2} n_{12,i,0} - \frac{1}{2} n_{21,j\ell} + \frac{1}{4} n_{12} ,$$

the element associated with the high level being

$$n_{12,i,1,j\ell} - \frac{1}{2} n_{12,i,1} - \frac{1}{2} n_{21,j\ell} + \frac{1}{4} n_{12} .$$

Consider the sum of these elements:

$$(n_{12,i,0,j\ell}+n_{12,i,1,j\ell}) - \frac{1}{2}(n_{12,i,0}+n_{12,i,1}) - n_{21,j\ell} + \frac{1}{2} n_{12}$$

which by use of equation (6.2.4) equals

$$n_{21,j\ell} - \frac{1}{2}(n_{12,i,0}+n_{12,i,1}) - n_{12,j\ell} + \frac{1}{2} n_{12} .$$

Since $n_{12,i,0} + n_{12,i,1} = n_{12}$ (the number of times an effect occurs at the high level plus the number of times at the low level equals $n_{12}$), this sum of the two elements is zero and $M_1Q_{12}M_2'$ can therefore be expressed in the simplified form

$$M_1Q_{12}M_2' = \tag{6.2.5}$$

$$\begin{bmatrix} q_{12,1,0,1,0} & q_{12,1,0,1,1} \cdots & q_{12,1,0,k_2,0} & q_{12,1,0,k_2,1} \\ -q_{12,1,0,1,0} & -q_{12,1,0,1,1} \cdots & -q_{12,1,0,k_2,0} & -q_{12,1,0,k_2,1} \\ \vdots & \vdots & \vdots & \vdots \\ q_{12,k_1,0,1,0} & q_{12,k_1,0,1,1} \cdots & q_{12,k_1,0,k_2,0} & q_{12,k_1,0,k_2,1} \\ -q_{12,k_1,0,1,0} & -q_{12,k_1,0,1,1} \cdots & -q_{12,k_1,0,k_2,0} & -q_{12,k_1,0,k_2,1} \end{bmatrix}$$

where $q_{12,i,0,j\ell} = n_{12,i,0,j\ell} - \frac{1}{2}\, n_{12,i,0} - \frac{1}{2}\, n_{21,j,\ell} + \frac{1}{4} n_{12}$.

Consider next the elements associated with the high and low levels of an effect on $V_2$ for any level of any effect on $V_1$. These elements, obtained from matrix (6.2.5) are denoted $\pm\, q_{12,i,0,j,1}$ and $\pm\, q_{12,i,0,j,0}$. Since considering either the high or the low level will give the same result, we consider the low level on $V_1$:

$$q_{12,i,0,j,0} = n_{12,ikj,0} - \frac{1}{2}\, n_{12,ik} - \frac{1}{2}\, n_{21,j0} + \frac{1}{4}\, n_{12} \;.$$

$$q_{12,i,0,j,1} = n_{12,ikj,1} - \frac{1}{2}\, n_{12,ik} - \frac{1}{2}\, n_{21,j,1} + \frac{1}{4}\, n_{12} \;.$$

Summing these two equations gives

$$(n_{12,ikj,0}+n_{12,ijk,1})-n_{12,ik} - \frac{1}{2}(n_{21,j,0}+n_{21,j,1}) + \frac{1}{2} n_{12}$$

which after equation (6.2.3) is used, gives

$$n_{12,ik}-n_{12,ik} - \frac{1}{2}(n_{21,j,0}+n_{21,j,1}) + \frac{1}{2} n_{12} .$$

For $V_2$ as for $V_1$, $n_{21,j,0} + n_{21,j,1} = n_{12}$ and therefore

$$q_{12,i,0,j,0} + q_{12,i,0,j,1} = 0$$

or

$$q_{12,i,0,j,0} = -q_{12,i,0,j,1} .$$

Using this fact along with the results in matrix (6.2.5) gives, after defining $q_{ij} = q_{12,i,0,j,0}$ $(i = 1,\ldots,k_1,$ $j = 1,\ldots,k_2)$,

$$M_1Q_{12}M_2 = \begin{bmatrix} q_{11} & -q_{11} & q_{12} & -q_{12} & \cdots & -q_{1k_2} \\ -q_{11} & q_{11} & -q_{12} & q_{12} & \cdots & q_{1k_2} \\ \vdots & \vdots & \vdots & \vdots & & \\ -q_{k_11} & q_{k_11} & -q_{k_12} & q_{k_12} & \cdots & q_{k_1k_2} \end{bmatrix} .$$

This can more easily be expressed as

$$M_1 Q_{12} M_2' = \begin{bmatrix} q_{11} & q_{12} & \cdots & q_{1k_2} \\ q_{21} & q_{22} & \cdots & q_{2k_2} \\ \vdots & \vdots & & \vdots \\ q_{k_1 1} & q_{k_1 2} & & q_{k_1 k_2} \end{bmatrix} \otimes (2I_2 - J_2) \; .$$

Consider now the value $q_{ij}$ ,

$$q_{ij} = n_{12,i,0,j,0} - \tfrac{1}{2} n_{12,i,0} - \tfrac{1}{2} n_{21,j,0} + \tfrac{1}{4}\, n_{12} \qquad (6.2.6)$$

= [the number of tc's in which effect i appears at the low level on $V_1$ while effect j is also at the low level on $V_2$]

$-\frac{1}{2}$ [the number of tc's in which i is at the low level on the $n_{12}$ units + the number of tc's in which j is at the low level] + $\frac{1}{4}$ [the number of tc's where $V_1$ and $V_2$ are both measured].

There are two situations to consider: the simple case where the $i^{th}$ effect on $V_1$ is equivalent to the $j^{th}$ effect on $V_2$ and the case where they are not equivalent. Obviously when the $i^{th}$ effect on $V_1$ = the $j^{th}$ effect on $V_2$ then

$$n_{12,i,0,j,0} = n_{12,i,0} = n_{21,j,0}$$

and thus

$$q_{ij} = \frac{1}{4} n_{12} \; . \qquad (6.2.7)$$

To determine the value of $q_{ij}$ when the $i^{th}$ effect on $V_1$ is not the $j^{th}$ effect on $V_2$ we will first return to some work done on the HMGLM(F) design. Recall from Chapter 4 that we assumed that there was no aliasing between effects of interest for each response and that effects influencing $V_1$ were not aliased with effects influencing $V_2$ unless of course the two effects were equal. For the HMGLM(F) design we showed that if the $i^{th}$ effect on $V_1$ was not the same as the $j^{th}$ effect on $V_2$ that $q_{ij} = 0$ (using the term $q_{ij}$ as just defined). We also found that when the $i^{th}$ and $j^{th}$ effects were identical $q_{ij} = \frac{1}{4} n_{ij}$, as was found here. In Chapter 4 we were working with the special case of the MGLM design where m = 0. Through our knowledge of the designs at m = 0, it will be easier to show how $M_1 Q_{12} M_2'$ changes as m changes.

We denote $q_{ij}$ for the HMGLM design by $q^*_{ij}$ with

$$q^*_{ij} = n^*_{12,i,0,j,0} - \frac{1}{2} n^*_{12,i,0} - \frac{1}{2} n^*_{21,j,0} + \frac{1}{4} n^*_{12} \; .$$

We are only interested here in values of $q_{ij}$ when effect

$i \neq$ effect $j$ since equation (6.2.7) covers the situation where $i = j$. Using $q^*_{ij}$ as a reference point will make it easier to determine $q_{ij}$ as $m$ changes. Consider first $m = 1$. There are several possible relationships between the levels of the $i^{th}$ and $j^{th}$ effects on tc, which will be used to denote the treatment combination applied to the unit not in common. Both effects could be at the high level on $tc_1$, or at the low level, or one could be at the high level while the other is at the low level. The question is how this affects $q_{ij}$. Suppose that both, effect $i$ on $V_1$ and effect $j$ on $V_2$, are at the high level on $tc_1$: Then

$$n_{12,i,0,j,0} = n^*_{12,i,0,j,0} ,$$

$$n_{12,i,0} = n^*_{12,i,0} ,$$

$$n_{21,j,0} = n^*_{21,j,0} ,$$

and of course $n_{12} = n^*_{12}-1$ since $n_{12} = n^*_{12}-m$. Thus

$$\begin{aligned} q_{ij} &= n^*_{12,i,0,j,0}-\tfrac{1}{2}n^*_{12,i,0}-\tfrac{1}{2}n^*_{21,j,0}+\tfrac{1}{4}(n^*_{12}-1) \\ &= q^*_{ij} - \tfrac{1}{4} = -\tfrac{1}{4} . \end{aligned} \tag{6.2.8}$$

Suppose i and j were both at the low level on $tc_1$. Then

$$n_{12,i,0,j,0} = n^*_{12,i,0,j,0} - 1, \quad n_{21,j,0} = n^*_{21,j,0}-1$$

$$n_{12,i,0} = n^*_{12,i,0} - 1, \quad \text{and} \quad n_{21,j,0} = n^*_{21,j,0} - 1 ,$$

thus

$$q_{ij} = (n^*_{12,i,0,j,0}-1)-\tfrac{1}{2}(n^*_{12,i,0}-1)-\tfrac{1}{2}(n^*_{21,j,0}-1)+\tfrac{1}{4}(n_{12}-1)$$

$$= q^*_{ij} - 1 + \frac{1}{2} + \frac{1}{2} - \frac{1}{4} = - \frac{1}{4} . \qquad (6.2.9)$$

Suppose now that on $tc_1$, i was at the low level and j was at the high level. Then

$$n_{12,i,0,j,0} = n^*_{12,i,0,j,0}, \; n_{12} = n^*_{12} - 1,$$

$$n_{12,i,0} = n^*_{12,i,0} - 1, \quad \text{and} \quad n_{21,j,0} = n^*_{21,j,0} .$$

Thus

$$q_{12} = q^*_{12} + \frac{1}{2} - \frac{1}{4} = \frac{1}{4} . \qquad (6.2.10)$$

The same result would have been attained had i been at the high level and j at the low level on $tc_1$.

We now define a $(k_1 \times k_2)$ matrix F which will allow us to condense the results just determined.

$$F = \begin{bmatrix} a_1b_1 & a_1b_2 & \cdots & a_1b_{k_2} \\ a_2b_1 & a_2b_2 & \cdots & a_2b_{k_2} \\ \vdots & \vdots & & \vdots \\ a_{k_1}b_1 & a_{k_1}b_2 & \cdots & a_{k_1}b_{k_2} \end{bmatrix} \qquad (6.2.11)$$

where

$a_i = 1$ if the $i^{th}$ effect on $V_1$ was at the low level on $tc_{1,1}$ ,

$=-1$ if it was at the high level $(i = 1,\ldots,k_1)$ ,

$b_j = 1$ if the $j^{th}$ effect on $V_2$ was at the low level on $tc_{1,2}$ ,

$=-1$ if it was at the high level $(j = 1,\ldots,k_2)$ .

(This method is appropriate when the effect is a main effect or an interaction where the convention of the high or low level of an interaction will again be used as it was defined in Chapter 2.) The matrix F is thus a matrix of positive and negative ones, being positive if both effects are at the same level and being negative otherwise.

Incorporating equations (6.2.7) - (6.2.10) gives the following general expression for the $M_1Q_{12}M_2'$ matrix with

$m = 1$:

$$M_1Q_{12}M_2' = \frac{1}{4}[s_2 2^{d_2 2} D - F] \otimes (2I_2 - J_2) \ , \qquad (6.2.12)$$

where D and F were defined in (4.2.27) and (6.2.11) respectively.

Consider now the case where $V_2$ is again measured on $s_2 2^{d_2 2}$ units but on two of the units $V_1$ is not measured, i.e., $m = 2$. The form of $q_{ij}$ (equation (6.2.6)) is applicable to this situation so our problem involves determining how $n_{12i0j0}$, $n_{12i0}$, $n_{21j0}$ change. Assume that the first unit where only $V_1$ is measured is the $x^{th}$ unit but for ease of notation the treatment combination will be denoted by $tc_1 = (tc_{1,1}, tc_{1,2})$. The second unit, the $y^{th}$ unit, has the treatment combination which will be denoted by $tc_2$. Once again the notation $n^*_{12,i,0,j,0}$, $n^*_{12i,0}$, $n^*_{21j,0}$ will be used to represent the values in $q^*_{ij}$ for a HMGLM design with the value of $q_{ij}$ for the CRMGLM design to be determined through the relationship with $q^*_{ij}$.

Consider a case where effect i on $V_1$ was at the low level on both $tc_{1,1}$ and $tc_{1,2}$ and effect j on $V_2$ was at the low level on both $tc_{1,2}$ and $tc_{2,2}$. Comparison of $q_{ij}$ to $q^*_{ij}$ gives

$$n_{12i,0,j,0} = n^*_{12i,0,j,0} - 2,\ n_{12} = n^*_{12} - 2,$$

$$n_{12i,0} = n^*_{12i,0} - 2,\ n_{21j,0} = n^*_{21,j,0} - 2.$$

Thus

$$q_{ij} = (n^*_{12i,0,j,0}-2)-\frac{1}{2}(n^*_{12i,0}-2+n^*_{21j,0}-2)+\frac{1}{4}(n^*_{12}-2)$$

$$= q^*_{ij} - 2 + 2 - \frac{1}{2} = -\frac{1}{2}\ . \qquad (6.2.13)$$

The value $q_{ij}$ can also be determined by using as a reference point the value of $q_{ij}$ denoted by $q_{ij*}$ that would have been obtained had a design been constructed with m = 1 with the one omitted unit having treatment combination $tc_1$. We then determine how $q_{ij*}$ changes when another unit is omitted, i.e., m = 2 and this unit has treatment combination $tc_2$. Thus

$$n_{12i,0,j,0} = n_{12i,0,j,0*} - 1,\ n_{12} = n_{12*} - 1$$

$$n_{12i,0} = n_{12i,0*} - 1, \text{ and } n_{21j,0} = n_{21j,0*} - 1$$

and solving for $q_{ij}$ yields

$$q_{ij} = q_{ij*} - \frac{1}{4} = -\frac{1}{4}$$

since $q_{ij*} = -\frac{1}{4}$ . This simple case with both effects at the low level on $tc_1$ and $tc_2$ was considered first for it is fairly easy to understand.

Consider now the case where effect i on $V_1$ is at the low level on $tc_{1,1}$ and effect j is at the highlevel on $tc_{1,2}$. On $tc_2$, effect i is at the high level while j is at the low level. For this situation

$$n_{12i,0,j,0} = n^*_{12i,0,j,0},\ n_{12} = n^*_{12} - 2$$

$$n_{12i,0} = n^*_{12i,0} - 1, \text{ and } n_{21j,0} = n^*_{21j,0} - 1 .$$

thus

$$q_{ij} = n^*_{12i,0,j,0} - \frac{1}{2}(n^*_{12i,0} - 1 + n^*_{21j,0} - 1) + \frac{1}{4}(n^*_{12} - 2)$$

$$= q^*_{ij} + 1 - \frac{1}{2} = \frac{1}{2} .$$

If the CRMGLM design with m = 1, where only $tc_1$ is left out, is used as the reference point rather than the HMGLM design, then, as found previously, $q_{ij*} = \frac{1}{4}$ . When we now consider leaving out the additional unit with treatment combination $tc_2$, then

$$n_{12i,0,j,0} = n_{12i,0,j,0*},\ n_{12} = n_{12*},$$

$$n_{12i,0} = n_{12i,0*}, \text{ and } n_{21j,0} = n_{21j,0*} - 1,$$

and thus

$$q_{ij} = q_{ij*} + \frac{1}{2} - \frac{1}{4} = \frac{1}{2} .$$

The matrix $M_1Q_{12}M_2'$ can therefore be expressed in a form which is an extension of (6.2.12):

$$M_1Q_{12}M_2' = \frac{1}{4}(s_2 2^{d_2}D-F_1-F_2) \otimes (2I_2-J_2)$$

where $F_1$ is determined by (6.2.11) using $tc_1$ to determine $a_i$ and $b_j$ and $F_2$ is determined in the same fashion from $tc_2$.

Following this general approach, this method is easily extended to any $m \leq s_2 2^{d_2}$, as given in the following lemma:

<u>Lemma 6.2.1</u> For a CRMGLM(F) design with $m \leq s_2 2^{d_2}$

$$M_1Q_{12}M_2' = \frac{1}{4}[s_2 2^{d_2}D - \sum_{k=1}^{m} F_k] \otimes (2I_2-J_2) \qquad (6.2.14)$$

where D is defined by matrix (6.2.11) which is associated with the $k^{th}$ omitted treatment combination $tc_k$ $(k = 1,\ldots,m)$. (When the term 'omitted' treatment combination is used, we are referring to a tc applied to a unit where $V_2$ is measured but not $V_1$, i.e., one of the m units that distinguishes this design from a HMGLM design. The importance of this omitted tc is that the off-diagonal covariance matrix is changed because this tc is not measured on a unit where $V_1$ is also measured. From this point of view this tc is actually omitted from the covariance structure and it was out of this context that the term 'omitted' was derived.)

It is interesting to now consider what would happen if, say, $m = 2^{d_2}$ and the m units were chosen so that an entire fraction of units on $V_2$ was not measured on units where $V_1$ was measured. This is of course equivalent to using a RMGLM design with $\alpha = 1$ and we would thus hope to attain the same value of $M_1Q_{12}M_2'$. We could also consider a case where all m units were not chosen from the same block but were picked so that these individual elements formed a complete fractional factorial. Care must be taken here to make sure that effects on $V_1$ are not aliased with effects on $V_2$ because of the units chosen. (If a block of units is chosen as in the RMGLM design then this aliasing is not a problem.) Complications can enter here if $2^{d_1} > 2^{d_2}$ because it is then possible that some effect influencing $V_1$ but not $V_2$, may be at the high level on all $2^{d_2}$ omitted units or possibly entirely at the low level (consider for example the effect B on the first 4 units in Example 4.2.1). As long as the levels of this effect occur with the high and low levels of other effects an equal number of times then this presents no problem.

Consider first the case where the $i^{th}$ effect on $V_1$ is not equal to the $j^{th}$ effect on $V_2$. On the m omitted units an effect, say, the $i^{th}$ effect, can appear at the low level either 0, $\frac{m}{2}$, or m times. If the $i^{th}$ effect appears at the low level either 0 or m times, then all effects on $V_2$ must appear $\frac{m}{2}$ times at the low level since a complete fraction was chosen. The following equivalences are thus valid

$$n_{12i,0,j,0} = n^*_{12i,0,j,0} - x(\tfrac{m}{2}),\quad n_{12} = n^*_{12} - m\ ,$$

$$n_{12i,0} = n_{12i,0} - xm, \text{ and } n_{21j,0} = n^*_{21j,0} - \frac{m}{2}\ ,$$

where $x = 0, \frac{1}{2}$, or 1. Therefore

$$q_{12} = q^*_{12} - x(\tfrac{m}{2}) + \frac{1}{2}\,xm + \frac{1}{2}\,\frac{m}{2} - \frac{m}{4} = 0$$

as was obtained for a RMGLM design when $i \neq j$.

Consider now the case where the $i^{th}$ effect on $V_1$ equals the $j^{th}$ effect on $V_2$. Since the $j^{th}$ effect appears in the complete fraction of $m = 2^{d_2}$ units $\frac{m}{2}$ times then so also does the $i^{th}$ effect on $V_1$. Therefore

$$n_{12i,0,j,0} = n^*_{12i,0,j,0} - \frac{m}{2}\ , \ n_{12} = n^*_{12} - m\ ,$$

$$n_{12i,0} = n^*_{12i,0} - \frac{m}{2}\ , \text{ and } n_{21j,0} = n^*_{21j,0} - \frac{m}{2}$$

and thus

$$q_{ij} = q^*_{ij} - \frac{m}{4}\ .$$

Upon combining this information we determine that $\sum_{k=1}^{m} F_m$ is a matrix of $k_{12}$ elements $\frac{m}{4} = 2^{d_2-2}$ with the remaining elements equal to zero. These non-zero elements are in the $(i,j)^{th}$ positions when the $i^{th}$ effect on $V_1$ is equivalent to the $j^{th}$ effect on $V_2$ ($i = 1,\ldots,k_1$, $j = 1,\ldots k_2$). Thus when this matrix is subtracted from the matrix $s_2 2^{d_2} D$, the same matrix that was found for the RMGLM design is obtained, as would be expected.

If we had considered $m = 2^{d_1}$ and removed a fraction of units on $V_1$ rather than $V_2$, then the same result would have been obtained. Also had we used $m = \alpha 2^{d_1}$ the variable x could now assume one of the values $0, \frac{1}{\alpha}, \frac{2}{\alpha}, \ldots, \frac{\alpha}{\alpha}, \frac{1}{2}$ but the same final result would be achieved.

Using $M_1 Q_{12} M_2'$ and equation (3.3.12), we can now determine a general form of $\mathrm{Cov}(\hat{\underline{\tau}}_1, \hat{\underline{\tau}}_2)$ to be:

$$\mathrm{Cov}(\hat{\underline{\tau}}_1,\hat{\underline{\tau}}_2) = \sigma_{12}D_1^-M_1Q_{12}M_2'D_2^- = \frac{4\sigma_{12}}{s_1 2^{d_1} s_2 2^{d_2}} (M_1Q_{12}M_2') .$$

The covariance matrix of estimable functions can now be found where $P_1$ and $P_2$ were defined in Section 4.2:

$$\begin{aligned}\mathrm{Cov}(CR) &= P_1\ \mathrm{Cov}(\hat{\underline{\tau}}_1,\hat{\underline{\tau}}_2)P_2' \\ &= \frac{2\sigma_{12}}{s_1 2^{d_1} s_2 2^{d_2}} [s_2 2^{d_2}D - \sum_{k=1}^{m} F_k].\end{aligned} \tag{6.2.15}$$

Matrix (6.2.1) can be completed by employing equations (6.2.2) and (6.2.15) giving $\mathrm{Var}(P\hat{\underline{\tau}})$ as

$$D(CR) = 2\begin{bmatrix} \dfrac{\sigma_{11}}{s_1 2^{d_1}} I_{k_1} & \dfrac{\sigma_{12}}{s_1 2^{d_1} s_2 2^{d_2}}(s_2 2^{d_2}D - \sum_{k=1}^{m} F_k)' \\ \dfrac{\sigma_{12}}{s_1 2^{d_1} s_2 2^{d_2}}(s_2 2^{d_2}D - \sum_{k=1}^{m} F_k) & \dfrac{\sigma_{22}}{s_2 2^{d_2}} I_{k_2} \end{bmatrix} \tag{6.2.16}$$

## 6.3 The Determinant of $\mathrm{Var}(P\hat{\underline{\tau}})$ in the CRMGLM(F) Design

In this section we shall attempt to find the determinant of $\mathrm{Var}(P\hat{\underline{\tau}})$, denoted $|D(CR)|$ for the two response CRMGLM design. Theorem 5.2.1, equation (5.2.2) will be employed to find $|D(CR)|$ using $D(CR)$ of equation (6.2.16)

$$|D(CR)| = 2^{k_1+k_2}\left|\frac{\sigma_{11}}{s_1 2^{d_1}} I_{k_1}\right|\left|\frac{\sigma_{22}}{s_2 2^{d_2}} I_{k_2}\right.$$

$$\left. - \left(\frac{\sigma_{12}}{s_1 2^{d_1} s_2 2^{d_2}}\right)^2 \left(\frac{s_1 2^{d_1}}{\sigma_{11}}\right) \cdot G' I_{k_2} G\right|$$

where $G = s_2 2^{d_2} D - \sum_{k=1}^{m} F_k$.

$$|D(CR)| = 2^{k_1+k_2}\left(\frac{\sigma_{11}}{s_1 2^{d_1}}\right)^{k_1}\left(\frac{\sigma_{22}}{s_2 2^{d_2}}\right)^{k_2}\left|I_{k_2} - \frac{\sigma_{12}^2}{s_1 2^{d_1} s_2 2^{d_2}\sigma_{11}\sigma_{22}} G'G\right|$$

$$= 2^{k_2^*}\left(\frac{\sigma_{11}}{s_1 2^{d_1}}\right)^{k_1}\left(\frac{\sigma_{22}}{s_2 2^{d_2}}\right)^{k_2}\left|I_{k_2} - \rho^2 \frac{1}{s_1 2^{d_1} s_2 2^{d_2}} G'G\right| \tag{6.3.1}$$

where $\rho^2 = \frac{\sigma_{12}^2}{\sigma_{11}\sigma_{22}}$ . We shall use the notation

$$|I_{k_2} - \rho^2 \frac{1}{s_1 2^{d_1} s_2 2^{d_2}} G'G| = (s_1 2^{d_1} s_2 2^{d_2})^{-k_2} |E|$$

where

$$E = s_1 2^{d_1} s_2 2^{d_2} I_{k_2} - \rho^2 G'G . \qquad (6.3.2)$$

The matrix G is dependent upon not only how many units are omitted from common measurement (m units), but also the relationships between the treatment combinations of these units. We would like to be able to express G as strictly a function of m and $n_{12}$, a situation allowing for a relatively straight forward approach to finding the optimal design. However, as just noted, G depends also upon the relationship between the treatment combinations. Since there are many possible choices of treatment combinations, it will be very hard to generalize the form of G'G.

Recall that we are interested in the CRMGLM designs so that they can be compared to the optimum HMGLM design. As m gets larger and larger, more and more money must be used for preparation of experimental units (the set-up cost associated with $\psi_0$). Thus $s_1^*$ and $s_2^*$ for a CRMGLM design will not be larger than $s_1$ and $s_2$ for a HMGLM design.

