APPLICATIONS OF THE CALCULUS FOR FACTORIAL ARRANGEMENTS AND ALLIED TOPICS

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INTRODUCTION AND SUMMARY

0.1 Introduction

This thesis deals primarily with the application of the calculus for factorial arrangements (Kurkjian and Zelen (1962, 1963)) to various designs. The thesis has been divided into six chapters. We have made extensive use of Kronecker products and various other results from matrix theory. The results in the first two chapters involve the use of projection operators.

In the first four chapters, different classes of factorial experiments have been studied by applying the calculus. Chapter 5 deals with another class of designs called repeated measurements designs (RMD's). It has been shown that the calculus for factorial arrangements serves as a powerful tool for studying the optimality properties of such designs under the possible presence of interaction. In Chapter 6, a class of designs very closely related to the RMD's has been investigated.

Section 0.2 contains a review of the literature on factorial experiments and RMD's. While reviewing the literature, we have restricted ourselves to the results pertaining to the topics discussed in this thesis. Section 0.3 presents a detailed chapterwise summary of this thesis. The motivation of the different chapters has been discussed and all main results have been quoted. Where necessary, the relevant definitions have been recalled. For ease of reference, the serial numbers of these theorems and definitions are the same as those in the main chapters.

It has been attempted to retain notational uniformity as far as practicable. The relevant notations have been explained in the beginning of each chapter.

0.2 A Brief Review of the Literature

Fisher (1935) introduced and popularized factorial designs. Among the early authors, Yates (1937) considered both symmetric and asymmetric factorial experiments and Bose and Kishen (1940) and Bose (1947) applied finite geometries to develop a mathematical theory for symmetric prime-powered factorials. Generalizations of the classical method due to Bose (1947) to asymmetric factorials were considered among others by White and Hultquist (1965), Raktoe (1969, 1970), Worthley and Banerjee (1974) and Sihota and Banerjee (1981). All but the latest of these were reviewed and discussed by Raktoe, Rayner and Chalton (1978). A related development was through the use of the DSIGN algorithm (Patterson (1976), Bailey (1977), Bailey, Gilchrist and Patterson (1977)). Recently, Voss (1986) and Voss and Dean (1987) investigated the relationship among these procedures with the objective of integrating them. Nair and Rao (1948) introduced balanced confounded designs for asymmetric factorials. These designs ensure balance with respect to each factorial effect and have orthogonal factorial structure (OFS) in the sense that the best linear unbiassed estimators (BLUEs) of estimable contrasts belonging to different factorial effects are uncorrelated. Further construction procedures for and combinatorial properties of balanced confounded designs were explored among others by Kramer and Bradley (1957), Zelen (1958), Kishen and Srivastava (1959), Das (1960), Paik and Federer (1973), and more recently by Lewis and Tuck (1985), Suen and Chakravarti (1985) and Gupta (1987).

Kurkjian and Zelen (1962, 1963) introduced a calculus for factorial arrangements which, as pointed out by Federer (1980), serves as a very powerful analytical tool in the

context of factorial designs. The calculus is extremely helpful in deriving characterizations, in a compact form, for balance and/or OFS in a general multifactor setting. In turn, these characterizations lead to useful construction procedures retaining high efficiency with respect to the factorial effects of interest.

Kurkjian and Zelen (1963) employed the calculus to obtain a sufficient condition for balance together with OFS for factorial experiments in block designs. Zelen and Federer (1964) extended their result to designs for two-way heterogeneity elimination. Kshirsagar (1966) established that the sufficient condition in Kurkjian and Zelen (1963) is also necessary for balance with OFS. The emphasis on balance, however, has a drawback that the resulting designs, although theoretically elegant, may become too large and hence expensive. Because of this reason, since the early seventies, work started on the conditions for OFS alone. John and Smith (1972) and Cotter, John and Smith (1973) obtained a sufficient condition for OFS in terms of a generalized- (g-) inverse of the intrablock matrix. Mukerjee (1979, 1980) gave necessary and sufficient conditions for OFS directly in terms of the intrablock matrix. These conditions, applicable to both block designs and designs for multiway elimination of heterogeneity, involve the checking of the commutativity of certain matrices with the intrablock matrix and, therefore, can be easily verified. Chauhan and Dean (1986) extended the results in Mukerjee (1980) to obtain characterizations for partial OFS. Some results from Mukerjee (1979, 1980) have been used in Chapters 1, 3, 4 and 5 of this thesis and there these have been stated as Lemmas 1.2.1, 1.3.4, 4.3.1 and 5.3.1.

The applications of the conditions for OFS, as mentioned in the last paragraph, in

the construction of factorial experiments in block designs have received considerable attention in recent years. These construction procedures generally fall into two broad categories, namely (a) the use of generalized cyclic designs and (b) the use of Kronecker or Kronecker-type products. The method (a) was developed by John (1973a, b), John and Dean (1975), Dean and John (1975), Dean and Lewis (1980) and several other researchers. This method has not been considered in the present thesis and we refer to John and Lewis (1983) and Street (1986) for a comprehensive list of references.

The alternative method (b) has been used by Mukerjee (1981, 1984, 1986) and Gupta (1983, 1985, 1986a). In this method the Kronecker product or some Kronecker-type product of certain varietal (i.e., single factor) designs are considered to generate a factorial design. Mukerjee (1981, 1984) and Gupta (1983) used this method to construct designs where the main effect efficiencies could be controlled by suitably choosing the varietal designs. Gupta (1985, 1986a) employed this method to control average efficiencies of interactions of all orders. Mukerjee (1986) used the Kronecker product and also some variants of it to control interaction efficiencies up to some suitable order. All these results deal with block designs.

In the context of row-column designs, John and Lewis (1983) and Lewis (1986) constructed and studied factorial experiments with OFS using the generalized cyclic procedure of construction. As for factorial designs for the elimination of heterogeneity in several directions, it appears that much work remained to be done. This problem has been considered in Chapter 1 of this thesis.

Most of the available results on the construction of factorial designs are on

equireplicate designs only. All of the references cited above deal with equireplicate designs. The same remark holds good also for most of the classical construction procedures (see e.g., Voss (1986)). Some results on non-equireplicate factorials are available in Puri and Nigam (1976, 1978). The properties of non-equireplicate Kronecker factorials have been investigated in Chapter 2.

The notion of efficiency-consistency in factorial designs was introduced by Lewis and Dean (1985). They showed that every equireplicate connected design with OFS is efficiency-consistent. Mukerjee and Dean (1986) extended this result to the case of disconnected designs and proved that the converse is also true. Thus they showed that efficiency-consistency provides a characterization for OFS. Some further results on efficiency-consistency were reported by Gupta (1986b). In Chapter 3, we consider an analogous concept, namely, that of estimability-consistency and prove its equivalence with the concept of regularity (Mukerjee (1979), Chauhan and Dean (1986), Chauhan (1987)) in factorial experiments.

A very interesting class of factorial experiments is the class where the levels of one factor represent different qualities of material and the levels of another factor represent different quantities of these qualities. Such experiments were first considered by Fisher (1935) where zero, single and double doses of certain fertilizers were applied and their yields studied. The interesting feature of these experiments, which make them different from ordinary factorials is that some of the level combinations, namely those where the quantitative factor is at the zero level, are indistinguishable. Another example of such an experiment was given by John and Quenouille (1977). There is not

much literature available on such designs and it seems that a definite mathematical formulation for this problem is lacking. This problem has been studied in Chapter 4.

We next turn to a class of designs called repeated measurements designs (RMD's). In such designs a number of treatments are applied sequentially to a number of experimental units over periods. Hedayat and Afsarinejad (1975) gave a general review of RMD's including a discussion on their practical applications and a comprehensive bibliography up to that stage. An interesting feature of these designs is that since the same experimental unit is repeatedly exposed to a number of treatments, the residual effect of a treatment in the following period is also an important source of variation together with the direct effect of a treatment in the period in which it is applied. In the field of optimal RMD's, the pioneering work is due to Hedayat and Afsarinejad (1978). Other important contributions are due to Cheng and Wu (1980), Magda (1980), Constantine and Hedayat (1982) and Kunert (1983, 1984a, b, 1985, 1987). Many of these authors considered the problem of universal optimality under fixed effects additive model incorporating direct and first order residual effects of treatments apart from effects due to units and periods. In proving the optimality results they used a fundamental tool due to Kiefer (1975). Some of these results were extended by Mukhopadhyay and Saha (1985) to the case of mixed effects additive models where the unit effects were random. All these authors assumed the absence of any interaction between the direct and residual effects. Under a non-additive model (i.e., where this interaction is incorporated in the model) some results on construction and analysis of such designs were given by Patterson (1968, 1970) and Kershner and

Federer (1981) – in this context, reference may also be made to the discussion by Federer following Hedayat (1981). Patterson (1973) considered some orthogonality results in this connection. For an excellent review of the literature on optimal RMD's up to that stage, we refer to Hedayat (1981). In Chapter 5, the calculus for factorial arrangements has been applied to examine the robustness of certain optimality results in RMD's under a non-additive model.

A class of designs very closely related to RMD's is the class of serially balanced sequences. These designs were introduced by Finney and Outhwaite (1955) to study experiments where a single experimental unit is exposed to a number of treatments in succession. Such designs are common in the field of biological assay and Finney (1956) discussed their practical applications. In this context, reference may also be made to Williams (1949). Methods of construction of such sequences were given by Sampford (1957). Sinha (1975) studied the A-, D-, and E-optimality of a class of these sequences which he called "standard sequences". Some optimality results on serially balanced sequences have been derived and related construction procedures have been discussed in Chapter 6 of this thesis.

The results in Chapters 5 and 6 are primarily concerned with optimal designs. The pioneering work in this field is due to Kiefer (1958, 1959, 1975), who introduced the notions of A-, D-, E-, ϕ_p and universal optimality. For ease of reference, we present below the definition of universal optimality:

Consider a function $\phi: B_{v,0} \to (-\infty, \infty]$, where $B_{v,0}$ is the collection of $v \times v$ nonnegative definite matrices with zero row and column sums. Let C_d denote the C-

matrix i.e., the intrablock matrix of a design d. Then, a design d^* is called universally optimal if it minimizes $\phi(C_d)$ over the competing designs we are interested in, for ϕ satisfying (i) ϕ is convex (ii) $\phi(bC)$ is non-increasing in the scalar $b \geq 0$, and (iii) ϕ is invariant under any simultaneous permutation of rows and columns of C.

Note that if d^* is universally optimal then it is A-, D- and E-optimal. Kiefer (1975) showed that a design d^* is universally optimal if d^* maximizes trace (C_d) over the competing class and C_{d^*} is completely symmetric.

As briefly outlined above, there has been a rapid growth in the literature on factorial designs and allied fields over the last four decades and a considerable interest is still continuing. For comprehensive reviews and further references on various aspects of factorial designs (including fractional replication, which has not been considered in this thesis) reference is made to Srivastava (1978), Raktoe, Hedayat and Federer (1981), Chatterjee (1982) and Street (1986).

0.3 Detailed Summary of the Thesis

<u>Definition 0.3.1.</u> A factorial design is said to have OFS if the best linear unbiassed estimators of estimable contrasts belonging to different factorial effects are orthogonal, i.e., uncorrelated so that the adjusted treatment sum of squares can be partitioned orthogonally into components corresponding to different factorial effects.

Definition 0.3.2. Let $A=(a_{ij})$ and $B=(b_{ij})$ be $m\times n$ and $p\times q$ matrices respectively. Then the Kronecker product $A\otimes B=(a_{ij}B)$ is an $mp\times nq$ matrix expressible as a partitioned matrix with $a_{ij}B$ as the $(ij)^{th}$ partition, $i=1,\ldots,m,j=1,\ldots,n$.

For the properties of Kronecker product we refer to Rao (1973a).

In chapters 1 to 4, whether the design is varietal or factorial, we have considered the fixed effects model with independent, homoscedastic errors and no block-treatment interaction.

Chapter 1: In Chapter 1 of this thesis, the Kronecker method is applied to construct equireplicate factorial designs for multiway elimination of heterogeneity. The designs constructed have OFS and lower bounds are given for their interaction efficiencies. Thus we extend the results of Mukerjee (1986) and Gupta (1986a) to the set-up of multiway heterogeneity elimination and in particular to row-column designs. In the context of block designs, these authors proved their results by explicitly evaluating certain eigen values. A direct generalization of this method becomes intractable in a setting for multiway heterogeneity elimination. Instead, our proofs are based on an approach using projection operators. Also, compared to Gupta (1985, 1986a), a broader definition of efficiency, viz the ϕ_p -efficiency, has been used.

Section 1.2 discusses the method of construction using the usual Kronecker product. We start with m equireplicate varietal designs D_1, D_2, \ldots, D_m each for t-way elimination of heterogeneity, the j^{th} design involving s_j treatments and n_j observations. Then the design D obtained by the Kronecker product of D_1, \ldots, D_m is a $s_1 \times s_2 \times \ldots \times s_m$ factorial design for t-way heterogeneity elimination. This method is easy to apply and as shown in Example 1.2.1, D may be an incomplete design and contain some empty 'cells'. The main result in this section is

Theorem 1.2.1. The design D has OFS.

Suppose the m factors in D are denoted by F_1, F_2, \ldots, F_m respectively. Then, a

typical factorial effect may be denoted by $F_1^{x_1} \dots F_m^{x_m} (= J(x), \text{ say})$ for $x = (x_1, \dots, x_m) \in \Omega$ where Ω is the set of all non-null m-component (0, 1) vectors.

The main result in Section 1.3 is

Theorem 1.3.1. For every $x = (x_1, \ldots, x_m) \in \Omega$ and every $p \ (0 \le p \le \infty)$,

$$E_p^x \ge \max_{1 \le j \le m} \{x_j H_p^j\}$$

where H_p^j is the ϕ_p -efficiency of the varietal design D_j and E_p^x is the ϕ_p -efficiency of D with respect to the factorial effect J(x).

In view of this theorem, factorial designs with high interaction efficiencies can be constructed if one starts with efficient varietal designs.

The Kronecker product method, though theoretically appealing, may sometimes lead to practical difficulties if a large number of factors are to be considered. This is because, in that case, D may involve a large number of observations. To overcome this difficulty, a construction method based on a modified version of the usual Kronecker product is discussed in Section 1.4. Example 1.4.1 illustrates this method. Let $D^{(g)}$ be a factorial design constructed by this restricted Kronecker product method of order g. Then we have

Theorem 1.4.1. The design $D^{(g)}$ has OFS.

Theorem 1.4.2. For $x = (x_1, \ldots, x_m) \in \Omega$ and every $p \ (0 \le p \le \infty)$,

$$E_p^x(g) \ge \max_{1 \le j \le m} \{x_j H_p^j\}$$

provided among x_1, \ldots, x_m at most g are unity; where H_p^j is as in Theorem 1.3.1 and $E_p^x(g)$ is the ϕ_p -efficiency of $D^{(g)}$ with respect to J(x).

These two theorems imply that this restricted Kronecker product method of order

g maintains OFS of the resulting design and controls the factorial effect efficiencies in $D^{(g)}$, for effects involving up to g factors, in terms of efficiencies of D_1, \ldots, D_m . This method is to be used in situations where m is large and the higher order interactions are relatively unimportant. The design $D^{(g)}$ involves a much lesser number of observations than D.

Chapter 2: After having considered Kronecker factorial designs in the equireplicate case, a very natural question arises as to what can be done in the non-equireplicate case. From the discussion in section 0.2 it is clear that so far non-equireplicate factorials have not received much attention. A reason for this may be that maintaining OFS becomes a problem when the number of replications vary and consequently the analysis of these designs and the study of the factorial effect efficiencies by the usual methods become difficult. On the other hand, the need for studying such factorial designs exists in order to give the experimenter more scope to study experiments in the different situations which arise in practice.

In Chapter 2 we have studied this problem. In Section 2.2 we begin with block designs. The usual Kronecker product is taken of m non-equireplicate connected designs D_1, \ldots, D_m with varying block sizes. The resulting design D is a non-equireplicate factorial design with varying block sizes.

In Section 2.3 it is shown that even in the non-equireplicate setting, the interaction efficiencies with respect to contrasts belonging to factorial effects in D can be controlled and high efficiencies ensured by suitably choosing the varietal designs D_1, \ldots, D_m . For $1 \le j \le m$, let $e_j(\mathbf{u}_j)$ be the efficiency (relative to the corresponding

completely randomized design) with which a treatment contrast with coefficient vector \mathbf{u}_j is estimated in D_j . Similarly, let $e(\mathbf{u}^x)$ be the efficiency with which a contrast belonging to the factorial effect J(x) and having a coefficient factor \mathbf{u}^x is estimated in D, where $\mathbf{u}^x = \bigotimes_{j=1}^m \mathbf{u}_j^{x_j}$ with $\mathbf{u}_j^{x_j} = \mathbf{u}_j$ if $x_j = 1, = 1_{s_j}$ if $x_j = 0$ $(1 \le j \le m)$. Here 1_{s_j} is an $s_j \times 1$ vector with all elements unity. Then we have:

Theorem 2.3.1.
$$e(\mathbf{u}^x) \geq \max_{j:x_j=1} e_j(\mathbf{u}_j)$$
, for each $x = (x_1, \dots, x_m) \in \Omega$.

This theorem extends the ideas in Gupta (1986a) and Mukerjee (1986) to a non-equireplicate set-up. The designs D_1, \ldots, D_m are left quite arbitrary and so the method is capable of generating factorial designs with a wide range of parameters.

It can be seen through examples that non-equireplicate factorials may not have OFS. We show in Section 2.4 that this does not really pose any serious problem in the analysis of D and Theorem 2.4.1 gives a simple formula for the evaluation of a g-inverse of the C-matrix.

In Section 2.5 the results of Sections 2.3 and 2.4 are extended to designs for multiway heterogeneity elimination. The results in these sections deal with efficiencies of individual contrasts in the factorial design D.

In Section 2.6 we consider complete sets of orthonormal contrasts belonging to different factorial effects and set lower bounds for ϕ_p -efficiencies of such sets of contrasts. The main theorem in this section is proved with reference to designs for multiway heterogeneity elimination and the corresponding results for block designs follow as special cases. We have

Theorem 2.6.1. For every $x = (x_1, \ldots, x_m) \in \Omega$ and every $p \ (0 \le p \le \infty)$,

$$E_p^x \ge \max_{1 \le j \le m} \{x_j H_p^j\},$$

where E_p^x is the ϕ_p -efficiency with respect to the factorial effect J(x) in D while H_p^j is the ϕ_p -efficiency of D_j .

Chapter 3: In Chapter 3 we study another property of factorial designs, namely, regularity. We give the following definition due to Mukerjee (1979).

Consider a $s_1 \times s_2 \times \ldots \times s_m$ possibly disconnected design d. Let C be the usual intrablock matrix of d, V^x denote the estimable space corresponding to J(x) and R(A) denote the row space of a matrix A. Then

<u>Definition 3.2.1.</u> d is regular if $R(C) \equiv \bigoplus_{x \in \Omega} V^x$ where \oplus denotes direct sum.

For discussion on the notion of regularity with examples we refer to Section 3.2.

In Section 3.3 we introduce the concept of estimability-consistency which is somewhat similar to that of efficiency-consistency as introduced by Lewis and Dean (1985). Let d be an $s_1 \times s_2 \times \ldots \times s_m$ factorial design. For any $x = (x_1, \ldots, x_m) \in \Omega$ let d_x be the design obtained from d by deleting the i^{th} digit from the treatment labels, for all i for which $x_i = 0, i = 1, \ldots, m$. Then we have:

Definition 3.3.1. d is estimability-consistent provided for each $x \in \Omega$, every contrast belonging to J(x) in d is estimable in d if and only if the corresponding contrast belonging to J(x) in d_x is estimable in d_x .

In Section 3.4 the main theorem is:

Theorem 3.4.1. An m-factor design, d, is estimability-consistent if and only if it is regular.

This result establishes the equivalence between regularity and estimabilityconsistency and thus provides a simple and intuitively appealing interpretation for
the somewhat abstract phenomenon of regularity.

In Section 3.5 we define the notion of partial estimability-consistency of order t. This concept is somewhat analogous to that of partial efficiency-consistency in Mukerjee and Dean (1986). The main result in this section is

Theorem 3.5.1. An m-factor design, d, is partially estimability-consistent of order $t \leq m$ if and only if it is regular of order t.

Chapter 4: In Chapter 4 we study factorial designs for quality-quantity interaction.

As discussed in Section 0.2, not much work has been done in this area. Recently, Cox (1984) posed a number of problems in experimental design and one of these problems related to the development of a systematic theory for the study of quality-quantity interaction.

Let d be a two-factor experiment where the first factor F_1 is quantitative and involves $s_1 + 1$ levels, say $0, 1, \ldots, s_1$ while the second factor F_2 is the qualitative factor, having s_2 levels, say $1, 2, \ldots, s_2$. The level combinations where F_1 is at the zero level, are indistinguishable so that there are only $s_1s_2 + 1 = v$ distinct level combinations. To take into account this special feature of the level combinations, in Section 4.2, the calculus for factorial arrangements has been substantially modified.

In Section 4.3 we find necessary and sufficient conditions for OFS.

Let d have an intrablock matrix of the form $C = \begin{pmatrix} \alpha & \beta' \\ \beta & H \end{pmatrix}$ where H is a square matrix of order s_1s_2 , the initial row and column of C correspond to the treatment 0

and the other rows and columns correspond to the other s_1s_2 level combinations in the lexicographic order. Let 1_n denote the $n \times 1$ unit vector. Then the first result states

Theorem 4.3.1. For d to have OFS, it is necessary and sufficient that

- (i) $\beta = \mathbf{u} \otimes \mathbf{1}_2$ for some s_1 -component vector \mathbf{u} and
- (ii) the matrix $H^* = H \alpha^{-1} \beta \beta'$ has structure K.

For the sake of completeness, we give the following definition (cf. Mukerjee (1979)) also:

Definition 4.2.2. A square matrix of order s_1s_2 is said to have structure K if it can be expressed as a linear combination of Kronecker products of proper matrices of orders s_1, s_2 respectively. Here a proper matrix is a square matrix with all row and column sums equal.

Next we show how designs with OFS in the present setting can be obtained from ordinary factorial designs with OFS. We start with an ordinary $(s_1 + 1) \times s_2$ factorial design d_o . Let d_o be connected with a C-matrix given by

$$C_0 = egin{bmatrix} C_{00} & C_{01} & \dots & C_{0s_1} \ \dots & \dots & \dots & \dots \ \dots & \dots & \dots & \dots \ C_{s_10} & C_{s_11} & \dots & C_{s_1s_1} \end{bmatrix}$$

where each C_{ij} is $s_2 \times s_2$ and the rows and columns of C_0 correspond to the $(s_1 + 1)s_2$ level combinations in d_0 in the lexicographic order.

A design d is derived from d_o by replacing the s_2 level combinations $01, 02, \ldots, 0s_2$ in d_o by a single treatment 0. Then we have:

Theorem 4.3.2. Let d_o be connected and have OFS with the C-matrix matrix as given above. Then the derived design d will have OFS if and only if for every $i, j (1 \le i, j \le s_1)$ the following holds

$$C_{i0} - \rho_{io}s_2^{-1}E_2 = C_{oj} - \rho_{oj}s_2^{-1}E_2$$

where $E_2 = \mathbf{1}_2 \mathbf{1}'_2$ and $C_{ij} \mathbf{1}_2 = C'_{ij} \mathbf{1}_2 = \rho_{ij} \mathbf{1}_2$, $0 \le i, j \le s_1$.

In Section 4.4 we consider the problem of intra-effect orthogonality. This may be of importance since interest may lie in the linear, quadradic, cubic, ... components of the first factor which is quantitative. A design will be said to have strong orthogonal factorial structure (SOFS) if it has OFS and admits intra-effect orthogonality with respect to main effect F_1 and interaction F_1F_2 (relative to F_1). The main result of this section is as follows:

Theorem 4.4.3. Let d be a connected two-factor design for the study of quality-quantity interaction. Then in order that d may have SOFS, it is necessary and sufficient that the C-matrix of d is of the form

$$C=lpha \left[egin{array}{cccc} 1 & -(s_1s_2)^{-1}\mathbf{1}_1'\otimes\mathbf{1}_2' \ -(s_1s_2)^{-1}\mathbf{1}_1\otimes\mathbf{1}_2 & I_1\otimes H_1+E_1\otimes H_2 \end{array}
ight],$$

where I_1 is the $s_1 \times s_1$ identity matrix, α is a positive constant and H_1 , H_2 are $s_2 \times s_2$ proper matrices with $H_1 \mathbf{1}_2 = (s_1 s_2)^{-1} (s_1 + 1) \mathbf{1}_2$.

Some construction procedures have been briefly discussed in Section 4.5. In Section 4.6, the extension of the above results to the multifactor case has been indicated.

Chapter 5: In Chapter 5 we consider repeated measurements designs (RMD's). As stated in Section 0.2, all the existing work on optimality of RMD's has been done

under an additive model. But in practical situations it is likely that an effect due to the interaction of direct and residual effects will be also present. This is illustrated by an example in John and Quenouille (1977). In Chapter 5 we have used non-additive models, by incorporating the direct-versus-residual interaction effect in the additive models assumed by the previous researchers. Two types of models are considered; the circular model (cf. Magda (1980)) where in each unit the residuals in the initial period are incurred from the last period; and the non-circular model (cf. Cheng and Wu (1980)) where there is no residual effect in the first period. For the sake of completeness we give some definitions (cf. Cheng and Wu (1980), Magda (1980)) below:

<u>Definition 5.2.1.</u> An RMD is called uniform if in each period the same number of units is assigned to each treatment and on each unit each treatment appears in the same number of periods.

An RMD where t treatments are applied sequentially to n units over p periods is abbreviated by RMD (t, n, p). The class of all such designs will be denoted by $\Omega_{t,n,p}$. If d is an RMD, let d(i,j) denote the treatment assigned by d in the i^{th} period to the j^{th} unit.

Definition 5.2.2. Under the non-circular model an RMD is called strongly balanced if the collection of ordered pairs $\{d(i-1,j), d(i,j)\}, 1 \le i \le p-1, 1 \le j \le n$, contains each ordered pair of treatments, distinct or not, the same number of times; under the circular model an RMD is called strongly balanced if the same holds considering ordered pairs $\{d(i-1,j), d(i,j)\}, 0 \le i \le p-1, 1 \le j \le n$.

A strongly balanced uniform RMD (t, n, p) is abbreviated SBURMD (t, n, p). Examples of such designs are given in Section 5.2.

Under the non-additive model the study of RMD's by the standard methods becomes rather involved. To overcome this difficulty, in Section 5.3 we have established a correspondence between factorial experiments and RMD's and shown how the application of the calculus for factorial arrangements is helpful in this context.

The principal result on the optimality of SBURMD's in Cheng and Wu (1980) states: "Under an additive non-circular model, a SBURMD (t, n, p) is universally optimal for the estimation of direct as well as residual effects over $\Omega_{t,n,p}$." (Cheng and Wu (1980), Theorem 3.1). We have the following result:

Theorem 5.4.1. Under a non-additive non-circular model, a SBURMD (t, n, p) is universally optimal over $\Omega_{t,n,p}$ for the estimation of direct effects.

Although by Theorem 5.4.1 the result of Cheng and Wu (1980) is robust for direct effects under the non-additive model, the same is not true for residual effects (cf. Example 5.4.1). For the estimation of residual effects we have the following result:

For any $d \in \Omega_{t,n,p}$, let S_{dh} be the set of units which receive the treatment h $(0 \le h \le t-1)$ in the last period. Then the following holds:

Theorem 5.4.2. Under a non-additive model a SBURMD (t, n, p) d^* allows orthogonal estimation of the residual effects contrasts and hence becomes universally optimal over $\Omega_{t,n,p}$ for the residual effects if

(i) for each h, h' ($0 \le h, h' \le t - 1$) there are exactly nt^{-2} units receiving the treatments h and h' in the initial and the last periods respectively and

(ii) for each h $(0 \le h \le t-1)$, in the collection of ordered pairs $\{d^*(i-1,j), d^*(i,j)\}$, $1 \le i \le p-1; j \in S_{d^*h}$, each ordered pair (h, h_2) $(0 \le h_2 \le t-1)$ occurs the same number (say ν_1) of times while each ordered pair (h_1, h_2) $(0 \le h_1, h_2 \le t-1; h_1 \ne h)$ occurs the same number (say ν_2) of times.

Cheng and Wu (1980) gave a method of construction of SBURMD's when $t^2|n$ and pt^{-1} is even. These designs satisfy the condition of Theorem 5.4.2. For the situation where $t^2|n$ and pt^{-1} is odd we suggest a method of constructing SBURMD's satisfying these conditions. This method works for all $t \neq 6$, this restriction being due to the fact that the method makes use of a pair of mutually orthogonal latin squares of order t. Thus Theorem 5.4.2 covers almost all situations where a SBURMD (t, n, p) may exist. Example 5.4.2 illustrates this method.

Next we show that if we ignore the conditions of Theorem 5.4.2, then we can give a method of construction of SBURMD (t, n, p) even when t = 6 and p/6 is odd. Thus the conditions $t^2|n$ and t|p (p > t) are shown to be both necessary and sufficient for the existence of a SBURMD (t, n, p).

In this section we also study the robustness of another result due to Cheng and Wu (1980). We show that this result is robust for residual effects only and not for direct effects. Let d_o be a strongly balanced RMD (t, n, p) which is uniform on the periods and is uniform on the units in the first p-1 periods. Then we have Theorem 5.4.3. Under a non-additive model d_o is universally optimal over $\Omega_{t,n,p}$ for

In Section 5.5 we study RMD's under the circular model. Let \overline{d} be a SBURMD

the estimation of residual effects.

(t, n, p) under such a model. The main result of Magda (1980) remains robust under a non-additive model and we have:

Theorem 5.5.1. Under a non-additive circular model, \overline{d} is universally optimal for the estimation of direct as well as residual effects over $\Omega_{t,n,p}$.

Turning to the problem of construction of SBURMD's in a circular setting it is clear that such a SBURMD exists only if t|n and t|p (p>t). We have:

Theorem 5.5.2. Under the circular model, if t|n and pt^{-1} is an even integer then a SBURMD (t, n, p) exists.

Example 5.5.1 illustrates this method of construction.

In Section 5.6 we show that the results in Theorems 5.4.1, 5.4.2, 5.5.1 and 5.5.2 remain robust under a mixed effect model where the unit effects are random.

Chapter 6: In the last chapter, i.e. Chapter 6 we study serially balanced sequences which are closely related to RMD's. These sequences are block designs where a number of treatments are applied successively to a single experimental unit. We first give the following definition:

Definition 6.2.7. A type $2^*(u)$ sequence of order v and length vu ($u \le v - 1$) is a closed chain of symbols (treatments) such that (i) each of the v distinct symbols occurs u times in the sequence, (ii) the sequence falls into u blocks each containing the v symbols once each, (iii) the direct effect versus first order residual effect incidence matrix is that of a symmetric balanced incomplete block design and (iv) each block ends with the same symbol.

To begin with, we consider the usual fixed effects model incorporating the block

effect, the direct effect and residual effect. Let C(n) be the class of all sequences with v symbols and length n. Then we have

Theorem 6.3.1. Within the class C(vu), a type $2^*(u)$ sequence, if it exists, is universally optimal for both direct and residual effects, under the model assumed, provided v > 2.

In Section 6.4 a method of constructing type $2^*(u)$ sequences has been given. This method has a fairly wide coverage and has been illustrated in Example 6.4.1.

In Section 6.5 we have studied the optimality of another class of sequences called type 1 sequences (cf. Definition 6.2.1) under a non-additive model analogous to the ones considered in Chapter 5, where the interaction between direct and residual effects is incorporated in the usual fixed effects model for studying such sequences. It has been shown that a type 1 sequence is equivalent to a v^2 factorial experiment and hence we have

Theorem 6.5.1. Under a non-additive model,

- (i) in a type 1 sequence best linear unbiassed estimators of direct effect contrasts are orthogonal to those of the residual and interaction effect contrasts and
- (ii) within the class $C(mv^2)$, a type 1 sequence of order v and index m, if it exists, is universally optimal for the estimation of direct effect contrasts.

Example 6.5.1 illustrates that a type 1 sequence may not be universally optimal for the estimation of residual effects. We have hence modified type 1 sequences and defined a class of sequences called type 1* sequences (cf. Definition 6.2.4) and then it has been shown that for such sequences, a result analogous to Theorem 6.5.1 holds

for the residual effects. These type 1* sequences can be constructed easily.

Section 6.6 deals with optimality properties of type 1 sequences under the usual additive model. The main results are:

Theorem 6.6.1. Under an additive model

- (i) in a type 1 sequence, the best linear unbiassed estimators of direct effect contrasts are orthogonal to those of the residual effect contrasts
- (ii) within the class $C(mv^2)$ a type 1 sequence of order v and index m, if it exists, is universally optimal for the estimation of direct effect contrasts.

Theorem 6.6.2. Under an additive model, a type 1 sequence is strongly optimal for the estimation of residual effects contrasts within the class of all designs having the same 'residual-effect-versus-block' incidence matrix.

Theorem 6.6.2 covers the result of Sinha (1975) as a special case since he essentially proved Theorem 6.6.2 for a particular class of type 1 sequences.

Chapter 1

KRONECKER FACTORIAL DESIGNS FOR MULTIWAY ELIMINATION OF HETEROGENITY

1.1 Introduction

In this chapter, the method of Kronecker products is applied to construct factorial designs for multiway elimination of heterogeneity, starting from some varietal (single factor) designs. This method gives designs with orthogonal factorial structure and at the same time, controls the interaction efficiencies in terms of efficiencies of the varietal designs.

A factorial design is said to have orthogonal factorial structure (OFS) if the best linear unbiassed estimators of estimable contrasts belonging to different factorial effects are orthogonal, i.e., uncorrelated so that the adjusted treatment sum of squares can be partitioned orthogonally into components corresponding to different factorial effects. A broad sufficient condition for OFS was obtained by John and Smith (1973) in the two-factor case and the result was extended to the multifactor case by Cotter, John and Smith (1972). Mukerjee (1979, 1980) gave necessary and sufficient conditions for OFS in easily verifiable forms.

The construction problem for factorial experiments in a block design with OFS has received considerable attention in recent years and two broad general procedures have emerged, namely (a) the use of generalized cyclic designs and (b) the use of Kronecker or Kronecker-type products of varietal designs. John (1973, a, b), Dean and John (1975) and Dean and Lewis (1986) have used method (a) for constructing

designs with *OFS* (see John and Lewis (1983) for a comprehensive list of references). The alternative approach (b) has been used extensively by Mukerjee (1981, 1984, 1986) and Gupta (1983, 1985, 1986a).

In the method (b), Kronecker or Kronecker-type products of m varietal designs, involving s_1, s_2, \ldots, s_m treatments respectively, generate an $s_1 \times s_2 \times \ldots \times s_m$ factorial design. Suitable choices of these products guarantee OFS in the resulting factorial design. Furthermore, it is possible to set lower bounds for interaction efficiencies in the resulting factorial design in terms of the efficiencies in the varietal designs one starts with. Consequently, by appropriately selecting these varietal designs, one can ensure an efficient estimation of contrasts belonging to the factorial effects of interest. This makes the method useful from a practical viewpoint. In addition, due to the comparatively easy availability of the varietal designs, this method is quite flexible and convenient to apply.

Mukerjee (1981, 1984) and Gupta (1983) considered methods of construction for factorial block designs with OFS employing Kronecker-type products controlling main effect efficiencies. In this context, mention may be made of Lewis and Dean (1985). Recently, in the two-factor case Gupta (1985) studied the interaction efficiencies in Kronecker designs. The results were extended in Gupta (1986a) where it was shown that by taking the ordinary Kronecker product of varietal designs, the average efficiencies of interactions of all orders can be controlled. Mukerjee (1986) employed the Kronecker product and also some variants of the Kronecker product to obtain factorial designs with OFS while controlling the Φ_p -efficiencies (cf. Kiefer

(1975)) of these interactions up to some suitable order. In the set up of two-way elimination of heterogeneity, Zelen and Federer (1964) applied the calculus for factorial arrangements to obtain conditions for OFS. Recently, John and Lewis (1983) and Lewis (1986) constructed and studied factorial experiments with OFS in row-column designs, using the generalized cyclic method of construction. As for designs eliminating heterogeneity in several directions, it appears that much work yet remains to be done though Mukerjee (1980) gave necessary and sufficient conditions for OFS of such designs.

This chapter aims at extending the results of Mukerjee (1986) and Gupta (1986a) to a set-up for multiway elimination of heterogeneity and thus, in particular to row-column designs also. For block designs, Mukerjee (1981, 1986) and Gupta (1985, 1986a) proved their results using explicit evaluation of certain eigenvalues. In the set-up of this chapter, a direct generalization of their method becomes intractable and so, instead of using eigenvalues, a more subtle approach involving projection operators has been adopted to simplify the derivation considerably. Also, compared to Gupta (1985, 1986a), a broader definition of efficiency has been used.

In sections 1.2 and 1.3 the ordinary Kronecker product is considered and it is shown that the resulting design has OFS while the Φ_p -efficiencies of interaction effects of all orders can be controlled in terms of the efficiencies of the component varietal designs. A disadvantage of this Kronecker product is that the resulting design becomes large if there are too many factors. As shown in section 1.4, this difficulty may be overcome by the use of a restricted form of the Kronecker product which exercises a

control over efficiencies of interactions up to a preassigned order. The use of such a restricted product may be justified since the higher order interactions are not usually of much practical importance especially when the number of factors is large.

1.2 The Method of Kronecker Product

Throughout this chapter, both for a varietal and a factorial design, the model assumed is the fixed effects model with independent, homoscedastic errors. Let D_1, D_2, \ldots, D_m be m varietal designs for t-way elimination of heterogeneity and let for $1 \leq j \leq m, D_j$ involve s_j treatments, n_j observations and have a design matrix

$$V_j = [Z_{j0}, Z_{j1}, \ldots, Z_{jt}],$$

where Z_{j0} is of order $n_j \times s_j$ and Z_{ja} is of order $n_j \times u_{ja} (1 \le a \le t), u_{ja}$ being the number of classes according to the a-th way of heterogeneity elimination. The columns of Z_{j0} correspond to the effects of the s_j treatments in D_j while for $1 \le a \le t$, the u_{ja} columns of Z_{ja} correspond to the effects of the u_{ja} classes according to the a-th way of heterogeneity elimination (see Example 1.2.1 for an illustration). So, for $0 \le a \le t$, in each row of Z_{ja} , exactly one element is unity and the others are all zero. Hence, denoting by $\mathbf{1}_n$ an $n \times 1$ vector with all elements unity,

$$Z_{j0}\mathbf{1}_{s_j}=Z_{j1}\mathbf{1}_{u_{j1}}=\cdots=Z_{jt}\mathbf{1}_{u_{jt}}=\mathbf{1}_{n_j}.$$
 (1.2.1)

Let D_j be equireplicate with common replication number r_j . So,

$$n_j = r_j s_j, Z'_{j0} \mathbf{1}_{n_j} = r_j \mathbf{1}_{s_j} , \quad Z'_{j0} Z_{j0} = r_j I_{s_j}, \qquad (1.2.2)$$

where I_n is the $n \times n$ identity matrix. The reduced normal equations for the treatment effects in D_j have the coefficient matrix given by, say,

$$C_j = Z'_{j0}(pr^{\perp}(Z_j))Z_{j0},$$
 (1.2.3)

where

$$Z_j = [Z_{j1}, \cdot \cdot \cdot, Z_{jt}],$$
 (1.2.4)

and for any matrix $L, pr^{\perp}(L) = I - pr(L)$ and $pr(L) = L(L'L)^{\perp}L'$ where $(L'L)^{\perp}$ is any generalized inverse of L'L.

The design D obtained by taking the Kronecker product of D_1, \ldots, D_m , has a design matrix

$$V = \begin{bmatrix} m \\ \bigotimes_{j=1}^m Z_{j0}, & \bigotimes_{j=1}^m Z_{j1}, \dots, & \bigotimes_{j=1}^m Z_{jt} \end{bmatrix}, \qquad (1.2.5)$$

where the symbol \otimes stands for Kronecker product. From the way of obtaining D from D_1, \ldots, D_m it is clear that if for $1 \leq j \leq m$, the treatment i_j occurs in the (l_{j1}, \ldots, l_{jt}) -th "cell" of D_j , then the treatment (i_1, \ldots, i_m) occurs in the $((l_{j1}, \ldots, l_{m1}), (l_{j2}, \ldots, l_{m2}), \ldots, (l_{jm1}, \ldots, l_{mm1}))$ -th "cell" of D. $(1 \leq l_{ja} \leq u_{ja}, 1 \leq a \leq t)$. Clearly D involves $\frac{m}{m} s_j (= v \text{ say})$ treatments, which are in effect v m-plets. Interpreting these as v factorial level combinations, D may be looked upon as an $s_1 \times s_2 \times \ldots \times s_m$ factorial design for t-way elimination of heterogeneity. D involves $m \choose j=1$ observations and is equireplicate with common replication number $m \choose j=1$ $r_j (= r \text{ say})$. The v columns of $m \choose j=1$ correspond to the effects of the v treatments and for $1 \leq a \leq t$, the columns of $m \choose j=1$ correspond to the classes according to the a-th way of heterogeneity elimination in D.

This method of obtaining factorial designs may be easily applied since the component varietal designs can be obtained comparatively readily. Also, the design D may be an incomplete design and as the following example illustrates, can contain empty cells.

Example 1.2.1. Construction of a 3 × 4 factorial row-column design.

Here
$$m = 2$$
, $s_1 = 3$, $s_2 = 4$, $t = 2$.

Let the two varietal row-column designs D_1 and D_2 be as follows.

Here $V_2 = (Z_{20}, Z_{21}, Z_{22})$, where

The columns of Z_{21} and Z_{22} correspond to the rows and columns respectively, in D_2 . Similarly, one may obtain explicit expressions for $V_1, Z_{10}, Z_{11}, Z_{12}$ considering the design D_1 .

The 3×4 factorial row-column design D is obtained as the Kronecker product design of D_1 and D_2 and is laid out in 8 rows and 12 columns as shown below. D has incomplete rows and columns and also some empty cells.

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02	01		00	12	11	_	10	22	21		20
03	_	02	01	13	- -	12	11	23		22	21
_	02	00	03		12	10	13		22	20	23
10	13	11	+	20	23	21	_	00	03	01	
12	11		10	22	21	_	20	02	01	-	00
13		12	11	23	-	22	21	03	<u> </u>	02	01
	12	10	13	<u> </u>	22	20	23	—	02	00	03

As in (1.2.3), the reduced normal equations for the treatment effects in D have the $v \times v$ coefficient matrix given by, say,

$$C = \begin{pmatrix} m \\ \bigotimes_{j=1}^{m} Z_{j0} \end{pmatrix}' \left(pr^{\perp}(Z) \right) \begin{pmatrix} m \\ \bigotimes_{j=1}^{m} Z_{j0} \end{pmatrix}, \qquad (1.2.6)$$

where

$$Z = \begin{bmatrix} m \\ \bigotimes_{j=1}^{m} Z_{j1}, \dots, \bigotimes_{j=1}^{m} Z_{jt} \end{bmatrix}. \tag{1.2.7}$$

In the following theorem it is proved that D has OFS. The proof is based on the application of a result due to Mukerjee (1980) and this result is stated as Lemma 1.2.1 below. A result on projection operators is also required which is established in Lemma 1.2.2.

Let Ω denote the set of all non-null m-component (0, 1)-vectors. For any $x = (x_1, \ldots, x_m) \in \Omega$, define

$$G^x = \bigotimes_{j=1}^m G_j^{x_j}, \qquad (1.2.8)$$

where

$$G_j^{x_j} = I_{s_j} \text{ if } x_j = 1, = \mathbf{1}_{s_j} \mathbf{1}'_{s_j} \text{ if } x_j = 0.$$
 (1.2.9)

Lemma 1.2.1 (Mukerjee (1980)). The design D has OFS if and only if for every $x \in \Omega, G^x$ commutes with C(i.e., CG^x is symmetric).

Lemma 1.2.2. Let $A_{10}, A_{11}, \ldots, A_{1t}$ and $A_{20}, A_{21}, \ldots, A_{2t}$ be two sets of t matrices each such that the matrices in the same set have the same number of rows. Let $A = [A_{11} \otimes A_{21}, \ldots, A_{1t} \otimes A_{2t}]$ and $A_1 = [A_{11}, \ldots, A_{1t}]$. Let

$$\mu(A_{20}) \subseteq \cap_{a=1}^t \mu(A_{2a}),$$
 (1.2.10)

where for any matrix $L, \mu(L)$ denotes the column space of L. Then,

$$(pr(A))(A_{10} \otimes A_{20}) = \{(pr(A_1))A_{10}\} \otimes A_{20}.$$

<u>Proof:</u> There exists a matrix $\Delta_1 = [\Delta'_{11}, \ldots, \Delta'_{1t}]'$, where for $1 \le a \le t$, the number of rows of Δ_{1a} equals the number of columns of A_{1a} , such that $A'_1A_1\Delta_1 = A'_1A_{10}$. Hence

$$(pr(A_1)) A_{10} = A_1 (A_1' A_1)^{-} A_1' A_{10} = A_1 \Delta_1 = \sum_{a=1}^{t} A_{1a} \Delta_{1a}$$
 (1.2.11)

and

$$A'(A_{10} \otimes A_{20}) = \begin{bmatrix} A'_{11}(\sum_{a=1}^{t} A_{1a} \triangle_{1a}) \otimes A'_{21} A_{20} \\ \vdots \\ A'_{1t}(\sum_{a=1}^{t} A_{1a} \triangle_{1a}) \otimes A'_{2t} A_{20} \end{bmatrix}, \qquad (1.2.12)$$

since $\mu(A_{1a}) \subseteq \mu(A_1)$, $1 \le a \le t$. Now, (1.2.10) implies that for $1 \le a \le t$, there exist matrices B_a such that

$$A_{20} = A_{2a}B_a (1.2.13)$$

and hence from (1.2.12), $A'(A_{10} \otimes A_{20})$ simplifies to $A'A\Delta$ where $\Delta = (\Delta'_{11} \otimes B'_1, \ldots, \Delta'_{1t} \otimes B'_t)'$. Consequently, by (1.2.11) and (1.2.13)

$$(pr(A)) (A_{10} \otimes A_{20}) = A(A'A)^{-} A' A \triangle = A \triangle = \sum_{a=1}^{t} (A_{1a} \otimes A_{2a}) (\triangle_{1a} \otimes B_{a})$$
$$= \sum_{a=1}^{t} (A_{1a} \triangle_{1a}) \otimes (A_{2a} B_{a}) = \{ (pr(A_{1})) A_{10} \} \otimes A_{20},$$

completing the proof.

Theorem 1.2.1. The design D has OFS.

<u>Proof:</u> Consider any $x = (x_1, ..., x_m) \in \Omega$. Without loss of generality (by a renaming of factors if necessary) it may be assumed that $x_j = 1$ for $1 \le j \le f$, and $x_j = 0$ for $f + 1 \le j \le m$. Then by (1.2.7) and (1.2.8),

$$G^x = G^{(1)} \otimes G^{(2)}, \ Z = [Z_1^{(1)} \otimes Z_1^{(2)}, \dots, Z_t^{(1)} \otimes Z_t^{(2)}],$$
 (1.2.14)

where

$$G^{(1)} = \underset{j=1}{\overset{f}{\otimes}} I_{s_{j}}, \ G^{(2)} = \underset{j=f+1}{\overset{m}{\otimes}} 1_{s_{j}} 1_{s_{j}}^{!}, \ \underset{j=1}{\overset{m}{\otimes}} Z_{ja} = Z_{a}^{(1)} \otimes Z_{a}^{(2)}, \ (0 \leq a \leq t),$$
and
$$Z_{a}^{(1)} = \underset{j=1}{\overset{f}{\otimes}} Z_{ja}, \ Z_{a}^{(2)} = \underset{j=f+1}{\overset{m}{\otimes}} Z_{ja}, \ (0 \leq a \leq t).$$

From (1.2.6),

$$CG^{x} = (\bigotimes_{j=1}^{m} Z_{j0})'(\bigotimes_{j=1}^{m} Z_{j0})G^{x} - (\bigotimes_{j=1}^{m} Z_{j0})'pr(Z)(\bigotimes_{j=1}^{m} Z_{j0})G^{x}, \qquad (1.2.16)$$

where by (1.2.14) and (1.2.15),

$$\left(\bigotimes_{j=1}^{m} Z_{j0} \right) G^{x} = \left(Z_{0}^{(1)} G^{(1)} \right) \otimes \left(Z_{0}^{(2)} G^{(2)} \right) = Z_{0}^{(1)} \otimes \left(Z_{0}^{(2)} G^{(2)} \right). \tag{1.2.17}$$

On simplification, using (1.2.1), and (1.2.15), for $1 \le a \le t$,

$$Z_0^{(2)}G^{(2)} = \bigotimes_{j=f+1}^m Z_{j0} \mathbf{1}_{s_j} \mathbf{1}'_{s_j}$$

$$= \bigotimes_{j=f+1}^m \mathbf{1}_{n_j} \mathbf{1}'_{s_j} = Z_a^{(2)} \left\{ \bigotimes_{j=f+1}^m \mathbf{1}_{u_{ja}} \mathbf{1}'_{s_j} \right\}. \tag{1.2.18}$$

Hence $\mu(Z_0^{(2)}G^{(2)}) \subseteq \cap_{a=1}^t \mu(Z_a^{(2)})$ and so, by (1.2.14), (1.2.15), (1.2.17), (1.2.18) and Lemma 1.2.2,

$$pr(Z)(\underset{j=1}{\overset{m}{\otimes}} Z_{j0})G^{x} = pr(Z)(Z_{0}^{(1)} \otimes Z_{0}^{(2)}G^{(2)}) = \{pr(Z^{(1)})Z_{0}^{(1)}\} \otimes \{Z_{0}^{(2)}G^{(2)}\}$$

$$= \left\{pr(Z^{(1)})Z_{0}^{(1)}\right\} \otimes \left\{\underset{j=f+1}{\overset{m}{\otimes}} \mathbf{1}_{n_{j}}\mathbf{1}'_{s_{j}}\right\}, \qquad (1.2.19)$$

where

$$Z^{(1)} = \left[Z_1^{(1)}, \dots, Z_t^{(1)} \right].$$
 (1.2.20)

Consequently, by (1.2.2), (1.2.14), (1.2.15), and (1.2.19),

$$\begin{pmatrix} \binom{m}{\otimes} Z_{j0} \end{pmatrix}' pr(Z) \begin{pmatrix} \binom{m}{\otimes} Z_{j0} \end{pmatrix} G^{x} = \begin{pmatrix} \binom{m}{\otimes} Z_{j0} \end{pmatrix}' \left\{ \left(pr(Z^{(1)}) Z_{0}^{(1)} \right) \otimes \begin{pmatrix} \binom{m}{\otimes} 1_{n_{j}} 1'_{s_{j}} \right) \right\}$$

$$= (Z_{0}^{(1)'} pr(Z^{(1)}) Z_{0}^{(1)}) \otimes (\bigotimes_{j=f+1}^{m} Z'_{j0} 1_{n_{j}} 1'_{s_{j}}) = (Z_{0}^{(1)'} pr(Z^{(1)}) Z_{0}^{(1)}) \otimes (\bigotimes_{j=f+1}^{m} r_{j} 1_{s_{j}} 1'_{s_{j}}).$$

Hence, from (1.2.1), (1.2.2), (1.2.15) and (1.2.16) it follows that

$$CG^{x} = \left(\prod_{j=1}^{m} r_{j} \right) G^{x} - \left(Z_{0}^{(1)'} pr(Z^{(1)}) Z_{0}^{(1)} \right) \otimes \left(\bigotimes_{j=f+1}^{m} r_{j} \mathbf{1}_{s_{j}} \mathbf{1}'_{s_{j}} \right), \tag{1.2.21}$$

which is symmetric. Therefore, the theorem follows from Lemma 1.2.1.