Therefore if $|D(CR)|$ is to be less than $|D(H)|$ then it must be due to the fact that the off-diagonal elements in G'G offset the loss in the diagonal elements when compared to the diagonal matrix D'D of the HMGLM design.

The determinant (6.3.2) is dominated by the main diagonal terms due to the magnitude of $(s_1 2^{d_1}, s_2 2^{d_2})$ in comparison to $(s_2 2^{d_2} - m)^2$. Thus for a constant m, for any particular $s_1$ and $s_2$, minimization of $|D(CR)|$ is equivalent to minimizing (6.3.2) which is analogous to maximizing the main diagonal elements of G'G. These points will be discussed further in relation to the following example.

Example 6.3.1 Consider the following situation: $v = 4$, $v_1 = 3$, $v_2 = 3$, $k_1 = 3$, $k_2 = 3$, $k_{12} = 2$, $d_1 = 3$, $d_2 = 2$, $s_1 = 3$, $s_2 = 5$. Assume that $V_1$ is affected by factors A, C, D and $V_2$ is affected by factors A, B, D and that we are interested in contrasts on only the main effects. In the following examples, $s_2 2^{d_2} D = \begin{bmatrix} 20 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 20 \end{bmatrix}$ and $|E| = |480\ I_3 - \rho^2\ G'G|$. The following are the matrices $X_1$ and $X_2$, the reduced design matrices for the two responses:

| | | | $V_1$ | | | | | | | $V_2$ | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $tc_1$ | A | | C | | D | | | A | | B | | D | | $tc_2$ |
| '1' | 1 | 0 | 1 | 0 | 1 | 0 | 1 | 1 | 0 | 1 | 0 | 1 | 0 | '1' |
| a | 0 | 1 | 1 | 0 | 1 | 0 | 2 | 0 | 1 | 0 | 1 | 1 | 0 | ab |
| ad | 0 | 1 | 1 | 0 | 0 | 1 | 3 | 0 | 1 | 1 | 0 | 0 | 1 | ad |
| d | 1 | 0 | 1 | 0 | 0 | 1 | 4 | 1 | 0 | 0 | 1 | 0 | 1 | bd |
| ac | 0 | 1 | 0 | 1 | 1 | 0 | 5 | 0 | 1 | 1 | 0 | 1 | 0 | a |
| c | 1 | 0 | 0 | 1 | 1 | 0 | 6 | 1 | 0 | 0 | 1 | 1 | 0 | b |
| cd | 1 | 0 | 0 | 1 | 0 | 1 | 7 | 1 | 0 | 1 | 0 | 0 | 1 | d |
| acd | 0 | 1 | 0 | 1 | 0 | 1 | 8 | 0 | 1 | 0 | 1 | 0 | 1 | abd |
| c | 1 | 0 | 1 | 0 | 1 | 0 | 9 | 1 | 0 | 1 | 0 | 1 | 0 | '1' |
| ac | 0 | 1 | 1 | 0 | 1 | 0 | 10 | 0 | 1 | 0 | 1 | 1 | 0 | ab |
| acd | 0 | 1 | 1 | 0 | 0 | 1 | 11 | 0 | 1 | 1 | 0 | 0 | 1 | ad |
| cd | 1 | 0 | 1 | 0 | 0 | 1 | 12 | 1 | 0 | 0 | 1 | 0 | 1 | bd |
| '1' | 1 | 0 | 0 | 1 | 1 | 0 | 13 | 1 | 0 | 0 | 1 | 1 | 0 | b |
| a | 0 | 1 | 0 | 1 | 1 | 0 | 14 | 0 | 1 | 1 | 0 | 1 | 0 | a |
| ad | 0 | 1 | 0 | 1 | 0 | 1 | 15 | 0 | 1 | 0 | 1 | 0 | 1 | abd |
| d | 1 | 0 | 0 | 1 | 0 | 1 | 16 | 1 | 0 | 1 | 0 | 0 | 1 | d |
| '1' | 1 | 0 | 1 | 0 | 1 | 0 | 17 | 1 | 0 | 1 | 0 | 1 | 0 | '1' |
| a | 0 | 1 | 1 | 0 | 1 | 0 | 18 | 0 | 1 | 0 | 1 | 1 | 0 | ab |
| ad | 0 | 1 | 1 | 0 | 0 | 1 | 19 | 0 | 1 | 1 | 0 | 0 | 1 | ad |
| d | 1 | 0 | 1 | 0 | 0 | 1 | 20 | 1 | 0 | 0 | 1 | 0 | 1 | bd |
| ac | 0 | 1 | 0 | 1 | 1 | 0 | 21 | | | | | | | |
| c | 1 | 0 | 0 | 1 | 1 | 0 | 22 | | | | | | | |
| cd | 1 | 0 | 0 | 1 | 0 | 1 | 23 | | | | | | | |
| acd | 0 | 1 | 0 | 1 | | 0 | 24 | | | | | | | |

Table 6.3.1 contains the appropriate $F_k$ matrices when the m omitted units include the $k^{th}$ unit with $tc_k = (tc_{k,1}, tc_{k,2})$, the tc applied to the whole unit and the respective tc affecting $V_1$ and $V_2$.

Table 6.3.1
F Matrices for Different CRMGLM Designs

| Unit # | Unit tc | F Matrix | | | Unit # | Unit tc | F Matrix | | |
|---|---|---|---|---|---|---|---|---|---|
| | | 1 | 1 | 1 | | | 1 | -1 | 1 |
| 1 | '1' | 1 | 1 | 1 | 13 | b | 1 | -1 | 1 |
| | | 1 | 1 | 1 | | | 1 | -1 | 1 |
| | | 1 | 1 | -1 | | | 1 | 1 | 1 |
| 2 | ab | -1 | -1 | 1 | 15 | abd | -1 | -1 | -1 |
| | | -1 | -1 | 1 | | | 1 | 1 | 1 |
| | | 1 | -1 | -1 | | | 1 | 1 | 1 |
| 4 | bd | 1 | -1 | -1 | 17 | '1' | 1 | 1 | 1 |
| | | -1 | 1 | 1 | | | 1 | 1 | 1 |
| | | 1 | 1 | -1 | | | 1 | 1 | -1 |
| 7 | cd | -1 | -1 | 1 | 18 | ab | -1 | -1 | 1 |
| | | -1 | -1 | 1 | | | -1 | -1 | 1 |
| | | 1 | 1 | 1 | | | 1 | -1 | 1 |
| 8 | abcd | 1 | 1 | 1 | 19 | ad | -1 | 1 | -1 |
| | | 1 | 1 | 1 | | | 1 | -1 | 1 |
| | | 1 | -1 | -1 | | | | | |
| 12 | bcd | -1 | 1 | 1 | | | | | |
| | | -1 | 1 | 1 | | | | | |

Some of these F matrices will be used in the following cases. They illustrate most of the different F matrices that are possible in this example.

In the following specific CRMGLM(F) cases of this example, contained in Table 6.3.2, the m tc's that are to be omitted in this specific case are given first. Their associated F matrices have just been enumerated. The G matrix is first determined and then the G'G matrix is found. We will denote the elements of G by $\{g_{ij}\}$ and the elements of G'G by $\{gg_{ij}\}$. Finally for each case, $|E|$ is found, first when $\rho^2 = 1$, then when $\rho^2 = .5$. Examples A through D have m = 1; examples E through J have m = 2; and examples K through O have m = 3.

There are several important things to be noted from these cases. First, $g_{11}$ and $g_{33}$ are always $s_2 2^{d_2} - m$. The $s_2 2^{d_2}$ portion of this term comes from the matrix $s_2 2^{d_2} D$ where the D matrix has zeros in all positions except for having unity elements in the (1,1) and (3,3) positions (since effects A and D influence both responses). The -m portion comes from $- \sum_{k=1}^{m} F_k$. Each $F_k$ always has a plus one in the (1,1) and (3,3) positions since effects A and D must be at the same level on $tc_{k,1}$ and $tc_{k,2}$.

Table 6.3.2

G, G'G, and $|E|$ for Different CRMGLM Designs

| Case | tc | G | | | G'G | | | $\lvert E(\rho^2 = 1.)\rvert$<br>$\lvert E(\rho^2 = .5)\rvert$ |
|---|---|---|---|---|---|---|---|---|
| A | $tc_1$=('1','1') | 19 | -1 | -1 | 363 | -17 | -37 | 5,830,400 |
| | | -1 | -1 | -1 | -17 | 3 | -17 | 42,431,200 |
| | | -1 | -1 | 19 | -37 | -17 | 363 | |
| | | 19 | -1 | 1 | 363 | -17 | 37 | 5,830,400 |
| B | $tc_2$=(a,ab) | 1 | 1 | -1 | -17 | 3 | 17 | 42,431,200 |
| | | 1 | 1 | 19 | 37 | 17 | 363 | |
| | | 19 | 1 | 1 | 363 | 17 | 37 | 5,830,400 |
| C | $tc_{12}$=(cd,bd) | 1 | -1 | -1 | 17 | 3 | -17 | 42,431,200 |
| | | 1 | -1 | 19 | 37 | -17 | 363 | |
| | | 19 | 1 | -1 | 363 | 17 | -37 | 5,830,400 |
| D | $tc_{19}$=(ad,ad) | 1 | -1 | 1 | 17 | 3 | 17 | 42,431,200 |
| | | -1 | 1 | 19 | -37 | 17 | 363 | |

Table 6.3.2 - (Continued)

| Case | tc | G | | | G'G | | | $\lvert E(\rho^2 = 1.)\rvert$ <br> $\lvert E(\rho^2 = .5)\rvert$ |
|---|---|---|---|---|---|---|---|---|
| | $tc_1$ | 18 | -2 | 0 | 324 | -36 | 0 | 11,089,920 |
| E | $tc_2$ | 0 | 0 | -2 | -36 | 4 | 0 | 47,930,880 |
| | | 0 | 0 | 18 | 0 | 0 | 328 | |
| | $tc_1$ | 18 | 0 | 0 | 324 | 0 | 0 | 11,032,320 |
| F | $tc_{12}$ | 0 | -2 | -2 | 0 | 8 | -32 | 47,750,880 |
| | | 0 | -2 | 18 | 0 | -32 | 328 | |
| | $tc_1$ | 18 | 0 | -2 | 328 | 0 | -72 | 8,529,920 |
| G | $tc_{19}$ | 0 | -2 | 0 | 0 | 4 | 0 | 47,111,680 |
| | | -2 | 0 | 18 | -72 | 0 | 328 | |
| | $tc_2$ | 18 | 0 | -2 | 332 | 0 | 68 | 8,294,400 |
| H | $tc_{12}$ | 2 | 0 | -2 | 0 | 0 | 0 | 46,771,200 |
| | | 2 | 0 | 18 | 68 | 0 | 332 | |

Table 6.3.2 - (Continued)

| Case | tc | G | | | G'G | | | $\lvert E(\rho^2 = 1.)\rvert$ <br> $\lvert E(\rho^2 = .5)\rvert$ |
|---|---|---|---|---|---|---|---|---|
| | $tc_1$ | 18 | -2 | -2 | 332 | -28 | -68 | 7,961,600 |
| I | $tc_8$=(acd,abd) | -2 | -2 | -2 | -28 | 12 | -28 | 46,076,800 |
| | | -2 | -2 | 18 | -68 | -28 | 332 | |
| | $tc_7$=(cd,d) | 18 | -2 | 2 | 332 | -28 | 68 | 7,961,600 |
| J | $tc_{18}$=(a,ab) | 2 | 2 | -2 | -28 | 12 | 28 | 46,076,800 |
| | | 2 | 2 | 18 | 68 | 28 | 332 | |
| | $tc_1$ | 17 | -1 | 1 | 291 | -19 | 31 | 15,733,760 |
| K | $tc_2$ | 1 | -1 | -3 | -19 | 3 | -15 | 52,733,440 |
| | $tc_{12}$ | 1 | -1 | 17 | 31 | -15 | 299 | |
| | $tc_1$ | 17 | -1 | -1 | 291 | -19 | -35 | 16,292,864 |
| L | $tc_2$ | 1 | -1 | -1 | -19 | 3 | 19 | 53,329,408 |
| | $tc_{19}$ | -1 | 1 | 17 | -35 | 19 | 291 | |

Table 6.3.2 - (Continued)

| Case | tc | G | | | G'G | | | $\lvert E(\rho^2 = 1.)\rvert$ / $\lvert E(\rho^2 = .5)\rvert$ |
|---|---|---|---|---|---|---|---|---|
| | $tc_1$ | 17 | -3 | -1 | 291 | -49 | -31 | 15,169,280 |
| M | $tc_8$ | -1 | -1 | -3 | -49 | 11 | -11 | 52,138,720 |
| | $tc_{18}$ | -1 | -1 | -17 | -31 | -11 | 299 | |
| | $tc_1$ | 17 | -3 | -3 | 307 | -33 | -93 | 9,465,600 |
| N | $tc_8$ | -3 | -3 | -3 | -33 | 27 | -33 | 48,568,800 |
| | $tc_{17}$=('1','1') | -3 | -3 | 17 | -93 | -33 | 307 | |
| | $tc_2$ | 17 | -3 | 3 | 307 | -33 | 93 | 9,465,600 |
| O | $tc_7$=(cd,d) | 3 | 3 | -3 | -33 | 27 | 33 | 48,568,800 |
| | $tc_{18}$ | 3 | 3 | 17 | 93 | 33 | 307 | |

Consider now $|E|$ in the first 4 cases of this example (A), (B), (C), (D). For any particular $\rho^2$, all the determinants are equal. We shall now look more closely at the $m = 1$ cases in an attempt to establish why these determinants are the same. Denote the matrix F by $\{f_{ij}\}$ and notice that

$$f_{11} = f_{33} = 1, \text{ and}$$

$$f_{13} = f_{31} = \begin{cases} 1 & \text{if effects A and D are both at the same level on the omitted tc,} \\ -1 & \text{if at different levels.} \end{cases}$$

We shall consider first the case where the effects not influencing both responses, B and C, are at the same level for the omitted tc and thus $f_{22} = 1$. With B and C at the same level then $f_{12} = f_{21}$ ( = a say) and $f_{23} = f_{32}$ (= b say). We denote the value of $f_{13}$ by c, allowing a general expression for F and G:

$$F = \begin{bmatrix} 1 & a & c \\ a & 1 & b \\ c & b & 1 \end{bmatrix} \quad \text{and} \quad G = \begin{bmatrix} n_{12} & -a & -c \\ -a & -1 & -b \\ -c & -b & n_{12} \end{bmatrix}.$$

This leads to

$$G'G = \begin{bmatrix} n_{12}+a^2+c^2 & -n_{12}a+a+bc & -2n_{12}c+ab \\ & 1+a^2+b^2 & -n_{12}b+ac+b \\ \text{(sym.)} & & n_{12}^2+b^2+c^2 \end{bmatrix}$$

$$E =$$

$$\begin{bmatrix} s_1 2^{d_1} s_2 2^{d_2} - \rho^2(n_{12}^2+a^2+c^2) & \rho^2(n_{12}a-bc-a) & \rho^2(2n_{k2}c-ab) \\ & s_1 2^{d_2} s_2 2^{d_2} - \rho^2(1+a^2+b^2) & \rho^2(n_{12}b-ac-b) \\ \text{(sym.)} & & s_1 2^{d_1} s_2 2^{d_2} - \rho^2(n_{12}^2+b^2+c^2) \end{bmatrix}$$

(6.3.3)

We now consider the elements of the matrix $E = \{e_{ij}\}$ with special attention given to the values and signs of these elements. Notice first that the diagonal elements of G'G are not influenced by the signs of a, b, and c, and thus the $e_{ii}$ values are not affected. We look now at how the off-diagonal elements of E change with respect to sign changes of a, b, and c. With the two effects B and C at the same level then:

$a = -1$ if A and B are at different levels on $tc_k$,
$\quad = 1$ otherwise,

$b = -1$ if C and D are at different levels on $tc_k$,
$\quad = 1$ otherwise,

$c = -1$ if A and D are at different levels on $tc_k$,
$\quad = 1$ otherwise.

When $c = 1$, then $a = b$ (= say $q = \pm 1$) and

$$e_{12} = \rho^2(qn_{12}-q-q) = \rho^2 q(n_{12}-2) \ , \qquad (6.3.4a)$$

$$e_{13} = \rho^2(2n_{12}-q^2) = \rho^2(2n_{12}-1), \text{ and} \qquad (6.3.4b)$$

$$e_{23} = \rho^2(qn_{12}-q-q) = \rho^2 q(n_{12}-2) \ . \qquad (6.3.4c)$$

When $c = -1$, then $a = -b$ (= say $q = \pm 1$) and

$$e_{12} = \rho^2(qn_{12}-q-q) = \rho^2 q(n_{12}-2) \ , \qquad (6.3.5a)$$

$$e_{13} = \rho^2(-2n_{12}+q^2) = -\rho^2(2n_{12}-1), \text{ and} \qquad (6.3.5b)$$

$$e_{23} = \rho^2(-qn_{12}+q+q) = -\rho^2 q(n_{12}-2) \ . \qquad (6.3.5c)$$

Two important things should be noted from the comparison of equations (6.3.4) and (6.3.5): (i) the absolute values of these off-diagonal terms are not changed by the different signs a, b, and c can assume for the situation described by these equations, and (ii) no matter what the signs of a, b, and c, the values of $e_{12}$, $e_{13}$, and $e_{23}$ are either all greater than zero, or one of these values is positive with the other two values being negative.

We consider now the situation where effects B and C occur at different levels on the omitted treatment combination and therefore $f_{22} = -1$. With B and C at different levels, then $f_{12} = -f_{21}$ (= a say) and $f_{32} = -f_{23}$ (= b say). We again denote $f_{13} = f_{31}$ by c and obtain the following general matrix expressions:

$$F = \begin{bmatrix} 1 & a & c \\ -a & -1 & -b \\ c & b & 1 \end{bmatrix} , \quad G = \begin{bmatrix} n_{12} & -a & -c \\ a & 1 & b \\ -c & -b & n_{12} \end{bmatrix} ,$$

$$G'G = \begin{bmatrix} n_{12}^2+a^2+c^2 & -an_{12}+a+bc & -2cn_{12}+ab \\ & 1+a^2+b^2 & -bn_{12}+ac+b \\ (\text{sym.}) & & n_{12}^2+b^2+c^2 \end{bmatrix} ,$$

$E =$

$$\begin{bmatrix} s_1 2^{d_1} s_2 2^{d_2} - \rho^2(n_{12}^2+a^2+c^2) & \rho^2(an_{12}-a-bc) & \rho^2(2cn_{12}-ab) \\ & s_1 2^{d_1} s_2 2^{d_2} - \rho^2(1+a^2+b^2) & \rho^2(bn_{12}-ac-b) \\ \text{(sym.)} & & s_1 2^{d_1} s_2 2^{d_2} - \rho^2(n_{12}^2+b^2+c^2) \end{bmatrix}$$

(6.3.6)

We shall once again consider the values and signs of the off-diagonal elements of E, our interest concerning how they change with respect to sign changes of a, b, and c. As before the main diagonal values, $e_{ii}$, are not affected by a sign change in a, b, or c. When the effects B and C are at different levels on the omitted treatment combinations, $tc_k$, then:

$a = -1$ if A and B are at different levels on $tc_k$,
$\quad = 1$ otherwise,

$b = -1$ if C and D are at the same level on $tc_k$,
$\quad = 1$ otherwise,

$c = -1$ if A and D are at different levels on $tc_k$,
$\quad = 1$ otherwise.

When $c = 1$, then $a = b$ (= say $q = \pm 1$) and

$$e_{12} = \rho^2(qn_{12}-q-q) = q\rho^2(n_{12}-2) \ , \qquad (6.3.7a)$$

$$e_{13} = \rho^2(2n_{12}-q^2) = \rho^2(2n_{12}-1), \text{ and} \qquad (6.3.7b)$$

$$e_{23} = \rho^2(qn_{12}-q-q) = q\rho^2(n_{12}-2) \ . \qquad (6.3.7c)$$

When $c = -1$, then $a = -b$ (= say $q = \pm 1$) and

$$e_{12} = \rho^2(qn_{12}-q-q) = q\rho^2(n_{12}-2) \qquad (6.3.8a)$$

$$e_{13} = \rho^2(-2n_{12}+q^2) = -\rho^2(2n_{12}-1), \text{ and} \qquad (6.3.8b)$$

$$e_{23} = \rho^2(-qn_{12}+q+q) = -q\rho^2(n_{12}-2) \ . \qquad (6.3.8c)$$

When comparing equations (6.3.7) and (6.3.8), as was previously noted for (6.3.4) and (6.3.5), the absolute values of the off-diagonal terms are identical. The same can be said for the comparison between (6.3.4), (6.3.5) and (6.3.7) (6.3.8). The main diagonal elements of (6.3.3) and (6.3.6) are also identical. When the signs of the off-diagonal elements are studied, $e_{12}$, $e_{13}$, and $e_{23}$ are found to be either all positive or only one is positive while the other two are negative. This once again agrees with the conclusions made when B and C were at the same level on $tc_k$.

Thus regardless of the relationship between the effects B and C, the elements of the matrix E, disregarding their signs, are the same. Denote the elements of this symmetric matrix E by

$$E = \begin{bmatrix} d & e & f \\ e & g & h \\ f & h & d \end{bmatrix} .$$

We have also shown that of the off-diagonal elements e, f, and h, either one is positive or all three are positive. We now wish to show that $|E|$ is the same for these cases. The possible matrices are

$$\text{(i)} \begin{bmatrix} d & e & f \\ e & g & h \\ f & h & d \end{bmatrix} , \qquad \text{(ii)} \begin{bmatrix} d & -e & -f \\ -e & g & h \\ -f & h & d \end{bmatrix} ,$$

$$\text{(iii)} \begin{bmatrix} d & -e & f \\ -e & g & -h \\ f & -h & d \end{bmatrix} , \text{ and } \text{(iv)} \begin{bmatrix} d & e & -f \\ e & g & -h \\ -f & -h & d \end{bmatrix} .$$

By multiplying certain rows and columns of matrices (ii), (iii), and (iv) by -1, we can show the determinant of these matrices to be equal to the determinant of the matrix (i): for matrix (ii), multiply the first row and column by -1; for matrix (iii), multiply the second row and column by -1;

and for matrix (iv), multiply the third row and column by -1. These operations make these matrices equivalent to matrix (i) and the operations have not changed the values of the determinants.

Therefore when m = 1, it does not matter which of the treatment combinations is omitted, when concerned with minimizing the determinant of the variance-covariance matrix of estimable functions, because $|D(CR)|$ is the same for each unit.

When the cases with m = 2 are considered (cases (E) through (J)), the $|E|$-values are no longer necessarily the same. Where the G matrices were very similar in the m = 1 cases, this is no longer true due to the fact that the $g_{ij}$ values can now assume the values (-2,0,2) (excluding $g_{11}$ and $g_{33}$). This of course changes the $gg_{ij}$ values even more drastically. Therefore, since the matrix G is determined by which tc's are omitted, then $|D(CR)|$ is dependent upon not only m, but also upon which tc's are omitted.

It should also be noted that cases (I) and (J) gave the same $|E|$ and that this value was less than $|E|$ given in any other case with m = 2. It was not by chance that (I) and (J) had the same $|E|$-value. Notice that in case (I), $F_1 = F_8$ and that in case (J), $F_7 = F_{18}$. Thus the values in the G matrices in both cases achieve their maximum absolute values, and the values in G'G apart from the signs, are the same.

For this example let us now consider

$$|E| = \left| \begin{bmatrix} 480 & 0 & 0 \\ 0 & 480 & 0 \\ 0 & 0 & 480 \end{bmatrix} - \rho^2 \; G'G \right|.$$

With the main diagonal terms $g_{jj} < 480$ for $m > 0$ or $\rho^2 < 1$ or $s_1 2^{d_1} \neq s_2 2^{d_2}$, the determinant of E is dominated by the main diagonal elements of E. Therefore, if we desire to minimize $|E|$ for any particular m, this is tantamount to maximizing the main diagonal elements of G'G since $\rho^2$ is a constant for any particular experiment. Recall that $gg_{jj} = \sum_{i=1}^{k_1} g_{ij}^2$ for $j = 1,\ldots,k$. Thus when chosing the m units to omit to maximize $gg_{jj}$ we must omit tc's that cause $g_{ij}$ to achieve its absolute maximum. This is exactly what is accomplished in cases (I) and (J). Obviously the only way to maximize every element of $\sum_{k=1}^{m} F_k$ is to choose the tc's so that all $F_k$'s are equal thus giving in general the following matrix:

$$\sum_{k=1}^{m} F_k = \begin{bmatrix} \pm m & \pm m & \cdots & \pm m \\ \vdots & \vdots & & \vdots \\ \pm m & \pm m & \cdots & \pm m \end{bmatrix}_{(k_1 \times k_2)} . \tag{6.3.9}$$

The case that is simplest and most easily identified is illustrated in case (I) where in the tc's all factors were either all at the high level or all at the low level giving each $F_k = J$ and thus $\Sigma F_k = mJ$. The other cases having the $F_k$'s equal give the same $|E|$ as does this case but this case is easiest to work with.

For these different cases where the 2 tc are chosen so that the F matrices are the same, it could be shown that the $|E|$ values are the same. A procedure analagous to the one used for the case m = 1 could be formulated with the a, b, and c values now being $\pm 2$'s. For the case m = 1 it may be trivially stated that all m F matrices are identical. This same type of procedure could also be used for larger values of m.