1.3 Lower Bounds for Efficiencies

The notion of efficiency as used in this chapter is the general Φp -efficiency (cf. Kiefer (1975)) and the definition is given below. For every $p, (0 \le p \le \infty)$ and every positive integer q, let $h_p^{(q)}$ be an extended real valued function defined over the class $\Gamma^{(q)}$ of $q \times q$ non-negative definite (n.n.d.) matrices such that for any $B \in \Gamma^{(q)}$ with eigenvalues $\lambda_i(B)$ $(1 \le i \le q)$,

$$h_p^{(q)}(B) = \{ \frac{q}{\pi} \lambda_i(B) \}^{\frac{1}{q}} \text{ when } p = 0,$$

$$= \{ q^{-1} \sum_{i=1}^{q} (\lambda_i(B))^{-p} \}^{-\frac{1}{p}} \text{ when } 0
$$= \min_{1 \le i \le q} \lambda_i(B) \text{ when } p = \infty,$$$$

provided the $\lambda_i(B)$'s are all positive. Otherwise, $h_p^{(q)}(B) = 0$, $(0 \le p \le \infty)$.

For $1 \leq j \leq m$, let P_j be an $(s_j - 1) \times s_j$ matrix such that $[s_j^{-\frac{1}{2}} 1_{s_j}, P_j']'$ is an orthogonal matrix. Then, the Φ_p -efficiency of the varietal design D_j is given by, say,

$$H_p^j = r_j^{-1} h_p^{(s_j - 1)}(P_j C_j P_j'), \quad (0 \le p \le \infty),$$
 (1.3.1)

where C_j is as in (1.2.3). If $p=0,1,\infty$, then this Φ_p -efficiency reduces to the standard D-,A-,E-efficiencies respectively.

In the factorial set-up, for any $x = (x_1, \ldots, x_m) \in \Omega$, define

$$P^x = \bigotimes_{j=1}^m P_j^{x_j}, \tag{1.3.2}$$

where for $1 \leq j \leq m$,

$$P_j^{x_j} = P_j \text{ if } x_j = 1, = s_j^{-\frac{1}{2}} \mathbf{1}'_{s_j} \text{ if } x_j = 0.$$
 (1.3.3)

Suppose the m factors in D are denoted by F_1, F_2, \ldots, F_m respectively. Then any typical factorial effect may be denoted by $F_1^{x_1} \ldots F_m^{x_m} (= J(x), \text{ say})$ for $x = (x_1, \ldots, x_m) \in \Omega$. Let τ be the $v \times 1$ vector of (factorial) treatment effects in D, arranged in lexicographic order. Then (cf. Kurkjian and Zelen (1963), Mukerjee (1981)) it may be seen that $P^x \tau$ represents a full set of orthonormal contrasts belonging to J(x). The number of rows in P^x will be $\prod_{j=1}^m (s_j - 1)^{x_j} (= \alpha(x), \text{ say})$ and let A_x denote the $\alpha(x) \times \alpha(x)$ coefficient matrix of the reduced normal equations for estimating $P^x \tau$ in D (cf. Kiefer (1975)) i.e., A_x is the information matrix for $P^x \tau$ in D. Then the Φ_p -efficiency of D with respect to the factorial effect J(x) is given by, say,

$$E_p^x = r^{-1} h_p^{(\alpha(x))}(A_x), \quad (0 \le p \le \infty). \tag{1.3.4}$$

The next theorem provides lower bounds for the efficiencies with respect to the different factorial effects in D in terms of the efficiencies of the designs D_1, \ldots, D_m . The following lemmas are needed in the proof. Lemmas 1.3.1 and 1.3.2 are well known (in these lemmas, for any matrix L, $\mu(L)$ denotes the column space of L). Lemma 1.3.3 follows from Poincare's separation theorem (cf. Rao (1973a, ch 1) and the proof is omitted here. Lemma 1.3.4 is due to Mukerjee (1986).

Lemma 1.3.1. Let A_{1j}, A_{2j} be matrices such that $\mu(A_{1j}) \subseteq \mu(A_{2j})$ $(1 \le j \le \omega)$. Then $\mu(\bigotimes_{j=1}^{\omega} A_{1j}) \subseteq \mu(\bigotimes_{j=1}^{\omega} A_{2j})$.

Lemma 1.3.2. Let A and B be matrices such that $\mu(A) \subseteq \mu(B)$. Then pr(B) - pr(A) is n.n.d.

Lemma 1.3.3. For $q \times q$ n.n.d. matrices A, B, if A - B is n.n.d., then

$$h_p^{(q)}(A) \ge h_p^{(q)}(B) \ (0 \le p \le \infty).$$

Lemma 1.3.4 (Mukerjee (1986)). If a factorial design has OFS then for each $x \in \Omega$, $A_x = P^x C P^{x'}$ where C is the usual C-matrix of the factorial design.

Theorem 1.3.1. For every $x = (x_1, \ldots, x_m) \in \Omega$, and every $p \ (0 \le p \le \infty)$,

$$E_p^x \geq \max_{1 \leq j \leq m} \{x_j H_p^j\}.$$

<u>Proof:</u> By Theorem 1.2.1 and Lemma 1.3.4, for every $x \in \Omega$, $A_x = P^x C P^{x'}$ where C is as in (1.2.6). As before, consider any $x = (x_1, \ldots, x_m) \in \Omega$ and let without loss of generality, $x_j = 1$ for $1 \le j \le f$ and $j \le j \le m$. Then by (1.2.8), (1.2.9), (1.3.2), (1.3.3)

$$P^{x} = (\bigotimes_{j=1}^{f} P_{j}) \otimes (\bigotimes_{j=f+1}^{m} s_{j}^{-\frac{1}{2}} \mathbf{1}'_{s_{j}}) = (\prod_{j=f+1}^{m} s_{j})^{-\frac{3}{2}} \{P^{(1)} \otimes (\bigotimes_{j=f+1}^{m} \mathbf{1}'_{s_{j}})\} G^{x}$$
 (1.3.5)

where

$$P^{(1)} = \bigotimes_{j=1}^{f} P_j. \tag{1.3.6}$$

By (1.2.8), (1.2.9), (1.2.21) and (1.3.5), it follows after some simplication that $A_x = P^x C P^{x'}$

$$= \left(\frac{\pi}{\pi} s_{j}\right)^{-\frac{3}{2}} P^{x} \left[\left(\frac{\pi}{\pi} r_{j}\right) G^{x} - \left(Z_{0}^{(1)'} pr(Z^{(1)}) Z_{0}^{(1)}\right) \otimes \left(\frac{\otimes}{j=f+1} r_{j} \mathbf{1}_{s_{j}} \mathbf{1}_{s_{j}}'\right)\right] \left[P^{(1)'} \otimes \left(\frac{\otimes}{j=f+1} \mathbf{1}_{s_{j}}\right)\right]$$

$$= \left(\frac{\pi}{j=f+1} r_{j}\right) \left[\left(\frac{f}{j=1} r_{j}\right) I_{\alpha(x)} - P^{(1)} Z_{0}^{(1)'} pr(Z^{(1)}) Z_{0}^{(1)} P^{(1)'}\right]. \tag{1.3.7}$$

By Lemma (1.3.1), $\mu(\bigotimes_{j=1}^f Z_{ja}) \subseteq \mu(Z_{1a} \otimes (\bigotimes_{j=2}^f I_{n_j})), 1 \leq \alpha \leq t$, and hence by

(1.2.4), (1.2.15) and (1.2.20),
$$\mu(Z^{(1)}) \subseteq \mu(Z_1 \otimes (\bigotimes_{j=2}^f I_{n_j}))$$
. So by Lemma 1.3.2,
$$pr\left\{ (Z_1) \otimes (\bigotimes_{j=2}^f I_{n_j}) \right\} - pr(Z^{(1)}) = \{ pr(Z_1) \} \otimes \left(\bigotimes_{j=2}^f I_{n_j}\right) - pr\left(Z^{(1)}\right)$$
 is n.n.d. (1.3.8)

From (1.2.2), (1.2.3), (1.2.15), (1.3.6) and the definition of the P_j matrices,

$$P_{1}C_{1}P'_{1} \otimes \left(\bigotimes_{j=2}^{f} r_{j}I_{s_{j-1}} \right) = r_{1}P_{1}P'_{1} \otimes \left(\bigotimes_{j=2}^{f} r_{j}I_{s_{j-1}} \right) - \left(P_{1}Z'_{10}pr(Z_{1})Z_{10}P'_{1} \right) \otimes \left(\bigotimes_{j=2}^{f} r_{j}I_{s_{j-1}} \right)$$

$$= \left(\prod_{j=1}^{f} r_{j} \right) I_{\alpha(x)} - \left(P_{1}Z'_{10}pr(Z_{1})Z_{10}P'_{1} \right) \otimes \left(\bigotimes_{j=2}^{f} P_{j}Z'_{j0}I_{n_{j}}Z_{j0}P'_{j} \right)$$

$$= \left(\prod_{j=1}^{f} r_{j} \right) I_{\alpha(x)} - P^{(1)}Z_{0}^{(1)'}(\{pr(Z_{1})\} \otimes \{\bigotimes_{j=2}^{f} I_{n_{j}}\})Z_{0}^{(1)}P^{(1)'}. \tag{1.3.9}$$

So from (1.3.7) and (1.3.9), it follows that

$$A_{x} - \left(\prod_{j=f+1}^{m} r_{j} \right) \left\{ (P_{1}C_{1}P_{1}') \otimes \left(\bigotimes_{j=2}^{f} r_{j}I_{s_{j-1}} \right) \right\}$$

$$= \left(\prod_{j=f+1}^{m} r_{j} \right) P^{(1)}Z_{0}^{(1)'} \left[\left\{ pr(Z_{1}) \right\} \otimes \left\{ \bigotimes_{j=2}^{f} I_{n_{j}} \right\} - pr(Z^{(1)}) \right] Z_{0}^{(1)}P^{(1)'}, \quad (1.3.10)$$

which is n.n.d. in view of the n.n.d.-ness of the right-hand member of (1.3.8).

Hence by Lemma (1.3.3),

$$h_p^{(\alpha(x))}(A_x) \ge h_p^{(\alpha(x))} \left[\begin{pmatrix} m \\ \pi \\ j=f+1 \end{pmatrix} r_j \right] \left\{ (P_1 C_1 P_1') \otimes \begin{pmatrix} f \\ \otimes \\ j=2 \end{pmatrix} r_j I_{s_j-1} \right\}$$

$$= \begin{pmatrix} m \\ \pi \\ j=2 \end{pmatrix} h_p^{(s_1-1)} \left(P_1 C_1 P_1' \right) \left(0 \le p \le \infty \right)$$

Dividing the above by $\prod_{j=1}^{m} r_j$, it is immediate from (1.3.1), (1.3.4) that

$$E_p^x \ge H_p^1 \ (0 \le p \le \infty).$$

Similarly, $E_p^x \ge H_p^j$ for $1 \le j \le f, 0 \le p \le \infty$ and hence

$$E_p^x \ge \max_{1 \le j \le m} \{x_j H_p^j\} \ (0 \le p \le \infty),$$

since $x_j = 0$ for $f + 1 \le j \le m$. This completes the proof.

Remarks:

- 1. Theorems 1.2.1 and 1.3.1 demonstrate that, even in the set-up of multiway heterogeneity elimination, the method of Kronecker product remains rather simple and useful from the practical point of view and is also theoretically appealing. By these theorems, it is clear, that, in order to construct a factorial design D, one has only to start with some varietal designs D₁,..., D_m and take their Kronecker product. This makes the construction of factorial designs for multiway heterogeneity elimination particularly simple since in practice, it is often much easier to construct varietal designs than factorial designs. Theorem 1.2.1 ensures that D has OFS. Theorem 1.3.1 shows how, by choosing the varietal designs D₁,..., D_m suitably, one can control and remain assured of the factorial effect efficiencies in the resulting design D in terms of the efficiencies of D₁,..., D_m. So, if one starts with efficient varietal designs, then their Kronecker product will generate a factorial design with high interaction efficiencies.
- 2. In particular, if J(x) represents a main effect (i.e., f = 1) then it is easy to see from the proof of Theorem 1.3.1 that equality holds in the lower bound given by Theorem 1.3.1, i.e., for $1 \le j \le m$, the efficiency of main effect F_j in D is equal to the efficiency of the corresponding varietal design D_j .
- 3. More interestingly, if J(x) represents an interaction involving two or more factors, then very often, one gets the satisfying observation that the actual value of E_p^x is much greater than the corresponding lower bound. For example, for the designs D_1 and D_2 in Example 1.2.1, it may be shown after computations that $P_1C_1P_1'=$

1.50 I_2 , $P_2C_2P_2'=2.00I_3$ where C_1 and C_2 are the C-matrices of D_1 and D_2 respectively and I_2 , I_3 are 2×2 and 3×3 identity matrices respectively.

Hence by (1.3.1) D_1 and D_2 are balanced with $H_p^1 = 0.75$, $H_p^2 = 0.6667$ $(0 \le p \le \infty)$.

Hence by Theorem 1.3.1, for the resulting factorial design D, one obtains

$$E_p^{10} \ge 0.75$$
, $E_p^{01} \ge 0.6667$, $E_p^{11} \ge 0.75$.

Actual computations show that while E_p^{01} , E_p^{10} attain the lower bounds, the true value of E_p^{11} is as high as .975. So, as this example suggests, the method of Kronecker product is likely to be particularly useful when emphasis lies on the efficient estimation of the interaction contrasts.

4. The property of Kronecker factorials, as considered in Theorem 1.3.1, has been termed 'faithfulness' by Mukerjee (1981, 1986) in the context of block designs.

1.4 The Restricted Kronecker Product

Although Theorems 1.2.1 and 1.3.1 make the Kronecker product method theoretically attractive, one practical difficulty may arise with this method when the number of factors, m, is large in the sense that the number of observations in D, namely $\frac{m}{\pi} n_j$, may become very large. To overcome this difficulty, this section considers a method of construction which guarantees OFS and at the same time exercises control over lower order interaction efficiencies. The fact that the higher order interaction efficiencies cannot be controlled by this method, does not detract from its merit since this method will be used when there is a large number of factors and in that situation the higher order interactions will usually not be of much interest. To that effect, a

modified version of the method of Kronecker product, called the "restricted Kronecker product" is considered below.

With notations as in section 1.2, suppose for $1 \le j \le m$, it is possible to partition Z_{ja} as

$$Z_{ja} = [Z'_{ja1}, Z'_{ja2}, \dots, Z'_{jaw_j}]', \qquad (1.4.1)$$

where for $1 \leq \ell \leq \omega_j, Z_{ja\ell}$ has $n_j \omega_j^{-1} (= \beta_j, \text{say})$ rows, such that

$$\mathbf{1}'_{\beta_j} Z_{ja1} = \mathbf{1}'_{\beta_j} Z_{ja2} = \dots = \mathbf{1}'_{\beta_j} Z_{jaw_j} (= \psi'_{ja}, \text{say}),$$

$$(1 \le a \le t; 1 \le j \le m)$$

$$(1.4.2)$$

$$\mathbf{1}'_{\beta_j} Z_{j0\ell} = (r_j \omega_j^{-1}) \mathbf{1}'_{s_j} \quad (1 \le \ell \le \omega_j, 1 \le j \le m). \tag{1.4.3}$$

By (1.2.1), (1.4.1), for $1 \le \ell \le \omega_j$, $1 \le j \le m$,

$$Z_{j0\ell} \mathbf{1}_{s_i} = Z_{j1\ell} \mathbf{1}_{u_{i1}} = \dots = Z_{jt\ell} \mathbf{1}_{u_{it}} = \mathbf{1}_{\beta_i}. \tag{1.4.4}$$

Also, recalling that for $1 \leq j \leq m$, each row of Z_{j0} contains exactly one element equal to unity and the rest zero, it follows from (1.4.1), (1.4.3) that

$$Z'_{j0\ell}Z_{j0\ell} = (r_j\omega_j^{-1})I_{s_j} \quad (1 \le \ell \le \omega_j; 1 \le j \le m).$$
 (1.4.5)

Physically, the partitioning (1.4.1) means that for $1 \leq j \leq m$, the varietal design D_j is partitioned into ω_j subdesigns such that each subdesign involves β_j observations, in each subdesign each of the s_j treatments is replicated $r_j \omega_j^{-1}$ times and the condition (1.4.2) holds. In many practical situations, such a partitioning can be attained in a natural way. An illustrative example will be given at the end of this section.

For matrices L_1, \ldots, L_{ω} having the same number of columns define $\bigcup_{i=1}^{\omega} L_i = [L'_1, \ldots, L'_{\omega}]'$. Then the restricted Kronecker product of order $g(\leq m)$ of the m varietal designs D_1, \ldots, D_m is defined to be a design $D^{(g)}$ with a design matrix

$$V^{(g)} = \bigcup_{(\gamma_1, \dots, \gamma_m)' \in T} \left[\bigotimes_{j=1}^m Z_{j0\gamma_j}, \bigotimes_{j=1}^m Z_{j1\gamma_j}, \dots, \bigotimes_{j=1}^m Z_{jt\gamma_j} \right],$$

where the union is taken over only a subset T of the $\frac{m}{\pi}\omega_j$ possible combinations $(\gamma_1,\ldots,\gamma_m)'$ such that the combinations included in T, written as columns, form an orthogonal array (possibly with variable symbols) with m rows, strength g and $\omega_1,\omega_2,\ldots,\omega_m$ symbols. (cf. Rao (1973b)).

As in section 1.2, $D^{(g)}$ may be interpreted as an $s_1 \times \ldots \times s_m$ factorial design for t-way elimination of heterogeneity and involving $\frac{m}{m} s_j$ treatments each replicated $N(\frac{m}{m} r_j \omega_j^{-1}) (= r^{(g)}, \text{ say})$ times, where N is the cardinality of T. Clearly, $D^{(g)}$ involves $N(\frac{m}{m} n_j \omega_j^{-1})$ observations and this number will be less than the number of observations, namely $\frac{m}{m} n_j$, in the ordinary Kronecker product design D, whenever $N < \frac{m}{j=1} \omega_j$, i.e., whenever the orthogonal array is non-trivial in the sense that all possible combinations $(\gamma_1, \ldots, \gamma_m)'$ do not occur as columns of T. In particular if g = m then the restricted Kronecker product reduces to the ordinary Kronecker product.

Theorems 1.4.1 and 1.4.2 below extend Theorems 1.2.1 and 1.3.1 respectively to the restricted Kronecker product set-up.

Theorem 1.4.1 The design $D^{(g)}$ has OFS.

Proof: Define

$$Q_{a} = \bigcup_{(\gamma_{1}, \dots, \gamma_{m})' \in T} \{ \bigotimes_{j=1}^{m} Z_{ja\gamma_{j}} \}, (0 \leq a \leq t), \tag{1.4.6}$$

and

$$Q = [Q_1, \dots, Q_t]. (1.4.7)$$

Then the reduced normal equations for the (factorial) treatment effects in $D^{(g)}$ have a $v \times v$ coefficient matrix given by, say,

$$C^{(g)} = Q_0' p r^{\perp}(Q) Q_0, \tag{1.4.8}$$

which is analogous to (1.2.6). As in Theorem 1.2.1, this theorem will also be proved by invoking Lemma 1.2.1 after establishing that $C^{(g)}G^x$ is symmetric for every $x \in \Omega$. Without loss of generality, consider $x = (x_1, \ldots, x_m) \in \Omega$ where $x_j = 1$ if $1 \le j \le j$ $j \le j$ and j = 0 if $j \le j$ if $j \le j$ so, as in (1.2.14), $j \le j$ because $j \le j$ let

$$Q_a^{(1)} = \bigcup_{(\gamma_1, \dots, \gamma_m)' \in T} \{ \bigotimes_{j=1}^f Z_{ja\gamma_j} \} \ (0 \le a \le t); \ Q^{(1)} = [Q_1^{(1)}, \dots, Q_t^{(1)}]. \tag{1.4.9}$$

From (1.4.8),

$$C^{(g)}G^{x} = Q_{0}'Q_{0}G^{x} - Q_{0}'pr(Q)Q_{0}G^{x}, \qquad (1.4.10)$$

where from (1.4.5) and (1.4.6),

$$Q'_{0}Q_{0} = \sum_{(\gamma_{1},...,\gamma_{m})' \in T} \{ \bigotimes_{j=1}^{m} Z'_{j0\gamma_{j}} Z_{j0\gamma_{j}} \} = \sum_{(\gamma_{1},...,\gamma_{m})' \in T} \{ \prod_{j=1}^{m} r_{j}\omega_{j}^{-1} \} \{ \bigotimes_{j=1}^{m} I_{s_{j}} \}$$

$$= N(\prod_{j=1}^{m} r_{j}\omega_{j}^{-1}) (\bigotimes_{j=1}^{m} I_{s_{j}}). \tag{1.4.11}$$

By (1.2.14), (1.2.15), (1.4.2), (1.4.4), (1.4.6) and (1.4.7) on simplification:

$$Q'Q_0G^x = \bigcup_{a=1}^t \left[\left\{ \sum_{(\gamma_1, \dots, \gamma_m)' \in T} \bigotimes_{j=1}^f \left(Z'_{ja\gamma_j} Z_{j0\gamma_j} \right) \right\} \otimes \left\{ \bigotimes_{j=f+1}^m \left(\psi_{ja} \mathbf{1}'_{s_j} \right) \right\} \right]. \quad (1.4.12)$$

Clearly, there exists a matrix $\Delta_1 = [\Delta'_{11}, \ldots, \Delta'_{1t}]'$, where the number of rows of Δ_{1a} equals the number of columns of $Q_a^{(1)}$ $(1 \le a \le t)$ such that

$$Q^{(1)'}Q^{(1)}\Delta_1 = Q^{(1)'}Q_0^{(1)}G^{(1)}. (1.4.13)$$

Now, defining

$$\Delta = \left[\Delta'_{11} \otimes (\bigotimes_{j=f+1}^{m} \mathbf{1}_{u_{j1}} \mathbf{1}'_{s_{j}})', \dots, \Delta'_{1t} \otimes (\bigotimes_{j=f+1}^{m} \mathbf{1}_{u_{jt}} \mathbf{1}'_{s_{j}})' \right]', \text{ we have}$$

$$Q'Q\Delta = \bigcup_{a=1}^{t} \left[\left\{ \sum_{(\gamma_1, \dots, \gamma_m)' \in T} \bigotimes_{j=1}^{f} \left(Z'_{ja\gamma_j} Z_{j0\gamma_j} \right) \right\} \otimes \left\{ \bigotimes_{j=f+1}^{m} \left(\psi_{ja} \mathbf{1}'_{s_j} \right) \right\} \right],$$

after some considerable algebra using (1.2.14), (1.2.15), (1.4.2), (1.4.4) (1.4.6), (1.4.7) and (1.4.13). Hence from (1.4.12), $Q'Q_0G^x = Q'Q\Delta$. Consequently,

$$Q_0' pr(Q) Q_0 G^x = Q_0' Q(Q'Q)^- Q' Q_0 G^x = Q_0' Q \triangle$$

$$= \left\{ Q_0^{(1)'} pr(Q^{(1)}) Q_0^{(1)} \right\} \otimes \left\{ \bigotimes_{j=f+1}^m (r_j \omega_j^{-1} \mathbf{1}_{s_j} \mathbf{1}'_{s_j}) \right\}, \quad (1.4.14)$$

after simplification using (1.4.3), (1.4.4), (1.4.6), (1.4.7) and (1.4.9) and the definition of Δ . From (1.4.10), (1.4.11) and (1.4.14) it follows that

$$C^{(g)}G^{x} = N(\prod_{j=1}^{m} r_{j}\omega_{j}^{-1})(\bigotimes_{j=1}^{m} I_{s_{j}})G^{x}$$

$$-\left\{Q_{0}^{(1)'}pr(Q^{(1)})Q_{0}^{(1)}\right\} \otimes \left\{\bigotimes_{j=f+1}^{m} r_{j}\omega_{j}^{-1}\mathbf{1}_{s_{j}}\mathbf{1}_{s_{j}}'\right\}, \quad (1.4.15)$$

which is symmetric and hence the proof is complete.

To prove our next result, i.e., the result stating lower bounds for the factorial effect efficiencies in $D^{(g)}$, the notations are as in section 1.3, the only change being that for any $x \in \Omega$, the coefficient matrix of the reduced normal equations for estimating $P^x \tau$ in $D^{(g)}$ is denoted by $A_x^{(g)}$ and accordingly, the Φ_p -efficiency of $D^{(g)}$ with respect to the factorial effect J(x) is denoted by

$$E_p^x(g) = r^{(g)-1} h_p^{(\alpha(x))} (A_x^{(g)}).$$

Theorem 1.4.2. For $x = (x_1 \dots x_m) \in \Omega$ and every $p \ (0 \le p \le \infty)$,

$$E_p^x(g) \ge \max_{1 \le j \le m} \{x_j H_p^j\},\,$$

provided among x_1, \ldots, x_m at most g are unity.

<u>Proof:</u> As before, without loss of generality consider $x=(x_1,\ldots,x_m)$ $\in \Omega$ where

 $x_j = 1 \text{ if } 1 \le j \le f; \ x_j = 0 \text{ if } f + 1 \le j \le m, \text{ and } f \le g.$

By Lemma 1.3.4, $A_x^{(g)} = P^x C^{(g)} P^{x'}$ where $C^{(g)} G^x$ is as in (1.4.15).

Since the combinations $(\gamma_1, \ldots, \gamma_m)'$ included in T form an orthogonal array with N assemblies and strength g (and hence with strength f, for $f \leq g$), it follows that for every $(\gamma_1, \ldots, \gamma_f)'$ $(1 \leq \gamma_j \leq \omega_j; 1 \leq j \leq f)$ there are exactly $N(\frac{f}{\pi} \omega_j)^{-1}$ combinations in T with the first f entries equal to $\gamma_1, \ldots, \gamma_f$, provided $f \leq g$. Hence by (1.4.1), (1.4.9), for any a, k $(0 \leq a, k \leq t)$,

$$Q_{a}^{(1)'}Q_{k}^{(1)} = \sum_{(\gamma_{1},...,\gamma_{m})'\in T} \left\{ \bigotimes_{j=1}^{f} \left(Z'_{ja\gamma_{j}} Z_{jk\gamma_{j}} \right) \right\}$$

$$= \left(N / \inf_{j=1}^{f} \omega_{j} \right) \sum_{\gamma_{1}=1}^{\omega_{1}} ... \sum_{\gamma_{f}=1}^{\omega_{f}} \left\{ \bigotimes_{j=1}^{f} \left(Z'_{ja\gamma_{f}} Z_{jk\gamma_{f}} \right) \right\}$$

$$= \left(N / \inf_{j=1}^{f} \omega_{j} \right) \bigotimes_{j=1}^{f} \left\{ \sum_{\gamma_{j=1}}^{\omega_{j}} Z'_{ja\gamma_{j}} Z_{jk\gamma_{j}} \right\}$$

$$= \left(N / \inf_{j=1}^{f} \omega_{j} \right) \bigotimes_{j=1}^{f} \left\{ Z'_{ja} Z_{jk} \right\}$$

$$= \left(N / \inf_{j=1}^{f} \omega_{j} \right) \left(\bigotimes_{j=1}^{f} Z'_{ja} \right) \left(\bigotimes_{j=1}^{f} Z_{jk} \right)$$

$$= \left(N / \inf_{j=1}^{f} \omega_{j} \right) Z_{a}^{(1)'} Z_{k}^{(1)}, \qquad (1.4.16)$$

whenever $f \leq g$ and $Z_a^{(1)}, Z_k^{(1)}$ are as in (1.2.15). By (1.2.15), (1.2.20), (1.4.9) and (1.4.16) it follows that

$$Q^{(1)'}Q^{(1)} = \left(N/\frac{f}{\pi}\omega_j\right)Z^{(1)'}Z^{(1)} , \quad Q^{(1)'}Q_0^{(1)} = \left(N/\frac{f}{\pi}\omega_j\right)Z^{(1)'}Z_0^{(1)}$$

whenever $f \leq g$. Therefore, for $f \leq g$,

$$Q_0^{(1)'}pr(Q^{(1)})Q_0^{(1)} = \left(N/\prod_{j=1}^f \omega_j\right) \left\{Z_0^{(1)'}pr(Z^{(1)})Z_0^{(1)}\right\}.$$

Hence from (1.4.15), for $f \leq g$

$$C^{(g)}G^{x} = \left\{ N \prod_{j=1}^{m} (r_{j}\omega_{j}^{-1}) \right\} G^{x}$$

$$- \left(N / \prod_{j=1}^{f} \omega_{j} \right) \left\{ Z_{0}^{(1)'} pr(Z^{(1)}) Z_{0}^{(1)} \right\} \otimes \left\{ \bigotimes_{j=f+1}^{m} r_{j}\omega_{j}^{-1} \mathbf{1}_{s_{j}} \mathbf{1}'_{s_{j}} \right\},$$

which is analogous to (1.2.21). The rest of the proof may now be completed along the line of proof of Theorem 1.3.1.

By Theorem 1.4.2, one can apply the method of restricted Kronecker product of order g to construct a factorial design for t-way heterogeneity elimination and control the factorial effect efficiencies in $D^{(g)}$, for effects involving up to g factors, in terms of the efficiencies of D_1, \ldots, D_m . In particular, if one wants to control only the main effect efficiencies then g=1 and T should represent an orthogonal array of strength 1 which can be obtained easily. If in addition, one wants to control the two-factor efficiencies also then g=2 and T should represent an orthogonal array of strength 2. This also poses no major combinatorial problem since orthogonal arrays of strength 2 are available in plenty (see e.g., Raghavaro (1971), ch 2).

As indicated earlier, in many situations there exists a natural way of attaining the partition (1.4.1) such that (1.4.2) and (1.4.3) are satisfied. For example, considering a set-up of row-column designs (i.e., t = 2), suppose D_j is a complete or an incomplete latin square which can be partitioned into disjoint transversals such that each transversal contains each of the s_j treatments in D_j exactly once. Then these transversals provide a natural way of attaining a partition (1.4.1) such that the conditions (1.4.2) and (1.4.3) hold. These considerations indicate that the method of restricted Kronecker product has a wide applicability. As an illustration an example

is given below.

Example 1.4.1 Construction of a $4 \times 5 \times 7$ factorial row-column design.

Here $s_1 = 4$, $s_2 = 5$, $s_3 = 7$. As the initial varietal row-column designs D_1, D_2, D_3 we take three incomplete latin squares given by

In each of these squares the cells will be denoted by ordered pairs $(y_1, y_2), (y_1, y_2 = 1, 2, ...)$. A partitioning of D_1 as in (1.4.1) which satisfies (1.4.2) and (1.4.3) with $\omega_1 = 3$, is given by the three sets of cells:

$$\{(1,1),(2,2),(3,3),(4,4)\},\ \{(1,2),(2,1),(3,4),(4,3)\},\ \{(1,3),(2,4),(3,1),(4,2)\}.$$

A similar partitioning of D_2 with $\omega_2 = 3$ is given by the three sets of cells:

$$\{(1,2),(2,3),(3,4),(4,5),(5,1)\},\ \{(1,4),(2,5),(3,1),(4,2),(5,3)\},\ \{(1,5),(2,1),(3,2),(4,3),(5,4)\},$$

and a partitioning of D_3 with $\omega_3 = 3$ is given by the three sets of cells:

$$\{(1,1),(2,2),(3,3),(4,4),(5,5),(6,6),(7,7)\},\$$

 $\{(1,3),(2,4),(3,5),(4,6),(5,7),(6,1),(7,2)\},\$
 $\{(1,6),(2,7),(3,1),(4,2),(5,3),(6,4),(7,5)\},\$

Note that $\omega_1 = \omega_2 = \omega_3 = 3$. Hence taking $T = \{(1,1,1), (1,2,2), (1,3,3), \dots \}$

(2,1,2),(2,2,3),(2,3,1),(3,1,3),(3,2,1),(3,3,2), which is an orthogonal array of strength 2, and applying the method of restricted Kronecker product (with g=2) one can get a $4 \times 5 \times 7$ factorial row column design, say $D^{(2)}$, which has OFS and in which the main effect and two-factor interaction efficiencies are controlled in the sense of Theorem 1.4.2. Since the cardinality of T is 9 and $\prod_{j=1}^{3} \omega_j = 27$, the number of observations required in $D^{(2)}$ is only one-thirds the number of observations required in the ordinary Kronecker product of D_1, D_2, D_3 .

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Chapter 2

NON-EQUIREPLICATE KRONECKER FACTORIAL DESIGNS

2.1 Introduction

Often practical situations arise when it becomes imperative to use designs with varying numbers of replication and varying block sizes. The need to study such designs has been advocated among others by Pearce (1964), Calinski (1971) and Hedayat and Federer (1974). While the literature on varietal block designs satisfying the above conditions is very rich, it appears that in the context of factorial designs, the problem of unequal replication has not received much attention.

The two important methods of constructing factorial designs, namely, the generalized cyclic method and the method of Kronecker or Kronecker-type products, have so far been used to construct equireplicate designs only. This can be noted from the various references given in the introduction of Chapter 1. In Chapter 1, we have applied the latter of the above two methods to construct equireplicate designs. Besides these two methods of construction, it appears that, most of the classical construction procedures for factorial designs also, do not consider the non-equireplicate case. The class of "general classical designs", which has been defined by Voss (1986) and shown to include the classes of designs generated by several confounding methods in the literature, is also equireplicate.

In the non-equireplicate set-up for factorial designs, among the very few references available, we would like to mention the papers by Puri and Nigam (1976, 1978). They studied $s_1 \times s_2 \times \ldots \times s_m$ balanced factorial experiments with a replication vector of

the form $\mathbf{r} = r(\mathbf{a}_1 \otimes \ldots \otimes \mathbf{a}_m)$, where, for $1 \leq j \leq m$, \mathbf{a}_j is a $s_j \times 1$ vector of relative replications of the j^{th} factor, and the symbol \otimes denotes Kronecker product. They discussed the analysis of such designs and studied their efficiencies together with some methods of construction.

A reason for the dearth of work in this area may be that maintaining OFS becomes a problem when the number of replications vary. Consequently, an analysis of these designs by the usual methods becomes difficult, rendering the study of the factorial effect efficiencies even more so. On the other hand, the necessity of constructing and studying factorial designs with varying replication numbers and varying block sizes remains, so as to give the experimenter more scope to study experiments in unconventional circumstances which arise in practice. One such very common situation is where the treatment combinations in a factorial experiment are not all equally expensive or easily available, making the use of equireplicate designs either too expensive or wasteful, if not altogether impossible. Thus the study of factorial designs with unequal numbers of replication, which allow estimation of important contrasts with desired efficiencies and admit a simple analysis, seems very pertinent.

In an attempt to fulfil this need to some extent, non-equireplicate Kronecker factorial designs are considered in this chapter. To motivate, we begin with block designs in section 2.2. Section 2.3 demonstrates how the interaction efficiencies may be controlled and high efficiencies achieved for the resulting factorial design, simply by suitably choosing the initial varietal designs. In section 2.4, it is shown that even though the resulting designs may not have OFS, they admit a simple analysis. In

section 2.5, the results have been extended to designs for multiway elimination of heterogeneity through the use of projection operators. Some further results have been presented in section 2.6. Finally, in section 2.7 some related open problems have been discussed.

2.2 Non-equireplicate Kronecker Factorials: Block Designs

Throughout the chapter, whether the design under consideration is varietal or factorial, the usual fixed effects intrablock model, with independent homoscedastic errors and no block treatment interaction, is assumed.

Let for $1 \leq j \leq m, D_j$ be a varietal design involving s_j varieties, n_j observations and having an $s_j \times b_j$ incidence matrix N_j . Let the varieties be labelled $0, 1, \ldots, s_j - 1$ and let $r_{j0}, r_{j1}, \ldots, r_{js_j-1}$ be their replication numbers respectively. Let $k_{j0}, k_{j1}, \ldots, k_{jb_j-1}$ be the block sizes in D_j . Let $\mathbf{r}_j = (r_{j0}, r_{j1}, \ldots, r_{js_j-1})', \mathbf{k}_j = (k_{j0}, k_{j1}, \ldots, k_{jb_j-1})', R_j = \text{Diag }(r_{j0}, r_{j1}, \ldots, r_{js_j-1}), K_j = \text{Diag }(k_{j0}, k_{j1}, \ldots, k_{jb_j-1})'$. The elements of \mathbf{r}_j or \mathbf{k}_j are not necessarily equal.

The reduced normal equations for the treatment effects in D_j have a coefficient matrix given by

$$C_j = R_j - N_j K_i^{-1} N_j'. (2.2.1)$$

The Kronecker product of D_1, \ldots, D_m is a design D with incidence matrix

$$N = \bigotimes_{j=1}^{m} N_j \tag{2.2.2}$$

where \otimes denotes Kronecker product. As in Chapter 1, by interpreting the $\frac{m}{m} s_j$ treatments in D as $\frac{m}{m} s_j$ factorial level combinations, D may be looked upon as an $s_1 \times s_2 \times \ldots \times s_m$ factorial design involving $\frac{m}{m} s_j (= v, \text{say})$ treatments in $\frac{m}{m} b_j (= b, m)$

say) blocks with $\frac{m}{m}$ n_j observations. The replication numbers and block sizes in D are given by the elements of the $v \times 1$ and $b \times 1$ vectors $\mathbf{r} = \mathbf{r}_1 \otimes \ldots \otimes \mathbf{r}_m$ and $\mathbf{k} = \mathbf{k}_1 \otimes \ldots \otimes \mathbf{k}_m$ respectively. Since the designs D_1, \ldots, D_m are not necessarily equireplicate nor proper, in D also, neither the replication numbers nor the block sizes are necessarily equal.

Let R and K be $v \times v$ and $b \times b$ diagonal matrices with diagonal elements given by the elements of the vectors \mathbf{r} and \mathbf{k} respectively, i.e., $R = \bigotimes_{j=1}^m R_j$ and $K = \bigotimes_{j=1}^m K_j$.

Then, by (2.2.1) and (2.2.2), the coefficient matrix of the reduced normal equations for the treatment effects in D is given by,

$$C = R - NK^{-1}N' = \bigotimes_{j=1}^{m} R_j - \left(\bigotimes_{j=1}^{m} N_j\right) \left(\bigotimes_{j=1}^{m} K_j^{-1}\right) \left(\bigotimes_{j=1}^{m} N_j'\right)$$
$$= \bigotimes_{j=1}^{m} R_j - \bigotimes_{j=1}^{m} (R_j - C_j) \tag{2.2.3}$$

2.3 Lower Bounds for Interaction Efficiencies

The efficiency with which a treatment contrast with the $s_j \times 1$ coefficient vector \mathbf{u}_j is estimated in D_j is defined as

$$e_{j}(\mathbf{u}_{j}) = \mathbf{u}_{j}^{\prime} R_{j}^{-1} \mathbf{u}_{j} / \mathbf{u}_{j}^{\prime} C_{j}^{-} \mathbf{u}_{j} \text{ if the contrast is estimable in } D_{j},$$

$$= 0 \qquad \text{otherwise}$$

$$(2.3.1)$$

where C_j^- is any generalized (g-) inverse of C_j . Clearly, the efficiency in (2.3.1) is based on a comparison of D_j with the corresponding (unblocked) completely randomized design having the same replication numbers as D_j . Also, (2.3.1) remains the same whatever be the choice of the g-inverse C_j^- .

In the factorial set-up, let τ be the $v \times 1$ vector of treatment effects in D, ar-

ranged lexicographically. Analogously to (2.3.1), the efficiency with which a treatment contrast $\mathbf{u}'\boldsymbol{\tau}$ is estimated in D is defined as

$$e(\mathbf{u}) = \mathbf{u}'R^{-1}\mathbf{u}/\mathbf{u}'C^{-1}\mathbf{u} \text{ if the contrast is estimable in } D$$

$$= 0 \qquad \text{otherwise}$$

$$(2.3.2)$$

Here also, the efficiency (2.3.2) is expressed relative to a (unblocked) completely randomized design having the same replication numbers as D. Again, (2.3.2) remains the same for every choice of the g-inverse C^- .

It may be seen that in D all main effect contrasts are estimable if and only if each of D_1, \ldots, D_m is connected. It is, therefore, assumed hereafter that each of D_1, \ldots, D_m is connected. This will imply that D is connected and hence ensure that all matrix inverses considered in the next two sections exist.

The following lemmas will be helpful. The proof of the first lemma is straight-forward and hence omitted. Let the column space of any matrix A be denoted by $\mu(A)$.

Lemma 2.3.1. For $1 \leq j \leq m$, let A_j, B_j be non-negative definite (n.n.d.) matrices such that $A_j - B_j$ is n.n.d. Then $\bigotimes_{j=1}^m A_j - \bigotimes_{j=1}^m B_j$ is n.n.d.

Lemma 2.3.2. Let A and B be n.n.d. matrices such that A-B is n.n.d. Then $\mu(B) \subseteq \mu(A)$ and for every matrix U satisfying $\mu(U) \subseteq \mu(B)$,

$$U'B^-U - U'A^-U$$
,

is n.n.d. where A^-, B^- are any generalized inverses of A, B respectively.

<u>Proof:</u> Since B is n.n.d., there exists some matrix L such that B = LL'. Again, since A - B is n.n.d., we have A - B = HH' for some matrix H. Hence, $A = (H L)(\frac{H'}{L'})$

and therefore it follows that $\mu(A) \equiv \mu(H \ L) \supseteq \mu(L) \equiv \mu(B)$. Hence the first part of the lemma.

Now let $\mu(\mathbf{U}) \subseteq \mu(B) \equiv \mu(L)$. Then $\mathbf{U} = LD$ for some matrix D. Hence $\mathbf{U}'B^{-}\mathbf{U} - \mathbf{U}'A^{-}\mathbf{U} = D'[L'(LL')^{-}L - L'(HH' + LL')^{-}L]D$. Since $L'(LL')^{-}L - L'(HH' + LL')^{-}L$ is clearly n.n.d., the lemma follows.

The next lemma follows as a corollary to Lemma 2.3.2.

Lemma 2.3.3. Let A and B be n.n.d. matrices such that A-B is n.n.d. Then $\mu(B) \subseteq \mu(A)$ and for every vector $\mathbf{u} \in \mu(B)$,

$$\mathbf{u}'B^{-}\mathbf{u} \geq \mathbf{u}'A^{-}\mathbf{u},$$

where A^-, B^- are any g-inverses of A, B respectively.

Let $\mathbf{1}_n$ denote the $n \times 1$ vector with all elements unity. For $1 \leq j \leq m$, let \mathbf{u}_j be any $s_j \times 1$ non-null vector satisfying $\mathbf{u}_j' \mathbf{1}_{s_j} = 0$, so that \mathbf{u}_j may be considered as the coefficient vector of a treatment contrast in D_j .

Considering now the $s_1 \times s_2 \times \ldots \times s_m$ Kronecker factorial design D, let Ω and J(x) be as defined in section 1.2 of Chapter 1. For any $x = (x_1, \ldots, x_m) \in \Omega$, define the $v \times 1$ vector

where
$$\mathbf{u}^x = \bigotimes_{j=1}^m \mathbf{u}_j^{x_j},$$

$$\mathbf{u}_j^{x_j} = \mathbf{u}_j \text{ if } x_j = 1; = \mathbf{1}_{s_j} \text{ if } x_j = 0.$$

Then, $\mathbf{u}^{x'}\boldsymbol{\tau}$ represents a typical contrast belonging to the factorial effect J(x) in D.

The following theorem sets a lower bound for $e(\mathbf{u}^x)$ and demonstrates that even in a non-equireplicate setting, high efficiencies with respect to contrasts belonging to

factorial effects in D can be ensured by suitably choosing the initial varietal designs D_1, \ldots, D_m .

Theorem 2.3.1. $e(\mathbf{u}^x) \ge \max_{j:x_j=1} e_j(\mathbf{u}_j)$, for each $x \in \Omega$.

<u>Proof:</u> For $1 \le j \le m$, let

where
$$L_j = \bigotimes_{f=1}^m L_{jf} \quad , \quad W_j = \bigotimes_{f=1}^m W_{jf} \quad ,$$

$$L_{jf} = W_{jf} = R_f \text{ if } f \neq j; L_{jj} = C_j, W_{jj} = R_j - C_j.$$

Note that for each j, $L_j = \bigotimes_{f=1}^m R_f - W_j$, so that by (2.2.3), $C - L_j = W_j - \bigotimes_{f=1}^m (R_f - C_f), \tag{2.3.5}$

which is n.n.d. by (2.3.4) and Lemma 2.3.1.

Now consider any $x=(x_1,\ldots,x_m)$ ϵ Ω . Without loss of generality, let $x_1=1$. Then by (2.3.3), (2.3.4), \mathbf{u}^x ϵ $\mu(L_1)$. But by (2.3.5), $C-L_1$ is n.n.d. Hence it follows from Lemma 2.3.3 that

$$\mathbf{u}^{x'}C^{-}\mathbf{u}^{x} \leq \mathbf{u}^{x'}L_{1}^{-}\mathbf{u}^{x} = \mathbf{u}^{x'}(C_{1}^{-} \otimes R_{2}^{-1} \otimes \ldots \otimes R_{m}^{-1})\mathbf{u}^{x}$$

$$= (\mathbf{u}_{1}^{\prime}C_{1}^{-}\mathbf{u}_{1}) \times \begin{bmatrix} m \\ \pi \\ j=2 \end{bmatrix} (\mathbf{u}_{j}^{x_{j}})^{\prime}R_{j}^{-1}\mathbf{u}_{j}^{x_{j}}, \qquad (2.3.6)$$

using (2.3.3) and (2.3.4). But by (2.3.3), noting that $x_1 = 1$,

$$\mathbf{u}^{x'} R^{-1} \mathbf{u}^{x} = \left(\mathbf{u}_{1}' R_{1}^{-1} \mathbf{u}_{1} \right) \times \left[\prod_{j=2}^{m} \left(\mathbf{u}_{j}^{x_{j}} \right)' R_{j}^{-1} \mathbf{u}_{j}^{x_{j}} \right].$$

Hence by (2.3.1), (2.3.2) and (2.3.6), $e(\mathbf{u}^x) \geq e_1(\mathbf{u}_1)$. Similarly, it may be shown that $e(\mathbf{u}^x) \geq e_j(\mathbf{u}_j)$ for every j such that $x_j = 1$. Hence the theorem.

Remarks:

1. Theorem 2.3.1 extends the basic ideas in Gupta (1986a) and Mukerjee (1986) to

a non-equireplicate set-up.

- 2. As remarked in Chapter 1, in this set-up also, the use of the method of Kronecker product results in factorial designs with a wide range of parameter values since the initial designs D_1, \ldots, D_m are left quite arbitrary. Thus the construction of factorial designs with varying replication numbers and block sizes become particularly easy.
- 3. In this set-up also, the method of Kronecker product is capable of controlling the interaction efficiencies in D. By an appropriate choice of D_1, \ldots, D_m , high efficiencies with respect to contrasts of interest may be achieved in D. Again, as in Chapter 1, it can be illustrated by examples that often the actual value of $e(\mathbf{u}^x)$ is much higher than the lower bound given in the theorem.

2.4 A Computation of C^-

It may be seen through examples that non-equireplicate Kronecker factorials rarely have OFS as they do not satisfy the necessary and sufficient condition for OFS as in Mukerjee (1979). But in spite of that, a method for computing a g-inverse of C, which does not require the inversion of large matrices, is available.

For $1 \leq j \leq m$, let T_j be an $(s_j-1)\times s_j$ matrix such that $(q_j\mathbf{r}_j, T_j')'$ is orthogonal, where $q_j = (\mathbf{r}_j'\mathbf{r}_j)^{-\frac{1}{2}}$. For $x = (x_1, \ldots, x_m) \in \Omega$, define

where
$$T_x = \bigotimes_{j=1}^m T_j^{x_j},$$

$$T_j^{x_j} = T_j \quad \text{if } x_j = 1 \quad , \quad = \mathbf{1}'_{s_j} \quad \text{if} \quad x_j = 0.$$

Let
$$T=(\ldots,T'_x,\ldots)'_{x~\epsilon~\Omega}, i.e., T=(T^{00\ldots 1'},\ldots,T^{11\ldots 1'})'.$$
 Let $\mathbf{1}=\mathbf{1}_{s_1}\otimes\ldots\otimes$

$$1_{s_m}, T^* = (1, T')'.$$

Lemma 2.4.1. The $v \times v$ matrix T^* is non-singular.

<u>Proof:</u> Note that $T^* = T_1^* \otimes ... \otimes T_m^*$, where $T_j^* = (\mathbf{1}_{s_j}, T_j')', (1 \leq j \leq m)$. From the definition of T_j it follows that each T_j^* is non-singular and hence the lemma.

<u>Lemma 2.4.2</u> For every $x, y \in \Omega, x \neq y, T_xCT'_y = 0$.

Proof: Consider $x = (x_1, \ldots, x_m) \in \Omega, y = (y_1, \ldots, y_m) \in \Omega, x \neq y$. By (2.2.3), (2.4.1)

$$T^{x}CT^{y'} = \bigotimes_{j=1}^{m} (T_{j}^{x_{j}} R_{j} T_{j}^{y'_{j}}) - \bigotimes_{j=1}^{m} (T_{j}^{x_{j}} (R_{j} - C_{j}) T_{j}^{y'_{j}}). \tag{2.4.2}$$

Since $x \neq y$, there exists at least one j such that $x_j \neq y_j$. Let without loss of generality, $x_k = 1, y_k = 0$. Then,

$$T_k^{x_k} R_k T_k^{y_k'} = T_k R_k \mathbf{1}_{s_k} = T_k \mathbf{r}_k = \mathbf{0},$$

$$T_k^{x_k}(R_k - C_k)T_k^{y_k'} = T_k(R_k - C_k)1_{s_k} = T_kR_k1_{s_k} = T_kr_k = 0,$$

by the definition of T_k and the fact that $C_k \mathbf{1}_{s_k} = \mathbf{0}$. Hence by (2.4.2) lemma follows.

Theorem 2.4.1 A g-inverse of C is given by

$$C^{-} = \sum_{x \in \Omega} T'_{x} (T_{x} C T'_{x})^{-1} T_{x}.$$

<u>Proof:</u> From the definition of the T_j matrices, $T_j \mathbf{r}_j = 0$ for each j and so by (2.4.1)

$$T_x C T_x' = T_x (C + \bigotimes_{i=1}^m \mathbf{r}_j \mathbf{r}_j') T_x'.$$

Since D is connected, $T_x(C + \bigotimes_{j=1}^m \mathbf{r}_j \mathbf{r}_j') T_x'$ is positive definite and hence $T_x C T_x'$ is also non-singular. Define the $v \times v$ matrices

$$L = \operatorname{Diag}\left(0, \underbrace{\ldots, T_x C T_x', \ldots}\right) \quad , L^* = \operatorname{Diag}\left(0, \underbrace{\ldots, (T_x C T_x')^{-1}, \ldots}\right).$$

Since C1=0, from Lemma 2.4.2 it follows that $T^*CT^{*'}=L$ and hence by Lemma 2.4.1., $C=T^{*-1}LT^{*'-1}$.