We look now at the cases where m = 3 to see if they support what was determined for m = 2. Here the G matrices are even more flexible with $g_{ij}$ assuming values (-3,-1,1,3) (excluding $g_{11}$ and $g_{33}$). The differences in the G'G matrices and thus in the $|E|$ values are even greater. Case (N) and (O) illustrate the choice of tc's giving the minimum values of $|E|$. Once again these are the cases having the $F_k$ matrices identical. The case m = 3 therefore supports the conclusions determined for m = 2. It is easy to visualize that this scheme would give the minimum $|E|$ value for not only this example but for all situations.

If we thus concern ourselves with the form of G

$$G = s_2 2^{d_2 2} D - m\, J_{k_1,k_2} \tag{6.3.10}$$

we have a lower bound for all $|E|$ values for some value m and more importantly it will also allow us to express $|D(CR)|$ as a function of $s_1$, $s_2$, and m so that an optimum design can be determined.

This method of selecting the m omitted treatment combinations for any particular $s_1$, $s_2$, and m creates a design whose $|D(CR)|$ value is less than or equal to $|D(CR)|$ given by another choice of m tc's. For some values of $s_1$, $s_2$, and m this may be a strict inequality. It is for this reason that this method of choosing the design will be said to give a 'lower bound' design. Situations where this is a strict inequality, occur for certain m values when, because of the number of experimental units, there are m tc's in the design which give the same F matrix. For the situation described in Example 6.3.1, if m > 3 then equation (6.3.10) gives a G matrix that cannot be realistically attained. This equation assumes that there are at least m tc's that give identical F matrices, when for this example there are a maximum of 3 units having these similar matrices. Even for these cases however we will continue to use the G matrix, (6.3.10). If it happens that a 'lower bound' design is optimum and that this design is not possible because of the comparative values $s_1$, $s_2$, and m then the actual situation must be considered and the optimal HMGLM design compared to the best possible CRMGLM design for this situation. This problem will be discussed in greater detail at a later point.

Now that we have determined a general expression for the G matrix which gives a lower bound for $|E|$ we can find a general form of $G'G$ and then the general form of E. At this point we can proceed to find $|E|$ which along with equation (6.3.1) gives the form of $|D(CR)|$ in terms of the variables $s_1$, $s_2$, and m, thus accomplishing the objective of this section.

To simplify the notation, we will assume that the $k_{12}$ unity elements of D will be the first $k_{12}$ diagonal elements. All that this assumes is that if we denote the $k_1$ effects influencing $V_1$ by $A_1,\ldots,A_{k_1}$ and the $k_2$ effects influencing $V_2$ by $B_1,\ldots,B_{k_2}$ then effect $A_j$ = effect $B_j$ $(j = 1,\ldots,k_{12})$. Thus this is strictly a matter of convenience and has no effect on the determinant $|E|$.

The result of this assumption is that the first $k_{12}$ diagonal elements of G are $n_{12}$ with the remaining $k_2$-$k_{12}$ elements and the off-diagonal elements being equal to -m. Thus

$$G = \left[\begin{array}{cccc|ccc} n_{12} & -m & \cdots & -m & -m & \cdots & -m \\ -m & n_{12} & & -m & -m & \cdots & -m \\ \vdots & & \ddots & & & & \\ -m & -m & \cdots & n_{12} & -m & \cdots & -m \\ \hline -m & -m & \cdots & -m & -m & \cdots & -m \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ -m & -m & \cdots & -m & -m & \cdots & -m \end{array}\right] \qquad (6.3.11)$$

where the dimension of the main diagonal matrices are $k_{12}\times k_{12}$ and $k_{(1)}\times k_{(2)}$ where $k_{1i} = k_i - k_{12}$ for i = 1,2. We can thus determine G'G and denote it as follows

$$G'G = \begin{bmatrix} gg_{11} & \cdots & gg_{1,k_2} \\ \vdots & & \vdots \\ gg_{k_2,1} & \cdots & gg_{k_2,k_2} \end{bmatrix}$$

where

$$gg_{ii} = n_{12}^2 + (k_1 - 1)m^2 \qquad i = 1,\ldots,k_{12}$$

$$gg_{i\ell} = -2mn_{12} + (k_1 - 2)m^2 \qquad \ell \neq i,\ \ell = 1,\ldots,k_{12}\ ,$$

$$gg_{ij} = gg_{ji} = -n_{12}m+(k_1-1)m^2 \qquad j = k_{12}+1,\ldots,k_2 \;,$$

$$gg_{jk} = k_1m^2 \qquad\qquad k = k_{12}+1,\ldots,k_2 \;.$$

Since $E = s_1 2^{d_1} s_2 2^{d_2} I_{k_2} - \sigma^2 G'G$, we denote E by

$$E = \left[\begin{array}{cccc|cccc} b & c & \cdots & c & & & & \\ c & b & & c & & & & \\ \vdots & & \ddots & \vdots & & aJ_{k_{12},k_{(2)}} & & \\ c & c & & b & & & & \\ \hline & & & & d & f & \cdots & f \\ & & & & f & d & & f \\ & aJ_{k_{(2)},k_{12}} & & & \vdots & & \ddots & \vdots \\ & & & & f & f & \cdots & d \end{array}\right] \qquad (6.3.12)$$

where

$$a = \rho^2[n_{12}m - (k_1-1)m^2]$$

$$b = s_1 2^{d_1} s_2 2^{d_2} - \rho^2[n_{12}^2 + (k_1-1)m^2] \;,$$

$$c = \rho^2[2mn_{12} - (k_1-2)m^2] \;,$$

$$d = s_1 2^{d_1} s_2 2^{d_2} - \rho^2[k_1m^2] \;,$$

$$f = -\rho^2 k_1 m^2 \;.$$

By using elementary row and column transformations it can be shown that

$$|E| = (b-c)^{k_{12}-1}(d-f)^{k_{(2)}-1} \cdot \{(b+(k_{12}-1)c)(d+(k_{(2)}-1)f)-k_{12}k_{(2)}a^2\}. \tag{6.3.13}$$

We shall now re-express (6.3.13) in terms of $s_1 2^{d_1}$, $s_2 2^{d_2}$, and m, rather than in terms of a, b, c, and d. We use equation (6.3.12) to obtain

$$\begin{aligned}|E| = {} & [s_1 2^{d_1} s_2 2^{d_2} - \rho^2 (s_2 2^{d_2})^2]^{k_{12}-1}[s_1 2^{d_1} s_2 2^{d_2}]^{k_2-k_{12}-1} \cdot \\ & \{(s_1 2^{d_1} s_2 2^{d_2})^2 - \rho^2 s_1 2^{d_1}(s_2 2^{d_2})^3 + 2\rho^2 k_{12} m s_1 2^{d_1}(s_2 2^{d_2})^2 \\ & - \rho^2 k_1 k_2 m^2 s_1 2^{d_1} s_2 2^{d_2} + \rho^4 (k_1-k_{12})(k_2-k_{12}) m^2 (s_2 2^{d_2})^2\}.\end{aligned} \tag{6.3.14}$$

When equation (6.3.14) is used in conjunction with equation (6.3.1), we can determine the general form of the determinant of $Var(P\hat{\underline{\tau}})$ for a CRMGLM(F) design as a function of m, $s_1$, and $s_2$:

$$\begin{aligned}|D(CR)| = {} & 2^{k_2^*}\left(\frac{\sigma_{11}}{s_1 2^{d_1}}\right)^{k_1}\left(\frac{\sigma_{22}}{s_2 2^{d_2}}\right)^{k_2}(s_1 2^{d_1} s_2 2^{d_2})^{-k_{12}-1}[s_1 2^{d_1} s_2 2^{d_2} - \\ & \rho^2 (s_2 2^{d_2})^2]^{k_{12}-1}\{(s_1 2^{d_1} s_2 2^{d_2})^2 - \rho^2 s_1 2^{d_1}(s_2 2^{d_2})^3 + \\ & 2\rho^2 k_{12} m s_1 2^{d_1}(s_2 2^{d_2})^2 - \rho^2 k_1 k_2 m^2 s_1 2^{d_1} s_2 2^{d_2} +\end{aligned}$$

$$\rho^4(k_1-k_{12})(k_2-k_{12})m^2(s_2 2^{d_2})^2 \ . \qquad (6.3.15)$$

Let us consider the artificial comparison of $|\mathrm{Var}(P\hat{\underline{\tau}})|$ for a CRMGLM design with $|\mathrm{Var}(P\hat{\underline{\tau}})|$ for the HMGLM design from which the CRMGLM design was formed by omitting m tc. In this comparison we consider $s_1$ and $s_2$ to be the same for both designs. We are completely ignoring the cost constraint and from this point of view the comparison may be said to be artificial, because if $\psi_0 > 0$ then using m extra units in the CRMGLM design would cause $s_1$ and $s_2$ for the CRMGLM design to be less than their respective values for the HMGLM design. The comparison, however, even disregarding cost, is of interest.

The $|\mathrm{Var}(P\hat{\underline{\tau}})|$ for a HMGLM design, denoted $|D(H)|$, was given in (5.2.9) and can be expressed as

$$|D(H)| = 2^{k_2^*}\left(\frac{\sigma_{11}}{s_1 2^{d_1}}\right)^{k_1}\left(\frac{\sigma_{22}}{s_2 2^{d_2}}\right)^{k_2}(s_1 2^{d_1} s_2 2^{d_2})^{-k_{12}-1}[s_1 2^{d_1} s_2 2^{d_2} - \rho^2(s_2 2^{d_2})^2]^{k_{12}-1}\, s_1 2^{d_1} s_2 2^{d_2}[s_1 2^{d_1} s_2 2^{d_2} - \rho^2(s_2 2^{d_2})^2]. \qquad (6.3.16)$$

It is of interest to compare (6.3.16) and (6.3.15) to determine when

$$|D(H)| - |D(CR)| > 0 \ . \qquad (6.3.17)$$

Inequality (6.3.17) is satisfied when

$$(s_1 2^{d_1} s_2 2^{d_2})^2 - \rho^2 s_1 2^{d_1}(s_2 2^{d_2})^3 - \{(s_1 2^{d_1} s_2 2^{d_2})^2 - \rho^2 s_1 2^{d_1}(s_2 2^{d_2})^3 + \rho^2 m s_1 2^{d_1} s_2 2^{d_2}[2k_{12}s_2 2^{d_2} - k_1 k_2 m + \rho^2(k_1-k_{12})(k_2-k_{12})m \frac{s_2 2^{d_2}}{s_1 2^{d_1}}]\} > 0,$$

or, after dividing out positive terms, when

$$mk_1k_2 > 2k_{12}s_2 2^{d_2} + \rho^2(k_1-k_{12})(k_2-k_{12})m \frac{s_2 2^{d_2}}{s_1 2^{d_1}} . \quad (6.3.18)$$

If $k_{12} = 0$ then (6.3.18) reduces to

$$mk_1k_2 > mk_1k_2[\rho^2 \frac{s_2 2^{d_2}}{s_1 2^{d_1}}]$$

which is true, giving $|D(H)| > |D(CR)|$ when comparing two designs, a HMGLM and a CRMGLM where on each of the designs $V_1$ is measured on $s_1 2^{d_1}$ units and $V_2$ is measured on $s_2 2^{d_2}$ units. Whether this CRMGLM design is the optimum MGLM design will depend upon $\psi_0$ which determines how much smaller $s_1^*$ and $s_2^*$ for the CRMGLM design would be than $s_1$ and $s_2$ for the HMGLM design. When $k_{12} \neq 0$ then whether or not (6.3.18) can be satisfied, will depend upon the values of the variables. Inspection of (6.3.18) indicates that the inequality is more likely to be satisfied when $s_2 2^{d_2}$ is relatively small.

Since these cases show that it may be possible that a CRMGLM(F) design could be a better design than the HMGLM design it therefore makes sense to attempt to determine a general form of the optimal CRMGLM(F) design.

We should note however that for the best CRMGLM design with parameters $s_1^*$, $s_2^*$, m, costing $\psi'$, there also exists a HMGLM design with parameters $s_1^*$, $s_2^*$, but costing only $\psi'-m\psi_0$. We have just seen how the determinants of these two designs compare (inequality (6.3.18)) but the optimal HMGLM design still has these things in its favor: (i) this HMGLM design being compared to the CRMGLM design is not necessarily the optimal HMGLM design costing $\psi'-m\psi_0$, and (ii) when we consider the additional $m\psi_0$, available to sample $V_1$ and $V_2$, an even better HMGLM design can be found.

## 6.4 Determination of the Optimal CRMGLM(F) Design

In the last section the general form of the determinant of $\text{Var}(P\hat{\underline{\tau}})$ was found for a CRMGLM design, equation (6.3.15). Some justification was also given for attempting to find the optimal CRMGLM design in that it may be better than the optimal HMGLM design. We shall approach this optimization problem along the same lines that were used for the HMGLM designs.

The CRMGLM design will be formed in the same manner we used previously: We start with a HMGLM design with the variables ordered so that $\psi_1/k_1 \leq \psi_2/k_2$. For some constant m, we assume that m treatment combinations can be chosen so that (6.3.10) is satisfied and a 'lower bound' CRMGLM design can be found. (We treat m as a constant and thus leave our optimization problem in terms of only $s_1$ and $s_2$.) We can therefore consider that the amount of money we now have for sampling $V_1$ and $V_2$ is $\psi'-m\psi_0$ if we wish to minimize $|D(CR)|$ with respect to $s_1$ and $s_2$. This will therefore be somewhat equivalent to the hierarchial problem for the total amount of money $\psi'-m\psi_0$. After determining the general form of the values of $s_1$ and $s_2$ to minimize $|D(CR)|$ for a general constant m, we shall consider different integer values of m to determine that value of m which gives the optimum CRMGLM design.

The cost equation for the CRMGLM design is given by

$$\psi' = \psi_0 m + \psi_1^* s_1 2^{d_1} + \psi_2 s_2 2^{d_2} . \tag{6.4.1}$$

We use the method of LaGrange to find the values of $s_1$ and $s_2$ to minimize $|D(CR)|$, equation (6.3.17), when restricted by the cost constraint (6.4.1):

$$L = c_1(s_1 2^{d_1})^{-k_1}(s_2 2^{d_2})^{-k_2}(s_1 2^{d_1} s_2 2^{d_2})^{-k_{12}-1}(s_1 2^{d_1} s_2 2^{d_2} -$$

$$\rho^2(s_2 2^{d_2})^2)^{k_{12}-1} H + \lambda(\psi'-m\psi_0-s_1 2^{d_1}\psi_1^*-s_2 2^{d_2}\psi_2), \tag{6.4.2}$$

where

$$H = (s_1 2^{d_1} s_2 2^{d_2})^2 - \rho^2 s_1 2^{d_1}(s_2 2^{d_2})^3 + m s_1 2^{d_1} s_2 2^{d_2} \rho^2 (2k_{12} s_2 2^{d_2} -$$

$$k_1 k_2 m) + m^2 (s_2 2^{d_2})^2 \rho^4 (k_1 - k_{12})(k_2 - k_{12}) \,, \qquad (6.4.3)$$

where $c_1 = 2^{k_2} \sigma_{11}^{k_1} \sigma_{22}^{k_2}$ (this term, being a constant with respect to $s_1$ and $s_2$, will not affect the values of $s_1$ and $s_2$ that minimize L and will therefore be eliminated from the equation).

We find the partial derivative of L with respect to $s_1$:

$$\frac{\partial L}{\partial s_1} = -k_1 2^{d_1} (s_1 2^{d_1})^{-k_1-1} (s_2 2^{d_2})^{-k_2} (s_1 2^{d_1} s_2 2^{d_2})^{-k_{12}-1}$$

$$(s_1 2^{d_1} s_2 2^{d_2} - \rho^2 (s_2 2^{d_2})^2)^{k_{12}-1} H - (k_{12}+1) 2^{d_1} (s_1 2^{d_1})^{-k_1}$$

$$(s_2 2^{d_2})^{-k_2} (s_1 2^{d_1} s_2 2^{d_2})^{-k_{12}-2} s_2 2^{d_2} (s_1 2^{d_1} s_2 2^{d_2} -$$

$$\rho^2 (s_2 2^{d_2})^2)^{k_{12}-1} H + (k_{12}-1) 2^{d_1} (s_1 2^{d_1})^{-k_1} (s_2 2^{d_2})^{-k_2}$$

$$(s_1 2^{d_1} s_2 2^{d_2})^{-k_{12}-1} s_2 2^{d_2} (s_1 2^{d_1} s_2 2^{d_2} - \rho^2 (s_2 2^{d_2})^2)^{k_{12}-2} H$$

$$+ 2^{d_1} (s_1 2^{d_1})^{-k_1} (s_2 2^{d_2})^{-k_2} (s_1 2^{d_1} s_2 2^{d_2})^{-k_{12}-1}$$

$$(s_1 2^{d_1} s_2 2^{d_2} - \rho^2 (s_2 2^{d_2})^2)^{k_{12}-1} H_1' - \lambda 2^{d_1} \psi_1^* \,,$$

where

$$\frac{\partial H}{\partial s_1} = 2^{d_1}H_1' = 2s_1 2^{d_1} 2^{d_1}(s_2 2^{d_2})^2 - \rho^2 2^{d_1}(s_2 2^{d_2})^3$$

$$+ 2m2^{d_1}k_{12}(s_2 2^{d_2})^2\rho^2 - 2^{d_1}k_1 k_2 m^2 s_2 2^{d_2}\rho^2.$$

Upon collection of terms $\frac{\partial H}{\partial s_1}$ further simplifies to:

$$\frac{\partial L}{\partial s_1} = 2^{d_1}(s_1 2^{d_1})^{-k_1-1}(s_2 2^{d_2})^{-k_2-1}(s_1 2^{d_1}s_2 2^{d_2})^{-k_{12}-2}$$

$$(s_1 2^{d_1}s_2 2^{d_2} - \rho^2(s_2 2^{d_2})^2)^{k_{12}-2}\ s_1 2^{d_1}(s_2 2^{d_2})^3$$

$$\{s_2 2^{d_2}\rho^2(k_1+k_{12}+1)H - s_1 2^{d_1}(k_1+2)H$$

$$+ [(s_1 2^{d_1})^2 - s_1 2^{d_1}s_2 2^{d_2}\rho^2]H_1'\} - \lambda 2^{d_1}\ \psi_1^*.$$

Equation (6.4.3) along with $H_1'$ are now included in $\frac{\partial L}{\partial s_1}$ which after collection of terms yields

$$\frac{\partial L}{\partial s_1} = 2^{d_1}(s_1 2^{d_1})^{-k_1}(s_2 2^{d_2})^{-k_2}(s_1 2^{d_1}s_2 2^{d_2})^{-k_{12}-2}$$

$$[s_1 2^{d_1}s_2 2^{d_2} - \rho^2(s_2 2^{d_2})^2]^{k_{12}-2}(s_2 2^{d_2})^2\{(s_1 2^{d_1})^3(s_2 2^{d_2})^2$$

$$(-k_1) + (s_1 2^{d_1})^2 s_2 2^{d_2}[k_1 k_2(k_1+1)m^2\rho^2]$$

$$+ (s_1 2^{d_1}s_2 2^{d_2})^2[-2k_{12}(k_1+1)m\rho^2] + (s_1 2^{d_1})^2(s_2 2^{d_2})^3$$

$$[(2k_1+k_{12})\rho^2]+s_1 2^{d_1}(s_2 2^{d_2})^2[-(k_1+2)(k_1-k_{12})(k_2-k_{12})m^2\rho^4$$

$$-\ k_1k_2(-_1+k_{12})m^2\rho^4]+s_1 2^{d_1}(s_2 2^{d_2})^3[2k_{12}(k_1+k_{12})m\rho^4]$$

$$+\ s_1 2^{d_1}(s_2 2^{d_2})^4[-(k_1+k_{12})\rho^4]+(s_2 2^{d_2})^3[(k_1+k_{12}+1)$$

$$(k_1-k_{12})(k_2-k_{12})m^2\rho^6]\} - \lambda 2^{d_1}\ \psi_1^*. \tag{6.4.4}$$

We shall employ the notation

$$\frac{\partial L}{\partial s_1} = 2^{d_1}\ L_1 - \lambda\ 2^{d_1}\ \psi_1^*\ .$$

We now consider $\frac{\partial L}{\partial s_2}$ , which after many intermediate steps reduces to the following:

$$\frac{\partial L}{\partial s_2} = 2^{d_2}(s_1 2^{d_1})^{-k_1}(s_2 2^{d_2})^{-k_2}(s_1 2^{d_1}s_2 2^{d_2})^{-k_{12}-2}(s_1 2^{d_1}s_2 2^{d_2} -$$

$$\rho^2(s_2 2^{d_2})^2)^{k_{12}-2}(s_2 2^{d_2})^2\{(s_1 2^{d_1})^4(s_2 2^{d_2})[-k_2] + (s_1 2^{d_1})^3$$

$$[k_1k_2(k_2+1)m^2\rho^2]+(s_1 2^{d_1})^3 s_2 2^{d_2}[-2k_2k_{12}m\rho^2]+(s_1 2^{d_1})^3$$

$$(s_2 2^{d_2})^2[(2k_2-k_{12})\rho^2]+(s_1 2^{d_1})^2 s_2 2^{d_2}[-k_2(k_1-k_{12})$$

$$(k_2-k_{12})m^2\rho^4-k_1k_2(k_2-k_{12}+2)m^2\rho^4]+(s_1 2^{d_1}s_2 2^{d_2})^2$$

$$[2k_{12}(k_2-k_{12}+1)m\rho^4]+(s_1 2^{d_1})^2(s_2 2^{d_2})^3[-(k_2-k_{12})\rho^4]+$$

$$(s_1 2^{d_1})(s_2 2^{d_2})^2[(k_2-k_{12}+1)(k_1-k_{12})(k_2-k_{12})m^2\rho^6]\} -\lambda 2^{d_2}\psi_2. \tag{6.4.5}$$

We can denote the above equation by

$$\frac{\partial L}{\partial s_2} = 2^{d_2} L_2 - \lambda\, 2^{d_2}\, \psi_2.$$

We now divide both sides of $\frac{\partial L}{\partial s_1} = 0$ by $2^{d_1}$. After solving $\frac{\partial L}{\partial s_2} = 0$ for $\lambda$ we substitute this $\lambda$ value back into $\frac{\partial L}{\partial s_1} = 0$ and obtain

$$L_1 - Y\, L_2 = 0$$

where $Y = \psi_1^*/\psi_2$. We can also use the cost equation (6.4.1) and solve for $s_2 2^{d_2}$ and attain

$$s_2 2^{d_2} = \frac{\psi'}{\psi_2} - m\,\frac{\psi_0}{\psi_2} - \frac{\psi_1^*}{\psi_2}\, s_1 2^{d_1} = c - Y\, s_1 2^{d_1} \tag{6.4.6}$$

where

$$c = \frac{\psi'}{\psi_2} - m\,\frac{\psi_0}{\psi_2}\,. \tag{6.4.7}$$

Substituting (6.4.6) into $L_1 - YL_2 = 0$, makes this equation a function of only $s_1$, allowing us to solve for $s_1$.

$$
\begin{aligned}
L_1-YL_2 = 0 = {} & (s_1 2^{d_1})^{-k_1-k_{12}-2}(c-Ys_1 2^{d_1})^{-k_2-k_{12}} \\
& [cs_1 2^{d_1}-Y(s_1 2^{d_1})^2-\rho^2(c-Ys_1 2^{d_1})^2]^{k_{12}-2}P(s_1) \ , \qquad (6.4.8)
\end{aligned}
$$

where

$$
\begin{aligned}
P(s_1) = {} & (c(s_1 2^{d_1})^3-Y(s_1 2^{d_1})^4)[k_1(c-s_1 2^{d_1}Y)+Yk_2 s_1 2^{d_1}] \\
& +(s_1 2^{d_1})^2 k_1 k_2 m^2 \rho^2 [(k_1+1)(c-s_1 2^{d_1}Y)-s_1 2^{d_1}(k_2+1)Y] \\
& -2[c(s_1 2^{d_1})^2-Y(s_1 2^{d_1})^3]\rho^2 k_{12} m[(k_1+1)(c-s_1 2^{d_1}Y) \\
& -k_2 Y s_1 2^{d_1}]+(s_1 2^{d_1})^2(c-Ys_1 2^{d_1})^2\rho^2[(2k_1+k_{12})(c-Ys_1 2^{d_1}) \\
& -s_1 2^{d_1}(2k_2-k_{12})Y]+(cs_1 2^{d_1}-Y(s_1 2^{d_1})^2)m^2\rho^4\{-(k_1-k_{12})(k_2-k_{12}) \\
& (k_2-k_{12})[(k_1+2)(c-s_1 2^{d_1}Y)-s_1 2^{d_1}k_2 Y]-k_1 k_2 \\
& [(k_1+k_{12})(c-s_1 2^{d_1}Y)-s_1 2^{d_1}(k_2-k_{12}+2)Y]\}+2s_1 2^{d_1} \\
& (c-Ys_1 2^{d_1})^2 k_{12} m\rho^4[(k_1+k_{12})(c-Ys_1 2^{d_1})-s_1 2^{d_1}(k_2-k_{12}+1)Y] \\
& +s_1 2^{d_1}(c-Ys_1 2^{d_1})^3\rho^4[-(k_1+k_{12})(c-Ys_1 2^{d_1})+s_1 2^{d_1} \\
& (k_2-k_{12})Y]+(c-s_1 2^{d_1}Y)^2(k_1-k_{12})(k_2-k_{12})m^2\rho^6[(k_1+k_{12}+1)
\end{aligned}
$$

$$(c-s_1 2^{d_1} Y)-s_1 2^{d_1}(k_2-k_{12}+1)Y] \, . \tag{6.4.9}$$

The only way that equation (6.4.8) can be satisfied is for $s_1 2^{d_1}$ or $s_2 2^{d_2}$ to equal $\pm$ infinity or for $P(s_1) = 0$. By virtue of the cost constraint, we shall be concerned only with those values of $s_1$ which are roots of $P(s_1) = 0$. After multiplication and collection of terms, $P(s_1)$ can be expressed as follows:

$$P(s_1) = p_0 + \sum_{j=1}^{5} p_j (s_1 2^{d_1})^j \, , \tag{6.4.10}$$

where

$$p_0 = (k_1+k_{12}+1)(k_1-k_{12})(k_2-k_{12})m^2\rho^6c^3 \, , \tag{6.4.11a}$$

$$\begin{aligned} p_1 = & -(k_1-k_{12})(k_2-k_{12})(k_1+2)m^2\rho^4c^2[\rho^2Y+1] \\ & -(2k_1+2k_{12}+k_2+2)(k_1-k_{12})(k_2-k_{12})m^2\rho^6Yc^2 \\ & -(k_1+k_{12})\rho^4c^2[c^2-2k_{12}mc+k_1k_2m^2] \, , \end{aligned} \tag{6.4.11b}$$

$$p_2 = (k_1+1)\rho^2 c[c^2-2k_{12}mc+k_1k_2m^2]+(2k_1+k_2+4)(k_1-k_{12})(k_2-k_{12})$$

$$m^2\rho^4 Yc(\rho^2Y+1)+(k_1+k_{12}+k_2+1)(k_1-k_{12})(k_2-k_{12})m^2\rho^6Y^2c$$

$$+(k_1+k_{12}-1)\rho^2c^3(\rho^2Y+1)-(k_1+k_{12}-1)k_1k_2m^2\rho^4Yc$$

$$+(3k_1+2k_{12}+k_2+1)\rho^4Yc(c^2-2k_{12}mc+k_1k_2m^2) \quad , \qquad (6.4.11c)$$

$$p_3 = -(k_1+k_2+2)(k_1-k_{12})(k_2-k_{12})m^2\rho^4Y^2(\ ^2Y+1)$$

$$-(6k_1+2k_2+2k_{12})\rho^2Yc^2(\rho^2Y+1)$$

$$-(k_1+k_2+2)k_1k_2m^2\rho^2Y(\rho^2Y+1)+2(2k_1+k_2+2)k_{12}m\rho^2Yc$$

$$(\rho^2Y+1)-(k_2+k_{12})\rho^4Y^2c+2(k_1+k_{12}+k_2)k_{12}m\rho^4Y^2c-k_1c^2,$$

$$(6.4.11d)$$

$$p_4 = (4k_1+3k_2+k_{12})\rho^2Y^2c(\rho^2Y+1)+(2k_1+k_2)Yc(\rho^2Y+1)$$

$$-\ 2(k_1+k_2+1)k_{12}m\rho^2Y^2(\rho^2Y+1) \quad , \qquad \text{and} \qquad (6.4.11e)$$

$$p_5 = -(k_1+k_2)Y^2(\rho^2Y+1)^2 \ . \qquad (6.4.11f)$$

For some particular value of m, the solution of the fifth order equation, $P(s_1) = 0$, (6.4.10), yields 5 roots of $s_1$, an odd number of which must be real. For each of these real roots we can use equation (6.4.6) to obtain the associated $s_2$ value thus defining a CRMGLM design. These $(s_1,s_2)$ values are the critical values of the design. Comparison of $|D(CR)|$ at these values to $|D(CR)|$ at the end point values allows us to determine the optimal CRMGLM(F) design. This optimal design will then be compared to the optimal HMGLM design to obtain finally the optimal MGLM design.