Also, C^- as in the statement of the theorem equals $T^{*'}L^*T^*$ and hence $CC^-C=$ C, as desired.

Remark: We note that for each $x \in \Omega$, $T^xCT^{x'}$ is a square matrix of order $\frac{\pi}{\pi}(s_j-1)^{x_j}(=\alpha(x), \text{say})$. So by Theorem 2.4.1, the analysis of D, which requires the evaluation of C^- , involves the inversion of matrices of order $\alpha(x), x \in \Omega$. This may lead to computational simplicity since the numbers $\alpha(x), x \in \Omega$, will be much smaller than v, the order of C. Even for a factorial design with OFS it may be seen that (cf. Mukerjee (1979)) the calculation of C^- will in general involve inversion of matrices of precisely the same orders, unless some further supplementary information is available on the design. Thus, although in a non-equireplicate situation the Kronecker factorial design may not have OFS, still its analysis does not pose any serious problem in terms of computational complexity.

2.5. Non-equireplicate Kronecker Factorial Designs for Multiway Heterogeneity Elimination.

The results of sections 2.3 and 2.4 may be extended to designs for multiway elimination of heterogeneity. As in Chapter 1, in this section also, we use the technique of projection operators as it simplifies the computations considerably in the context of multiway heterogeneity elimination.

Let D_1, \ldots, D_m be m non-equireplicate varietal designs for t-way elimination of heterogeneity. We assume that D_1, \ldots, D_m are connected in order to ensure that the Kronecker factorial design D is also connected. Using notations similar to those in Chapter 1, let the design matrix of D_j , for $1 \leq j \leq m$, be

$$V_j = [Z_{j0}, Z_{j1}, \ldots, Z_{jt}],$$

where Z_{j0} is of order $n_j \times s_j$ and Z_{ja} is of order $n_j \times u_{ja} (1 \le a \le t), u_{ja}$ being the number of classes according to the a-th way of heterogeneity elimination. Let for $1 \le j \le m, r_{j0}, r_{j1}, \ldots, r_{js_j-1}$ be the replication numbers of the s_j treatments $0, 1, \ldots, s_j - 1$ respectively. Then, for $1 \le j \le m$,

$$Z'_{j0}Z_{j0} = \text{Diag}(r_{j0}, r_{j1}, \dots, r_{js_{j}-1}) = R_{j}(\text{say})$$

$$Z'_{j0}\mathbf{1}_{n_{j}} = (r_{j0}, \dots, r_{js_{j}-1})' = \mathbf{r}_{j}(\text{say})$$

$$(2.5.1)$$

Let for any matrix L, pr(L) and $pr^{\perp}(L)$ be as in Chapter 1.

Then, the reduced normal equations for the treatments effects in D_j have the coefficient matrix

$$C_j = Z'_{j0} \left(pr^{\perp}(Z_j) \right) Z_{j0},$$
 (2.5.2)

where

$$Z_j = (Z_{j1}, \dots, Z_{jt}).$$
 (2.5.3)

As shown in Chapter 1, the reduced normal equations for the treatment effects in the Kronecker design D will have the $v \times v$ coefficient matrix

where
$$Z_0 = Z_0' p r^{\perp}(Z) Z_0$$

$$Z_0 = \bigotimes_{j=1}^m Z_{j0} \quad , \quad Z = \left(\bigotimes_{j=1}^m Z_{j1}, \dots, \bigotimes_{j=1}^m Z_{jt}\right)$$

$$(2.5.4)$$

The following theorem extends Theorem 2.3.1 to this set-up for multiway heterogeneity elimination. The efficiency of a contrast is defined, as usual, relative to the corresponding completely randomized design, as in section 2.3.

Theorem 2.5.1 $e(\mathbf{u}^x) \ge \max_{j:x_j=1} e_j(\mathbf{u}_j)$, for each $x \in \Omega$.

Proof: From (2.5.1) and (2.5.4), $C = \bigotimes_{f=1}^{m} R_f - Z_0' pr(Z) Z_0$. Defining the matrices L_j and W_j as in (2.3.4), it follows that

$$C - L_j = W_j - Z_0' pr(Z) Z_0.$$
 (2.5.5)

Define

$$Z^* = \left[Z_{11} \otimes \begin{pmatrix} \bigotimes_{j=2}^m I_{n_j} \end{pmatrix}, \dots, Z_{1t} \otimes \begin{pmatrix} \bigotimes_{j=2}^m I_{n_j} \end{pmatrix} \right] = Z_1 \otimes \begin{pmatrix} \bigotimes_{j=2}^m I_{n_j} \end{pmatrix}.$$

Then, by Lemmas 2.3.1 and 2.3.2, $\mu(Z) \subseteq \mu(Z^*)$ and so $pr(Z^*) - pr(Z)$ is n.n.d. Hence $Z_0'pr(Z^*)Z_0 - Z_0'pr(Z)Z_0$ is n.n.d. But from the definitions of Z_0 and Z^* it follows that

$$Z'_{0}pr(Z^{*})Z_{0} = Z'_{10}pr(Z_{1})Z_{10} \otimes \begin{pmatrix} \bigotimes_{j=2}^{m} Z'_{j0} Z_{j0} \end{pmatrix}$$

$$= \{Z'_{10}Z_{10} - Z'_{10}pr^{\perp}(Z_{1})Z_{10}\} \otimes \begin{pmatrix} \bigotimes_{j=2}^{m} Z'_{j0} Z_{j0} \end{pmatrix}$$

$$= (R_{1} - C_{1}) \otimes \begin{pmatrix} \bigotimes_{j=2}^{m} R_{j} \end{pmatrix} \text{ by (2.5.1) and (2.5.2)}$$

$$= W_{1} \text{ by (2.3.4)}.$$

So, by (2.5.5), $C - L_1$ is n.n.d. Similarly, $C - L_j$ is n.n.d. for every $1 \le j \le m$. Now, the proof of the theorem proceeds along the line of proof of Theorem 2.3.1. Remarks:

1. The proof of Theorem 1.3.1 of Chapter 1 can be simplified using the arguments used in proving Theorem 2.5.1. However, the proof of Theorem 1.3.1 as given in Chapter 1 remains useful since it can be extended to the case of restricted Kronecker products which lead to smaller and economical designs (vide section 1.4). On the other hand, it appears that the above proof of Theorem 2.5.1 cannot be

extended to such situations.

2. As remarked in section 2.3, in the context of multiway heterogeneity elimination also, high efficiencies with respect to contrasts belonging to factorial effects in D can be ensured by suitably choosing the initial non-equireplicate varietal designs D_1, \ldots, D_m . Often, the actual values of $e(\mathbf{u}^x)$ are much higher than the stated lower bound.

The following lemma extends Lemma 2.4.2 to the context of multiway heterogeneity elimination. It is clear that an extension of Theorem 2.4.1 to the present set-up follows from this lemma. Notations are used as in section 2.4, while C is as in (2.5.4).

<u>Lemma 2.5.1</u> For every $x, y \in \Omega, x \neq y, T_xCT'_y = 0$.

Proof: Let $x = (x_1, \ldots, x_m), y = (y_1, \ldots, y_m)$. Since $x \neq y$, without loss of generality let $x_m = 1, y_m = 0$.

Now, since $T_m^{x_m}R_mT_m^{y_m'}=T_mR_m\mathbf{1}_{s_m}=T_m\mathbf{r}_m=\mathbf{0}$, we have

$$T_x C T_y' = T_x (\bigotimes_{i=1}^m R_i) T_y' - T_x Z_0' pr(Z) Z_0 T_y',$$
 (2.5.6)

where

$$T_x(\bigotimes_{j=1}^m R_j)T_y' = \bigotimes_{j=1}^m T_j^{x_j} R_j T_j^{y_j'} = 0.$$
 (2.5.7)

Again, $Z_0T'_y=\begin{pmatrix} m-1\\ \otimes\\ j=1\end{pmatrix}Z_{j0}T_j^{y'_j}\otimes \mathbf{1}_{n_m}$ since $y_m=0$ and $Z_{m0}\mathbf{1}_{s_j}=\mathbf{1}_{n_m}$. Hence from Lemma 1.2.2 of Chapter 1 and remembering that $\mathbf{1}_{n_m}\ \epsilon\ \mu(Z_{ma})$ for $1\leq a\leq t$, it follows that

$$pr(Z)(Z_0T_y') = \{pr(Z^{(m-1)})(\bigotimes_{j=1}^{m-1} Z_{j0}T_j^{y_j'})\} \otimes \mathbf{1}_{n_m}, \qquad (2.5.8)$$

where
$$Z^{(m-1)} = \begin{bmatrix} m-1 \\ \otimes \\ j=1 \end{bmatrix} Z_{j1}, \dots, \begin{bmatrix} m-1 \\ \otimes \\ j=1 \end{bmatrix} Z_{jt}$$
. Again,

context.

$$T_{x}Z'_{0} = T_{x} \begin{pmatrix} m \\ \otimes \\ j=1 \end{pmatrix} Z'_{j0} = \begin{pmatrix} m-1 \\ \otimes \\ j=1 \end{pmatrix} T'_{j}Z'_{j0} \otimes (T_{m}Z'_{m0}). \tag{2.5.9}$$

From (2.5.8), (2.5.9) and noting that $T_m Z'_{m0} 1_{n_m} = T_m \mathbf{r}_m = 0$, it follows that $T_x Z_0' pr(Z) Z_0 T_y' = 0$. This together with (2.5.6) and (2.5.7) proves the lemma. Remark: The same remarks as presented after Theorem 2.4.1 hold good in the present

Some Further Results

In this chapter, we have so far considered the problem of setting lower bounds for efficiencies of individual contrasts in non-equireplicate Kronecker factorial designs. As in Chapter 1, one may also consider complete sets of orthonormal contrasts belonging to different factorial effects and then set lower bounds for Φ_p -efficiencies of such complete sets of contrasts. In this section, we consider this latter problem with reference to designs for multiway heterogeneity elimination. From the results obtained below, corresponding results for block designs will follow as a special case.

We assume as before that each of the varietal designs D_1, \ldots, D_m is connected as this will guarantee the connectedness of D.

The definition of Φ_p -efficiency as given below follows as a natural extension of that considered in Chapter 1. For any $v \times v$ positive definite (p.d.) matrix A with eigenvalues $\lambda_1(A), \ldots, \lambda_v(A)$, let

$$h_p^* (A) = \left(\frac{1}{v} \sum_{i=1}^v (\lambda_i(A))^p\right)^{\frac{1}{p}}, \quad 0
$$= \left(\frac{v}{\pi} \lambda_i(A)\right)^{\frac{1}{v}}, \quad \text{for } p = 0$$

$$= \max_i \lambda_i(A), \quad \text{for } p = \infty$$$$

For $1 \leq j \leq m$, the Φ_p -efficiency of D_j is defined as

$$H_p^j = \frac{h_p^* \left(P_j R_j^{-1} P_j' \right)}{h_p^* \left(P_j C_j^{-} P_i' \right)} \quad , \quad 0 \le p \le \infty$$
 (2.6.1)

where P_j is as defined in Chapter 1, C_j is as in (2.5.2), R_j is as in (2.5.1) and C_j^- is any g-inverse of C_j .

Similarly, for any $x=(x_1,\ldots,x_m)$ $\in \Omega$, the Φ_p -efficiency with respect to the factorial effect J(x) in D is defined as

$$E_p^x = \frac{h_p^* \left[P^x \left(\bigotimes_{j=1}^m R_j^{-1} \right) P^{x'} \right]}{h_p^* \left[P^x C^- P^{x'} \right]}$$
(2.6.2)

where P^x is as in (1.3.2) of Chapter 1, C is as in (2.5.4) and C^- is any g-inverse of C.

Since D_1, \ldots, D_m are connected, the matrices in (2.6.1) and (2.6.2) are p.d. Also note that the dispersion matrix of $P^x\hat{\tau}$ in D is given by $\sigma^2 P^x C^- P^{x'}$, where σ^2 is the constant error variance. Both definitions of H_p^j and E_p^x are based on comparisons with the corresponding completely randomized designs.

The following lemma will be used.

<u>Lemma 2.6.1</u> Let A and B be p.d. matrices such that A - B is n.n.d. Then

$$h_p^*(A) \ge h_p^*(B).$$

<u>Proof:</u> The proof follows from Lemma 1.3.3 of Chapter 1 after noting that for every $v \times v$ p.d. matrix A, $h_p^*(A) = \left\{h_p^{(v)}(A^{-1})\right\}^{-1}$ where $h_p^{(v)}(\cdot)$ is as defined in section 1.3 of Chapter 1.

The following theorem provides lower bounds for the Φ_p -efficiencies in D in terms of the Φ_p -efficiencies of D_j .

Theorem 2.6.1 For every $x = (x_1, \ldots, x_m) \in \Omega$ and every $p \ (0 \le p \le \infty)$,

$$E_p^x \ge \max_{1 \le j \le m} \left\{ x_j H_p^j \right\}.$$

<u>Proof:</u> Consider any $x = (x_1, ..., x_m) \in \Omega$. Without loss of generality, let $x_1 = 1$. Then, it can be proved along the line of proof of Theorem 2.5.1 that $C - L_1$ is n.n.d.

Since D_1, \ldots, D_m are connected, $\mu(P^{x'}) \subseteq \mu(L_1)$ and hence by Lemma 2.3.2, $P^x L_1^- P^{x'} - P^x C^- P^{x'}$ is n.n.d. Hence by Lemma 2.6.1

$$h_p^*(P^xC^-P^{x'}) \le h_p^*(P^xL_1^-P^{x'}).$$

Hence, by (2.3.4) and (2.6.2), and noting that $x_1 = 1$,

$$\begin{split} E_p^x &\geq \frac{h_p^* \left[P^x \left(\underset{j=1}{\overset{m}{\otimes}} R_j^{-1} \right) P^{x'} \right]}{h_p^* \left[P^x L_1^- P^{x'} \right]} \\ &= \frac{h_p^* \left(P_1 R_1^{-1} P_1' \right) \underset{j=2}{\overset{m}{\pi}} h_p^* \left(P_j^{x_j} R_j^{-1} P_j^{x_j'} \right)}{h_p^* \left(P_1 C_1^- P_1' \right) \underset{j=2}{\overset{m}{\pi}} h_p^* \left(P_j^{x_j} R_j^{-1} P_j^{x_j'} \right)} \\ &= H_p^1 \text{ by (2.6.1).} \end{split}$$

Similarly, $E_p^x \ge H_p^j$ for every j such that $x_j = 1$. This completes the proof.

Remark: The theorem demonstrates that even in the context of non-equireplicate

Kronecker designs for multiway elimination of heterogeneity, one can achieve high Φ_p -efficiencies for the design D by starting with suitably efficient varietal designs. Again, the actual Φ_p -efficiency attained is often much greater than the lower bound.

2.7 Discussion

Remark. The necessary and sufficient condition for block designs to have OFS is due to Mukerjee (1979) and the result has been stated as Lemma 1.2.1 in Chapter 1. It may be easily verified that the condition is not satisfied for non-equireplicate Kronecker factorials. In fact, if we consider a factorial experiment laid out in an (unblocked) completely randomized design, then it can be easily verified that this design will have OFS if and only if it is equireplicate. Thus it appears that even if a non-equireplicate factorial block design has OFS, then such orthogonality is not a very natural property of the design but somewhat artifically enforced through the introduction of suitable blocks. A similar remark also holds good in a setting for multiway heterogeneity elimination. So it seems debatable whether OFS is at all a natural phenomenon in a non-equireplicate setting. And, anyway, as sections 2.3-2.6 show, the lack of OFS in this case does not pose any major problem in either attaining high interaction efficiencies or in ensuring a simple analysis.

Although the method of Kronecker product is capable of producing small and hence economically viable designs with a moderate number of factors, the size of the design may become too large with a large number of factors. In the equireplicate case Gupta (1983), Mukerjee (1981, 1986) considered some variants of the ordinary Kronecker product to construct smaller designs ensuring high efficiencies only for

the lower order interactions. In the case of multiway elimination of heterogeneity in the equireplicate case Mukerjee and Sen (1987) considered a similar variant of the Kronecker product which has been presented in Chapter 1. Unfortunately, in the non-equireplicate setting, it may be seen that analogues of Theorem 2.3.1 do not hold with such modifications. It seems that this problem deserves further attention.

Chapter 3

ESTIMABILITY-CONSISTENCY AND ITS EQUIVALENCE WITH REGULARITY IN FACTORIAL EXPERIMENTS

3.1 Introduction

In the context of factorial designs, disconnected designs are of importance. This is because a factorial design becomes disconnected when certain contrasts are completely confounded. Mukerjee (1979) introduced the concept of regular disconnected designs and obtained conditions for orthogonal factorial structure of disconnected regular designs. More results on regularity of factorial designs are available in Mukerjee (1980), Chauhan and Dean (1986), Mukerjee and Dean (1986) and Chauhan (1987).

Lewis and Dean (1985) introduced the notion of efficiency-consistency in factorial designs. They established that every equireplicate connected design with orthogonal factorial structure (OFS) is efficiency-consistent. This result was extended to the case of disconnected designs by Mukerjee and Dean (1986) and they proved its converse and some further results. Thus OFS was shown to be necessary and sufficient for efficiency-consistency and so efficiency consistency provided a characterisation for OFS. Some further results on efficiency-consistency were obtained by Gupta (1986b).

In this chapter we introduce the concept of estimability-consistency which is somewhat analogous to that of efficiency-consistency. It is shown that estimability-consistency provides a characterization for regularity. This result seems to be of interest from the practical viewpoint as it provides an appealing interpretation for the somewhat abstract phenomenon of regularity.

Section 3.2 of this chapter discusses the concept of regularity and its implications. In Section 3.3 estimability-consistency is defined and related results are proved. Section 3.4 establishes the characterization for regularity in terms of estimabilityconsistency. Section 3.5 deals with the equivalence of partial estimability-consistency with regularity of a certain order.

3.2 The Notion of Regularity and Some Preliminaries

Throughout the chapter, the fixed effects intrablock model with independent homoscedastic errors and no block-treatment interaction is assumed.

Consider a $s_1 \times s_2 \times \ldots \times s_m$ factorial block design, d, which may be possibly disconnected. The design d is assumed to be neither equireplicate nor proper. Let Ω be as in the previous chapters and $v = \frac{m}{\pi} s_i$. Let a typical factorial effect be denoted, as usual, by J(x) for $x \in \Omega$.

Let C be the usual intrablock matrix of d. Let V^x denote the estimable space corresponding to J(x). For any matrix A let R(A) denote its row space. Then, clearly, $R(C) \supseteq \bigoplus_{x \in \Omega} V^x \text{ where } \oplus \text{ denotes direct sum.}$

We state the following definition of regularity.

<u>Definition 3.2.1.</u> (Mukerjee (1979)). An m-factor design d, is regular if

$$R(C) \equiv \bigoplus_{x \in \Omega} V^x$$
.

While a connected design is always regular, the same cannot be said about disconnected designs. As seen in Mukerjee (1979), in regular designs, when OFS holds, the adjusted treatment sum of squares can be partitioned orthogonally into components corresponding to different factorial effects. But such a partitioning is not possible

in irregular disconnected designs. In fact, in the latter case, the estimable contrasts belonging to factorial interactions do not span the space of all possible estimable contrasts and hence the adjusted treatment sum of squares will contain a component due to some estimable contrasts which can be attributed to none of the factorial effects. This makes such designs wasteful in the sense that they achieve estimability of these unimportant contrasts at the cost of the important ones. For further discussion on the practical relevance of regularity, we refer to Mukerjee (1979).

The following example serves as an illustration.

Example 3.2.1. Consider the following single replicate 2³ experiments in 2 blocks.

$$D_1: \{(0,0,0),(0,0,1),(0,1,0),(1,0,0)\} \{(1,1,0),(0,1,1),(1,0,1),(1,1,1)\}$$

$$D_2: \{(0,0,0),(0,0,1),(1,0,0),(1,0,1)\} \{(0,1,0),(0,1,1),(1,1,0),(1,1,1)\}$$

Here $s_1 = 2, s_2 = 2, s_3 = 2$. Both D_1 and D_2 are disconnected with rank (C) = 6 for both designs.

It can be shown that for $D_1, V^{001} = V^{010} = V^{100} = V^{111} = \{0\}$ while contrasts belonging to J(110), J(101) and J(011) are estimable. Thus for D_1

$$\operatorname{rank} \big\{ \underset{x \in \Omega}{\oplus} V^x \big\} = 3 < \operatorname{rank} (C).$$

Hence D_1 is an irregular design and some useless contrasts are estimable.

On the other hand, with D_2 , contrasts belonging to the 6 interactions J(001), J(100), J(011), J(101), J(110) and J(111) are estimable and hence D_2 is a regular disconnected design.

3.3 Estimability-Consistency

Let τ denote the $v \times 1$ vector of factorial treatment effects in d arranged lex-

icographically. Consider any $x = (x_1, \ldots, x_m) \in \Omega$. Let d_x be the design obtained from d by deleting the i^{th} digit from the treatment labels for all i for which $x_i = 0, i = 1, \ldots, m$. Thus d_x will involve $\prod_{i=1}^m s_i^{x_i} (= v_x, \text{say})$ treatment combinations and let τ_x denote the vector of the v_x factorial treatment effects, arranged lexicographically.

Lewis and Dean (1985) defined d to be efficiency-consistent if the efficiencies of all estimable contrasts belonging to J(x) in d are equal to the efficiencies of the corresponding contrasts in d_x , for each $x \in \Omega$. Analogous to this definition we introduce the concept of estimability-consistency. We first give the following notations:

For $j=1,\ldots,m$ let $\mathbf{1}_j$ denote the $s_j\times 1$ vector with all elements unity, $E_j=\mathbf{1}_j\mathbf{1}_j'$ and I_j denotes the $s_j\times s_j$ identity matrix. For $x\in\Omega$, define the matrices

$$W^x = \bigotimes_{j=1}^m W_j^{x_j} \tag{3.3.1a}$$

where \otimes denotes Kronecker product and for $j = 1, \ldots, m$,

$$W_i^{x_j} = I_j - s_i^{-1} E_j \text{ if } x_j = 1, = s_i^{-1} E_j \text{ if } x_j = 0$$
 (3.3.1b)

and

$$S^x = \bigotimes_{j=1}^m S_j^{x_j} \tag{3.3.2a}$$

where for $j = 1, \ldots, m$,

$$S_j^{x_j} = I_j \text{ if } x_j = 1, = 1'_j \text{ if } x_j = 0$$
 (3.3.2b)

For every $x \in \Omega$, from the way d_x is obtained from d, it is clear that the intrablock matrix of d_x becomes $S^x C S^{x'} = C_x$ (say).

Note that for every $x \in \Omega$, the rows of W^x span the space of all contrasts, not necessarily estimable, belonging to J(x) in d and the rows of $W^xS^{x'}$ span the space

of all contrasts belonging to J(x) in d_x . Also, for each $x \in \Omega$, it is possible to define a correspondence between the contrasts belonging to J(x) in d and d_x such that for any $q \neq 0$, the contrast $q'W^x\tau$ belonging to J(x) in d corresponds to the contrast $q'W^xS^{x'}\tau_x$ belonging to J(x) in d_x and conversely.

Lemma 3.3.1. Let $q'W^x\tau$ be a contrast belonging to J(x) in d. Then the estimability of $q'W^x\tau$ in d implies the estimability of the corresponding contrast $q'W^xS^{x'}\tau_x$ in d_x .

<u>Proof:</u> Since $q'W^x\tau$ is estimable in d, there exists a $v\times 1$ vector u such that

$$\mathbf{q}'W^x = \mathbf{u}'C \tag{3.3.3}$$

Postmultiplying both sides of (3.3.3) by $S^{x'}$ it follows that $q'W^xS^{x'}$ belongs to $R(CS^{x'})$. Since C is n.n.d. \exists a matrix B such that C = BB'. Hence

 $R(CS^{x'}) \equiv R(BB'S^{x'}) \subseteq R(B'S^{x'}) \equiv R(S^xBB'S^{x'}) \equiv R(S^xC\ S^{x'}) \equiv R(C_x).$

Hence $q'W^xS^{x'}$ belongs to $R(C_x)$ and $q'W^xS^{x'}\tau_x$ is estimable in d_x . Q.E.D.

Remark: In general, the converse of Lemma 3.3.1 is not true as may be seen through examples. Thus considering the design D_1 in Example 3.2.1, the contrast representing the main effect of the first factor is not estimable in D_1 although the corresponding contrast is easily seen to be estimable in the subdesign d_{100} obtained from D_1 . In fact, Theorem 3.4.1 in section 3.4 shows that all irregular designs provide such examples. A factorial design for which the converse of Lemma 3.3.1 also holds will be called estimability-consistent. We thus have the following definition:

Definition 3.3.1. An m-factor design, d, is called estimability-consistent provided for each $x \in \Omega$, every contrast belonging to J(x) in d is estimable in d if and only if the corresponding contrast belonging to J(x) in d_x is estimable in d_x .

3.4 Equivalence of Regularity and Estimability-Consistency

In the following Theorem 3.4.1 we shall show that the two notions of regularity and estimability-consistency are equivalent. Since the latter concept seems much more simpler than the former, this result is useful in providing a simple and straightforward interpretation for the rather involved concept of regularity in terms of estimability-consistency.

The following lemmas will be used in proving the main theorem.

Lemma 3.4.1. The m-factor design, d, is regular if and only if

$$R(CW^x) \subseteq R(C) \ \forall \ x \in \Omega,$$
 (3.4.1)

where C is as usual the intrablock matrix of d.

<u>Proof:</u> Only If Suppose d is regular. Since W^x spans the space of all contrasts belonging to J(x) in d, for all $x \in \Omega, V^x \subseteq R(W^x)$. So for each $x \in \Omega$ there exists a matrix L_x such that

$$V^x \equiv R(L_x W^x). \tag{3.4.2}$$

But $V^x \subseteq R(C)$ by definition and so by (3.4.2)

$$R(L_x W^x) \subseteq R(C) \ \forall \ x \in \Omega.$$
 (3.4.3)

Now, since d is regular, by Definition 3.2.1 and (3.4.2), there exists matrices H_x ($x \in \Omega$) such that $C = \sum_{x \in \Omega} H_x L_x W^x$. Hence observing that $W^x W^y = W^x$ if x = y, = 0 if $x \neq y$, it follows that

$$CW^x = H_x L_x W^x.$$

Consequently $R(CW^x) \subseteq R(L_xW^x)$, and by (3.4.3) the 'only if' part of the lemma

follows.

If: Suppose (3.4.1) holds. Then clearly

$$R(CW^x) \subseteq R(W^x) \cap R(C) \equiv V^x, \tag{3.4.4}$$

by the definition of V^x . Let I be the $v \times v$ identity matrix and E be the $v \times v$ matrix with all elements unity. Then, from (3.3.1a) and (3.3.1b), $\sum_{x \in \Omega} W^x = I - v^{-1}E$ and noting that CE = 0, we have $C = \sum_{x \in \Omega} CW^x$. This together with (3.4.4) implies that $R(C) \subseteq \bigoplus_{x \in \Omega} V^x$ where \bigoplus denotes the direct sum. Hence, remembering that for every design $R(C) \supseteq \bigoplus_{x \in \Omega} V^x$, we have $R(C) \equiv \bigoplus_{x \in \Omega} V^x$. Thus the 'if' part of the lemma follows.

Lemma 3.4.2. The m-factor design, d, is regular if and only if

$$R(CZ^x) \subseteq R(C) \ \forall \ x \in \Omega$$
, where $Z^x = S^{x'}S^x$.

Proof: Note that from (3.3.2a) and (3.3.2b) it follows that

$$Z^x = \bigotimes_{j=1}^m Z_j^{x_j}$$
, where $Z_j^{x_j} = I_j$ if $x_j = 1, = E_j$ if $x_j = 0$.

The proof follows from Lemma 3.4.1 after noting that for each x, Z^x is a linear combination of E and W^y for $y \in \Omega$ and for each x, W^x is a linear combination of E and Z^y for $y \in \Omega$.

Theorem 3.4.1. The m-factor design, d, is estimability-consistent if and only if it is regular.

Proof: If Let the design d be regular. Then by Lemma 3.4.2,

$$R(CZ^x) \subseteq R(C), \ \forall \ x \in \Omega$$
 (3.4.5)

To show that d is estimability-consistent, for any $x \in \Omega$ consider the subdesign d_x . In view of Lemma 3.3.1 it will be enough to show that the estimability of the contrast $\mathbf{q}'W^xS^{x'}\boldsymbol{\tau}_x$ ($\mathbf{q}\neq\mathbf{0}$) belonging to J(x) in d_x implies the estimability of the corresponding contrast $\mathbf{q}'W^x\boldsymbol{\tau}$ in d.

Consider any contrast $q'W^xS^{x'}\tau_x$ $(q \neq 0)$ which is estimable in d_x . Then, for some vector \mathbf{u} , since the intrablock matrix of d_x is given by $S^xCS^{x'}$,

$$\mathbf{q}'W^x S^{x'} = \mathbf{u}' S^x C S^{x'}. \tag{3.4.6}$$

Now, from (3.3.1a), (3.3.1b) and (3.3.2a), (3.3.2b) it follows that $W^x S^{x'} S^x = \frac{v}{v_x} W^x$. Hence, postmultiplying both sides of (3.4.6) by S^x , one obtains

$$\mathbf{q}'W^{x} = \frac{v_{x}}{v}\mathbf{u}'S^{x}CS^{x'}S^{x} = \frac{v_{x}}{v}\mathbf{u}'S^{x}CZ^{x}.$$

Hence $q'W^x \in R(CZ^x) \subseteq R(C)$ by (3.4.5) and so $q'W^x\tau$ is estimable in d. This proves the 'if' part.

Only If This part will be proved by induction along the line of Mukerjee and Dean (1986). Let d be estimability-consistent. For u = 1, ..., m, define

$$\Omega_u = \{x : x \in \Omega, x \text{ contains exactly } u \text{ unit digits}\}.$$

Consider any $x \in \Omega_1$. Then from the definition of the matrices Z^x and W^x it is easy to see that for some non-zero constants ℓ_x and m_x , $Z^x = \ell_x W^x + m_x E$.

Since CE = 0, one gets

$$CZ^x = \ell_x CW^x \tag{3.4.7}$$

Again, since $Z^x S^{x'} = \frac{v}{v_x} S^{x'}$, by postmultiplying both sides of (3.4.7) by $S^{x'}$ one has $\frac{v}{v_x} C S^{x'} = \ell_x C W^x S^{x'}.$

Since $\ell_x \neq 0$ this implies that

$$R(CW^xS^{x'}) \equiv R(CS^{x'}) \equiv R(S^xCS^{x'})$$
 since C is non-negative definite $\equiv R(C_x)$, remembering that $C_x = S^xCS^{x'}$

This implies that $R(CW^x) \subseteq R(C)$ since the design d is estimability-consistent. So, by (3.4.7) $R(CZ^x) \subseteq R(C) \ \forall \ x \in \Omega_1$.

To apply the method of induction, suppose that $R(CZ^x) \subseteq R(C)$, $\forall x \in \Omega_1 \cup \Omega_2 \cup \ldots \cup \Omega_g$ $(1 \leq g < m)$ and consider $x \in \Omega_{g+1}$. Defining $\Omega(x) = \{y : y \in \Omega, y \neq x, y_i \leq x_i, i = 1, \ldots, m\}$, from the definition of Z^x and W^x it follows that

$$Z^{x} = f_{x}W^{x} + \sum_{y \in \Omega(x)} f_{y}Z^{y} + k_{x}E,$$

where $f_x(\neq 0), f_y$ ($y \in \Omega(x)$) and k_x are constants. Then, as before, remembering that CE = 0, one gets

$$CZ^{x} = f_{x}CW^{x} + \sum_{y \in \Omega(x)} f_{y}CZ^{y}.$$
 (3.4.8)

Now, by definition, $\Omega(x) \subseteq \Omega_1 \cup \Omega_2 \cup \ldots \cup \Omega_g$ and hence by induction hypothesis,

$$R(CZ^y) \subseteq R(C) \ \forall \ y \in \Omega(x).$$

Hence there exist matrices G_y such that

$$f_y C Z^y = G_y C \quad \forall \quad y \in \Omega(x). \tag{3.4.9}$$

Postmultiplying both sides of (3.4.8) by $S^{x'}$ and using (3.4.9) and remembering that $Z^x S^{x'} = \frac{v}{v_x} S^{x'}$, we have

$$f_x C W^x S^{x'} = \frac{v}{v_x} C S^{x'} - \sum_{y \in \Omega(x)} G_y C S^{x'}.$$

Since $f_x \neq 0$ this implies that

$$R(CW^xS^{x'}) \subseteq R(CS^{x'})$$

$$\equiv R(S^xCS^{x'}) \text{ since } C \text{ is non-negative definite}$$

$$\equiv R(C_x).$$

This implies that $R(CW^x) \subseteq R(C)$ since d is estimability-consistent, which, together with (3.4.8), (3.4.9) implies that $R(CZ^x) \subseteq R(C) \ \forall \ x \in \Omega_{g+1}$.

Thus by induction, $R(CZ^x) \subseteq R(C) \ \forall \ x \in \Omega$, and by Lemma 3.4.2 the design d is regular. Q.E.D.

3.5 Partial Estimability-Consistency

Mukerjee and Dean (1986) proved certain equivalence theorems connecting partial efficiency-consistency and partial orthogonal factorial structure. The analogues of some of their results can be proved in the present context.

Definition 3.5.1. An m-factor design d is partially estimability-consistent of order t provided for every $x \in \Omega_1 \cup \Omega_2 \cup \ldots \cup \Omega_t$, every contrast belonging to J(x) in d is estimable in d if and only if the corresponding contrast belonging to J(x) in d_x is estimable in d_x .

Theorem 3.5.1. An m-factor design, d, is partially estimability-consistent of order $t \leq m$ if and only if it is regular of order t.

The proof of the theorem follows the line of proof of Theorem 3.4.1 and is hence omitted. In the above, the definition of regularity of order t is as in Mukerjee (1980) where some discussion on the implications of such regularity is also available.

Remark: It is hard to carry out the equivalence relations as in Theorems 3.4.1, 3.5.1 any further. For example, one may define partial estimability-consistency and partial regularity with respect to individual interactions (along the line of Chauhan and Dean (1986) who considered orthogonal factorial structure with respect to individual interactions), but it is believed that they will no more be equivalent.

Chapter 4

FACTORIAL DESIGNS FOR QUALITY-QUANTITY INTERACTION 4.1 <u>Introduction</u>

Sometimes in a factorial experiment, the levels of one factor represent different qualities of material while the levels of another factor represent different quantities of these qualities. Such experiments were first considered by Fisher (1935) in the context of factorial experiments where zero, single and double doses of certain fertilizers were applied and the yield was studied. Another interesting example was given by John and Quenouille (1977) where they experimented with three forms of milk applied at three different protein levels, the lowest level being zero. The important feature of these experiments, which make them different from ordinary factorials is that some of the level combinations, namely those where the quantitative factor is at the zero level, are indistinguishable. This necessitates a substantial modification of the standard calculus for factorial arrangements (cf. Kurkjian and Zelen (1963)). Incidentally, it may be remarked that recently, Cox (1984) posed a number of open problems in experimental design and one of these problems related to the development of a systematic theory for the study of such quality-quantity interaction.

This chapter aims at developing a mathematical formulation for this problem. Necessary and sufficient conditions for inter- and intra-effect orthogonality and also for some other kinds of orthogonality relevant in this situation are considered. Some construction procedures have been discussed subsequently in Section 4.5. To avoid notational complexity, only the two-factor case has been considered in detail. In

the last section of the chapter, the extension to the multifactor case has also been indicated.

4.2 Notation and Preliminaries

Throughout the chapter, the model assumed is the usual fixed effects model, with independent homoscedastic errors and no block-treatment interaction.

Consider a two-factor set-up in factors F_1 and F_2 . Here F_1 is the quantitative factor and involves $s_1 + 1$ levels $0, 1, 2, \ldots s_1$ while F_2 is the qualitative factor having s_2 levels $1, 2, \ldots, s_2$. It may be emphasized that the levels of F_1 need not be necessarily equispaced.

When F_1 is applied at the 0 level, all the levels of F_2 become equivalent since the level combinations $01, \ldots, 0s_2$ become, in effect, indistinguishable. So these s_2 level combinations may be considered to represent a single level combination, say 0. Thus instead of $(s_1 + 1)s_2$ level combinations as in usual factorial experiments, there are only $s_1s_2 + 1 (= v \text{ say})$ distinct level combinations, namely 0 and ij $(1 \le i \le s_1, 1 \le j \le s_2)$. Clearly, the typical level combination ij denotes that the level j of the qualitative factor is applied at the quantitative level i $(1 \le i \le s_1, 1 \le j \le s_2)$.

Let the $v \times 1$ vector $\tau = (\tau_0, \tau_{11}, \dots, \tau_{1s_2}, \dots, \tau_{s_11}, \dots, \tau_{s_1s_2})'$ represent the fixed effects due to these v level combinations. Let $\overline{\tau}_i = s_2^{-1} \sum_{j=1}^{s_2} \tau_{ij}$ for $1 \leq i \leq s_1$, and $\overline{\tau}_0 = \tau_0$. Then, a typical contrast belonging to main effect F_1 is of the form $\ell = \sum_{i=0}^{s_1} \ell_i \ \overline{\tau}_i$ where $\sum_{i=0}^{s_1} \ell_i = 0$ and the ℓ_i 's are not all zeros.

For i=1,2, let $\mathbf{1}_i$ be the $s_i \times 1$ vector with all elements unity and let P_i be an $(s_i-1)\times s_i$ matrix such that $(s_i^{-\frac{1}{2}}\mathbf{1}_i,P_i')'$ is orthogonal. Note that for a $s_1\times s_2$ usual

factorial experiment, a complete set of orthonormal contrasts belonging to the main effect of the first factor has a coefficient matrix $(P_1 \otimes s_2^{-\frac{1}{2}} \mathbf{1}_2')$. So, it follows that, in the present set-up, a complete set of orthonormal contrasts belonging to main effect F_1 is given by $P^{10}\tau$ where the $s_1 \times v$ matrix P^{10} is defined as

$$P^{10} = \begin{bmatrix} -[(v-1)/v]^{\frac{1}{2}} & [v(v-1)]^{-\frac{1}{2}} \mathbf{1}_{1}' \otimes \mathbf{1}_{2}' \\ \mathbf{0} & s_{2}^{-\frac{1}{2}} P_{1} \otimes \mathbf{1}_{2}' \end{bmatrix}.$$
(4.2.1*a*)

Similarly full sets of orthonormal contrasts belonging to main effect F_2 and interaction F_1F_2 are given by $P^{01}\tau$ and $P^{11}\tau$ respectively, where

$$P^{01} = \begin{bmatrix} \mathbf{0} & s_1^{-\frac{1}{2}} \mathbf{1}_1' \otimes P_2 \end{bmatrix} , P^{11} = \begin{bmatrix} \mathbf{0} & P_1 \otimes P_2 \end{bmatrix}. \tag{4.2.1b}$$

These matrices P^{10} , P^{01} , and P^{11} are obtained by suitable modifications of the corresponding matrices in an ordinary factorial setting and they take care of the special structure of the level combinations as mentioned above. Also, $P^{10}P^{01'}=0$, $P^{10}P^{11'}=0$, so that, as in the case of ordinary factorials, in this case also, the contrasts belonging to different factorial effects are mutually orthogonal.

We state the following definitions.

<u>Definition 4.2.1.</u> A square matrix will be called proper if all its row and column sums are equal.

Definition 4.2.2. (Mukerjee (1979)). A square matrix of order $s_1 s_2$ will be said to have structure K if it can be expressed as a linear combination of Kronecker products of proper matrices of orders s_1, s_2 respectively.

4.3 Conditions for Orthogonal Factorial Structure

Let the v level combinations be arranged in a connected block design d, the $v \times v$ intrablock matrix of d being denoted by

$$C = \begin{bmatrix} \alpha & \beta' \\ \beta & H \end{bmatrix},$$
 (4.3.1)

where H is a square matrix of order $v-1 (=s_1s_2)$, the initial row and column of C correspond to the treatment 0 and the other rows and columns correspond to the other v-1 level combinations in the lexicographic order. Let $\Omega = \{01, 10, 11\}$. In order to derive conditions for OFS of d, we shall use a result due to Mukerjee (1979) for traditional factorials. The result is stated as Lemma 4.3.1 for the two-factor case. Lemma 4.3.1 (Mukerjee (1979)). A $s_1 \times s_2$ factorial experiment arranged in a connected block design will have OFS if and only if the C-matrix of the design commutes with $W^x = P^{x'}P^x$ for all $x \in \Omega$.

The following theorem obtains a necessary and sufficient condition for OFS of d.

Theorem 4.3.1. For d to have OFS, it is necessary and sufficient that with reference to (4.3.1),

- (i) $\beta = \mathbf{u} \otimes \mathbf{1}_2$ for some s_1 -component vector \mathbf{u} and
- (ii) the matrix $H^* = H \alpha^{-1}\beta\beta'$ has structure K.

<u>Proof:</u> Since d is connected, clearly $\alpha>0$ and so H^* is well-defined. From the definition of W^x and (4.2.1a, b) it follows that $\sum_{x \in \Omega} W^x = I - v^{-1}E$ where I is the $v \times v$ identity matrix and E is the $v \times v$ matrix with all elements unity. Hence, by Lemma 4.3.1 and remembering that CE=EC=0, it follows that d has OFS if and

only if

$$W^{01}C = CW^{01}$$
 , $W^{11}C = CW^{11}$. (4.3.2)

To prove the necessity of the conditions of the theorem, let d have OFS. Then (4.3.2) holds. Define

$$L^{01} = s_1^{-\frac{1}{2}} \mathbf{1}_1' \otimes P_2$$
, $L^{10} = P_1 \otimes s_2^{-\frac{1}{2}} \mathbf{1}_2'$, $L^{11} = P_1 \otimes P_2$, $A^x = L^{x'} L^x$ for $x \in \Omega$.

Then from (4.2.1b) it follows that

$$W^{01} = \begin{bmatrix} 0 & 0' \\ 0 & A^{01} \end{bmatrix} , W^{11} = \begin{bmatrix} 0 & 0' \\ 0 & A^{11} \end{bmatrix}.$$

So, with C as in (4.3.1), conditions (4.3.2) imply that

$$A^{01} \beta = 0$$
, $A^{11} \beta = 0$, (4.3.3a)

$$A^{01} H = H A^{01}, \quad A^{11} H = H A^{11}.$$
 (4.3.3b)

From (4.3.3a) it follows that

$$L^{01'}L^{01}\beta = 0$$
, $L^{11'}L^{11}\beta = 0 \implies L^{01}\beta = 0$, $L^{11}\beta = 0$

since $L^{01}L^{01'}$ and $L^{11}L^{11'}$ are identity matrices of appropriate orders. Consequently $\boldsymbol{\beta}$ ϵ ortho complement of row space $\begin{pmatrix} L^{01} \\ L^{11} \end{pmatrix}$

$$\Longrightarrow eta \ \epsilon \ \mathrm{row \ space} \ igg(rac{L^{10}}{L^{00}} igg) \ \mathrm{where} \ L^{00} = \left[s_1^{-\frac{1}{2}} \mathbf{1}_1' \otimes s_2^{-1} \mathbf{1}_2' \right],$$

and hence the necessity of condition (i) follows.

Again, from (4.3.3a, b),

$$A^{01}H^* = H^*A^{01}$$
 , $A^{11}H^* = H^*A^{11}$. (4.3.4)

Since CE = EC = 0, from (4.3.1) it follows that H^* is a proper matrix with all row

and column sums equal to zero. Also, since

$$\sum_{x \in \Omega} A^x = I_1 \otimes I_2 - (s_1 s_2)^{-1} (E_1 \otimes E_2),$$

where $E_i = \mathbf{1}_i \mathbf{1}_i'$ for i = 1, 2; (4.3.4.) implies that $A^{10}H^* = H^*A^{10}$. Thus, H^* commutes with A^x for all $x \in \Omega$. Noting that A^x is idempotent for $x \in \Omega$, one can write $H^* = \sum_{x \in \Omega} A^x H^* A^x$. Then, remembering that H^* is a proper matrix, the necessity of condition (ii) follows readily along the line of proof of Lemma 3.1 of Mukerjee (1979).

The sufficiency of (i) and (ii) follows by retracing the above steps. Q.E.D.

In the context of ordinary factorial designs, the literature on general methods of construction ensuring OFS is very rich. The balanced confounded designs as considered by Nair and Rao (1948) may be seen to possess OFS. For the methods of construction using generalized cyclic designs and Kronecker products, various references are given in Chapter 1 of this thesis.

Therefore, since ordinary factorial designs with *OFS* are readily available, in this chapter we now explore the conditions under which factorial designs with *OFS* in the present setting may be derived from them.

The following lemma will be helpful.

<u>Lemma 4.3.2.</u> Let

$$B = \begin{bmatrix} B_{11} & B_{12} & \dots & B_{1v_1} \\ B_{21} & B_{22} & \dots & B_{2v_1} \\ \vdots & & \vdots & & \\ B_{v_11} & B_{v_12} & \dots & B_{v_1v_1} \end{bmatrix},$$

where each B_{ij} is $v_2 \times v_2$, be a square matrix of order $v = v_1 v_2$. Then B has structure

K if and only if

(a) each B_{ij} is a proper matrix and

(b)
$$\sum_{h=1}^{v_1} B_{ih} = \sum_{h=1}^{v_1} B_{hj}$$
 for each $i, j \ (1 \le i, j \le v_1)$.

The proof of this lemma may be derived from Lemma 4.3.1.

Let d_o be an ordinary $(s_1+1)\times s_2$ factorial experiment arranged in a block design involving level combinations denoted by ij ($0 \le i \le s_1, 1 \le j \le s_2$). Suppose a design d is derived from d_o by replacing the s_2 level combinations $01, \ldots, 0s_2$ in d_o by a single treatment 0. We will now investigate the conditions under which d, when viewed as a design for studying quality-quantity interaction, will have OFS.

Let d_o be connected and let the C-matrix of d_o be given by

$$C_{0} = \begin{bmatrix} C_{00} & C_{01} & \dots & C_{0s_{1}} \\ C_{10} & C_{11} & \dots & C_{1s_{1}} \\ \vdots & & & \vdots \\ C_{s_{1}0} & C_{s_{1}1} & \dots & C_{s_{1}s_{1}} \end{bmatrix} = \begin{bmatrix} C_{00} & C^{(01)} \\ C^{(10)} & C^{(11)} \end{bmatrix}, \qquad (4.3.5)$$

say, where each C_{ij} is $s_2 \times s_2$ and the rows and columns of C_0 correspond to the $(s_1+1)s_2$ level combinations in d_o in the lexicographic order. Suppose that d_o has OFS as an ordinary factorial design. Then, by Mukerjee (1979), C_0 will have structure K and so by Lemma 4.3.2,

$$C_{ij}\mathbf{1}_2 = C'_{ij}\mathbf{1}_2 = \rho_{ij}\mathbf{1}_2, \quad 0 \le i, j \le s_1$$
 (4.3.6a)

$$C_{ij}\mathbf{1}_{2} = C'_{ij}\mathbf{1}_{2} = \rho_{ij}\mathbf{1}_{2}, \quad 0 \le i, j \le s_{1}$$

$$\sum_{h=0}^{s_{1}} C_{ih} = \sum_{h=0}^{s_{1}} C_{hj}, \quad 0 \le i, j \le s_{1}$$

$$(4.3.6b)$$

for some constants $\{\rho_{ij}\}$. Again, since the row sums and column sums of C_0 are all

zero, from (4.3.6a) it follows that

$$\sum_{h=0}^{s_1} \rho_{ih} = \sum_{h=0}^{s_1} \rho_{hj} = 0 \quad , \quad 0 \le i, j \le s_1.$$
 (4.3.6c)

The following theorem gives the required conditions.

Theorem 4.3.2. Let d_o be connected and have OFS. Then the derived design d will have OFS if and only if, with reference to (4.3.5) and (4.3.6a), for every $i, j (1 \le i, j \le s_1)$ the following holds:

$$C_{i0} - \rho_{i0} s_2^{-1} E_2 = C_{0j} - \rho_{0j} s_2^{-1} E_2$$
(4.3.7)

<u>Proof:</u> The connectedness of d_o implies that of d. In view of the kind of merger of treatments used to derive d from d_o it follows that the C-matrix of d is of the form

$$\begin{bmatrix} \mathbf{1}_{2}' & \mathbf{0}' \\ \mathbf{0} & I_{1} \times I_{2} \end{bmatrix} C_{0} \begin{bmatrix} \mathbf{1}_{2} & \mathbf{0}' \\ \mathbf{0} & I_{1} \times I_{2} \end{bmatrix}$$

$$= \begin{bmatrix} \mathbf{1}_{2}' C_{00} \mathbf{1}_{2} & \mathbf{u}' \otimes \mathbf{1}_{2}' \\ \mathbf{u} \otimes \mathbf{1}_{2} & C^{(11)} \end{bmatrix}$$

$$(4.3.8)$$

by (4.3.5) and (4.3.6a), where $\mathbf{u}' = (\rho_{01}, \dots, \rho_{0n})$.

Comparing this with (4.3.1) it can be seen that the condition (i) in Theorem 4.3.1 is clearly satisfied. So, by the same theorem, d will have OFS if and only if the matrix H^* has structure K.

Now,
$$H^* = \begin{bmatrix} H_{11}^* & H_{12}^* & \dots & H_{1s_1}^* \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & \\ & & & \\$$

where

$$H_{ij}^* = C_{ij} - (1_2'C_{00}1_2)^{-1}(C_{i0}1_2)(1_2'C_{0j})$$

$$= C_{ij} - (\rho_{00}s_2)^{-1}\rho_{i0}\rho_{0j}E_2, \quad 1 \le i, j \le s_1,$$
(4.3.9)

on simplification using (4.3.6a).

Again, by (4.3.6a) and (4.3.9), H_{ij}^* is a proper matrix for every $i, j (1 \le i, j \le s_1)$. So, by Lemma (4.3.2), H^* will have structure K if and only if for every $i, j (1 \le i, j \le s_1)$,

$$\sum_{h=1}^{s_1} H_{ih}^* = \sum_{h=1}^{s_1} H_{hj}^*. \tag{4.3.10}$$

But, by (4.3.6c) and (4.3.9),

$$\sum_{h=1}^{s_1} H_{ih}^* = \sum_{h=1}^{s_1} C_{ih} - (\rho_{00} s_2)^{-1} \rho_{i0} (\sum_{h=1}^{s_1} \rho_{0h}) E_2$$

$$= \sum_{h=0}^{s_1} C_{ih} - C_{i0} + s_2^{-1} \rho_{i0} E_2,$$

and similarly,

$$\sum_{h=1}^{s_1} H_{hj}^* = \sum_{h=0}^{s_1} C_{hj} - C_{0j} + s_2^{-1} \rho_{0j} E_2.$$

Hence from (4.3.6b) it follows that (4.3.10) holds if and only if (4.3.7) holds for every $i, j \ (1 \le i, j \le s_1)$ Q.E.D.