Let us now consider the end point values for this design. At one end point, (a), $s_1$ is as large as possible (and thus $s_2$ is as small as possible) and at the other end point (b) $s_1 2^{d_1} = s_2 2^{d_2}$. In the HMGLM designs, these points occurred where (a) $s_2 = 0$ and (b) $s_1 2^{d_1} = s_2 2^{d_2}$, i.e., an MDM design. In this design however, we have indirectly assumed that we have at least m units of $V_2$ and that $n_{12} = s_2 2^{d_2} - m$. At end point (a), $n_{12} = 0$ with $s_2 > 0$ and this is therefore an RMGLM design. Since we know that the optimal RMGLM is the HMGLM design we need not compare our CRMGLM designs at the real critical values to end point (a) because when we find the best CRMGLM design, we will be comparing it to the best HMGLM design anyway. We will thus ignore end point (a). End point b however is possible and must be considered. At this end point $s_1 2^{d_1} = s_2 2^{d_2}$ and

$n_{12} = s_2 2^{d_2} - m$. Thus

$$s_i = \frac{\psi' - m\psi_0}{\psi_2^*} 2^{-d_i} \text{ for } i = 1,2 \ . \qquad (6.4.12)$$

The value of $|D(CR)|$ must be found at this end point and compared to the values of $|D(CR)|$ at the real solutions of $P(s_1) = 0$ with the design giving the lowest $|D(CR)|$ value being the optimum CRMGLM design for this value of m.

## 6.5 The Solution of the Polynomial $P(s_1)$

We have not been able to simplify equation (6.4.10) any further and have thus been unable to determine any general expression for the roots of this equation. Therefore we cannot determine a general equation representing the values $(s_1, s_2)$ that give the optimum CRMGLM design for a particular value of m. To solve this problem, a computer program has been written to find and evaluate the roots of the fifth order equation (6.4.10). In this section, the approach taken to this problem is outlined and a description of the method of polynomial solution used in the program is given. Since we have treated m as a constant, we are actually finding the optimal CRMGLM design for a specific m. It is therefore necessary to consider the different possible m values and then compare the $|D(CR)|$ values for the optimum designs found for each m. For a particular m, the program first solves the polynomial determining the 5 roots. We consider only the real roots of $s_1$ and using these values solve for the corresponding $s_2$ value. These two values must be checked to make sure that they are admissible. To be admissible: (i) $s_1$ must be real, (ii) $s_1, s_2 > 0$, (iii) $s_2 2^{d_2} \geq m$, and (iv) $s_1 2^{d_1} \geq s_2 2^{d_2}$. This fourth condition is required because in our derivation of $|D(CR)|$ we have assumed that $s_1 2^{d_1} \geq s_2 2^{d_2}$ and thus $|D(CR)|$ is valid only under these circumstances. This consideration is discussed in greater detail in the next section. If it should happen that none of our critical values are admissible, then our best design for this value of m will be the end point design (b). (This is analagous to the optimal HMGLM derivations: When the solution did not give admissible roots, the end point design, the MDM design, was optimal.) We can then evaluate $|D(CR)|$ for the particular m and each admissible critical value $(s_1, s_2)$. These $|D(CR)|$ values along with the $|D(CR)|$ value for the design formed by using the end point (b) values, $s_1 2^{d_1} = s_2 2^{d_2} = n_{12}+m$, can be compared. The design that generates the smallest $|D(CR)|$ value is the best CRMGLM design for this particular m. We do this for other m values and then compare the designs optimal for each m.

The optimal design is also determined when $m = 0$. It can be easily seen that at $m = 0$ the LaGrangian function L, equation (6.4.2), is the same as L for the HMGLM design used in Chapter 5. The optimal CRMGLM design when m = 0 is therefore the HMGLM design. The end point (b) design, the MDM design, is also found and the $|D(MD)|$ is determined.

Therefore when we compare the best designs for the different m values, including m = 0, we are finding the optimal MGLM design because we are comparing the optimal RMGLM design (either the HMGLM or the MDM design) to the best CRMGLM design.

The computer program has the capacity to iterate through a range of values of m, m = 0,1,...,mmax and to find the optimal CRMGLM design for each m. The value mmax is entered by the experimenter. In the next section we will discuss how the value mmax should be chosen and why.

This program has variable output options. It can output only admissible designs along with $|\mathrm{Var}(P\hat{\underline{\tau}})|$ values, or it can output the inadmissible designs in addition to the admissible designs. These inadmissible designs are outputted in groups that were inadmissible for the same reason. A third option is to output all steps to computation, showing how quickly the polynomial solving algorithm converged to the roots and many of the intermediate steps. These intermediate results basically concern the solution of the polynomial roots and are thus not really necessary from the design point of view. Thus this option is not recommended due partly to its length and partly to the fact that it is not necessary to our determination of the optimal design.

Rather than giving the determinant of $\mathrm{Var}(P\hat{\underline{\tau}})$ for each design, which will be a rather small number, the reciprocal of the determinant is determined apart from the constant term $2^{k_2^*} \sigma_{11}^{k_1} \sigma_{22}^{k_2}$. This was done for two reasons: (i) the values are directly comparable to those values outputted in the HMGLM program, and (ii) the reciprocals are larger than unity and are easier to compare. The optimal design is thus the design which gives the largest $\frac{1}{|D(CR)|}$ values.

A listing of this program along with the input instructions are given in Appendix 2. The program that determined the optimal HMGLM design and then checked to make sure that the design with $s_1 = c^+ s_2 2^{d_2 - d_1}$ was optimal, should be run prior to this program. The HMGLM program has the output option of punching data cards in the format to be used as input to the CRMGLM program. Thus after running the HMGLM program to find the optimal HMGLM design we are then ready to run the CRMGLM program to see if a CRMGLM design exists that gives a smaller $|\mathrm{Var}(P\hat{\underline{\tau}})|$ value (or a larger reciprocal) then does the HMGLM design. In this fashion the optimal MGLM design is determined.

A brief description will now be given of the method used to solve the polynomial. The strong point of this program is that in addition to being very accurate, it supplies its own initial estimates. Its accuracy stems from the facts that

(i) it uses two very efficient methods to obtain the roots, (ii) these methods use the entire original polynomial, i.e., the polynomial is not reduced as each root is found, a procedure which compounds the round-off error, and (iii) it is written in double precision. Both (ii) and (iii) work toward reducing the rounding error, the major problem in obtaining accurate answers.

The quotient-difference (QD) algorithm is employed first. This algorithm, although slow in convergence, furnishes simultaneous approximations to all zeros of a polynomial. Only the original real coefficients are required, no initial approximations are necessary. Due to its slow rate of convergence, the QD algorithm is used to furnish rough first approximations to be used in two very efficient algorithms, the Newton method and the Bairstow method.

The QD algorithm converges to the absolute values of roots. When it converges to a single real root then this value is used as a first approximation in Newton's method. Newton's algorithm always converges when the starting point is "sufficiently close" to the solution, generally in four or less iterations. The initial approximation from the QD algorithm is more than "sufficiently close". When several zeros of the polynomial have the same absolute value, as happens every time a polynomial with real coefficients has a pair of complex conjugate zeros, then the QD algorithm gives approximations to the coefficients of a quadratic equation that can be used by the Bairstow algorithm. This algorithm is also accurate and fast in its convergence to the true quadratic polynomial which can then be solved using the quadratic equation.

The combination of these three algorithms as a method of solving polynomial equations was suggested by Henrici (1964) and more extensive descriptions of these three algorithms can also be found there.

## 6.6 Interpretation, Explanation, and Discussion of Results

This section contains a potpourri of ideas, observations, and justifications. An explanation is given as to why we have assumed that the optimal CRMGLM design has $V_1$ as the MFOR. The fact that we have used a lower bound CRMGLM design is then discussed and some of its short comings are pointed out along with when these short comings are most prevalent. Finally the variable mmax is discussed with observations given as to what range of values of m need be considered and in what range of m-values the lower bound design may lose its effectiveness.

An assumption, that has been made without any real explanation as to why it has been made or as to whether it is justifiable, concerns whether the optimal CRMGLM design must have $s_1 2^{d_1} \geq s_2 2^{d_2}$. After ordering the variables as was done for the HMGLM design, i.e., $\psi_1/k_1 \leq \psi_2/k_2$, we have conducted our derivations as if $s_1 2^{d_1} \geq s_2 2^{d_2}$. Since our derivations assumed that $s_1 2^{d_1} \geq s_2 2^{d_2}$, then if our polynomial solution arrived at a root $s_1$ which gave $s_1 2^{d_1} < s_2 2^{d_2}$, then this root had to be discounted and considered inadmissible. Had we been able to attain a general solution to $P(s_1)$ and thus determined an equation for the optimal sample sizes then we could have analyzed these equations when $V_2$ was the MFOR to see if the equations could give any admissible roots. We could have thus solved the problem in a manner analagous to our proof that $V_2$ could not be the MFOR for an optimal HMGLM design.

Some simulations have been conducted in an attempt to disprove this assumption that $V_1$ must be the MFOR. The CRMGLM program does not assume that $\psi_1/k_1 \leq \psi_2/k_2$, it only assumes that the design has $s_1 2^{d_1} \geq s_2 2^{d_2}$. We can therefore just switch subscripts and input these values into the program to see if an admissible design can be found with our new variables. Suppose that after reordering the responses so that $\psi_1/k_1 > \psi_2/k_2$, we can find an admissible optimal CRMGLM design having $s_1 2^{d_1} > s_2 2^{d_2}$. We will then have disproved our previous assumption that when $\psi_1/k_1 \leq \psi_2/k_2$, $V_1$ must be the MFOR. In all situations considered, after the reordering, no admissible designs were found with

$s_1 2^{d_1} > s_2 2^{d_2}$. The only admissible designs, when trying to force $V_2$ to be the MFOR, were found at end point (b) where $s_2 2^{d_2} = s_1 2^{d_1} = n_{12} - m$.

We return now to our standard notation of the variables where $\psi_1/k_1 \leq \psi_2/k_2$. As further justification as to why $V_1$ is the MFOR we consider our numbering relationship. The ratios $\psi_i/k_i$ $(i = 1,2)$ show basically "cost per information". With one unit sampled on $V_i$ at a cost of $\psi_i$ we obtain information on $k_i$ effects. It still makes sense, as it did for the HMGLM design, that when restricted by a cost constraint we would measure more often those responses where we can get the most information for our money. This is exactly the situation here when $V_1$ is the MFOR.

When we also think along the lines of continuity, we know that for HMGLM designs (CRMGLM designs with $m = 0$) and for RMGLM designs (certain CRMGLM designs with $m = \alpha 2^{d_2}$, $\alpha = 1,\ldots,s_2$) the MFOR is $V_1$. It might also be felt that this can be extended to the designs with the value m between the m-values of the RMGLM designs.

The most convincing argument for this numbering of responses is the "information per cost" approach. The simulation consideration is not presented as a reason but more as supporting evidence.

We wish to now consider what happens to our lower bound design as m gets larger. The best way to begin this topic is to return to the general form of the G matrix

$$G = s_2 2^{d_2} D - \sum_{k=1}^{m} F_k \ .$$

Denote by $m_*$ the number of units whose treatment combinations generate the F matrix, $F = J_{k_1,k_2}$ for a particular design where $V_2$ is measured on $s_2 2^{d_2}$ units. When $m > m_*$ the matrix G no longer represents a G matrix generated by a possible design for this situation. This was the reason that the procedure by which we assumed that the tc's to be omitted would be chosen was said to give a lower bound design. When $m > m_*$ we can still choose the first $m_*$ by the convention advocated previously, giving

$$\sum_{k=1}^{m} F_k = \sum_{k=1}^{m_*} F_k + \sum_{k=m_*+1}^{m} F_k = m_* J + \sum_{k=m_*+1}^{m} F_k \ . \qquad (6.6.1)$$

(When $m = m_*+1$ an example of a true $\sum_{k=1}^{m} F_k$ for a situation similar to that in Example 6.3.1 would be

$$\sum_{k=1}^{m} F_k = \begin{bmatrix} a & a & b \\ b & b & a \\ b & b & a \end{bmatrix}$$

where $a = m_*+1$ and $b = m_*-1$. In Example 6.3.1 $m_* = 3$ and if $m = 4$ and the four omitted units are the $1^{st}$, $2^{nd}$, $7^{th}$ and

$18^{th}$ units then this exact $\Sigma F_k$ matrix is attained.) As $(m-m_*)$ gets larger, the $\sum_{k=1}^{m} F_k$ matrix gets further and further away from what our lower bound design assumes it to be. As $\Sigma F$ becomes increasingly different, the G'G matrix and $|E|$ value become even more markedly different than the G'G and $|E|$ for the lower bound design. $|E|$ for the real design will be greater than $|E|$ for the lower bound design.

Therefore when $m > m_*$, the determinant for the lower bound design, $|D(CR)|_{LB}$, is less than $|D(CR)|$ for the best realistic design that could be determined. The questions arise: When can this be harmful? When must special care be taken? The lower bound design assumes that in equation (6.6.1)

$$\sum_{k=m_*+1}^{m} F_k = (m-m_*)J \tag{6.6.2}$$

when in fact in the best realistic design most of the elements in $\sum_{k=m_*+1}^{m} F_k$ will be less than $(m-m_*)$. There can thus be certain situations where a $CRMGLM_{LB}$ design can appear to be optimal (having $m > m_*$) but in actuality a CRMGLM design cannot be constructed for this m value which is anywhere close to being optimal. Recall that we stated that $|E|$ is generally dominated by the main diagonal terms. For a lower bound design the diagonal terms are given by

$$e_{ii} = s_1 2^{d_1} s_2 2^{d_2} - \rho^2[(s_2 2^{d_2} - m)^2 + (k_1-1)m^2] \qquad (6.6.3a)$$

if the $i^{th}$ effect on $V_2$ also influences $V_1$ $(i = 1,\ldots,k_2)$,

$$= s_1 2^{d_1} s_2 2^{d_2} - \rho^2 k_1 m^2 \text{ , otherwise.} \qquad (6.6.3b)$$

When $m \leq m_*$ the basic effect of increasing m is the reduction of $n_{12}$ $(= s_2 2^{d_2} - m)$ with the overall effect of enlarging $e_{ii}$. When $s_1 2^{d_1}$ is not much larger than $s_2 2^{d_2}$ then for $m_* < m < \frac{1}{2}(s_2 2^{d_2})$, the effect of $(k_1-1)m^2$ can be very strong, reducing $e_{ii}$, which along with the off-diagonal terms may make it appear that a CRMGLM design is optimum. This term $(k_1-1)m^2$ as illustrated in equation (6.6.2) is the result of using the lower bound design, the actual value from a real design would be less than $(k_1-1)m^2$ while the off-diagonal term would also be smaller.

Consider now the situation where $s_1 2^{d_1}$ is much larger than $s_2 2^{d_2}$. Now the larger m will not have the same overpowering effect that it had before. The $s_1 2^{d_1} s_2 2^{d_2}$ portion of $e_{ii}$ still dominates $|E|$ and there is therefore less chance that a lower bound design will appear optimal when its corresponding CRMGLM design really is not.

In the preceding derivations we have ignored one very important aspect that makes this lower bound design appear to be a little better than it actually is. As m gets larger, $s_1$ and $s_2$ must get smaller due to the smaller amount of money that can be allocated to sampling $V_1$ and $V_2$. Although this would make $|E|$ smaller it does not make $|D(CR)|$ smaller because

$$|D(CR)| = (s_1 2^{d_1})^{-(k_1+k_2)} (s_2 2^{d_2})^{-2k_2} |E|.$$

This discussion points out the fact that if after running the program, a CRMGLM design with $m > m_*$ is found to be better than the optimal HMGLM design then before the CRMGLM design is accepted as optimal it should be investigated further. This program really gives an indication as to when the HMGLM design can be accepted as optimal and when more work is required.

Next we consider $|D(CR)|$ for a real design and examine a property of these designs which occurs when the m omitted units include certain specific groups of units. Recall that when an entire fraction of units, say $2^d$ units, was omitted, then $\sum_{k=1}^{2^d} F_k = 2^d D$, i.e., all elements of the matrix are zeros except for $k_{12}$ values of $2^d$. All of the other elements were zero because, due to the orthogonality of the design, each effect occurred with other effects an equal number of times at the high and low level, i.e., there are an equal number of plus and minus ones at a given position in the $2^d$ F matrices. This situation corresponds to a RMGLM design.

We consider the matrix $\Sigma F_k$ for a real situation as m increases. Until m exceeds $m_*$, units can be chosen to be omitted so that all elements of $\Sigma F$ continue to increase in size. But when $m > m_*$, units can no longer be chosen so that all elements of F uniformly increase. Some elements will increase; some will decrease.

We will now consider some different cases which will illustrate some facts about and give us a better feel for the size of mmax to be used. Consider a situation where $m = m(-)+2^d$ and the $2^d$ units make up an entire fraction. We start with a HMGLM design and omit m units or we could equivalently consider starting with a RMGLM desing leaving out m(-) units. Consider two designs, design A having $m = 2^{d_2}+m(-)$ and design B having $m = m(-)$ where these m(-) units are the same for both designs. Assume that for both designs $s_1$ and $s_2$ are the same and we now compare the G matrices. For design A

$$\sum_{k=1}^{m} F_k = 2^{d_2}D + C$$

where C denotes the sum of the F matrices for the m(-) separate units. For design B

$$\sum_{k=1}^{m(-)} F_k = C.$$

The corresponding G matrices are

$$G_A = (s_2-1)2^{d_2}D - C,$$

$$G_B = s_2 2^{d_2}D - C .$$

Obviously the elements of $G_A'G_A$ will be smaller than those of $G_B'G_B$. Thus the elements of

$$E_A = s_1 2^{d_1} s_2 2^{d_2} I_k - G_A'G_A$$

will be larger, especially the dominating main diagonal elements, than the elements of $E_B$. Thus $|E_A| > |E_B|$ and the design B will always be better than design A.

The point to be made is that when m is so big or is chosen so that it includes a complete fraction of $2^d$ units, then the orthogonality of these $2^d$ units defeats the purpose of adding the additional $2^d$ units to try to attain a better design. We have just shown that a better design can be found when only $m-2^d$ units are used. Thus when we consider a very large m, we can be defeating our purpose.

We now consider another important fact about the value of m. Recall that

$$\sum_{k=1}^{s_2 2^{d_2}} F_k = s_2 2^{d_2} D . \tag{6.6.4}$$

Consider a design A with $m_A = m(-)$ units where $m(-) < \frac{1}{2} s_2 2^{d_2}$.

Consider another design B with $m_B = s_2 2^{d_2} - m(-)$ and the $m_B$ units omitted are the units that were not omitted in design A. These designs will be called reciprocal designs. For design A we denote $F_A = \sum_{k=1}^{m} F_k = \{f_{ijA}\}$ by C and thus from (6.6.4) for design B

$$F_B = \sum_{k=1}^{m} F_k = s_2 2^{d_2} D - C \ .$$

Therefore apart from the $k_{12}$ elements of $F_A$ and $F_B$ (those elements equivalent to the $k_{12}$ unity elements of D) $f_{ijA} = -f_{ijB}$.

From working with these designs it has become obvious that even when we assume that $s_1$ and $s_2$ are the same for both reciprocal designs that design A with $m_A < \frac{1}{2} s_2 2^{d_2}$ will be a better design than design B because $|E_A| < |E_B|$. Let us illustrate this point by referring to a situation as described in Example 6.3.1. In reference to design A

$$F_A = \begin{bmatrix} m(-) & f_1 & f_2 \\ f_3 & f_4 & f_5 \\ f_2 & f_6 & m(-) \end{bmatrix} \quad \text{and} \quad G_A = \begin{bmatrix} s_2 2^{d_2} - m(-) - f_1 & & -f_2 \\ -f_3 & -f_4 & -f_5 \\ -f_2 & -f_6 & s_2 2^{d_2} - m(-) \end{bmatrix}$$

and

$$G_A'G_A =$$

$$\begin{bmatrix} [s_2 2^{d_2}-m(-)]^2+f_2^2+f_3^2 & -f_1(s_2 2^{d_2}-m(-))+f_3f_4+f_2f_6 & -2f_2(s_2 2^{d_2}-m(-))+f_3f_5 \\ & f_1^2+f_4^2+f_6^2 & -f_6(s_2 2^{d_2}-m(-))+f_1f_2+f_4f_5 \\ (\text{sym.}) & & (s_2 2^{d_2}-m(-))+f_2^2+f_5^2 \end{bmatrix}$$

For design B,

$$F_B = \begin{bmatrix} s_2 2^{d_2}-m(-) & -f_1 & -f_2 \\ -f_3 & -f_4 & -f_5 \\ -f_2 & -f_6 & s_2 2^{d_2}-m(-) \end{bmatrix} \quad \text{and} \quad G_B = \begin{bmatrix} m(-) & f_1 & f_2 \\ f_3 & f_4 & f_5 \\ f_2 & f_6 & m(-) \end{bmatrix}$$

and

$$G_B'G_B = \begin{bmatrix} m(-)^2+f_2^2+f_3^2 & f_1m(-)+f_3f_4+f_2f_6 & 2f_2m(-)+f_3f_5 \\ & f_1^2+f_4^2+f_5^2 & f_6m(-)+f_1f_2+f_4f_5 \\ (\text{sym.}) & & m(-)^2+f_2^2+f_5^2 \end{bmatrix}.$$

These matrices are needed to determine E. Recall that

$$E = s_1 2^{d_1} s_2 2^{d_2} I_{k_2} - \rho^2 G'G$$

and we wish to find $|E|$. Since $s_2 2^{d_2} - m(-) > m(-)$, the main diagonal terms of $G_A'G_A$ are greater than the corresponding terms of $G'G$, $|E|$ will be dominated by the diagonal elements of E. Since design A gives larger diagonal elements of $G'G$ than does B, it follows that $G_A'G_A$ does more to offset the diagonal elements $s_1 2^{d_1} s_2 2^{d_2}$ than does B, i.e., the determinant of E will be less for design A than B. Even though some off-diagonal elements of $G_B'G_B$ may be greater than their corresponding elements in $G_A'G_A$, this contribution towards a reduction in $|E_B|$ will not be as significant as the reduction in the main diagonal elements accomplished by the reciprocal design A. Another point favoring design A is that the sample sizes $s_{1A}$ and $s_{2A}$ will be larger than $s_{1B}$ and $s_{2B}$ because less money need be allocated for set-up costs since $m_A < m_B$.