Remark. There are various choices of d_o for which (4.3.7) holds. In particular, if d_o is a balanced confounded design in the sense of Nair and Rao, it can be verified that condition (4.3.7) holds. An example will be considered in section 4.5.

4.4 Some More Results on Orthogonality

In this section we consider the problem of intra-effect orthogonality. In factorial designs, the problem of intra-effect-orthogonality, in addition to that of inter-effect-orthogonality or OFS which has been considered above, is often of importance. We

shall consider the

- (i) intra-effect orthogonality with respect to main effect F_1 and
- (ii) intra-effect orthogonality with respect to interaction F_1F_2 relative to the factor F_1 .

Adopting the notation of section 4.2, we have:

<u>Definition 4.4.1.</u> Intra-effect-orthogonality holds with respect to main effect F_1 if the BLUE's of mutually orthogonal contrasts among the $\overline{\tau}_i$'s are uncorrelated.

Since F_1 is a quantitative factor, intra-effect orthogonality with respect to main effect F_1 will ensure an orthogonal splitting of the sum of square due to F_1 into linear, quadratic, cubic components and so on.

Let $\mu = \sum_{i=0}^{s_1} \mu_i \overline{\tau}_i$ and $\mu^* = \sum_{i=0}^{s_1} \mu_i^* \overline{\tau}_i$, with $\sum_{i=0}^{s_1} \mu_i = \sum_{i=0}^{s_1} \mu_i^* = 0$, be two contrasts among the $\overline{\tau}_i$'s. They will be called mutually orthogonal if $\sum_{i=0}^{s_1} \mu_i \mu_i^* = 0$.

Observe that if μ and μ^* are mutually orthogonal contrasts when considered as functions of the $\overline{\tau}_i$'s, they do not remain orthogonal when considered as functions of τ_o and $\tau_{ij} (1 \leq i \leq s_1, 1 \leq j \leq s_2)$ unless either μ_o or μ_o^* is zero. In other words, intra-effect-orthogonality with respect to F_1 calls for zero correlation among BLUE's of contrasts belonging to main effect F_1 , which, when looked upon as contrasts among the $\overline{\tau}_i$'s are mutually orthogonal but will not necessarily remain so when looked upon as contrasts among the original treatment effects. It is this special feature which makes the problem of intra-effect orthogonality in the present set-up different from the corresponding problem in ordinary factorials.

We have the following result:

: : :

Theorem 4.4.1. Let d, a design for studying quality-quantity interaction, be connected and have OFS. Then in order that intra-effect orthogonality with respect to main effect F_1 may hold in d it is necessary and sufficient that for some $\delta(>0)$ the following holds:

$$P^{10}CP^{10'} = \delta \begin{bmatrix} (s_1s_2+1)/(s_1+1) & 0' \\ 0 & I_{s_1-1} \end{bmatrix}.$$

<u>Proof:</u> Let $\tau^* = (\overline{\tau}_o, \overline{\tau}_1, \dots, \overline{\tau}_{s_1})'$. Any full set of orthonormal contrasts among the elements of τ^* will be of the form $G\tau^*$ where G is an $s_1 \times (s_1 + 1)$ matrix satisfying

 ϵ being an $(s_1 + 1) \times 1$ vector with all elements unity.

But with τ as in section 4.2, one may write $\tau^* = M\tau$ where

$$M = \begin{bmatrix} 1 & 0' \\ & & \\ 0 & s_2^{-1} I_1 \otimes \mathbf{1}_2' \end{bmatrix}. \tag{4.4.2}$$

Clearly, the elements of $G\tau^* = GM\tau$ are contrasts belonging to main effect F_1 . But since $P^{10}\tau$ gives a complete set of orthonormal contrasts belonging to main effect F_1 it follows that row space of GM is a subspace of row space of P^{10} . Since $P^{10}P^{10'} = I_1$ (see (4.2.1a), this implies that

$$GM = GMP^{10'}P^{10}.$$

So the BLUE of $G\tau^*$ is given by

$$G\hat{\tau}^* = GM\hat{\tau} = GMP^{10'}P^{10}\hat{\tau}.$$
 (4.4.3)

Now, following the line of proof of Theorem 3.4 in Mukerjee (1979) we have as follows: Let the reduced normal equations under the assumed model be in usual nota-

tions: $C\tau=Q$. Then since d has OFS, from Lemma 4.3.1 it follows that $P^{10}C=P^{10}CP^{10'}P^{10}$ and so,

$$P^{10}CP^{10'}P^{10}\tau = P^{10}Q.$$

Hence noting that $P^{10}CP^{10'}$ is non-singular since d is connected,

$$P^{10}\hat{\tau} = (P^{10}CP^{10'})^{-1}P^{10}Q.$$

Thus Disp $(P^{10}\hat{\tau}) = \sigma^2(P^{10}CP^{10'})^{-1}$, σ^2 being the error variance. Therefore, by (4.4.3), Disp $(G\hat{\tau}^*) = \sigma^2 U(G)$, where the $s_1 \times s_1$ matrix U(G) is given by

$$\mathbf{U}(G) = GMP^{10'}(P^{10}CP^{10'})^{-1}P^{10}M'G'.$$

Now, to prove the necessity of the stated condition, suppose intra-effect orthogonality holds with respect to main effect F_1 . Then, U(G) is a diagonal matrix for every G as defined above in (4.4.1). Hence, for any such fixed G, and for every $s_1 \times s_1$ orthogonal matrix G^* , $U(G^*G)$ is diagonal. Consequently, for any G satisfying (4.4.1), U(G) must be a constant times the identity matrix. Let

$$\mathbf{U}(G) = GMP^{10'}(P^{10}CP^{10'})^{-1}P^{10}M'G' = \delta_1 I_1, \tag{4.4.4}$$

the constant δ_1 being positive since $\mathbf{U}(G)$ is positive definite for a connected d.

From (4.2.1a), (4.4.1), (4.4.2) it follows after some simplification that

$$P^{10}M'G'GMP^{10'} = s_2^{-1} \begin{bmatrix} (s_1s_2 + 1)/(s_1 + 1) & \mathbf{0}' \\ & & & \\ \mathbf{0} & I_{s_1 - 1} \end{bmatrix}. \tag{4.4.5}$$

Premultiplying and postmultiplying both sides of (4.4.4) by $P^{10}M'G'$ and $GMP^{10'}$ respectively and applying (4.4.5), the necessity of the stated condition follows.

The proof of the sufficiency part is straightforward and hence omitted here.

Since the factor F_1 is quantitative and the factor F_2 is qualitative, one may be interested in having an orthogonal splitting of the SS due to interaction F_1F_2 relative to F_1 . For such a study, let

$$\eta = (\tau_{11}, \ldots, \tau_{1s_2}, \ldots, \tau_{s_11}, \ldots, \tau_{s_1s_2})'.$$

Then, by (4.2.1b), every contrast belonging to the interaction F_1F_2 will be a linear combination of the elements of $(P_1 \otimes P_2)\eta$.

Definition 4.4.2. Intra-effect orthogonality holds with respect to interaction F_1F_2 relative to the factor F_1 if the BLUE's of $\{(\mathbf{m}_1'P_1)\otimes P_2\}_{\eta}$ and $\{(\mathbf{m}_2'P_1)\otimes P_2\}_{\eta}$ are uncorrelated for every choice of mutually orthogonal non-null vectors $\mathbf{m}_1, \mathbf{m}_2$ of order $s_1 - 1$.

Under such orthogonality, it is possible to have an orthogonal splitting of the SS due to interaction F_1F_2 into components corresponding to (linear F_1) $\times F_2$, (quadratic F_1) $\times F_2$, (cubic F_1) $\times F_2$ and so on.

We have the following theorem.

Theorem 4.4.2. Let d be a connected two-factor design with OFS for the study of quality-quantity interaction. Then in d intra-effect orthogonality holds with respect to interaction F_1F_2 relative to the factor F_1 if and only if $P^{11}CP^{11'}$ is of the form $I_{s_1-1}\otimes B$ for some matrix B of order s_2-1 .

The proof of this theorem is straightforward and hence omitted.

So far three kinds of orthogonality have been considered, inter-effect orthogonality and the two intra-effect orthogonalities given by Definitions 4.4.1 and 4.4.2. A design for which all these three kinds of orthogonality hold simultaneously will be said to

have strong orthogonal factorial structure (SOFS). Combining Theorems 4.3.1, 4.4.1 and 4.4.2 we obtain the following.

Theorem 4.4.3. Let d be a connected two-factor design for the study of quality-quantity interaction. Then in order that d may have SOFS, it is necessary and sufficient that the C-matrix of d is of the form

$$C = \alpha \begin{bmatrix} 1 & -(s_1 s_2)^{-1} \mathbf{1}_1' \otimes \mathbf{1}_2' \\ -(s_1 s_2)^{-1} \mathbf{1}_1 \otimes \mathbf{1}_2 & I_1 \otimes H_1 + E_1 \otimes H_2 \end{bmatrix}, \qquad (4.4.6)$$

where α is a positive constant and H_1, H_2 are $s_2 \times s_2$ proper matrices with

$$H_1 \mathbf{1}_2 = (s_1 s_2)^{-1} (s_1 + 1) \mathbf{1}_2.$$
 (4.4.7)

The proof of this theorem is given in the appendix.

Remark. The condition (4.4.7) is non-trivial in the sense that it is not guaranteed by the condition (4.4.6). The following is an example of a design which has a C-matrix of the form (4.4.6) but for which (4.4.7) does not always hold.

Example 4.4.1. Let d be a design arranged in b blocks involving $s_1s_2 + 1$ treatments such that in each block treatment 0 is applied r times and every other level combination ij $(1 \le i \le s_1, 1 \le j \le s_2)$ is applied exactly once. Then the C-matrix of d will be given by

$$C = \begin{bmatrix} \frac{brs_1s_2}{r+s_1s_2} & -\frac{br}{r+s_1s_2} \mathbf{1}_1' \otimes \mathbf{1}_2' \\ -\frac{br}{r+s_1s_2} \mathbf{1}_1 \otimes \mathbf{1}_2 & bI_1 \otimes I_2 - \frac{b}{r+s_1s_2} E_1 \otimes E_2 \end{bmatrix}.$$

Thus, clearly C is of the form (4.4.6) whatever be the choice of r with $H_1 = \frac{r+s_1s_2}{rs_1s_2}I_2$. So condition (4.4.7) holds if and only if $r = s_2$.

4.5 Construction of Designs with OFS for the Study of Quality-Quantity Interaction

For construction of designs with OFS in the present set-up, the method of construction starting from a suitable ordinary factorial with OFS becomes very helpful in view of Theorem 4.3.2. As remarked at the end of Section 4.3, this theorem holds in particular if d_0 , the $(s_1 + 1) \times s_2$ ordinary factorial one starts with, is a balanced confounded design (Nair and Rao (1948)). Moreover, if d_0 be a balanced confounded design, then it can be seen that the resulting design d satisfies the conditions of Theorem 4.4.3 and therefore has SOFS. The following example serves as an illustration of this construction procedure.

Example 4.5.1. Suppose a design d for the study of quality-quantity interaction and having OFS is to be constructed involving 9 treatments.

Let $s_1 = 2, s_2 = 4$ and suppose one starts with a two-factor 3×4 balanced confounded design d_o . d_o will be laid out in 16 blocks as follows, the 12 treatment combinations being of the form $ij, 0 \le i \le 2, 1 \le j \le 4$.

Block	1:	01	11	21	Block	9:	03	11	23
	2:	01	12	22		10:	03	12	24
	3:	01	13	23		11:	03	13	21
	4:	01	14	24		12:	03	14	22
	5:	02	11	22		13:	04	11	24
	6:	02	12	23		14:	04	12	21
•	7:	02	13	24		15:	04	13	22
	8:	02	14	21		16:	04	14	23

The C-matrix of d_o is given by

$$C_0 = \frac{1}{3} \begin{bmatrix} 8I_4 & -E_4 & -E_4 \\ -E_4 & 8I_4 & -4I_4 \\ -E_4 & -4I_4 & 8I_4 \end{bmatrix}$$

and clearly condition (4.3.7) of Theorem 4.3.2 holds.

The required design d for study of quality-quantity interaction consists of the following blocks:

Block	1:	0	11	21	Block	9:	0	11	23
	2:	0	12	22		10:	0	12	24
	3:	0	13	23		11:	0	13	21
	4:	0	14	24		12:	0	14	22
	5:	0	11	22		13:	0	11	24
	6;	0	12	23		14:	0	12	21
	7:	0	13	24		15:	0	13	22
	8:	0	14	21		16:	0	14	23

d will have OFS by Theorem 4.3.2.

Again the C-matrix of d will be

$$C = \frac{32}{3} \begin{bmatrix} 1 & -\frac{1}{8} \mathbf{1}_{2}' \otimes \mathbf{1}_{4}' \\ -\frac{1}{8} \mathbf{1}_{2} \otimes \mathbf{1}_{4} & \frac{3}{8} (I_{1} \otimes I_{2}) - \frac{1}{8} E_{1} \otimes I_{2} \end{bmatrix}$$

and so it can be seen that both the conditions of Theorem 4.4.3 also hold. Hence d has SOFS.

As an alternative method of construction, we may start with 2 equireplicate connected varietal designs say d_1 and d_2 , involving s_1+1 and s_2 treatments respectively. Let d_o be the $(s_1+1)\times s_2$ design obtained as the Kronecker product of d_1 and d_2 . Then by Mukerjee (1981), d_o will have OFS as an ordinary factorial design. The C-matrix of d_{\circ} will be given by

$$C = R^{(1)} \otimes R^{(2)} - (R^{(1)} - C^{(1)}) \otimes (R^{(2)} - C^{(2)}),$$

where $C^{(1)}$ and $C^{(2)}$ are the C-matrices and $R^{(1)}$ and $R^{(2)}$ are the diagonal matrices of replication numbers of d_1 and d_2 respectively. So it easily follows that d_o satisfies condition (4.3.7) if

$$c_{01}^{(1)} = c_{02}^{(1)} = \ldots = c_{0s}^{(1)},$$

where $c_{0i}^{(1)}(1 \le i \le s_1)$ are the off-diagonal elements of the initial row of $C^{(1)}$. In such situations, the design d, obtained from d_0 as in Section 4.3, will have OFS by Theorem 4.3.2.

In view of the results in Mukerjee (1981, 1986), it is anticipated that the main effect and interaction efficiencies in d_0 , and hence those in d_0 , may be controlled by suitably choosing the varietal designs d_1 and d_2 . In particular, if d_1 be variance-balanced in the sense of having all off-diagonal elements of $C^{(1)}$ equal, then an application of Theorem 4.4.3 shows that the design d obtained from d_0 , the Kronecker product of d_1 and d_2 , will have SOFS. Also, instead of the Kronecker product, one may also obtain d_0 by the Khatri-Rao product of d_1 and d_2 and then obtain d from it.

4.6 Extension to the Multifactor Situation

Before concluding, we indicate an approach for a possible extension of the results to a multifactor situation. Let there be k pairs of factors (F_{j1}, F_{j2}) $(1 \le j \le k)$, where the levels of F_{j2} represent different qualities and those of F_{j1} represent various quantities of these qualities. Suppose that when F_{j1} is at the zero level the levels of F_{j2} become equivalent. Therefore, if F_{j1} has $(s_{j1}+1)$ levels and F_{j2} has s_{j2} levels then the

number of distinguishable level combinations of F_{j1} and F_{j2} becomes $(s_{j1}s_{j2}+1)=v_j$ (say). Consequently, the total number of distinct level combinations in the experiment becomes $\frac{k}{j=1}v_j$.

For $1 \leq j \leq k, i = 1, 2$, let 1_{ji} be the $s_{ji} \times 1$ vector with all elements unity and let P_{ji} be an $(s_{ji} - 1) \times s_{ji}$ matrix such that $(s_{ji}^{-\frac{1}{2}} 1_{ji}, P'_{ji})'$ is orthogonal. For $1 \leq j \leq k$, let $P^{10}(j), P^{01}(j), P^{11}(j)$ be defined as

$$P^{10}(j) = \begin{bmatrix} -[(v_{j-1})/v_j]^{\frac{1}{2}} & [v_j(v_{j-1})]^{-\frac{1}{2}} \mathbf{1}'_{j1} \otimes \mathbf{1}'_{j2} \\ 0 & s_{j2}^{-\frac{1}{2}} P_{j1} \otimes \mathbf{1}'_{j2} \end{bmatrix},$$

$$P^{01}(j) = \begin{bmatrix} \mathbf{0} & s_{j1}^{-\frac{1}{2}} \mathbf{1}'_{j1} \otimes P_{j2} \end{bmatrix}, \quad P^{11}(j) = \begin{bmatrix} \mathbf{0} & P_{j1} \otimes P_{j2} \end{bmatrix}.$$

Let $P^{00}(j)$ be the v_j -component row vector with each element $v_j^{-\frac{1}{2}}$ for $1 \leq j \leq k$.

A typical factorial effect will be denoted by $F_{11}^{x_{11}}F_{12}^{x_{21}}F_{21}^{x_{22}}F_{22}^{x_{22}}\dots F_{k1}^{x_{k1}}F_{k2}^{x_{k2}}$, where $(x_{11}, x_{12}, x_{21}, x_{22}, \dots, x_{k1}, x_{k2})$ is a non-null binary vector. It may be seen that the space of all contrasts belonging to this factorial effect is spanned by the rows of the matrix $P^{x_{11}x_{12}}(1) \otimes P^{x_{21}x_{22}}(2) \otimes \dots \otimes P^{x_{k1}x_{k2}}(k)$. For example, if k = 2, then the rows of $P^{10}(1) \otimes P^{11}(2)$ span the space of all contrasts belonging to the factorial effect $F_{11}F_{21}F_{22}$.

From the definition of the $P^{10}(j)$, $P^{01}(j)$ and $P^{11}(j)$ matrices $(1 \le j \le k)$, it is easy to see that contrasts belonging to different factorial effects are mutually orthogonal. Now, Theorems 4.3.1, 4.4.1, 4.4.2 and 4.4.3 can be extended to this multifactor set-up proceeding along the line of proofs of these theorems. The notations will however be somewhat involved for general k.

Appendix

Proof of Theorem 4.4.3. To prove the necessity of the stated condition, it is enough to show that it is a consequence of those in Theorems 4.3.1, 4.4.1 and 4.4.2. Let d have SOFS. Then by Theorem 4.3.1, the C-matrix of d can be written as

$$C = \begin{bmatrix} \alpha & \mathbf{u}' \otimes \mathbf{1}'_2 \\ \mathbf{u} \otimes \mathbf{1}_2 & H^* + \alpha^{-1} \mathbf{u} \mathbf{u}' \otimes E_2 \end{bmatrix}, \tag{4.A.1}$$

where H^* has structure K. Since each row sum of C is zero it follows that

$$\alpha + s_2 \mathbf{u}' \mathbf{1}_1 = 0 \tag{4.A.2}$$

$$H^*(\mathbf{1}_1 \otimes \mathbf{1}_2) = 0. (4.A.3)$$

From (4.2.1a) and (4.A.1) - (4.A.3), after some algebra

$$P^{10}CP^{10'} = \begin{bmatrix} \frac{\alpha v}{s_1 s_2} & -\sqrt{\frac{v s_2}{v-1}}(P_1 \mathbf{u})' \\ -\sqrt{\frac{v s_2}{v-1}}(P_1 \mathbf{u}) & s_2^{-1}(P_1 \otimes \mathbf{1}_2')\{H^* + \alpha^{-1} \mathbf{u} \mathbf{u}' \otimes E_2\}(P_1' \otimes \mathbf{1}_2) \end{bmatrix} (4.A.4)$$

Since d has SOFS, by Theorem 4.4.1, it follows from (4.A.4) that

$$P_1\mathbf{u} = \mathbf{0},\tag{4.A.5}$$

and for some $\delta > 0$,

$$\frac{\alpha v}{s_1 s_2} = \delta \frac{v}{s_1 + 1},\tag{4.A.6}$$

$$s_2^{-1}(P_1 \otimes \mathbf{1}_2')H^*(P_1' \otimes \mathbf{1}_2) = \delta I_{s_1-1}.$$
 (4.A.7)

Clearly, by (4.A.5), $\mathbf{u} = u\mathbf{1}_1$, for a scalar u, which by (4.A.2) equals $-(s_1s_2)^{-1}\alpha$.

Hence

$$\mathbf{u} = -(s_1 s_2)^{-1} \alpha \mathbf{1}_1. \tag{4.A.8}$$

Since d has SOFS, by (4.2.1b), (4.A.1), (4.A.5) and Theorem (4.4.2),

$$(P_1 \otimes P_2)H^*(P_1' \otimes P_2') = I_{s_1-1} \otimes B,$$
 (4.A.9)

for some matrix B. Since H^* has structure K, it may be seen from (4.A.3), (4.A.7), (4.A.9) that

$$H^* = I_1 \otimes H_1^* + E_1 \otimes H_2^*, \tag{4.A.10}$$

where H_1^*, H_2^* are $s_2 \times s_2$ proper matrices. Let $H_1^*1_2 = h_11_2$. Then from (4.A.6), (4.A.7), (4.A.10) it follows that $h_1 = \alpha(s_1 + 1)/(s_1s_2)$. It is now clear from (4.A.1), (4.A.8), (4.A.10) that if d has SOFS then C must be of the form

$$C = \alpha \begin{bmatrix} 1 & -(s_1s_2)^{-1}\mathbf{1}_1' \otimes \mathbf{1}_2' \\ -(s_1s_2)^{-1}\mathbf{1}_1 \otimes \mathbf{1}_2 & I_1 \otimes H_1 + E_1 \otimes H_2 \end{bmatrix},$$

where H_1, H_2 are proper matrices of order s_2 and $H_11_2 = \{(s_1 + 1)/(s_1s_2)\}1_2$. This proves the necessity of the stated condition. The sufficiency is obvious.

Chapter 5

OPTIMAL REPEATED MEASUREMENTS DESIGNS UNDER INTERACTION

5.1 Introduction

In some experiments a number of treatments are applied sequentially over periods to each of the experimental units. Designs for studying such experiments are known as repeated measurements designs (RMD's). The interesting feature of these designs is that since the same experimental unit is exposed repeatedly to a sequence of treatments, the "residual effect" of a treatment in the following period is also an important source of variation along with its "direct effect" in the period in which it is applied.

Hedayat and Afsarinejad (1975) have given a general review of RMD's including a discussion of their practical applications and a comprehensive bibliography up to that stage. The pioneering work in the area of optimal RMD's is also due to Hedayat and Afsarinejad (1978). Other significant contributions, covering the optimality and constructional aspects, were made by Cheng and Wu (1980), Magda (1980), Constantine and Hedayat (1982) and Kunert (1983, 1984, a, b, 1985, 1987). We refer to Hedayat (1981) for an excellent review of the literature on optimal RMD's. Applying a fundamental tool due to Kiefer (1975), many of these authors considered the problem of universal optimality under the usual fixed effects additive model incorporating direct and first order residual effects of treatments apart from effects due to units and periods.

In practical situations, however, it is likely that an effect due to the interaction of direct and residual effects will also be present. John and Quenouille (1977, pp. 211-214) analyzed a practical example on grass yields where such an interaction turned out to be significant. Interesting results on the problems of construction and analysis under such non-additive models were obtained by Patterson (1968, 1970) and Kershner and Federer (1981). In this connection, reference should be made to the discussion by Federer following Hedayat (1981). Patterson (1973) considered some orthogonality conditions in this context.

In sections 5.4 and 5.5 of this chapter, we investigate how far the optimality results in Cheng and Wu (1980) and Magda (1980) remain robust when the direct versus residual effects interaction is taken into account. It may be remarked that under such a non-additive model it becomes rather involved to prove the optimality results using the standard methods of analysis of RMD's. To overcome this difficulty, we establish a correspondence between factorial experiments and RMD's in section 5.3 and then use the calculus for factorial arrangements to prove the results.

In sections 5.4 and 5.5 some new constructions of optimal *RMD*'s have also been discussed. Section 5.6 shows that the optimality results also remain robust when the underlying model is a mixed effects model where the effects due to units may be random.

5.2 Notations and Definitions

We follow the notations and definitions as in Hedayat and Afsarinejad (1978), Cheng and Wu (1980) and Magda (1980). An RMD with n experimental units

 $1, 2, \ldots, n; \ p \text{ periods } 0, 1, \ldots, p-1 \text{ and } t \text{ treatments } 0, 1, \ldots, t-1 \text{ will be abbreviated}$ by RMD(t, n, p) and the class of all such designs will be denoted by $\Omega_{t,n,p}$. If d is an RMD, let d(i,j) denote the treatment assigned by d in the i^{th} period to the j^{th} unit. Let y_{ij} be the response under d(i,j). The observations are assumed to be uncorrelated and homoscedastic. The underlying model is called circular if in each unit the residuals in the initial period are incurred from the last period. Otherwise, i.e., if there is no residual effect in the first period, the model is called non-circular.

Taking the direct versus residual effect interaction into account, the circular model is given by,

$$E(y_{ij}) = \mu + \alpha_i + \beta_j + \xi_{d(i,j)d(i-1,j)}, \quad (0 \le i \le p-1, 1 \le j \le n)$$
 (5.2.1)

where i-1 is reduced mod p and the unknown constants μ , α_i , β_j represent respectively the general mean, the i^{th} period effect and the j^{th} unit effect. The unknown constant $\xi_{h_1h_2}(0 \le h_1, h_2 \le t-1)$ represents the effect produced when the treatment h_1 is applied in the current period with the treatment h_2 being applied in the immediately preceding period.