The preceding attempts to show that there is no reason to consider designs with $m > \frac{1}{2} s_2 2^{d_2}$, because these CRMGLM designs are known to have a reciprocal design that is a better design.

So far we have discussed some occurrances of CRMGLM designs for different ranges of values of m. The choice of mmax to be used in the program can be approached from two points of view: We can choose the value of mmax to be less than $\frac{1}{2} s_2 2^{d_2}$ so that the values of m considered give designs that are relatively close to realistic designs. (A suggested value is mmax = $\frac{1}{4} s_2 2^{d_2}$.) Another approach would be to choose mmax = $\frac{1}{2} s_2 2^{d_2}$ since we have seen that the optimal CRMGLM design will not have m > $s_2 2^{d_2 - 1}$. The problem is that the larger m becomes, the worse the lower bound CRMGLM design is as an "estimate" of the best real CRMGLM design at this m value. It is therefore quite likely that this design might appear better than the optimal HMGLM design when in fact this is not possible. When mmax is so large a problem that can arise, aside from the lower bound design determinant being far from that of a real design, is that $|D(CR)|_{LB}$ may be negative. This is due to the off-diagonal elements which, for the lower bound design, are much larger than they would be in a real design. Since D(CR) is a positive definite variance-covariance matrix, it cannot have a negative determinant.

Naturally by choosing mmax = $\frac{1}{2} s_2 2^{d_2}$, all the designs are given that would be investigated had mmax been made smaller.

We must not forget however that the larger m-values must be accepted with a great deal of caution.

In summary, we have considered several properties of CRMGLM designs which give us a better insight into the choice of mmax. We need not select mmax $> \frac{1}{2} s_2 2^{d_2}$ for we have seen that when $m > \frac{1}{2} s_2 2^{d_2}$, there exists a reciprocal design that is a better design. If $m \leq m_*$, and if a lower bound CRMGLM design is better than the optimal HMGLM design, then the optimal MGLM design is this CRMGLM design. There is no problem when $m \leq m_*$; for then the lower bound design is a realistic design. When $m > m_*$, care must be taken that we do not accept as optimal a lower bound design which may not be realistic. (As an estimate of $m_*$ that can be obtained without writing out an entire design and analyzing each $F_k$, one might use the smallest integer $\hat{m}_*$ such that

$$\hat{m}_* \geq s_2 2^{d_2 - d}$$

where $d = \max(d_1, d_2)$.) The lower bound CRMGLM design has its best chance of being accepted when $s_1 2^{d_1}$ is not much bigger than $s_2 2^{d_2}$. This point along with the structure of the diagonal elements of G'G imply that when $s_1 2^{d_1}$ and $s_2 2^{d_2}$ are close together and small, then chances are that a realistic CRMGLM design may be optimal.

We have been referring to the $s_1$ and $s_2$ values of the best CRMGLM design for a particular m before we even run the program. Since we first use the program to find the optimal RMGLM design, we determine $s_1$ and $s_2$ for the optimal HMGLM design before we use the CRMGLM program. These values for the HMGLM design will be fairly close to the values for the CRMGLM design and can therefore be used.

Even if we have not been able to prove conclusively that we have determined the optimal MGLM design, we have at least accomplished something. For a given situation we can now determine, for most cases, when the conventional MDM design is not the optimal design, and in these cases we can at least suggest a design which, if not optimal, is at least a better design to be used.

# CHAPTER VII

## SUGGESTIONS FOR FURTHER RESEARCH

The preceding chapters uncover several areas which may provide fruitful paths for further inquiry. This chapter briefly outlines possible future investigations into these areas.

As was true for the trace criterion, the work with the determinant criterion is equally applicable to factorial experiments where each factor has more than two levels. Similarly a further extension which would concern both the trace and the determinant criteria pertains to applications involving mixed factorial experiments. The derivation of the optimal design with respect to the trace criterion should be relatively straightforward as one need not be concerned with the off-diagonal covariance matrices of $\mathrm{Var}(P\hat{\underline{\tau}})$. However, these covariance matrices become important when one deals with optimality with respect to the determinant criterion. With individual responses being affected by different sets of factors and with the separate factors having different numbers of levels, some intriguing problems are introduced which may require a different approach to some of the proofs.

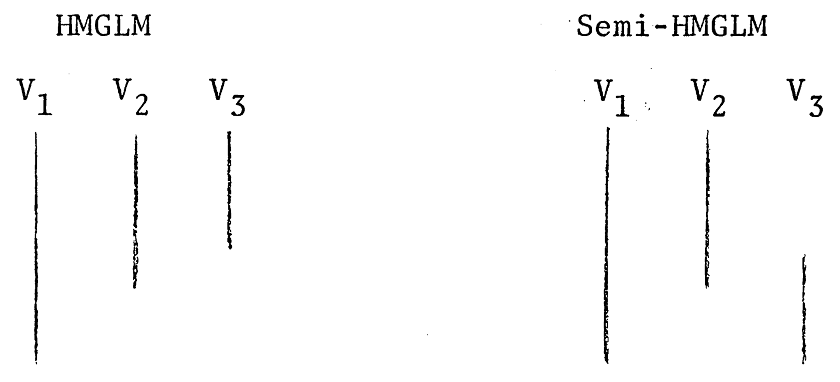
In addition to factorial experiments an interesting and useful extension of this work could include BIB and PBIB designs.

Another consideration for further investigation would employ different cost constraints from which a different set of optimal designs will be found. A frequently occurring cost relationship which can be illustrated by many real life examples is one in which the costs of measuring the responses are not independent, i.e., $\psi_i$ is not independent of $\psi_j$. Quite often for example, the cost of measuring $V_1$ on some unit may be less when $V_j$ is also measured on that unit.

One matter into which further investigation is needed is the determination of the optimal two-response CRMGLM designs. An initial goal, improving on our findings so far, would be to find, for those situations where $m > m_*$, an approximation better than the lower bound design assumed in Chapter 6, i.e., determine a lower bound design applicable to those situations where the previous lower bound design provides only a poor approximation. The further goal would be to determine the exact optimal design for each value of m. Hopefully the optimal MGLM can then be found conclusively. If only the initial goal can be realized, then we will be assured of a design at least as good as and possibly better than the one we can now determine.

One obvious extension of this work concerns designs that are optimum with respect to the determinant criterion. We have dealt with some specific p-response situations, but we need to extend to p responses the general results found for two responses. Due to the difficulty in determining a general form of the determinant, this may require first extending to a 3-response case, leading possibly to a proof by induction.

When extending these results to $p > 2$ responses, a new type of design can be formulated which we will call a Semi-Hierarchial MGLM design. It can be illustrated for a 3-response case as follows:



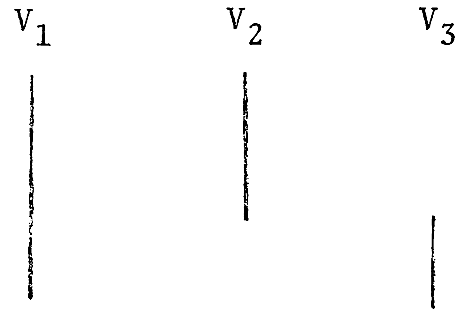

This semi-HMGLM design has some characteristics similar to the 2-response CRMGLM design in that

$$n_{23} \neq \min(s_2 2^{d_2}, s_3 2^{d_3})$$

However, the important distinction is that the cost of the two designs is the same since $n_{1i} = s_i 2^{d_i}$ for $i = 2,3$. It is possible that a change in the off-diagonal covariance matrices could lead to a smaller $|\mathrm{Var}(P\hat{\underline{\tau}})|$. Although we feel that the

CRMGLM designs will have very limited applications in the two response case since the HMGLM design is almost always the optimal design, the form of their off-diagonal covariance matrices in $\mathrm{Var}(P\hat{\underline{\tau}})$ will be applicable to the Semi-HMGLM designs. It is therefore conceivable that for certain $p > 2$ response situations, because the costs of the two designs are equivalent, the Semi-HMGLM design may be optimum. Notice that for the Semi-HMGLM design the main diagonal variance-covariance matrices and hence the trace criterion would not be affected. Thus the Semi-HMGLM design would then also be an optimal design under the trace criterion.

There exist circumstances where a Semi-HMGLM design must be used. Two possible examples follow: (i) There exist situations where only q of the p responses can be measured on an experimental unit (where $q < p$). This could be a situation where due to a time element only q responses can be measured before the experimental unit changes. (ii) A second case could involve a destructive sampling situation. Suppose that of three responses, the first can always be measured without affecting the other responses; but when $V_2$ is measured $V_3$ can no longer be measured; and when $V_3$ is measured, $V_2$ can no longer be measured. This would generate a Semi-HMGLM design similar to the following illustration:




A drawback to using these optimal designs is that when optimizing with respect to the trace criterion, a prior estimate of the variance of each response $\sigma_{ii}$ is required. With optimization with respect to the determinant criterion, an 'a priori' estimate of $\rho^2$ is needed. This generally requires that either similar experiments have previously been conducted under similar situations, or that possibly a pilot study was initiated. An approach that seems both interesting and sensible would be to set up the experiment in a sequential fashion. Using a portion of the allocated money, a MDM design with $s_1^*$ and $s_2^*$, could be formulated and conducted. From this design the variance estimates can be obtained, and using these estimates, the optimal HMGLM design with $s_1$ and $s_2$, can then be determined. The original design could then be augmented, and as long as $s_2 > s_2^*$, the optimal design can be used. If $s_2 < s_2^*$, then even though the optimal design cannot be formulated, we at least make use of a design better than the MDM design. This approach would be suitable when there is plenty of time and enough money that we are able to employ an original MDM design large enough to obtain reasonable variance estimates.

Not only do we hope that the results of this paper will provide a basis for future investigations, but furthermore we hope that the practicality of these designs will inspire others not only to use them but also to give consideration to the cost aspect of designing experiments.

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## APPENDIX I

## ABBREVIATIONS, MATRIX NOTATION, AND THEOREMS USED IN THE TEXT

Abbreviations:

| | |
|---|---|
| SM | Standard Multiresponse |
| GIM | General Incomplete Multiresponse |
| HM | Hierarchial Multiresponse |
| MDM | Multiple Design Multiresponse |
| MGLM | More General Linear Multivariate |
| HMGLM | Hierarchial More General Linear Multiresponse |
| RMGLM | Restricted More General Linear Multiresponse |
| CRMGLM | Complementary Restricted More General Linear Multiresponse |
| lhs | left hand side |
| rhs | right hand side |
| tc | treatment combination |
| MFOR | Most Frequently Observed Response |
| tr(A) | the trace of a square matrix A |
| $\det(A) = \|A\|$ | the determinant of a square matrix A |

Matrix Notation:

Generally a capital letter refers to a matrix. A lower case letter is a constant unless underlined in which case it is a column vector.

$I_n$ an n×n identity matrix

$J_{n,m}$ an n×m matrix of ones

$J_n = J_{n,n}$

$\underline{j}_n = J_{n,1}$

$O_{n,m}$ an n×m matrix of zeros

$\underline{0}_n = 0_{n,1}$

Assume A and C are (j×k) matrices, B is an (n×m) matrix, D is a (p×p) matrix, and E is a (p×p) matrix of full rank.
A ⊗ B is a kronecker product matrix of dimension (jn×km) such that

$$A \otimes B = \begin{bmatrix} a_{11}B & \cdots & a_{1k}B \\ \vdots & & \vdots \\ a_{j1}B & \cdots & a_{jk}B \end{bmatrix}$$

A * C is a Hadamard product matrix of dimension j k such that

$$A * C = \begin{bmatrix} a_{11}c_{11} & \cdots & a_{1k}c_{1k} \\ & & \\ a_{j1}c_{j1} & \cdots & a_{jk}c_{jk} \end{bmatrix} .$$

$A'$ denotes the transpose of A.

$E^{-1}$ denotes the inverse of E, i.e., $EE^{-1} = E^{-1}E = I_p$.

$D^-$ denotes generalized inverse of D, i.e., $DD^-D = D$.

Theorems:

<u>Theorem 1</u>: If A, B, C, and D are matrices of dimensions $(n_1 \times n_2)$, $(m_1 \times m_2)$, $(n_2 \times n_3)$, and $(m_2 \times m_3)$ respectively, then

$$(A \otimes B)(C \otimes D) = (AC \otimes BD).$$

<u>Theorem 2</u>: If $C = A \otimes B$ then $C^- = A^- \otimes B^-$.

<u>Theorem 3</u>: If A is a matrix such that the sum of each of the elements of any row or column equals zero, then a generalized inverse of A is

$$A^- = (A + \varepsilon J)^{-1}$$

for any non-zero constant $\varepsilon$.

<u>Theorem 4</u>: (Marcus and Minc(1964)) If A and B are real non-negative symmetric $(n \times n)$ matrices, then

$$|A * B| + |A||B| \geq |A| \prod_{i=1}^{n} b_{ii} + |B| \prod_{i=1}^{n} a_{ii} .$$

Cauchy's Inequality (or the Cauchy-Schwarz inequality):

For any real numbers $a_1, \ldots, a_n, b_1, \ldots, b_n$

$$(\sum_{i=1}^{n} a_i^2)(\sum_{i=1}^{n} b_i^2) \geq (\sum_{i=1}^{n} a_i b_i)^2$$

where equality is attained when $a_i = \alpha b_i$ $(i = 1,\ldots,n)$ for any constant $\alpha$.

APPENDIX II

## COMPUTER PROGRAMS

The first program listed here was described in Section 3.6. After finding the optimal design, with respect to the trace criterion, having real numbered solutions $s_1,\ldots,s_p$ this program determines the integer values $s_1,\ldots,s_p$ giving the best integer design. To use this program the following input cards are necessary:

| Card # | Cols. | Input Format | Variable Name | Description |
|---|---|---|---|---|
| 1 | 1-10 | I10 | IP | Number of responses |
| | 11-20 | F10.0 | YO | Set-up cost, $\psi_0$ |
| | 21-30 | F10.0 | TC | Amount of money available, $\psi'$ |
| | 31-40 | F10.0 | P | Number of levels of a factor |
| | 41-50 | F10.0 | PC | % over $\psi'$ allowable, express %/100 |
| | 51-60 | I10 | IWRIT | If IWRIT = 0, then all designs are outputted. Otherwise only the optimal design is outputted. |
| 2 | 1-10<br>11-20<br>etc. | 8F10.0 | S(I) | Read the optimum $s_i$ values, no more than 8 per card ($i = 1,\ldots,IP$) |

| Card # | Cols. | Input Format | Variable Name | Description |
|---|---|---|---|---|
| 3 | 1-10 etc. | 8F10.0 | Y(I) | The costs $\psi_i$ $(i = 1,\ldots,IP)$ |
| 4 | 1-10 etc. | 8F10.0 | K(I) | The number of effects of interest $k_i$ $(i = 1,\ldots,IP)$ |
| 5 | 1-10 etc. | 8F10.0 | V(I) | The estimates of $_{ii}$ $(i = 1,\ldots,IP)$ |
| 6 | 1-10 etc. | 8I10 | ID(I) | $ID(I) = d_i = v_i - f_i$ $(i = 1,\ldots,IP)$ |

```
C
C     THIS PROGRAM TAKES THE OPTIMAL REAL NUMBER S(I) VALUES
C        AND ROUNDS UP AND BACK LOOKING AT ALL POSSIBLE
C        COMBINATIONS OF THE ROUNDED INTEGER VALUES, TO
C        FIND THE OPTIMUM INTEGER DESIGN UNDER THE
C        TRACE CRITERION.
C
C
      DIMENSION S(25),Y(25),K(25),V(25),ID(25),SR(25,2),
     1OPT(2,27),IPL(25),IJ(25)
      COMMON J1,J2,J3,J4,J5,J6,J7,J8,J9,J10,J11,J12,J13,
     1J14,J15,J16,J17,J18,J19,J20,J21,J22,J23,J24,J25
      REAL*4 K
      EQUIVALENCE (J1,IPL(1))
      DATA OPT/54*0.0/
C
C     READ # RESPONSES,SET-UP COST,TOTAL AMT. MONEY,
C        # OF LEVELS, % OVER TOTAL COST ALLOWABLE, IWRIT:
C        IF IWRIT=0 THEN ALL DESIGNS ARE WRITTEN OUT
C
      READ(5,5) IP,YO,TC,P,PC,IWRIT
    5 FORMAT (I10,4F10.0,I10)
      WRITE(6,7) IP,YO,TC,P
    7 FORMAT(//,10X,'NUMBER OF RESPONSES',I4,5X,'SET UP ',
     1'COST',F7.2,5X,'TOTAL COST',F8.2,5X,'NUMBER OF LEVE',
     2'LS PER FACTOR',F5.0,///)
C
C     READ NUMBER OF BLOCKS
C
      READ(5,10) (S(I),I=1,IP)
   10 FORMAT(8F10.0)
      WRITE(6,11) (S(I),I=1,IP)
   11 FORMAT(10X,'REAL OPTIMUM NUMBERS OF BLOCKS',/,15X,
     17F15.4,3(/,20X,6F15.4))
C
C     READ IN COSTS Y(I), # TERMS K(I),VARIANCE V(I),
C        FRACTION SIZES  ID(I) = V-F
C
      READ(5,10)(Y(I),I=1,IP)
      READ(5,10)(K(I),I=1,IP)
      READ(5,10)(V(I),I=1,IP)
      READ(5,12)(ID(I),I=1,IP)
   12 FORMAT(8I10)
      WRITE(6,13)(Y(I),I=1,IP)
   13 FORMAT(///,10X,'MEASUREMENT COSTS FOR EACH RESPONSE',
     1/,15X,7F15.4,3(/,20X,6F15.4))
      WRITE(6,14)(K(I),I=1,IP)
   14 FORMAT(//,10X,'NUMBER OF TERMS UNDER STUDY',/,15X,
     1 11F10.0,/,20X,10F10.0,/,20X,4F10.0)
      WRITE(6,16) (V(I),I=1,IP)
```

```
   16 FORMAT(///,10X,'VARIANCES',/,15X,11F10.2,/,20X,
     110F10.2,/,20X,4F10.2)
      WRITE(6,17) (ID(I),I=1,IP)
   17 FORMAT(///,10X,' D(I) = V(I) - F(I) , THE NUMBER OF',
     1' FACTORS MINUS THE FRACTION SIZE',/,15X,19I6,/,
     220X,6I6)
      WRITE(6,18)
   18 FORMAT(////)
C
C     ROUND S(I)'S UP AND BACK,SET NUMBER LEVELS OF S = 2
C        FOR I = 1,...,IP
C
      DO 15 I=1,IP
      J = S(I)
      SR(I,1) = J
      SR(I,2) = J + 1
   15 IPL(I) = 2
      IF(IP .EQ. 25) GO TO 25
      IPP1 = IP + 1
      DO 20 I=IPP1,25
   20 IPL(I) = 1
   25 TMAX1 = .1E15
      TMAX2 = .1E15
      CMAX1 = TC
      CMAX2 = TC *(PC + 1.)
      DO 150 I25 = 1,J25
      IJ(25) = I25
      DO 150 I24 = 1,J24
      IJ(24) = I24
      DO 150 I23 = 1,J23
      IJ(23) = I23
      DO 150 I22 = 1,J22
      IJ(22) = I22
      DO 150 I21 = 1,J21
      IJ(21) = I21
      DO 150 I20 = 1,J20
      IJ(20) = I20
      DO 150 I19 = 1,J19
      IJ(19) = I19
      DO 150 I18 = 1,J18
      IJ(18) = I18
      DO 150 I17 = 1,J17
      IJ(17) = I17
      DO 150 I16 = 1,J16
      IJ(16) = I16
      DO 150 I15 = 1,J15
      IJ(15) = I15
      DO 150 I14 = 1,J14
      IJ(14) = I14
      DO 150 I13 = 1,J13
```

```
      IJ(13) = I13
      DO 150 I12 = 1,J12
      IJ(12) = I12
      DO 150 I11 = 1,J11
      IJ(11) = I11
      DO 150 I10 = 1,J10
      IJ(10) = I10
      DO 150 I9  = 1,J9
      IJ( 9) = I9
      DO 150 I8  = 1,J8
      IJ( 8) = I8
      DO 150 I7  = 1,J7
      IJ( 7) = I7
      DO 150 I6  = 1,J6
      IJ( 6) = I6
      DO 150 I5  = 1,J5
      IJ( 5) = I5
      DO 150 I4  = 1,J4
      IJ( 4) = I4
      DO 150 I3  = 1,J3
      IJ( 3) = I3
      DO 150 I2  = 1,J2
      IJ( 2) = I2
      DO 150 I1  = 1,J1
      IJ( 1) = I1
      T = 0.0
      C = 0.0
      DO 30 J=1,IP
      T=(P*(P-1.)*K(J)*V(J))/((P**ID(J))*SR(J,IJ(J)))+T
   30 C = Y(J) *(P**ID(J)) * SR(J,IJ(J)) + C
C
C     FIND THE MFOR, AFTER ROUND OFF IT MAY NOT BE V(1)
C
      XNO = SR(1,IJ(1)) * (P**ID(1))
      DO 35 J=2,IP
      XTRY = SR(J,IJ(J))*(P**ID(J))
      IF(XNO .LT. XTRY) XNO = XTRY
   35 CONTINUE
      C = C + YO*XNO
      IF (C .GT. CMAX1) GO TO 75
      IF (T .GE. TMAX1) GO TO 45
      TMAX1 = T
      OPT(1,26) = T
      OPT(1,27) = C
      DO 40 I=1,IP
   40 OPT(1,I) = SR(I,IJ(I))
   45 IF (IWRIT .NE. 0) GO TO 150
      WRITE(6,50) T,C,(SR(I,IJ(I)),I=1,IP)
   50 FORMAT(3X,F15.4,8X,F10.2,5X,18F5.0,/,83X,7F5.0)
      GO TO 150
```

```
 75 IF (C .GT. CMAX2) GO TO 100
    IF (T .GE. TMAX2) GO TO 85
    TMAX2 = T
    OPT(2,26) = T
    OPT(2,27) = C
    DO 80 I=1,IP
 80 OPT(2,I) = SR(I,IJ(I))
 85 IF (IWRIT .NE. 0) GO TO 150
    WRITE(6,90) T,C,(SR(I,IJ(I)),I=1,IP)
 90 FORMAT(7X,F15.4,4X,F10.2,5X,18F5.0,/,83X,7F5.0)
    GO TO 150
100 IF (IWRIT .NE. 0) GO TO 150
    WRITE(6,110)T,C,(SR(I,IJ(I)),I=1,IP)
110 FORMAT(11X,F15.4,F10.2,5X,18F5.0,/,83X,7F5.0)
150 CONTINUE
    WRITE(6,200)CMAX1,OPT(1,27),OPT(1,26),(OPT(1,I),
   1I=1,IP)
200 FORMAT('1',10(/),5X,'OPTIMAL DESIGN WHEN THE TOTAL ',
   1'AMOUNT OF MONEY THAT CAN BE SPENT IS',F9.2,//,10X,
   2'COST',10X,'TRACE',10X,'NUMBER OF TIMES FRACTIONS AR'
   3,'E REPLICATED',//,5X,F9.2,F15.4,10X,18F5.0,/,49X,
   47F5.0)
    WRITE(6,210) CMAX2,OPT(2,27),OPT(2,26),(OPT(2,I),
   1I=1,IP)
210 FORMAT(///,10X,'WHEN',F9.2,' IS ALLOCATED',//,5X,
   1F9.2,F15.4,10X,18F5.0,/,49X,7F5.0)
999 STOP
    END
```

The next program was described in Section 5.9. The parameters describing the experimental situation are read into the program which then determines the optimal HMGLM design under the determinant criterion. The program checks around the critical point $(s_1(+),s_2(+))$ to make sure that this point maximizes the reciprocal of $|\mathrm{Var}(P\hat{\underline{\tau}})|$. The program also punches out cards to be used as input to the program that determines the optimal CRMGLM design. To use this program the following input cards are necessary:

| Card # | Cols. | Input Format | Variable Name | Description |
|---|---|---|---|---|
| 1 | 1-3 | I3 | NOVS | Number of variable sets, different situations to be read in |
| | 4-6 | I3 | IJEND | Number of iterations to be made, changing the $\rho^2$ value. (If IJEND = 0, it assumes IJEND = 10). |
| | 7-11 | F5.0 | P2D10 | Amount $\rho^2$ is changed each iteration. If P2D10 = 0 it assumes P2D10 = $\rho^2/10$. |
| | 12-15 | I4 | IM | This is the value punched as the MMAX value as the input to the CRMGLM program. |
| Repeat the next card NOVS times | | | | |
| 2 | 1-10 | F10.0 | V1 | $k_1$ |
| thru NOVS+1 | 11-20 | F10.0 | V2 | $k_2$ |

| Card # | Cols. | Input Format | Variable Name | Description |
|---|---|---|---|---|
| | 21-30 | F10.0 | V12 | $k_{12}$ |
| | 31-40 | D10.0 | Y0 | $\psi_0$ |
| | 41-50 | D10.0 | Y1 | $\psi_1$ |
| | 51-60 | D10.0 | Y2 | $\psi_2$ |
| | 61-70 | D10.0 | YTC | $\psi'$ |
| | 71-80 | D10.0 | P2 | $\rho^2$ |

```
C
C
C     THIS PROGRAM CALCULATES THE OPTIMUM HMGLM(F) DESIGN
C        FOR A SITUATION THAT WILL BE READ IN.   THE PROGRAM
C        HAS THE CAPACITY TO CHANGE THE RHO SQUARED VALUES
C        LEAVING OTHER VALUES CONSTANT, WHICH IS USEFUL WHEN
C        CHECKING MANY SETS OF VALUES.  IT ALSO PUNCHES OUT
C        INPUT CARDS TO BE USED IN A PROGRAM THAT COMPARES
C        THIS HMGLM(F) DESIGN TO VARIOUS MGLM(F) DESIGNS.
C
C
      IMPLICIT  REAL*8 (A-H,O-U,W-Z)
      REAL*8   N2P,N1M,N2M,N1,N2,M1,M2,M,N,NP,NM,N1P
      DIMENSION DN(5),DM(5)
C
C
C     READ IN NOVS - THE NUMBER OF SETS OF VARIABLES TO BE
C        READ IN AND FOR WHICH THE OPTIMUM DESIGN IS
C        COMPUTED.
C       IJEND - THE NUMBER OF ITERATIONS TO BE MADE CHANGING
C        THE ORIGINAL VALUE OF RHO SQUARED,  IF IJEND = 0
C        THEN IT SETS IJEND =10 ;
C       P2D10  - THE AMOUNT P2 (RHO SQUARED) CHANGES EACH
C        ITERATION, IF 0 THEN P2D10 = P2 / 10   ;
C       IM  - THE MAX M VALUE TO BE PUNCHED AS INPUT DATA
C        FOR THE NEXT PROGRAM.
C
C
      READ(5,1) NOVS,IJEND,P2D10,IM
    1 FORMAT(2I3,F5.0,I4)
      IF(IJEND .EQ. 0) IJEND = 10
      IF(IM .EQ. 0) IM=4
      IJPLIM = 1000000
      IJNUM = 0
      NOBAD1 = 0
      NOBAD2 = 0
      NOBAD3 = 0
      DO 200 IJ=1,NOVS
C
C
C     DENOTE THE NUMBER OF FACTORS UNDER STUDY (K1,K2,K12)
C        BY V1, V2, V12;
C       Y0 - THE SET UP OR PREPARATION COST;
C       Y1,Y2 - THE COSTS OF RESPONSES 1 AND 2
C       YTC - THE TOTAL AMOUNT OF MONEY AVAILABLE;
C       P2 - RHO SQUARED
C
C
      READ(5,5) V1,V2,V12,Y0,Y1,Y2,YTC,P2
    5 FORMAT(3F10.0,5D10.0)
```

```
      KKK=0
      IV1  =  V1
      IV2  =  V2
      IV12=  V12
      Y1S  =  Y0  +  Y1
C
C
C     THE TERM W IN THE DISSERTATION IS REFERRED TO AS Y IN
C        THE PROGRAM.  IN WRITE STATEMENTS IT WILL BE
C        WRITTEN OUT AS W.
C
C
      Y = (Y1S/V1)/(Y2/V2)
      IF(P2D10 .NE. 0.0) GO TO 6
      P2D10 = P2 / 10.
    6 P2 = P2 + P2D10
      DO 200 IJ2 = 1,IJEND
      KKK=0
      P2 = P2 - P2D10
      WRITE(6,7) V1,V2,V12,Y0,Y1,Y2,YTC,P2
    7 FORMAT('1',//,3X,'K1=',F3.0,
     1              3X,'K2=',F3.0,3X,'K12=',F3.0,3X,'Y0=',D13.
                       6,3X,'Y1=',D
     213.6,3X,'Y2=',D13.6,3X,'YTC =',D13.6,3X,'P2=',D13.6)
      IF (V2 .EQ. V12) GO TO 11
      A = 2.*(1. + V12/V1) - (1. - V12/V2)
      B = SQRT((1. + V12/V1)*((1. + V12/V1) - (1. -V12/V2)))
      C = (1. - V12/V2)**2
      YP=(A + B*2.) / (P2*C)
      YM=(A - B*2.) / (P2*C)
      WRITE(6,10) Y,YM,YP
   10 FORMAT(//,5X,'WE OBTAIN REAL ROOTS FOR N1 WHEN W > W(+
                       ) OR W < W(-
     1) WHERE',/,10X,'W =',D13.6,10X,'W(-) =',D13.6,10X,'W(+
                       ) =',D13.6)
      PLIM = (A - 2.*B)/(Y*C)
      GO TO 14
   11 F = 4. * (1. + V2/V1)
      YM = 1. /(F*P2)
      PLIM = 1. / (F*Y)
      WRITE(6,13) Y,YM
   13 FORMAT(//,5X,'WE OBTAIN REAL ROOTS FOR N1 WHEN W < W(-
                       ) WHERE,  W
     1=',D13.6,3X,'AND  W(-) =',D13.6)
   14 WRITE(6,15) PLIM
   15 FORMAT(/,5X,'IF P2 <',D13.6,'  THEN W < W(-) ')
      IF (P2 .LE. PLIM) GO TO 19
      WRITE(6,17) P2,PLIM
   17 FORMAT(///,' *** P2 =',D13.6,' IS GREATER THAN P2 LIMI
                       T =',D13.6,'
```

```
  1 THUS WE WILL NOT HAVE REAL ROOTS FOR N1 OR N2.',/,10X
                   ,'WE THEREFO
  2RE USE THE  MDM DESIGN (N1=N2).  ***',//)
   KKK=1
   GO TO 57
19 COND = 1. / (2. - P2*(1. - V12/V2))
   WRITE(7,302)
302 FORMAT(' 6 1',/,' 1')
   IJNUM = IJNUM + 1
   WRITE(7,305) V1,V2,V12,P2,YTC,Y0,Y1,Y2,IJNUM
305 FORMAT(3F5.0,F5.3,4F10.1,13X,I7)
   WRITE(7,308) IM
308 FORMAT(I2)
   IF(IJ2 .EQ. IJEND) WRITE(7,305) V1,V2,V12,PLIM,YTC,Y0,
                   Y1,Y2,IJPLIM
   IF (V2 .EQ. V12) COND = .5
   WRITE(6,20) COND
20 FORMAT(/,5X,'IF W <',D13.6,'  THIS IS A SUFFICIENT CON
                   DITION THAT
  1C+ > 1 ')
   BY2= (1. - P2*(1. + V12/V1))/(1. - P2*(1. - V12/V2))
   P2CP = V1/(V1 + V12)
   WRITE(6,25) BY2,P2CP
25 FORMAT (/,5X,'IF THE ABOVE CONDITION IS NOT SATISFIED
                   THE W MUST F
  1ALL IN THE INTERVAL(0,',D13.6,')',/,8X,'WHERE THIS SEC
                   OND NUMBER I
  2S > 0 IF P2 < ',D13.6)
   WRITE(6,30) COND,BY2
30 FORMAT(/,5X,'A NECESSARY CONDITION THAT C- >1 IS THAT
                   W <',D13.6,'
  1 ALSO W MUST BE OUTSIDE THIS INTERVAL (0,',D13.6,')')
   A = 1. + Y*(1. -V12/V2)*P2
   B =DSQRT(A**2 - 4.*Y*P2*(1.+V12/V1))
   CP = (A+ B)/(2*Y)
   CM = (A- B)/(2*Y)
   N2P =YTC/(CP*Y1S + Y2)
   N2M =YTC/(CM*Y1S + Y2)
   N1P = N2P * CP
   N1M = N2M * CM
   WRITE(6,35) CP,N1P,N2P,CM,N1M,N2M
35 FORMAT(//,5X,'C(+)=',D13.6,10X,'N1=', D13.6,10X,'N2 ='
                   ,D13.6,
  1         /,5X,'C(-)=',D13.6,10X,'N1=', D13.6,10X,'N2 ='
                   ,D13.6)
   IF (CP .LE. 1.0) WRITE(6,36)
   IF (CM .GE. 1.0) WRITE(6,37)
36 FORMAT(2(' ****',/))
37 FORMAT(' * *',/,'  * *')
   DCP = (N1P**IV1)*(N2P**IV2)*((N1P/(N1P-P2*N2P))**IV12)
```

```
      DCM = (N1M**IV1)*(N2M**IV2)*((N1M/(N1M-P2*N2M))**IV12)
      WRITE(6,40) DCP,DCM
   40 FORMAT(/,10X,'D(C+) =',D20.12,15X,'D(C-)=',D20.12)
      WRITE(6,45)
   45 FORMAT  (/,5X, 'CONSIDERING SOME VALUES AROUND N1 AND
                    N2',/)
      DO 50 I=1,5
      N1 = N1P - .003 + I*.001
      M1 = N1M - .003 + I*.001
      N2 = (YTC - Y1S*N1)/Y2
      M2 = (YTC - Y1S*M1)/Y2
      DN(I) = (N1**IV1)*(N2**IV2)*((N1/(N1-P2*N2))**IV12)
      DM(I) = (M1**IV1)*(M2**IV2)*((M1/(M1-P2*M2))**IV12)
   50 WRITE(6,55) N1,N2,DN(I),M1,M2,DM(I)
   55 FORMAT(2(5X,'N1=',D13.6,3X,'N2 =',D13.6,3X,'D=',D19.12
                    ))
      DO 310 I=1,5
      IF (DN(I) .GT. DN(3)) GO TO 315
      IF (DM(I) .LT. DM(3)) GO TO 315
  310 CONTINUE
      GO TO 57
C
C
C     A WARNING IS WRITTEN TO MAKE IT EASIER TO SPOT AN
C        UNUSUAL SOLUTION.
C
C
  315 WRITE(6,62)
      WRITE(6,320)
  320 FORMAT(/,' EITHER DET(C+) IS NOT A MAX OR DET(C-) IS N
                    OT A MIN',/)
      WRITE(6,63)
      NOBAD1 = NOBAD1 + 1
   57 M = YTC/(Y1S + Y2)
      DSM = M**(IV1+IV2) * (1./(1.-P2))**IV12
      WRITE(6,60) M,DSM
   60 FORMAT(//,5X,'FOR THE  MDM DESIGN, N=',D13.6,10X,'D=',
                    D20.12)
      IF (KKK .EQ. 1) GO TO 199
      IF(DSM .LE. DCP) GO TO 59
      WRITE(6,62)
      WRITE(6,330) CP
  330 FORMAT(/,' DET(MDM) INVERSE IS LESS THAN DET(C+)',
     1 ' WHERE C+ =',F8.5,/)
      WRITE(6,63)
      NOBAD2 = NOBAD2 + 1
      IF(CP .GE. 1) NOBAD3 = NOBAD3 + 1
   59 A= V1 + (Y1S/Y2)*P2*(2.*V1 + V2 + V12)
      B = V1**2 + 2.*V1*Y1S*P2*(2.*V1 +V2+V12)/Y2 +((Y1S*P2)
                    **2)*((V1+V2
```

```
  1)**2 + (V1+V12)**2)/(Y2**2) + 2.*(V1+V2)*(V1+V12)*((Y1
                 S*P2/Y2)**2
  2-2.*(Y1S/Y2)*P2*(1. +P2*Y1S/Y2))
   C= 2.*Y1S*(V1+V2)*(1. +P2*Y1S/Y2)/Y2
   IF(B .GE. 0.) GO TO 64
   WRITE(6,62)
62 FORMAT(//,1X,5('**********'))
   WRITE(6,61) B
61 FORMAT   (' **** SQRT NEGATIVE NUMBER,  B =',D16.8)
   WRITE(6,63)
63 FORMAT(1X,5('**********'),//)
   B =DABS(B)
64 NP =(YTC/Y2) * (A +DSQRT(B))/C
   NM =(YTC/Y2) * (A -DSQRT(B))/C
   WRITE(6,65) NP,NM
65 FORMAT(//,5X,'FOR THE CASE WHERE WE EXPRESS N1 IN TERM
                 S OF N2 WE F
  1IND THE ROOTS FOR N1 TO BE  N1(+)=',D13.6,3X,'N1(-)=',
                 D13.6)
   N=NP
100 F=(YTC -Y1S*N)/Y2
   DF = -Y1S/Y2
   G = N - F*P2
   DG = 1. + P2*Y1S/Y2
   DH = (V1+V12)*F*G + V2*N*DF*G - V12*N*F*DG
   D2 = (V1+V12-1.)*F*G*DH + G*DF*(V2-1.)*N*DH- (V12+1.)*
                 DG*N*F*DH -
  2(V12+1.)*DG*N*F*DH + N*F*G*((V1+V12)*DF*G +(V1+V12)*F*
                 DG + V2*DF*G
  3 + V2*N*DF*DG - V12*F*DG - V12*N*DF*DG)
   D2N = (N**(IV1+IV12-2)) * (F**(IV2-2))*((1./G)**(IV12+
                 2))*D2
   WRITE(6,105) N,D2,D2N
105 FORMAT(10X,'FOR N=',D13.6,'  THE DETERMINANT IGNORING
                 THE CONSTANT
  1 VARIANCES IS',D20.12,5X,'D =',D20.12)
   IF(N .EQ. NM) GO TO 110
   N = NM
   GO TO 100
110 CONTINUE
   N1 = N1P
   N2 = N2P
190 A=(N1**(IV1+IV12-2))*(N2**(IV2-2))*((1./(N1-P2*N2))**
                 (IV12+2))
   D2N1=(N2**2)*(V1*N1-P2*N2*(V1+V2))*(N1*(V1-1.)-P2*N2*(
                 V1+V2-1.))
  1 +V12*P2*N1*(N2**3)
   D2N2 = (N1**2)*(V2*N1-P2*N2*(V2-V12))*(N1*(V2-1.)-P2*N
                 2*(V2-V12-1.
  1)) + (N1**3)*N2*P2*V12
```

```
      D2N1N2=N1*N2*(V1*N1-P2*N2*(V1+V12))*(N1*V2-P2*N2*(V2-V
                    12)) - ((N1+
     1N2)**2)*P2*V12
      DISTM = A*D2N1
      DINV2 = (D2N1*D2N2 -(D2N1N2**2))*(A**2)
      WRITE(6,195) N1,N2,DISTM,DINV2,D2N1,D2N2,D2N1N2
  195 FORMAT(///,5X,'TWO VARIABLES, N1=',D13.6,' , N2=',D13.
                    6, 3X, '2ND
     1PARTIAL W.R.T. N1=',D20.12,3X,'JACOBIAN=',D20.12,/,10X
                    ,'FOR THE TE
     2RMS MINUS THE CONSTANT TERM,  PARTIAL N1=',D20.12,5X,'
                    PARTIAL N2='
     3,D20.12,/,50X,'PARTIAL N1 N2 =',D20.12)
      IF(N1 .EQ. N1M) GO TO 199
      N1 = N1M
      N2 = N2M
      GO TO 190
  199 WRITE(6,201) IJNUM
  201 FORMAT(///,1X,I4)
  200 CONTINUE
C
C
C     AFTER GOING THRU MANY CASES, POSSIBLY WITH ITERATION
C        ON P2, THE UNUSUAL CASES WERE KEPT COUNT OF, AND
C        THE TOTALS ARE NOW PRINTED.
C
C
      WRITE(6,350) NOBAD1,NOBAD2,NOBAD3
  350 FORMAT('1',///,5X,'THE NUMBER OF TIMES THAT EITHER DET
                    (C+) WAS NOT
     1 A MAX OR DET(C-) WAS NOT A MIN',I5,///,5X,'THE NUMBER
                     OF TIMES DE
     2T(MDM) > DET(C+)',I5,//,10X,'WHERE C+ WAS >1 ',I5,'  T
                    IMES')
      WRITE(7,352) IJNUM
  352 FORMAT(I3)
  999 STOP
      END
```

The next program was also described in Section 5.9. This program is analogous to the first program described in this appendix except that this program determines the best integer design when the optimization criterion is the minimization of $|\mathrm{Var}(\hat{P\underline{\tau}})|$. If there are more than two responses, then the program determines the best integer design maximizing

$$f = (s_1 2^{d_1})^{k_1} \ldots (s_p 2^{d_p})^{k_p}$$

as discussed in Chapter 4. Input cards to this program are as follows:

| Card # | Cols. | Input Format | Variable Name | Description |
|---|---|---|---|---|
| 1 | 1-10 | I10 | IP | Number of responses |
| | 11-20 | F10.0 | Y0 | $\psi_0$ |
| | 21-30 | F10.0 | TC | $\psi'$ |
| | 31-40 | F10.0 | PC | % over $\psi'$ allowable, express %/100 |
| | 41-50 | I10 | IWRIT | If IWRIT = 0 all designs are outputted |
| 2 | 1-10 etc. | 8F10.0 | S(I) | $s_i$ (i = 1,...,IP) |
| 3 | 1-10 etc. | 8F10.0 | Y(I) | $\psi_i$ (i = 1,...,IP) |

| Card # | Cols. | Input Format | Variable Name | Description |
|---|---|---|---|---|
| 4 | 1-10 etc. | 8I10 | IK(I) | $k_i$ (i = 1,...,IP) |
| 5 | 1-10 etc. | 8I10 | ID(I) | $d_i$ (i = 1,...,IP) |
| 6 | 1-10 | F10.0 | P2 | $\rho^2$ |
| | 11-12 | I2 | IK12 | $k_{12}$ . |

```
C
C     THIS PROGRAM TAKES THE OPTIMAL REAL NUMBER S(I) VALUES
C        AND ROUNDS UP AND BACK LOOKING AT ALL POSSIBLE
C        COMBINATIONS OF THE ROUNDED INTEGER VALUES, TO
C        FIND THE OPTIMUM INTEGER DESIGN UNDER THE
C        DETERMINANT CRITERION.
C
C
      COMMON /BLK/ S,Y,CMAX1,CMAX2,IK,ID,IP,IWRIT
      COMMON /BLK1/ TWO,TC,PC,YO
      DIMENSION TWO(25)
      DIMENSION S(25),Y(25),IK(25),ID(25),OPT(2,27)
      REAL K
      DATA OPT/54*0.0/
C
C     READ # RESPONSES,SET-UP COST,TOTAL AMT. MONEY,
C        % OVER TOTAL COST ALLOWABLE,    IWRIT:
C        IF IWRIT=0 THEN ALL DESIGNS ARE WRITTEN OUT
C
      READ(5,5) IP,YO,TC,PC,IWRIT
    5 FORMAT (I10,3F10.0,I10)
      WRITE(6,7) IP,YO,TC
    7 FORMAT(//,10X,'NUMBER OF RESPONSES',I4,5X,'SET UP ',
     1'COST',F7.2,5X,'TOTAL COST',F8.2,///)
C
C     READ NUMBER OF BLOCKS
C
      READ(5,10) (S(I),I=1,IP)
   10 FORMAT(8F10.0)
      WRITE(6,11) (S(I),I=1,IP)
   11 FORMAT(10X,'REAL OPTIMUM NUMBERS OF BLOCKS',/,15X,
     17F15.4,3(/,20X,6F15.4))
C
C     READ IN COSTS Y(I), # TERMS K(I),
C        FRACTION SIZES  ID(I) = V-F
C
      READ(5,10)(Y(I),I=1,IP)
      READ(5,12)(IK(I),I=1,IP)
      READ(5,12)(ID(I),I=1,IP)
   12 FORMAT(8I10)
      WRITE(6,13)(Y(I),I=1,IP)
   13 FORMAT(///,10X,'MEASUREMENT COSTS FOR EACH RESPONSE',
     1/,15X,7F15.4,3(/,20X,6F15.4))
      WRITE(6,14)(IK(I),I=1,IP)
   14 FORMAT(//,10X,'NUMBER OF TERMS UNDER STUDY',/,15X,
     1 11I10,/,20X,10I10,/,20X,4I10)
      WRITE(6,17) (ID(I),I=1,IP)
   17 FORMAT(///,10X,' D(I) = V(I) - F(I) , THE NUMBER OF',
     1' FACTORS MINUS THE FRACTION SIZE',/,15X,19I6,/,
     220X,6I6)
```

```
      WRITE(6,18)
   18 FORMAT(////)
      DO 19 I = 1,IP
   19 TWO(I) = 2.**ID(I)
      IF(IP .EQ.2) GO TO 40
      GO TO 50
   40 CALL VAR2(OPT)
      GO TO 60
   50 CALL VARP(OPT)
   60 CONTINUE
      WRITE(6,200)CMAX1,OPT(1,27),OPT(1,26),(OPT(1,I),
     1I=1,IP)
  200 FORMAT('1',10(/),5X,'OPTIMAL DESIGN WHEN THE TOTAL ',
     1'AMOUNT OF MONEY THAT CAN BE SPENT IS',F9.2,//,10X,
     2'COST',10X,'TRACE',10X,'NUMBER OF TIMES FRACTIONS AR'
     3,'E REPLICATED',//,5X,F9.2,F15.4,10X,18F5.0,/,49X,
     47F5.0)
      WRITE(6,210) CMAX2,OPT(2,27),OPT(2,26),(OPT(2,I),
     1I=1,IP)
  210 FORMAT(///,10X,'WHEN',F9.2,' IS ALLOCATED',//,5X,
     1F9.2,F15.4,10X,18F5.0,/,49X,7F5.0)
  999 STOP
      END




      SUBROUTINE VAR2(OPT)
C
C     THIS SUBROUTINE DETERMINES THE OPTIMIM INTEGER RMGLM
C        DESIGN TO MINIMIZE THE VARIANCE-COVARIANCE
C        DETERMINANT.  THIS IS ONLY USED WHEN P=2 RESPONSES
C
      COMMON /BLK/ S,Y,CMAX1,CMAX2,IK,ID,IP,IWRIT
      COMMON /BLK1/ TWO,TC,PC,YO
      DIMENSION S(25),Y(25),IK(25),ID(25),OPT(2,27)
      DIMENSION RS(2,5)
      DIMENSION TWO(25)
      READ(5,10) P2,IK12
   10 FORMAT(F10.0,I2)
      WRITE(6,20) P2,IK12
   20 FORMAT(10X,'RHO SQUARED =',F7.4,10X,'K12 =',I4,///)
      DMAX1 = .1E15
      DMAX2 = .1E15
      CMAX1 = TC
      CMAX2 = TC * (PC + 1.)
      Y1 = Y(1)
      Y2 = Y(2)
      DO 50 I=1,2
```

```
      J = S(I)
      KJ = -2
      DO 50 I2 = 1,5
      RS(I,I2) = J + KJ
   50 KJ = KJ + 1
      DO 100 I1 = 1,5
      DO 100 I2 = 1,5
      IF(RS(2,I2)*TWO(2) .GT. RS(1,I1)*TWO(1)) GO TO 55
      XMA = RS(1,I1)
      XMI = RS(2,I2)
      IMA = 1
      GO TO 60
   55 XMA = RS(2,I2)
      XMI = RS(1,I1)
      IMA = 2
   60 IMI = 3 - IMA
      XA = XMA * TWO(IMA)
      XI = XMI * TWO(IMI)
      D=(XA**(IK(IMA)+IK12))*(XI**IK(IMI))/(XA-P2*XI)**IK12
      C=Y0*XA+Y1*RS(1,I1)*TWO(1)+Y2*RS(2,I2)*TWO(2)
      IF(C .GT. CMAX1) GO TO 75
      IF (D .GT. DMAX1) GO TO 65
      DMAX = D
      OPT(1,26) = D
      OPT(1,27) = C
      OPT(1,1) = RS(1,I1)
      OPT(1,2) = RS(2,I2)
   65 IF(IWRIT .NE. 0) GO TO 100
      WRITE(6,70) D,C,RS(1,I1),RS(2,I2)
   70 FORMAT(3X,F15.4,8X,F10.2,2(5X,F5.0))
      GO TO 100
   75 IF(C .GT. CMAX2) GO TO 80
      IF(D .GT. DMAX2) GO TO 80
      DMAX2 = D
      OPT(2,26) = D
      OPT(2,27) = C
      OPT(2,1) = RS(1,I1)
      OPT(2,2) = RS(2,I2)
   80 IF(IWRIT .NE. 0) GO TO 100
      WRITE(6,85) D,C,RS(1,I1),RS(2,I2)
   85 FORMAT(7X,F15.4,8X,F10.2,2(5X,F5.0))
  100 CONTINUE
      SMDM = TC / (Y0 + Y1 + Y2)
      IMDM1 = SMDM / TWO(1)
      IMDM2 = SMDM / TWO(2)
      R1 = FLOAT(IMDM1) * TWO(1)
      R2 = FLOAT(IMDM2) * TWO(2)
      RM = R1
      IF(R1 .GT. R2) RM = R2
      DM = RM ** (IK(1)+IK(2)) / (1. - P2)
```

```
      WRITE(6,110) DM,RM
  110 FORMAT(//,'  MDM DESIGN',5X,F15.4,5X,F5.0,//)
  999 RETURN
      END




      SUBROUTINE VARP(OPT)
C
C     THIS SUBROUTINE FINDS THE INTEGER DESIGN TO MAXIMIZE
C        THE FUNCTION F.  THIS SUBROUTINE IS USED
C        WHENEVER P > 2 RESPONSES
C
      COMMON /BLK/ S,Y,CMAX1,CMAX2,IK,ID,IP,IWRIT
      COMMON /BLK1/ TWO,TC,PC,YO
      COMMON J1,J2,J3,J4,J5,J6,J7,J8,J9,J10,J11,J12,J13,
     1J14,J15,J16,J17,J18,J19,J20,J21,J22,J23,J24,J25
      DIMENSION S(25),Y(25),IK(25),ID(25),OPT(2,27)
      DIMENSION SR(25,2),SRS(25),IPL(25),IJ(25)
      DIMENSION TWO(25)
      EQUIVALENCE (J1,IPL(1))
C
C     ROUND S(I)#S UP AND BACK,SET NUMBER LEVELS OF S = 2
C        FOR I = 1,...,IP
C
      DO 15 I=1,IP
      J = S(I)
      SR(I,1) = J
      SR(I,2) = J + 1
   15 IPL(I) = 2
      IF(IP .EQ. 25) GO TO 25
      IPP1 = IP + 1
      DO 20 I=IPP1,25
   20 IPL(I) = 1
   25 FMAX1 = .001
      FMAX2 = .001
      CMAX1 = TC
      CMAX2 = TC *(PC + 1.)
      DO 150 I25 = 1,J25
      IJ(25) = I25
      DO 150 I24 = 1,J24
      IJ(24) = I24
      DO 150 I23 = 1,J23
      IJ(23) = I23
      DO 150 I22 = 1,J22
      IJ(22) = I22
      DO 150 I21 = 1,J21
      IJ(21) = I21
```

```
      DO 150 I20 = 1,J20
      IJ(20) = I20
      DO 150 I19 = 1,J19
      IJ(19) = I19
      DO 150 I18 = 1,J18
      IJ(18) = I18
      DO 150 I17 = 1,J17
      IJ(17) = I17
      DO 150 I16 = 1,J16
      IJ(16) = I16
      DO 150 I15 = 1,J15
      IJ(15) = I15
      DO 150 I14 = 1,J14
      IJ(14) = I14
      DO 150 I13 = 1,J13
      IJ(13) = I13
      DO 150 I12 = 1,J12
      IJ(12) = I12
      DO 150 I11 = 1,J11
      IJ(11) = I11
      DO 150 I10 = 1,J10
      IJ(10) = I10
      DO 150 I9  = 1,J9
      IJ( 9) = I9
      DO 150 I8  = 1,J8
      IJ( 8) = I8
      DO 150 I7  = 1,J7
      IJ( 7) = I7
      DO 150 I6  = 1,J6
      IJ( 6) = I6
      DO 150 I5  = 1,J5
      IJ( 5) = I5
      DO 150 I4  = 1,J4
      IJ( 4) = I4
      DO 150 I3  = 1,J3
      IJ( 3) = I3
      DO 150 I2  = 1,J2
      IJ( 2) = I2
      DO 150 I1  = 1,J1
      IJ( 1) = I1
      F = 1
      C = 0.0
      DO 30 J=1,IP
      IJK = IJ(J)
      F = F *((SR(J,IJK)*TWO(J)) ** IK(J))
   30 C = Y(J) * TWO(J) * SR(J,IJK) + C
C
C     FIND THE MFOR, AFTER ROUND OFF IT MAY NOT BE V(1)
C
      IJK1 = IJ(1)
```

```
      XNO = SR(1,IJK1) * TWO(1)
      DO 35 J=2,IP
      IJK = IJ(J)
      XTRY = SR(J,IJK) * TWO(J)
      IF(XNO .LT. XTRY) XNO = XTRY
   35 CONTINUE
      C = C + YO*XNO
      IF (C .GT. CMAX1) GO TO 75
      IF (F .LT. FMAX1) GO TO 45
      FMAX1 = F
      OPT(1,26) = F
      OPT(1,27) = C
      DO 40 I=1,IP
      IJK = IJ(J)
   40 OPT(1,I) = SR(I,IJK)
   45 IF (IWRIT .NE. 0) GO TO 150
      DO 47 I=1,IP
      IJK = IJ(I)
   47 SRS(I) = SR(I,IJK)
      WRITE(6,50) F,C,(SRS(I),I=1,IP)
   50 FORMAT(3X,F15.4,8X,F10.2,5X,18F5.0,/,83X,7F5.0)
      GO TO 150
   75 IF (C .GT. CMAX2) GO TO 100
      IF (F .LT. FMAX2) GO TO 85
      FMAX2 = F
      OPT(2,26) = F
      OPT(2,27) = C
      DO 80 I=1,IP
      IJK = IJ(I)
   80 OPT(2,I) = SR(I,IJK)
   85 IF (IWRIT .NE. 0) GO TO 150
      DO 87 I = 1,IP
      IJK = IJ(I)
   87 SRS(I) = SR(I,IJK)
      WRITE(6,90) F,C,(SRS(I),I=1,IP)
   90 FORMAT(7X,F15.4,4X,F10.2,5X,18F5.0,/,83X,7F5.0)
      GO TO 150
  100 IF (IWRIT .NE. 0) GO TO 150
      DO 105 I = 1,IP
      IJK = IJ(I)
  105 SRS(I) = SR(I,IJK)
      WRITE(6,110) F,C,(SRS(I),I=1,IP)
  110 FORMAT(11X,F15.4,F10.2,5X,18F5.0,/,83X,7F5.0)
  150 CONTINUE
  999 RETURN
      END
```

This last program was described in Section 6.6. It determines the optimal CRMGLM design for either a single value of m or for a range of values of m (m = 0,1,...,MMAX). The program is basically a polynomial solver and can be used independently for this purpose by specifying certain values for input parameters. Input to this program is as follows:

| Card # | Cols. | Input Format | Variable Name | Description |
|---|---|---|---|---|
| 1 | 1-3 | I3 | NUMITR | The number of iterations or sets of data to be read in |
| | 31-35 | I5 | IWRITE | = 0, all steps toward calculation of determinant outputted.<br>< 6 (≠ 0), outputs admissible and inadmissible designs<br>> 6, outputs admissible designs. |
| Repeat the following group of cards NUMITR times. | | | | |
| 2 | 1-2 | I2 | N | the number of coefficients (= the order of the polynomial + 1) |
| | 3-4 | I2 | IJK | = 0 read in polynomial coefficients, this ignores design and just solves polynomial<br>≠ 0 reads in parameters to calculate polynomial to solve for the optimal design. |

| Card # | Cols. | Input Format | Variable Name | Description |
|---|---|---|---|---|
| If IJK = 0 then | | | | |
| 3a | 1-10 etc. | 8D10.0 | C(1,I) | read in the N polynomial coefficient |
| The rest of the cards assume IJK $\neq$ 0 | | | | |
| 3b | 1-2 | I2 | IJK2 | = 0, reads in only 1 m value and calculates the optimal design at that value<br>> 0, iterates for m = 0,1,...,MMAX |
| 4 | 1-5 | F5.0 | V1 | $k_1$ |
| | 6-10 | F5.0 | V2 | $k_2$ |
| | 11-15 | F5.0 | V12 | $k_{12}$ |
| | 16-20 | F5.0 | RHO | $\rho^2$ |
| | 21-30 | F10.0 | YT | $\psi'$ |
| | 31-40 | F10.0 | YO | $\psi_0$ |
| | 41-50 | F10.0 | Y1 | $\psi_1$ |
| | 51-60 | F10.0 | Y2 | $\psi_2$ |
| | 76-80 | I5 | KNUM | an arbitrary numbering system that can be used so that these designs are easily compared with those of the HMGLM program. |
| If IJK2 = 0 then | | | | |
| 5a | 1-5 | F5.0 | M | the one value of m to be evaluated |
| If IJK2 > 0, then | | | | |
| 5b | 1-2 | I2 | MMAX | the program determines the optimal CRMGLM designs for m = 0,1,...,MMAX. |

```
C
C
C     THIS PROGRAM COMPARES THE OPTIMUM HMGLM(F) DESIGN TO
C        MGLM(F) DESIGNS WITH 1,2,...,M OBSERVATIONS
C        MEASURED ON V(2) BUT NOT V(1).
C
C
      REAL*8 X,C,R,PX,Q,E,AA,T,BAIR,RTFINK,ROOT1,ROOT2,ROOTI
                    ,ROOTIM,RAT,
     1REAL,U,V,UE,VE,D,DSQRT,DABS,BAD,AG
      REAL*8 XN1,XN2
      REAL*4 M
      DIMENSION X(400),C(3,11),Q(75,10),E(75,11),T(11,11),AA
                    (11),BAIR(2,
     115),D(3,11)
      COMMON E,Q,X,T,C,D,BAIR,AA,AG,N,IKE
      REAL*8 XXX,D1,D2,DET
      DIMENSION XXX(11,2),DET(100,4),JDET(100)
      COMMON XXX,DET,JI,IDET,JDET,IWRITE
      COMMON V1,V2,V12,YT,Y0,Y1,Y2,RHO
C
C
C     READ NUMITR - THE NUMBER OF SETS OF DATA TO BE READ IN
C       IWRITE = 0 WRITES OUT ALL STEPS TOWARD CALCULATION
C        OF THE DETERMINANT FOR THE MGLM(F) DESIGN,
C       IWRITE < 6 WRITES OUT INADMISSABLE MGLM'S BUT NOT
C        ALL STEPS
C       IWRITE > 6 WRITES OUT ONLY ADMISSABLE VALUES
C
C
      READ(5,3) NUMITR,IWRITE
    3 FORMAT(I3,27X,I5)
      DO 600 MITER = 1,NUMITR
C
C
C     READ THE NUMBER OF COEFFICIENTS, IF IJK = 0 READ
C        COEFFICIENTS ;  IF IJK .NE. 0 READ IN VALUES FROM
C        WHICH COEFFICIENTS WILL BE CALCULATED.  IJK=0 CAN
C        BE USED WHEN COEFFICIENTS ARE ALREADY CALCULATED.
C
C
      READ(5,20) N,IJK
   20 FORMAT(2I2)
      IF(IJK .EQ. 0) GO TO 10
      IDET = 0
C
C
C     IF IJK2 NEGATIVE  ITERATE THE TWO POLYNOMIALS BETWEEN
C        N1 AND M (DO NOT ADVISE ITS USE DUE TO THE FACT
C        THAT A VERY PRECISE FIRST ESTIMATE IS REQUIRED);
```

```
C         IJK2  ZERO THEN ONLY ONE M VALUE WILL BE READ IN
C         IJK2 POSITIVE THEN M = 0,1,2,3,...
C
C
      READ(5,2) IJK2
    2 FORMAT(I2)
C
C
C     READ IN  V1, V2, V12 - THE NUMBER OF FACTORS OF
C         INTEREST FOR EACH RESPONSE, AND IN COMMON. IN THE
C         DISSERTATION THESE ARE DENOTED BY K1, K2, K12.
C         WHEN THESE VALUES ARE WRITTEN OUT THEY WILL BE
C         WRITTEN AS K1, K2, K12.
C        RHO - RHO SQUARED ;
C        YO - SET-UP COST;
C        Y1, Y2 - COST OF MEASURING RESPONSES V(1), V(2);
C        YT - TOTAL AMOUNT OF MONEY AVAILABLE;
C        KNUM - A NUMBERING SYSTEM TO HELP COMPARE THESE
C         RESULTS TO PREVIOUS PROGRAM RESULTS
C
C
      READ(5,5) V1,V2,V12,RHO,YT,YO,Y1,Y2,KNUM
    5 FORMAT(4F5.0,4F10.0,15X,I5)
      IF(IWRITE .NE. 0) GO TO 9
      WRITE(6,7) V1,V2,V12,RHO,YO,Y1,Y2,YT,KNUM
    7 FORMAT('1',//,5X,'K1 =',F3.0,10X,'K2 =',F3.0,10X,'K12
                    =',F3.0,10X,
     1'RHO SQ. =',F9.6,//,5X,'YO =',F13.6,9X,'Y1 =',F13.6,9X
                    ,'Y2 =',F13.
     26,9X,'YT =',F13.6,20X,I5)
    9 IF(IJK2) 300,400,500
C
C
C     READ IN COEFFICIENTS IF KNOWN
C
C
   10 READ(5,1)(C(1,I),I=1,N)
    1 FORMAT(8D10.0)
      CALL CALPOL
      GO TO 600
C
C
C     READ IN THE INITIAL ESTIMATE OF M (THIS METHOD IS NOT
C         SUGGESTED.)
C
C
  300 READ(5,305) M
  305 FORMAT(F5.0)
      XNB = YT / (YO+Y1+Y2)
      IF(IWRITE .EQ. 0) WRITE(6,506)
```

```
      CALL DETERM(XNB,0.0)
      DO 390 IZ=1,10
      CALL NPOLY(M)
      CALL CALPOL
      NM1 = N - 1
      NREAL = 0
      DO 320 I1=1,NM1
      IF(XXX(I1,2) .NE. 0.0) GO TO 320
      IF(XXX(I1,1) .LE. 0.0) GO TO 320
      XN1 = XXX(I1,1)
      XN2 = (YT -M*Y0 - XN1*(Y0+Y1)) / Y2
      IF(XN2 .GT. XN1) GO TO 310
      IF(XN2 .LT.  M ) GO TO 310
      IF(IWRITE .EQ. 0) WRITE(6,308)
  308 FORMAT(///)
      CALL DETERM(XN1,M)
      XN1R = XN1
      NREAL = NREAL + 1
      GO TO 320
  310 IF(IWRITE .NE. 0) GO TO 320
      WRITE(6,315) XN1,XN2,M
  315 FORMAT(//,15X,'WILL NOT USE ROOT WITH XN1 =',F8.4,
     1'  BECAUSE XN2 =',F8.4,'  AND M =',F8.4)
  320 CONTINUE
      IF(NREAL .NE. 0) GO TO 340
      IF(IWRITE .NE. 0) GO TO 600
      WRITE(6,998)
  998 FORMAT('1')
      WRITE(6,330) IZ
  330 FORMAT('1',/////,' STOP ITERATION OF N1 AND M ON STEP'
                    ,I3)
      WRITE(6,335)
  335 FORMAT(//,10X,49HALL N1'S ARE EITHER NOT REAL OR THEY
                    ARE NEGATIVE
     1,' OR THEY ARE NOT FEASABLE')
      GO TO 600
  340 IF (NREAL .GT. 1) GO TO 345
      IF(IWRITE .EQ. 0) WRITE(6,341)
  341 FORMAT('1',8('***'),//,' THERE IS MORE THAN 1 FEASAB',
     1'LE VALUE FOR N1, THE LAST OF WHICH IS BEING USED',
     2 //,1X,8('***'),////)
  345 XN1 = XN1R
      CALL MPOLY(XN1)
      CALL CALPOL
      NM1 = N - 1
      DO 350 I1=1,NM1
      IF(XXX(I1,2) .NE. 0.0) GO TO 350
      IF(XXX(I1,1) .LT. 0.0) GO TO 350
      M= XXX(I1,1)
      CALL DETERM(XN1,M)
```

```
      IF(IWRITE .EQ. 0) WRITE(6,998)
      GO TO 390
  350 CONTINUE
      IF(IWRITE .EQ. 0) WRITE(6,998)
      M = 0.0
      CALL NPOLY (M)
      CALL CALPOL
      CALL DETERM(XN1,M)
      IF(IWRITE .NE. 0) GO TO 600
      WRITE(6,330) IZ
      WRITE(6,355)
  355 FORMAT(//,10X,34HALL THE M'S ARE EITHER NOT REAL OR,
     118H THEY ARE NEGATIVE)
      GO TO 600
  390 CONTINUE
      GO TO 949
C
C
C     READ IN M.  N1 WILL BE COMPUTED FOR ONLY THIS M VALUE.
C
C
  400 READ(5,405) M
  405 FORMAT(F5.0)
      CALL NPOLY(M)
      CALL CALPOL
      CALL DETERM(XN1,M)
      GO TO 600
C
C
C     N1 IS COMPUTED FOR M = 0,1,2,3, ... , MMAX
C
C
  500 READ(5,505) MMAX
  505 FORMAT(I2)
      XNB = YT / (Y0+Y1+Y2)
      IF(IWRITE .EQ. 0) WRITE(6,506)
  506 FORMAT(//,10X,'DETERMINANT FOR M.D.M. DESIGN',/)
      CALL DETERM(XNB,0.0)
      MMAXP1 = MMAX + 1
      DO 550 I=1,MMAXP1
      M = I - 1
      IF(I .EQ. 1) GO TO 508
      XNB1 = (YT - Y0*M) / (Y0 + Y1 + Y2)
      CALL DETERM(XNB1,M)
  508 CALL NPOLY(M)
      CALL CALPOL
      NM1 = N - 1
      NREAL = 0
      IF(IWRITE .EQ. 0) WRITE(6,510)
  510 FORMAT(///,5X,'THE INVERSE OF THE DETERMINANT OF THE V
                      AR.-COV. MAT
```

```
  1RIX IS FOUND (THE VARIANCES WHICH ARE CONSTANTS ARE IG
                 NORED).',/,
  210X,'MAXIMIZING THE INVERSE OF THE DETERMINANT CORRESP
                 ONDS TO MINI
  3MIZING THE DETERMINANT.',//)
   DO 530 I1=1,NM1
   IF(XXX(I1,2) .NE. 0.0) GO TO 530
   IF(XXX(I1,1) .LE. 0.0) GO TO 530
   XN1 = XXX(I1,1)
   CALL DETERM(XN1,M)
   NREAL = 1
530 CONTINUE
   IF(IWRITE .EQ. 0) WRITE(6,998)
   IF(NREAL .EQ. 1) GO TO 550
   IF(IWRITE .NE. 0) GO TO 600
   WRITE(6,535) M
535 FORMAT(////,5X,'STOP ITERATION WHEN M =',F4.1)
   WRITE(6,335)
   GO TO 600
550 CONTINUE
949 WRITE(6,910)
910 FORMAT(//,5X,'PARAMETERS FOR THE MODEL')
   WRITE(6,917) V1,V2,V12,RHO,Y0,Y1,Y2,YT,KNUM
917 FORMAT(    //,7X,'K1 =',F3.0,10X,'K2 =',F3.0,10X,'K12
                 =',F3.0,20X,
  1'RHO SQ. =',F9.6,//,7X,'Y0 =',F13.6,9X,'Y1 =',F13.6,9X
                 ,'Y2 =',F13.
  26,9X,'YT =',F13.6,15X,I5,///)
   WRITE(6,920)
920 FORMAT(5X,'ADMISSABLE OPTIMAL DESIGN SIZES FOR VARYING
                 M VALUES',/
  1/)
   DO 950 IDEE = 1,IDET
   IF(JDET(IDEE) .NE. 0) GO TO 950
   WRITE(6,19) (DET(IDEE,I),I=1,4)
 19 FORMAT(10X,'DETERMINANT =',D16.8,3X,'WHERE:   N1 =',F8
                 .4,4X,'N2 ='
  1,F8.4,4X,'M =',F5.1,//)
950 CONTINUE
   IF(IWRITE .GT. 6) GO TO 980
   WRITE(6,955)
955 FORMAT(///,5X,'INADMISSABLE SIZES,  N2 =0  OR N2 > N1'
                 ,//)
   DO 960 IDEE = 1,IDET
   IF(JDET(IDEE) .NE. 1) GO TO 960
   WRITE(6,19) (DET(IDEE,I),I=1,4)
960 CONTINUE
   WRITE(6,930)
930 FORMAT(///,5X,'INADMISSABLE SIZES,  M > N2',//)
   DO 970 IDEE = 1,IDET
```

```
      IF(JDET(IDEE) .NE. 2) GO TO 970
      WRITE(6,19) (DET(IDEE,I),I=1,4)
  970 CONTINUE
  980 WRITE(6,998)
  600 CONTINUE
  999 STOP
      END




      SUBROUTINE CALPOL
C
C     THIS SUBRCUTINE ASSUMES THAT THE COEFFICIENTS HAVE
C        BEEN SPECIFIED AND THEN PRINTS AND CALLS THE
C        CORRECT SUBROUTINES.
C
C
      REAL*8 X,C,R,PX,Q,E,AA,T,BAIR,RTFINK,ROOT1,ROOT2,ROOTI
                    ,ROOTIM,RAT,
     1REAL,U,V,UE,VE,D,DSQRT,DABS,BAD,AG
      REAL*8 XN1,XN2
      REAL*4 M
      DIMENSION X(400),C(3,11),Q(75,10),E(75,11),T(11,11),AA
                    (11),BAIR(2,
     115),D(3,11)
      COMMON E,Q,X,T,C,D,BAIR,AA,AG,N,IKE
      REAL*8 XXX,D1,D2,DET
      DIMENSION XXX(11,2),DET(100,4),JDET(100)
      COMMON XXX,DET,JI,IDET,JDET,IWRITE
      COMMON V1,V2,V12,YT,Y0,Y1,Y2,RHO
      IF(IWRITE .NE. 0) GO TO 10
      WRITE(6,2)
    2 FORMAT(////,'       ORIGIONAL COEFFICIENTS WERE ',//)
      WRITE(6,3)(C(1,I),I=1,N)
    3 FORMAT( 6X,D16.8)
   10 JI = 1
      CALL QD
      IF (AG .EQ. 0) GO TO 33
      IF(IWRITE .NE. 0) GO TO 33
      WRITE (6,4) AG
    4 FORMAT(/////,'  COEFFICIENTS WHEN CHANGED BY A FACTOR
                    OF ',F3.0,
     1' , WERE:',/)
      WRITE (6,3)(AA(I),I=1,N)
   33 RETURN
      END
```

```
      SUBROUTINE NPOLY(M)
C
C       CALCULATE THE COEFFICIENTS FOR THE 5TH ORDER EQUATION
C          SOLVING DET(NON HIERARCHIAL) DESIGN
C
C
C
      REAL*8 X,C,R,PX,Q,E,AA,T,BAIR,RTFINK,ROOT1,ROOT2,ROOTI
                  ,ROOTIM,RAT,
     1REAL,U,V,UE,VE,D,DSQRT,DABS,BAD,AG
      REAL*4 M
      DIMENSION X(400),C(3,11),Q(75,10),E(75,11),T(11,11),AA
                  (11),BAIR(2,
     115),D(3,11)
      COMMON E,Q,X,T,C,D,BAIR,AA,AG,N,IKE
      REAL*8 XXX,D1,D2,DET
      DIMENSION XXX(11,2),DET(100,4),JDET(100)
      COMMON XXX,DET,JI,IDET,JDET,IWRITE
      COMMON V1,V2,V12,YT,Y0,Y1,Y2,RHO
      N=6
      Y=(Y0+Y1)/Y2
      F=YT/Y2 - M*Y0/Y2
      RYP=RHO*Y + 1.
      C(1,1) = -(V1+V2)*(Y**2)*(RYP**2)
      C(1,2) = (4.*V1+3.*V2+V12)*RHO*(Y**2)*F*RYP + (2.*V1+V
                  2 )*Y*F*RYP
     1-2.*(V1+V2+1.)*V12*M*RHO*(Y**2)*RYP
      C(1,3) = -(V1+V2+2.)*(V1-V12)*(V2-V12)*((M*RHO*Y)**2)*
                  RYP - (6.*V1
     1+2.*V2+2.*V12)*RHO*Y*RYP*(F**2) - (V1+V2+2.)*V1*V2*(M*
                  *2)*RHO*Y*RY
     2P + 2.*(2.*V1+V2+2.)*V12*M*RHO*Y*F*RYP - (V2+V12)*((RH
                  O*Y*F)**2) +
     3 2.*(V1+V12+V2)*V12*M*F*((RHO*Y)**2) - V1*(F**2)
      C(1,4) = (V1+1.)*RHO*F*(F**2-2.*V12*M*F + V1*V2*(M**2)
                  ) + (2.*V1+V
     12+4.)*(V1-V12)*(V2-V12)*((M*RHO)**2)*Y*F*RYP + (V1+V12
                  +V2+1.)*(V1-
     3V12)*(V2-V12)*((M*RHO*Y)**2)*RHO*F + (V1+V12-1.)*RHO*(
                  F**3)*RYP -
     4 (V1+V12-1.)*V1*V2*((M*RHO)**2)*Y*F + (3.*V1 +2.*V12+V
                  2+1.)*(RHO**
     52)*Y*F*((F**2)-2.*V12*M*F+V1*V2*(M**2))
      C(1,5) = -(V1-V12)*(V2-V12)*(V1+2.)*((M*RHO*F)**2)*RYP
                   - (2.*V1+2.
     1*V12+V2+2.)*(V1-V12)*(V2-V12)*(M**2)*(RHO**3)*Y*(F**2)
                   - (V1+V12)*
```

```
     2((RHO*F)**2)*(F**2-2.*V12*M*F + V1*V2*(M**2))
      C(1,6) = (V1+V12+1.)*(V1-V12)*(V2-V12)*((M*RHO*F)**2)*
                    RHO*F
      IF(IWRITE .NE. 0) GO TO 20
      WRITE(6,5) M
    5 FORMAT(//,' COEFFICIENTS OF N1 WITH M =',F10.5,//)
      WRITE(6,10) (C(1,I),I=1,N)
   10 FORMAT(7(2X,D16.8))
   20 RETURN
      END
```

```
      SUBROUTINE MPOLY(XN1)
C
C
C     THIS SUBROUTINE COMPUTES THE COEFFICIENTS OF THE J TH
C        ORDER POLYNOMIAL IN M WHERE A VALUE OF N1 = XN1
C        IS PLUGGED INTO THE POLYNOMIAL
C
C
      REAL*8 X,C,R,PX,Q,E,AA,T,BAIR,RTFINK,ROOT1,ROOT2,ROOTI
                    ,ROOTIM,RAT,
     1REAL,U,V,UE,VE,D,DSQRT,DABS,BAD,AG
      REAL*8 XN1,XN2
      REAL*8 A3,A2,A1,A0
      DIMENSION X(400),C(3,11),Q(75,10),E(75,11),T(11,11),AA
                    (11),BAIR(2,
     115),D(3,11)
      COMMON E,Q,X,T,C,D,BAIR,AA,AG,N,IKE
      REAL*8 XXX,D1,D2,DET
      DIMENSION XXX(11,2),DET(100,4),JDET(100)
      COMMON XXX,DET,JI,IDET,JDET,IWRITE
      COMMON V1,V2,V12,YT,Y0,Y1,Y2,RHO
      N = 5
      Y = (Y0 + Y1)/Y2
      RHO2 = RHO**2
      DX = YT/Y2 - Y* XN1
      YZ = Y0/Y2
      V1V2 = (V1 - V12) * (V2 - V12)
      A3= -(YZ**2)*(V2 - 2.)*V1V2*RHO2
      A2=DX*YZ*(V2-4.)*V1V2*RHO2 - XN1*YZ*(V2-1.)*V1*V2*RHO
                   - 2.*XN1*
```

```
   1 (YZ**2)*(V2-1.)*V12*RHO - XN1*(YZ**3)  *(V2-V12)*RHO
    A1 = 2.*(DX**2)*V1V2*RHO2 -2.*XN1*DX*V1*V2*RHO +2.*XN1
                  *DX*YZ*
   1 (V2-2.)*V12*RHO -((XN1*YZ)**2)*V2 +2.*XN1*(YZ**2)*DX*
                  (V2-V12)*RHO
    A0 = 2.*XN1*(DX**2)*V12*RHO + (XN1**2)*DX*YZ*V2 -XN1*(
                  DX**2)*YZ*
   1 (V2-V12)*RHO
    DDX = XN1 - RHO * DX
    RY = RHO * YZ
C
C     THESE ARE THE COEFFICIENTS OF THE POLYNOMIAL IN M
C
    C(1,1) = A3*RY + (YZ**3)*(V12-1.)*V1V2*(RHO**3)
    C(1,2) = A3*DDX + A2*RY + 2.*XN1*(YZ**3)*V12*(V12-1.)*
                  RHO2 + XN1*
   1 (YZ**2)*(V12-1.)*V1*V2*RHO2 -2.*(YZ**2)*DX*(V12-1.)*V
                  1V2*(RHO**3)
    C(1,3) = A2*DDX + A1*RY - 4.*XN1*(YZ**2)*DX*V12*(V12-1
                  .)*RHO2 -XN1
   1 *YZ*DX*(V12-1.)*V1*V2*RHO2 + YZ*(DX**2)*(V12-1.)*V1V2
                  *(RHO**3)
    C(1,4) = A1*DDX + A0*RY + 2.*XN1*(DX**2)*YZ*V12*(V12-1
                  .)*RHO2
    C(1,5) = A0*DDX
    IF(IWRITE .NE. 0) GO TO 20
    WRITE(6,5) XN1
  5 FORMAT(//,' COEFFICIENTS OF M WITH N1 =',F10.5,//)
    WRITE(6,10) (C(1,I),I=1,N)
 10 FORMAT(7(2X,D16.8))
 20 RETURN
    END




    SUBROUTINE DETERM(XN1,M)
C
C     CALCULATE THE INVERSE OF THE DETERMINANT OF THE
C        VARIANCE-COVARIANCE MATRIX.
C
C
    REAL*8 X,C,R,PX,Q,E,AA,T,BAIR,RTFINK,ROOT1,ROOT2,ROOTI
                  ,ROOTIM,RAT,
   1REAL,U,V,UE,VE,D,DSQRT,DABS,BAD,AG
    REAL*8 XN1,XN2
    REAL*4 M
    DIMENSION X(400),C(3,11),Q(75,10),E(75,11),T(11,11),AA
                  (11),BAIR(2,
```

```
     115),D(3,11)
      COMMON E,Q,X,T,C,D,BAIR,AA,AG,N,IKE
      REAL*8 XXX,D1,D2,DET
      DIMENSION XXX(11,2),DET(100,4),JDET(100)
      COMMON XXX,DET,JI,IDET,JDET,IWRITE
      COMMON V1,V2,V12,YT,YO,Y1,Y2,RHO
      IDET = IDET + 1
      XN2 = (YT - YO*M - (YO+Y1)*XN1) / Y2
      IV1 = V1
      IV2 = V2
      IV12= V12
C
C
C     CHECK N1 AND N2 VALUES, AND IF O THEN AVOID COMPUTING
C        THE DETERMINANT.
C
C
      IF (DABS(XN2) .LT. .1D-5) GO TO 5
      IF (DABS(XN1) .LT. .1D-5) GO TO 10
      D1 = (XN1 ** (IV1+IV12+1)) * (XN2**(IV2+IV12+1))
      D2 = (XN2**IV12)*((XN1-RHO*XN2)**(IV12-1))*((XN1**2)*X
                  N2 - RHO*
     1XN1*(XN2**2) + M*XN1*RHO*(2.*V12*XN2-V1*V2*M) + ((M*RH
                  O)**2)*XN2*
     2(V1-V12)*(V2-V12))
      GO TO 14
    5 XN2 = 0.0
      GO TO 11
   10 XN1 = 0.0
   11 DET(IDET,1) = 0.0
      GO TO 15
   14 DET(IDET,1) = D1 / D2
   15 DET(IDET,2) = XN1
      DET(IDET,3) = XN2
      DET(IDET,4) = M
      JDET(IDET) = 0
      IF((XN2 - XN1) .GT. .1D-3) JDET(IDET) = 1
      IF (  XN2      .LT. .1D-3) JDET(IDET) = 1
      IF ( M .GT. XN2) JDET(IDET) = 2
      IF(IWRITE .NE. 0) GO TO 20
      WRITE(6,19) (DET(IDET,I),I=1,4)
   19 FORMAT(10X,'DETERMINANT =',D16.8,3X,'WHERE:   N1 =',F8
                  .4,4X,'N2 ='
     1,F8.4,4X,'M =',F8.4,//)
   20 RETURN
      END
```

```
      SUBROUTINE QD
C
C
C     THIS SUBROUTINE USES THE Q. D. ALGORITHM TO FIND
C        SIMULTANEOUS APPROXIMATIONS TO ALL ZEROS OF A
C        POLYNOMIAL.
C
C
      REAL*8 X,C,R,PX,Q,E,AA,T,BAIR,RTFINK,ROOT1,ROOT2,ROOTI
                    ,ROOTIM,RAT,
     1REAL,U,V,UE,VE,D,DSQRT,DABS,BAD,AG
      DIMENSION X(400),C(3,11),Q(75,10),E(75,11),T(11,11),AA
                    (11),BAIR(2,
     115),D(3,11)
      COMMON E,Q,X,T,C,D,BAIR,AA,AG,N,IKE
      REAL*8 XXX,D1,D2,DET
      DIMENSION XXX(11,2),DET(100,4),JDET(100)
      COMMON XXX,DET,JI,IDET,JDET,IWRITE
      CALL TEST
      NS1=N-1
C
C     INITIAL VALUES FOR Q.D. ARE FOUND
C
      Q(1,1) = -AA(2)/AA(1)
       DO 2 I=2,NS1
      Q(1,I) = 0.0D0
    2 E(1,I) = AA(I+1) / AA(I)
       DO 4 I=1,75
      E(I,1) =0.0D0
    4 E(I,N) =0.0D0
      IF(IWRITE .EQ. 0) WRITE(6,24)
   24 FORMAT('0',//,5X,'QD ALGORITHM',//)
C
C
C     Q.D. ITERATION
C
C
      DO 10 I=2,50
      DO 6 J=1,NS1
      Q(I,J) = E(I-1,J+1) - E(I-1,J) + Q(I-1,J)
      IF (J .EQ. 1) GO TO 6
      E(I,J) = (Q(I,J)/Q(I,J-1)) * E(I-1,J)
    6 CONTINUE
      DO 11 J=2,NS1
      IF (DABS(E(I,J)) .LE. .1D-10)  E(I,J)=0.0D0
   11 CONTINUE
      DO 9 KK=1,N
      IF(E(I,KK) .NE. 0.0D0) GO TO 10
    9 CONTINUE
```

```
      IF(IWRITE .NE. 0) GO TO 50
      WRITE(6,71)
   71 FORMAT(//,10X,'ITERATION STOPPED BEFORE 50TH ITERATION
     1                ',//)
      WRITE (6,25) I,(Q(I,L),L=1,NS1)
   50 DO 27 KK=1,NS1
      Q(75,KK) = Q(I,KK)
      Q(74,KK) = Q(I-1,KK)
   27 E(75,KK) = E(I,KK)
      GO TO 14
   10 CONTINUE
      DO 110 I=51,75
      DO 106 J=1,NS1
      Q(I,J) = E(I-1,J+1) - E(I-1,J) + Q(I-1,J)
      IF (J .EQ. 1) GO TO 106
      E(I,J) = (Q(I,J)/Q(I,J-1)) * E(I-1,J)
  106 CONTINUE
      IF(IWRITE .NE. 0) GO TO 51
      WRITE (6,25) I,(Q(I,L),L=1,NS1)
      WRITE(6,26)(E(I,L),L=1,N)
   25 FORMAT(' Q',I2,7(5X,F13.7))
   26 FORMAT(' E  ',7(F14.9,4X))
   51 DO 111 J=2,NS1
      IF (DABS(E(I,J)) .LE. .1D-10)  E(I,J)=0.0D0
  111 CONTINUE
      DO 109 KK=1,N
      IF(E(I,KK) .NE. 0.0D0) GO TO 110
  109 CONTINUE
      DO 127 KK=1,NS1
      Q(75,KK) = Q(I,KK)
      Q(74,KK) = Q(I-1,KK)
  127 E(75,KK) = E(I,KK)
      GO TO 14
  110 CONTINUE
C
C     LIM(Q(N,I)) GOES TO ITH ROOT AS N GOES TO INFINITY
C
   14 KICK=0
      IF(IWRITE .EQ. 0) WRITE(6,23)
   23 FORMAT ('1')
      DO 20 I=2,N
      IKE=I-1
C
C
C     THE PROGRAM HAD CHECKED AGAINST .1D-05 .  ON SOME
C        POLYNOMIALS 75 ITERATIONS OF Q.D. IS NOT ENOUGH
C        TO ALLOW E < .1D-05 .  THUS THE VALUE WAS CHANGED
C        TO .1D-02 .  IN REAL SITUATIONS THESE E'S SHOULD
C        BE CHECKED TO MAKE SURE THE ROOTS ARE CONVERGING.
C        WHEN THE MODULUS OF REAL AND IMAGINARY ROOTS ARE
```

```
C          CLOSE IT TAKES A LONG TIME TO CONVERGE.
C
C       IF YOU HAVE N ROOTS AND NOT ALL ARE PRINTED OUT IT IS
C          BECAUSE SEVERAL REAL AND IMAGINARY ROOTS HAVE
C          MODULUSES VERY CLOSE TOGETHER.
C
C
        IF(DABS(E(75,I)) .GT. .1D-02) GO TO 18
        IF(KICK .EQ. 1) GO TO 16
        KICK=0
C
C
C       IF Q.D. HAS CONVERGED TO A ROOT THEN USE THIS AS FIRST
C          APPROXIMATION IN NEWTONS ALGORITHM.
C
C
        BAD=Q(75,IKE)
        CALL NEWT(BAD)
        GO TO 20
C
C
C       IF IT HAS NOT CONVERGED TO A ROOT THEN TWO VALUES WILL
C          BE USED AND THESE VALUES APPROXIMATE THE
C          COEFFICIENTS OF A QUADRATIC EQUATION
C
C
C       SINCE U AND V ARE APPROX. TO THE POLYNOMIAL
C                   (X**2) - U X + V = 0
C          AND BAIRSTOWS METHOD WANTS THE VALUES A AND B FROM
C          THE EQUATION:
C                      (X**2) - A X - B = 0
C          THEN A = U  AND  B= -V.  THUS WHEN BAIRST IS
C          CALLED, THE VALUES +U AND -V ARE SENT.   THE
C          NEGATIVE OF THE TWO VALUES FORND IN BAIRST ARE
C          RETURNED AND THEN SENT TO QUAD .
C
C
   16   U= Q(75,I-2) + Q(75,I-1)
        V = -Q(74,I-2) * Q(75,I-1)
        CALL BAIRST(U,V)
        CALL QUAD(U,V)
        KICK  =   0
        GO TO 20
   18   KICK=1
   20   CONTINUE
        RETURN
        END
```

```
      SUBROUTINE TEST
C
C
C     THIS SUBROUTINE CHECKS TO SEE IF ALL COEFFICIENTS ARE
C        NON-ZERO.
C
C
      REAL*8 X,C,R,PX,Q,E,AA,T,BAIR,RTFINK,ROOT1,ROOT2,ROOTI
                     ,ROOTIM,RAT,
     1REAL,U,V,UE,VE,D,DSQRT,DABS,BAD,AG
      DIMENSION X(400),C(3,11),Q(75,10),E(75,11),T(11,11),AA
                     (11),BAIR(2,
     115),D(3,11)
      COMMON E,Q,X,T,C,D,BAIR,AA,AG,N,IKE
      REAL*8 XXX,D1,D2,DET
      DIMENSION XXX(11,2),DET(100,4),JDET(100)
      COMMON XXX,DET,JI,IDET,JDET,IWRITE
      AG=0.0D0
   12 DO 1 I=1,N
      IF(DABS(C(1,I)) .LE. .1D-09) GO TO 10
    1 CONTINUE
      DO 2 I=1,N
    2 AA(I) = C(1,I)
      RETURN
C
C
C     THIS PART OF SUBROUTINE IS USED WHEN A COEFFICIENT=0 .
C        (SEE HERRICI P. 173 .)  THE Q.D. METHOD WORKS ONLY
C        WITH NON-ZERO COEFFICIENTS.
C
C
   10 AG = AG+1.D0
      DO 11 I=1,N
   11 T(1,I) = C(1,I)
      NS1=N-1
      DO 15 I=1,NS1
      T(I+1,1) = C(1,1)
      NA1SI = N+1-I
      DO 15 J=2,NA1SI
   15 T(I+1,J)= AG * T(I+1,J-1) + T(I,J)
      T(N+1,1) = C(1,1)
      DO 16 I=1,N
      NA2SI = N+2-I
   16 AA(I) = T(NA2SI,I)
      DO 18 I=1,N
      IF (DABS(AA(I)) .LE. .1D-5) GO TO 10
   18 CONTINUE
   17 RETURN
      END
```

```
      SUBROUTINE NEWT(BAD)
C
C
C
C     THIS SUBROUTINE USES NEWTONS ALGORITHM TO CONVERGE
C        TO REAL ROOTS.
C
C
      REAL*8 X,C,R,PX,Q,E,AA,T,BAIR,RTFINK,ROOT1,ROOT2,ROOTI
                    ,ROOTIM,RAT,
     1REAL,U,V,UE,VE,D,DSQRT,DABS,BAD,AG
      DIMENSION X(400),C(3,11),Q(75,10),E(75,11),T(11,11),AA
                    (11),BAIR(2,
     115),D(3,11)
      COMMON E,Q,X,T,C,D,BAIR,AA,AG,N,IKE
      REAL*8 XXX,D1,D2,DET
      DIMENSION XXX(11,2),DET(100,4),JDET(100)
      COMMON XXX,DET,JI,IDET,JDET,IWRITE
      X(1) = BAD
      J = 1
   50 R = X(J)
C
C
C     CALL SUBROUTINE TO COMPUTE FX AND ITS DERIVATIVE AT R
C
C
      CALL DOIT (R)
      PX = X(J) - R
C
C
C     CHECK TO SEE IF ROOT IS STILL CONVERGING
C
C
      IF ((DABS(X(J) - PX)) .LE. .1D-14 )  GO TO 75
C
C     SEE IF YOU HAVE ITERATED 400 TIMES YET
C
      IF (J .EQ. 400) GO TO 75
      J = J+1
      X(J) = PX
      GO TO 50
   75 X(J) = PX
      ROOT1 = X(J) + AG
      IF(IWRITE .EQ. 0) WRITE(6,1) IKE,ROOT1,J
    1 FORMAT ('0 X(',I2,')  =',F17.8,10X,'NEWTONS METHOD, NU
                    MBER OF ITER
```

```
     1ATIONS WAS ',I3,//)
      XXX(JI,1) = ROOT1
      XXX(JI,2) = 0.0
      JI = JI + 1
   76 RETURN
      END




      SUBROUTINE DOIT (R)
C
C
C     COMPUTES F(X) AND F'(X) FOR SOME VALUE OF X.
C
C
      REAL*8 X,C,R,PX,Q,E,AA,T,BAIR,RTFINK,ROOT1,ROOT2,ROOTI
                   ,ROOTIM,RAT,
     1REAL,U,V,UE,VE,D,DSQRT,DABS,BAD,AG
      REAL*8 XN1,XN2
      DIMENSION X(400),C(3,11),Q(75,10),E(75,11),T(11,11),AA
                   (11),BAIR(2,
     115),D(3,11)
      COMMON E,Q,X,T,C,D,BAIR,AA,AG,N,IKE
      REAL*8 XXX,D1,D2,DET
      DIMENSION XXX(11,2),DET(100,4),JDET(100)
      COMMON XXX,DET,JI,IDET,JDET,IWRITE
      DO 1 I=1,N
    1 D(1,I)=AA(I)
      D(2,1) = D(1,1)
C
C
C     COMPUTE F(X)
C
C
      DO 100 I = 2,N
      IS1 = I - 1
  100 D(2,I) = R* D(2,IS1) + D(1,I)
      NS1 = N-1
      D(3,1) = D(2,1)
C
C
C     COMPUTE F'(X)
C
C
      DO 101 K = 2,NS1
      KS1 = K - 1
  101 D(3,K) = R * D(3,KS1) + D(2,K)
      IF (DABS(D(3,NS1)) .LE. .1D-12) GO TO 102
```

```
      R = D(2,N) / D(3,NS1)
      GO TO 69
  102 R = 0.000
   69 RETURN
      END





      SUBROUTINE BAIRST(U,V)
C
C
C     THIS SUBROUTINE USING THE QUADRATIC FACTOR
C        APPROXIMATIONS FROM THE Q.D. ALGORITHM, CONVERGES
C        TO THE TRUE QUADRATIC POLYNOMIAL.  IN SUBROUTINE
C        QUAD THIS QUADRATIC POLYNOMIAL IS SOLVED.
C
C
      REAL*8 X,C,R,PX,Q,E,AA,T,BAIR,RTFINK,ROOT1,ROOT2,ROOTI
                   ,ROOTIM,RAT,
     1REAL,U,V,UE,VE,D,DSQRT,DABS,BAD,AG
      DIMENSION X(400),C(3,11),Q(75,10),E(75,11),T(11,11),AA
                   (11),BAIR(2,
     115),D(3,11)
      COMMON E,Q,X,T,C,D,BAIR,AA,AG,N,IKE
      REAL*8 XXX,D1,D2,DET
      DIMENSION XXX(11,2),DET(100,4),JDET(100)
      COMMON XXX,DET,JI,IDET,JDET,IWRITE
      NA2 = N + 2
      NA1 = N + 1
      NS1 = N - 1
      K=0
      BAIR(1,1) = 0.D0
      BAIR(1,2) = 0.D0
      BAIR(2,2) = 0.D0
      BAIR(2,1) = 0.D0
    2 DO 1 I=3,NA2
      IS1 = I-1
      IS2 = I-2
      BAIR(1,I) = AA(IS2) + U*BAIR(1,IS1) + V*BAIR(1,IS2)
    1 BAIR(2,I)=BAIR(1,I) + U*BAIR(2,IS1) + V*BAIR(2,IS2)
      IF (DABS(BAIR(1,NA2)) .LE. .1D-10)  GO TO 3
      IF (DABS(BAIR(1,NA1)) .LE. .1D-10)  GO TO 3
      K=K+1
      IF (K .EQ. 400) GO TO 3
      UE =(BAIR(1,NA2)*BAIR(2,NS1) -BAIR(1,NA1)*BAIR(2,N))/(
                   BAIR(2,N)**2
     1 - BAIR(2,NA1) * BAIR(2,NS1))
      VE =(BAIR(1,NA1)*BAIR(2,NA1) -BAIR(1,NA2)*BAIR(2,N))/(
                   BAIR(2,N)**2
```

```
    1 - BAIR(2,NA1)*BAIR(2,NS1))
      U = U + UE
      V = V + VE
      GO TO 2
    3 J = K
      U = -U
      V = -V
      IF(IWRITE .EQ. 0) WRITE(6,25)
   25 FORMAT(/)
      RETURN
      END




      SUBROUTINE QUAD(U,V)
C
C
C     THIS SUBROUTINE EXECUTES THE QUADRATIC FORMULA.
C
C
      REAL*8 X,C,R,PX,Q,E,AA,T,BAIR,RTFINK,ROOT1,ROOT2,ROOTI
                    ,ROOTIM,RAT,
     1REAL,U,V,UE,VE,D,DSQRT,DABS,BAD,AG
      DIMENSION X(400),C(3,11),Q(75,10),E(75,11),T(11,11),AA
                    (11),BAIR(2,
     115),D(3,11)
      COMMON E,Q,X,T,C,D,BAIR,AA,AG,N,IKE
      REAL*8 XXX,D1,D2,DET
      DIMENSION XXX(11,2),DET(100,4),JDET(100)
      COMMON XXX,DET,JI,IDET,JDET,IWRITE
      IKES1 = IKE-1
      REAL = -U/2 +AG
      RAT = U**2 - 4*V
      IF (RAT) 14,20,22
   14 ROOTI = (DSQRT(-RAT))/2.D0
      ROOTIM = -ROOTI
      IF(IWRITE .NE. 0) GO TO 16
      WRITE (6,15) IKES1,REAL,ROOTI
   15 FORMAT ('   X(',I2,')      REAL PART =',D17.8,/,7X,'IMAG
                    INARY PART =
     1',D17.8,//)
      WRITE (6,15) IKE,REAL,ROOTIM
   16 XXX(JI,1) = REAL
      XXX(JI,2) = ROOTI
      JI = JI + 1
      XXX(JI,1) = REAL
      XXX(JI,2) = ROOTIM
      JI = JI + 1
```

```
   GO TO 30
20 ROOT1 = REAL
   ROOT2 = REAL
   GO TO 24
22 RTFINK = (DSQRT(RAT))/2.D0
   ROOT1 = REAL + RTFINK
   ROOT2 = REAL - RTFINK
   IF(IWRITE .NE. 0) GO TO 26
24 WRITE (6,25) IKES1,ROOT1
   WRITE (6,25) IKE,ROOT2
25 FORMAT('  X(',I2,') = ',D17.8,10X,' QUADRATIC FORMULA,
                       REAL ROOTS'
  1,//)
26 XXX(JI,1) = ROOT1
   XXX(JI,2) = 0.0
   JI = JI + 1
   XXX(JI,1) = ROOT2
   XXX(JI,2) = 0.0
   JI = JI + 1
30 RETURN
   END
```

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OPTIMAL HIERARCHIAL FACTORIAL DESIGNS: THE MULTIPLE DESIGN MULTIRESPONSE CASE WITH COST CONSTRAINTS

BY

Samuel V. Givens

(ABSTRACT)

In designing multivariate experiments, it will often be the case that different responses have different design matrices. This most often occurs when certain responses are not influenced by various factors. If not all responses are measured on each observational unit, this gives rise to the More General Linear Multiresponse (MGLM) design.

For a factorial experiment, denote by V a variance-covariance matrix of estimable functions of the parameters of any effects one wishes to study. Optimal designs are found that minimize the trace of V when the size of the design is restricted by a total cost constraint, thus minimizing the average variance of each estimable function. It is shown that Hierarchial MGLM designs (HMGLM), a subset of the MGLM designs, need only be considered. In a HMGLM design a hierarchy of the responses $V_1,\dots,V_{p'}$ can be found such that if $i < j$ ($i,j = 1,\dots,p'$), $V_i$ should be measured on at least as many experimental units as $V_j$ is measured and $V_j$ is measured only on units where $V_i$ is also measured. Given the costs and 'a priori' variance estimates, optimal

designs for $2^V$ factorial experiments are found where $k_i$ effects are under study for $V_i$. The procedure is then extended to include $p^V$ factorial experiments.

We consider next the minimization of the determinant of V as a criterion for optimality. This criterion results in the confidence ellipsoids for the estimable functions to be of minimum volume. Due to the difficulty in defining the off-diagonal covariance matrices of V for the general class of MGLM designs, certain well-defined subclasses were considered where the covariance matrices of these designs could be found in general. First a rather natural subclass of MGLM designs, called Restricted MGLM designs (RMGLM), was investigated. HMGLM designs are a subclass of RMGLM designs, as are Multiple Design Multiresponse (MDM) designs which assume that all responses are measured on each experimental unit.

The general situation, assuming p' responses, was investigated first. Due to difficulty in finding the determinant of the matrix V, a general solution for the optimal RMGLM design was found for only certain specific situations.

In an attempt to ease the difficulty in determining the general form of det(V), the two-response case was considered. The optimal RMGLM design was then determined for more general situations. Finally, the complement subclass (CRMGLM designs) of the RMGLM designs in the class of MGLM designs was investigated for two-response situations. The optimal MGLM design can then be determined by comparing the optimal RMGLM and CRMGLM designs. For most situations, the optimal CRMGLM design can be found, but for those situations where it cannot be found, the optimal RMGLM design (a HMGLM design) can still be determined, giving a design at least as good as, and often better than, the generally accepted MDM design.