For the non-circular model, $E(y_{ij})$ is as in (5.2.1) for $1 \le i \le p-1, 1 \le j \le n$, while for i = 0,

where
$$E(y_{0j}) = \mu + \alpha_i + \beta_j + \tau_{d(0,j)} \qquad (1 \le j \le n)$$

$$\tau_{h_1} = t^{-1} \sum_{h_2=0}^{t-1} \xi_{h_1 h_2} \qquad (0 \le h_1 \le t-1)$$

$$(5.2.2)$$

Definition 5.2.1. An RMD will be called uniform if in each period the same number of units is assigned to each treatment and on each unit each treatment appears in the

same number of periods.

Definition 5.2.2. Under the non-circular model an RMD is called strongly balanced if the collection of ordered pairs $\{d(i-1,j),d(i,j)\}, 1 \leq i \leq p-1, 1 \leq j \leq n$, contains each ordered pair of treatments, distinct or not, the same number, say λ , of times; under the circular model an RMD is called strongly balanced if the same holds considering ordered pairs $\{d(i-1,j),d(i,j)\}, 0 \leq i \leq p-1, 1 \leq j \leq n$.

A strongly balanced uniform RMD(t,n,p) will be abbreviated by SBURMD (t,n,p). We consider two illustrative examples given below with rows and columns identified with periods and units respectively. Example 5.2.1 is a SBURMD(2,4,4) under the non-circular model with $\lambda = 3$, while Example 5.2.2 is a SBURMD(2,4,4) under the circular model with $\lambda = 4$.

Example 5.2.1	${f units}$				Example 5.2.2 ur					
	0	0	1	1		0	1	1	0	
	0	1	0	1		1	0	0	1	
periods	0	1	1	0	periods	1	0	0	1	
	1	1	0	0		0	1	1	0	
	1	0	1	0						
	1	0	0	1						

5.3 Application of the Calculus for Factorial Arrangements in the Analysis of RMD's

Since we take into account the interaction between the direct and first order residual effects of treatments, it appears convenient to apply the calculus for factorial arrangements, introduced by Kurkjian and Zelen (1962) and which has been extensively used in the previous chapters of this thesis.

Consider the $t^2 = v$ (say) treatment combinations $(h_1, h_2), 0 \le h_1, h_2 \le t - 1$,

such that the first (second) member of each combination represents the treatment contributing a direct (first order residual) effect to an experimental unit. The direct and first order residual effects of treatments may then be looked upon as the main effects of factors, say, F_1 and F_2 (each at t levels) respectively while their interaction is given by the interaction F_1F_2 . Thus, under this interpretation, an RMD(t, n, p) becomes equivalent to a t^2 factorial experiment laid out in p rows and n columns.

For any positive integer a, let I_a be the $a \times a$ identity matrix, $\mathbf{1}_a$ be an $a \times 1$ vector with all elements unity and $E_a = \mathbf{1}_a \mathbf{1}_a^t$. Define the $v \times 1$ vector

$$\boldsymbol{\xi} = (\xi_{00}, \xi_{01}, \dots, \xi_{0t-1}, \dots, \xi_{t-10}, \xi_{t-11}, \dots, \xi_{t-1t-1})'.$$

Then, by (5.2.1), (5.2.2), for a design $d \in \Omega_{t,n,p}$, the coefficient matrix for the reduced normal equations for ξ , under both the circular and the non-circular models, is of the form

$$C_d^{(v \times v)} = V_d - n^{-1} N_d N_d' - p^{-1} M_d M_d' + (np)^{-1} (N_d \mathbf{1}_p) (N_d \mathbf{1}_p)', \tag{5.3.1}$$

where

$$V_{d} = \sum_{i=0}^{p-1} \sum_{j=1}^{n} \ell_{ij} \ell'_{ij}, \ N_{d}^{(v \times p)} = \left(\sum_{j=1}^{n} \ell_{oj}, \dots, \sum_{j=1}^{n} \ell_{p-1,j}\right),$$

$$M_{d}^{(v \times n)} = \left(\sum_{i=0}^{p-1} \ell_{i1}, \dots, \sum_{i=0}^{p-1} \ell_{in}\right);$$
(5.3.2)

$$\ell_{ij} = \mathbf{e}_{d(i,j)} \otimes \mathbf{e}_{d(i-1,j)} \quad (0 \le i \le p-1, 1 \le j \le n)$$
 (5.3.3)

for the circular model;

$$\ell_{ij} = \mathbf{e}_{d(i,j)} \otimes \mathbf{e}_{d(i-1,j)} \quad (1 \le i \le p-1, 1 \le j \le n)$$

$$\ell_{0j} = t^{-1} \mathbf{e}_{d(0,j)} \otimes \mathbf{1}_{t} \qquad (1 \le j \le n)$$

$$(5.3.4)$$

for the non-circular model; e_h is a $t \times 1$ vector with 1 in the h^{th} position and zero elsewhere. As usual, \otimes denotes Kronecker product.

The typical contrasts belonging to main effect F_1 , main effect F_2 and interaction F_1F_2 are respectively of the forms $(\omega_1\otimes 1_t)'\xi$, $(1_t\otimes \omega_2)'\xi$, $(\omega_1\otimes \omega_2)'\xi$, where ω_1,ω_2 are any $t\times 1$ non-null vectors satisfying $\omega_1'1_t=\omega_2'1_t=0$.

We shall use a result by Mukerjee (1980) which has been stated as Lemma 1.2.1 in Chapter 1 of this thesis. In the present context of 2-factor designs we use the following simplified version of Lemma 1.2.1.

Lemma 5.3.1. In a two-factor design d, contrasts belonging to main effect $F_1(F_2)$ are estimable orthogonally to those belonging to main effect $F_2(F_1)$ and interaction F_1F_2 if and only if $G_1(G_2)$ commutes with the C-matrix of d, where $G_1 = I_t \otimes E_t$, $G_2 = E_t \otimes I_t$.

5.4 Optimality Results Under the Non-Circular Model

Throughout this section, the underlying model is the non-circular model described in Section 5.2. The aim is to examine the robustness of the main results in Section 3 of Cheng and Wu (1980) and to develop some further results.

Let d^* be a SBURMD(t, n, p). Cheng and Wu (1980, Theorem 3.1) proved the universal optimality of d^* over $\Omega_{t,n,p}$ for the estimation of direct as well as first order residual effects. Theorem 5.4.1 below establishes the robustness of their findings for the direct effects under a non-additive setting.

Theorem 5.4.1. Under a non-additive model, d^* is universally optimal over $\Omega_{t,n,p}$ for the estimation of direct effects.

<u>Proof:</u> In view of Theorem 3.1 of Cheng and Wu (1980), it is enough to show that in d^* , under the non-additive model, contrasts belonging to main effect F_1 are estimable orthogonally to those belonging to main effect F_2 and interaction F_1F_2 . So,

by Lemma 5.3.1 it is enough to show that $G_1C_{d^*}$ is symmetric.

Let $\mathbf{1} = \mathbf{1}_t \otimes \mathbf{1}_t$, $E = E_t \otimes E_t$. By (5.3.4) and the definition of a SBURMD(t, n, p), it follows that for d^*

$$\sum_{j=1}^{n} \ell_{oj} \ell'_{oj} = nt^{-3} (I_t \otimes E_t), \quad \sum_{i=1}^{p-1} \sum_{j=1}^{n} \ell_{ij} \ell'_{ij} = n(p-1)t^{-2} (I_t \otimes I_t),
\sum_{j=1}^{n} \ell_{oj} = nt^{-2} \mathbf{1}, \quad \sum_{i=1}^{p-1} \sum_{j=1}^{n} \ell_{ij} = n(p-1)t^{-2} \mathbf{1},
G_1(\sum_{j=1}^{n} \ell_{ij}) = nt^{-1} \mathbf{1}(0 \le i \le p-1), \quad G_1(\sum_{i=0}^{p-1} \ell_{ij}) = pt^{-1} \mathbf{1}(1 \le j \le n).$$
(5.4.1)

Hence by (5.3.2), after simplification,

$$V_{d^*} = nt^{-3}(I_t \otimes E_t) + n(p-1)t^{-2}(I_t \otimes I_t),$$

$$N_{d^*} \mathbf{1}_p = npt^{-2}\mathbf{1}, \ G_1 N_{d^*} N'_{d^*} = n^2 pt^{-3} E, \ G_1 M_{d^*} M'_{d^*} = np^2 t^{-3} E.$$

$$(5.4.2)$$

From (5.3.1) it now follows that $G_1C_{d^*}$ is symmetric. Q.E.D.

Remarks:

1. Though the result of Cheng and Wu remains robust for direct effects under a non-additive setting, the same is not true for residual effects. It is clear that as in Theorem 5.4.1, a SBURMD d^* will be universally optimal over $\Omega_{t,n,p}$ for the residual effects under the non-additive model provided d^* allows orthogonal estimation of the residual effect contrasts, i.e., by Lemma 5.3.1, provided $G_2C_{d^*}$ is symmetric. But not all SBURMD's satisfy this criterion. The following example serves to illustrate this.

Example 5.4.1. Consider the designs d_1^* and d_2^* each of which is a SBURMD (2,4,6)

On computation using (5.3.1) we have

$$C_{d_{1}^{*}} = \frac{1}{12} \begin{bmatrix} 41 & -5 & -14 & -22 \\ -5 & 41 & -22 & -14 \\ -14 & -22 & 45 & -9 \\ -22 & -14 & -9 & 45 \end{bmatrix}, C_{d_{2}^{*}} = \frac{1}{12} \begin{bmatrix} 37 & -2 & -16 & -19 \\ -2 & 37 & -19 & -16 \\ -16 & -19 & 37 & -2 \\ -19 & -16 & -2 & 37 \end{bmatrix}.$$

It can now be shown that

$$G_2C_{d_1^*} = rac{1}{12} egin{bmatrix} 27 & -27 & 31 & -31 \ -27 & 27 & -31 & 31 \ 27 & -27 & 31 & -31 \ -27 & 27 & -31 & 31 \ \end{bmatrix},$$

$$G_2C_{d_2^*} = rac{1}{12} egin{bmatrix} 21 & -21 & 21 & -21 \ -21 & 21 & -21 & 21 \ 21 & -21 & 21 & -21 \ -21 & 21 & -21 & 21 \end{bmatrix}.$$

Hence by Lemma 5.3.1, while d_2^* allows estimation of the residual effects orthogonally to direct effects and direct versus residual effect interaction, d_1^* does not. In fact, a direct computation shows that d_1^* is inferior to d_2^* in so far as the estimation of the (single) residual effect contrast is concerned.

2. From Remark 1 it is clear that the problem of identifying those SBURMD's which allow orthogonal estimation of the residual effect contrasts becomes non-trivial. Essentially, this calls for a combinatorial characterization of the commutativity of G_2 and C_{d^*} . But, in general, it appears that such a characterization may become too involved to be helpful in actual construction of d^* and so we

look for simpler sufficient conditions. In the special case $n=t^2$ and p=2t Patterson (1973) considered sufficient conditions in this regard. See also Berenblut (1964). In the following theorem we give a more general set of sufficient conditions with a very wide coverage.

For any $d \in \Omega_{t,n,p}$, let S_{dh} be the set of units which receive the treatment h (0 $\leq h \leq t-1$) in the last period. Then the following holds.

Theorem 5.4.2. Under a non-additive model, a SBURMD(t, n, p) d^* allows orthogonal estimation of the residual effects contrasts and hence becomes universally optimal over $\Omega_{t,n,p}$ for the residual effects if:

- (i) for each h, h' ($0 \le h, h' \le t 1$), there are exactly nt^{-2} units receiving the treatments h and h' in the initial and the last periods respectively, and
- (ii) for each h ($0 \le h \le t 1$), in the collection of ordered pairs $\{d^*(i 1, j), d^*(i, j)\}, 1 \le i \le p 1, j \in S_{d^*h}$ each ordered pair (h, h_2) ($0 \le h_2 \le t 1$) occurs the same number (say ν_1) of times while each ordered pair (h_1, h_2) ($0 \le h_1, h_2 \le t 1, h_1 \ne h$) occurs the same number (say ν_2) of times.

The proof of this theorem is given in the Appendix.

Remarks:

- 1. If d^* satisfies condition (ii) of Theorem 5.4.2 then by recalling the definition of a SBURMD, one may count in two ways the number of times each treatment appears in S_{d^*h} to get $\nu_1 = n(p-t)t^{-3}$ and $\nu_2 = npt^{-3}$.
- 2. From the definition of a SBURMD it is clear that a SBURMD(t, n, p) exists

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only if $t^2|n$ and t|p with p > t. Theorem 5.4.2 covers almost all situations where a SBURMD may exist. If $t^2|n$ and pt^{-1} is even, then Theorem 3.2 of Cheng and Wu (1980) gives a method of construction of SBURMD(t,n,p). It may be checked that in this case the designs constructed by their method satisfy the conditions of Theorem 5.4.2 and are hence universally optimal for the residual effects under the non-additive model. It may be remarked that in particular if $n = t^2$ and p = 2t then this finding also follows from the sufficient conditions in Patterson (1973).

3. It may be easily verified that d₂* of Example 5.4.1 satisfies the conditions (i) and
(ii) of Theorem 5.4.2 with ν₁ = 2 and ν₂ = 3.

Turning to the situation where $t^2|n$ and pt^{-1} is odd, let $pt^{-1} = 2m + 1 (m \ge 1)$ and consider the following method of construction which is successful for $t \ne 6$. First let $t \ne 2, 6$. Then a pair of mutually orthogonal latin squares, say, Q_1 and Q_2 , of order t exists. Let $0, 1, \ldots, t-1$ be the entries of Q_1 and Q_2 , q_{uh} be the h^{th} column of Q_u , $g_h = h\mathbf{1}_t$; and $\Gamma_h = (\mathbf{q}_{1h}, \mathbf{q}_{2h}, \mathbf{g}_h), (0 \le h \le t-1, u = 1, 2)$. Let $\Gamma = \begin{pmatrix} \Gamma_0, \Gamma_1, \ldots, \Gamma_{t-1} \end{pmatrix}$. If t = 2, let $\Gamma = \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{pmatrix}$, For $t \ne 6$, let

$$B_0 = \begin{bmatrix} 0 & 1 & \dots & t-1 \\ 0 & 0 & \dots & 0 \end{bmatrix}',$$

and for $1 \le h \le t-1$, let B_h be obtained by adding $h \pmod{t}$ to each element of B_0 . Let $B = (B_0, B_1, \ldots, B_{t-1})$ and define the $t \times p$ array $A_0 = (\Gamma, B, \ldots, B)$ where the array B is repeated m-1 times in A_0 . Let A_h be obtained by adding $h \pmod{t}$ to

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each element of A_o .

Then the $p \times t^2$ array $A = (A'_0, A'_1, \dots, A'_{t-1})$, with columns and rows identified with units and period respectively, is seen to be a $SBURMD(t, t^2, p)$ and it can be easily checked that A satisfies the conditions of Theorem 5.4.2. A SBURMD(t, n, p) satisfying these same conditions is obtained considering nt^{-2} copies of A together. Since such a design satisfies the conditions of Theorem 5.4.2, it follows that it is universally optimal over $\Omega_{t,n,p}$ for the residual effects under the non-additive model.

The above method is essentially a method of differences and the choice of Γ for t=2 has been made by trial and error. The design d_2^* in Example 5.4.1 was constructed by this method. Another detailed example is presented below.

Example 5.4.2. Let t = 3, n = 9, p = 15. One may take

$$Q_1 = egin{bmatrix} 0 & 1 & 2 \ 1 & 2 & 0 \ 2 & 0 & 1 \end{bmatrix} \ ext{and} \ \ Q_2 = egin{bmatrix} 0 & 1 & 2 \ 2 & 0 & 1 \ 1 & 2 & 0 \end{bmatrix},$$

$$B = \begin{bmatrix} 0 & 0 & 1 & 1 & 2 & 2 \\ 1 & 0 & 2 & 1 & 0 & 2 \\ 2 & 0 & 0 & 1 & 1 & 2 \\ B_0 & B_1 & B_2 \end{bmatrix}, \Gamma = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 1 & 2 & 0 & 2 & 0 & 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 0 & 2 & 1 & 1 & 0 & 2 \end{bmatrix}.$$

So $A_0 = (\Gamma, B)$ and the arrays A_1 and A_2 are formed by adding 1 and 2 (mod3) respectively to each element of A_0 . The 15 × 9 array $A = (A'_0, A'_1, A'_2)$ shown on the next page is a SBURMD satisfying the conditions of Theorem 5.4.2.

Remarks:

- 1. By Theorems 5.4.1, 5.4.2 and the discussion above, under a non-additive non-circular model a SBURMD(t, n, p), which is universally optimal over $\Omega_{t,n,p}$ for both the direct and the residual effects, exists whenever $t^2|n,t|p$ (p>t), except when t=6 and p is an odd multiple of 6. Since our method of construction used a pair of mutually orthogonal latin squares of order t, the restriction $t \neq 6$ was unavoidable.
- 2. If one ignores the conditions of Theorem 5.4.2, then as indicated below, a SBURMD(t,n,p) exists even when t=6 and $\frac{p}{6}$ is an odd integer, provided $t^2|n$ as usual.

Let
$$p=(2m+1)6 \ (m\geq 1).$$
 Define the 36×1 vector
$$\delta=(0,1,2,3,4,5,1,2,3,4,5,0,\dots,5,0,1,2,3,4)',$$

and the 36×2 matrix

Construct the $36 \times (2m+1)$ array $L_0 = (\Delta, \Delta, \ldots, \Delta, \delta)$, where the array Δ is repeated m times. Let L_h be obtained by adding h(mod 6) to each element of L_0 ($0 \le h \le 5$). Then the $p \times 36$ array $L = (L_0, L_1, \ldots, L_5)'$, with columns and rows interpreted as before, gives a SBURMD(6, 36, (2m+1)6). A SBURMD(6, n, (2m+1)6) is obtained by considering n/36 copies of L. This design does not satisfy the conditions of Theorem 5.4.2 and hence nothing can be said about its optimality for the residual effects under a non-additive model.

3. Remark 2 together with the preceding method of construction and Theorem 3.2 of Cheng and Wu (1980), establish that the conditions $t^2|n,t|p$ (p>t) are not only necessary but also sufficient for the existence of a SBURMD(t,n,p).

Before concluding this section on non-circular models, the robustness of another result in Cheng and Wu (1980) will be examined.

Let d_0 be a strongly balanced RMD(t, n, p) which is uniform on the periods and is uniform on the units in the first p-1 periods. In their Theorem 3.3, Cheng and Wu (1980) show that such a design is universally optimal over $\Omega_{t,n,p}$ for both the direct and first order residual effects under an additive model. We have the following: Theorem 5.4.3. Under a non-additive model, d_0 is universally optimal over $\Omega_{t,n,p}$ for the estimation of residual effects.

The proof follows the line of proof of Theorem 5.4.1 and is omitted. It may be noted that the corresponding result does not hold for the estimation of direct effects.

This is because $G_1C_{d_0}$ is not always symmetric as the following example illustrates. Example 5.4.3. Consider the design d_0 which is a strongly balanced RMD(2, 4, 7) uniform on the periods and uniform on the units in the first 6 periods.

On computation of C_{d_0} it can be shown that $G_1C_{d_0}$ is not symmetric and so d_0 may not be universally optimal for direct effects over $\Omega_{2,4,7}$.

5.5 Some Further Remarks

Throughout this section the underlying model is circular. Let \overline{d} be a SBURMD (t,n,p) under such a model. Magda (1980) considered the optimality of \overline{d} over $\Omega_{t,n,p}$ under an additive circular model. In his main result (Theorem 3.1), Magda (1980) proved that under such a model \overline{d} is universally optimal over $\Omega_{t,n,p}$ for both direct and residual effects. The next theorem proves the robustness of his result under a non-additive model.

Theorem 5.5.1. Under a non-additive model, \overline{d} is universally optimal over $\Omega_{t,n,p}$ for the estimation of direct as well as residual effects.

<u>Proof:</u> The proof follows the line proof of Theorem 5.4.1 and essentially checks that both $G_1C_{\overline{d}}$ and $G_2C_{\overline{d}}$ are symmetric.

Turning to the problem of construction, note that for the existence of an SBURMD's in a circular setting, it is necessary that t|n and t|p (p>t).

Theorem 5.5.2. Under the circular model, if t|n and pt^{-1} is an even integer then a SBURMD(t, n, p) exists.

Proof: First let t be even and define the $2t \times 1$ vector $\Phi_0 = (0, t-1, 1, t-2, \dots, t-1, 0)'$. Note that each of $0, 1, \dots, t-1$ occurs twice in Φ_0 and also among the differences $\{f_1 - f_0, f_2 - f_1, \dots, f_{2t-1} - f_{2t-2}, f_0 - f_{2t-1}\}$ (mod t), f_u being the u^{th} element of Φ_0 ($0 \le u \le 2t-1$).

Let Φ_h be the vector obtained by adding h(mod t) to each element of Φ_0 (1 $\leq h \leq t-1$). Then the $2t \times t$ array $[\Phi_0, \Phi_1, \dots, \Phi_{t-1}]$, with columns and rows identified with units and periods respectively, gives a SBURMD(t, t, 2t). A SBURMD(t, n, p) is obtained taking nt^{-1} and $\frac{1}{2}pt^{-1}$ copies of this $2t \times t$ array along the directions of the units and periods respectively. The proof for odd t follows in a similar manner starting from the $2t \times 1$ vector $(0, 1, t-1, 2, t-2, \dots, t-2, 2, t-1, 1, 0)'$ instead of Φ_0 . Q.E.D.

Example 5.5.1. The designs $\overline{d}_1, \overline{d}_2$ in this example are constructed by the above method and represent a SBURMD (4, 4, 8) and a SBURMD (5, 5, 10) respectively.

	units							units				
		0	1	2	3			0	1	2	3	4
\overline{d}_1 :	periods	3	0	1	2	\overline{d}_2 :	periods	1	2	3	4	0
	-	1		3				4	0	1	2	3
		2	3	0	1			2	3	4	0	1
		2	3	0	1	•		3	4	0	1	2
		1	2	3	0			3	4	0	1	2
		3	0	1	2			2	3	4	0	1
		0	1	2	3	•		4	0	1	2	3
						•		1	2	3	4	0
							•	0	1	2	3	4

When t|n and pt^{-1} is an odd integer, it has recently been shown by Roy (1985)

that a SBURMD(t, n, p) exists provided t = 0, 1, or 3 (mod 4). However, such a design may be non-existent if $t = 2 \pmod{4}$, e.g., as a complete enumeration reveals, a SBURMD(2, 2, 6) is non-existent.

Remarks

- 1. Restricting to a subclass of Ω_{t,n,p}, under the non-circular model, Cheng and Wu (1980, Theorems 3.4, 3.5) proved two more optimality results on SBURMD's. These results are in terms of minimization of the variance of the best linear unbiassed estimator of every contrast belonging to the direct (residual) effects over the subclass of equireplicate designs (the subclass of designs equireplicate in the first p-1 periods). Under the circular model, Magda (1980, Theorem 3.2) proved a similar result. It can be seen that these results remain robust under the non-additive model whenever the relevant orthogonality properties, as in Sections 5.4 and 5.5 hold.
- 2. Hedayat and Afsarinejad (1978), Cheng and Wu (1980) and Magda (1980) also derived universal optimality results on uniform RMD's which are balanced in the sense that each treatment never precedes itself but precedes each other treatment the same number of times. With notations as in Section 5.3 under a non-additive model this means that the treatment combinations (h, h) (0 ≤ h ≤ t − 1) never appear in such a design so that not all contrasts belonging to direct or residual effects remain estimable. Therefore, the optimality results on balanced uniform RMD's become non-robust under a non-additive model.
- 3. Throughout this chapter, the underlying model was non-additive but the empha-

sis was on the optimal estimation of the direct or residual effects, i.e. the main effects, contrasts. If interest lies also in the optimal estimation of the interaction contrasts then, some other, possibly larger, designs should be tried.

5.6 Optimality Results Under a Mixed Effects Model

Recently, Mukhopadhyay and Saha (1983) extended the optimality results of Cheng and Wu (1980) and Magda (1980) to mixed effects (but additive) models where the unit effect was considered random. In this section we show that some of the results of Mukhopadhyay and Saha (1983) remain robust under a non-additive model, i.e., equivalently we show that the results in Theorems 5.4.1 and 5.4.2 remain true even under a mixed effects model.

The circular non-additive mixed effects model is given by

$$y_{ij} = \mu + \alpha_i + b_j + \xi_{d(i,j)d(i-1,j)} + e_{ij}, (0 \le i \le p-1, 1 \le j \le n)$$
 (5.7.1)
where $y_{ij}, \mu, \alpha_i, \xi_{d(i,j)d(i-1,j)}$ are as in 5.2.1. For $1 \le j \le n, b_j$ represents the j^{th} unit effect and we assume that the $n \times 1$ vector $\mathbf{b} = (b_1, \dots, b_n) \sim N(0, \sigma_1^2 I_n)$.
 $\mathbf{e} = (\dots e_{ij} \dots)$ represents the error vector and let $\mathbf{e} \sim N(0, \sigma^2 I_{np})$, \mathbf{b} and \mathbf{e} being uncorrelated.

The non-circular non-additive mixed effects model follows similarly from 5.2.2. For a design $d \in \Omega_{t,n,p}$, the coefficient matrix of the reduced normal equations for ξ , under both these two models is given by

$$\begin{split} C_{d} = & \sigma^{-2} \sum_{i=0}^{p-1} \sum_{j=1}^{n} \ell_{ij} \ell'_{ij} - a \sum_{j=1}^{n} \binom{p-1}{\sum i=0} \ell_{ij} \binom{p-1}{\sum i=0} \ell'_{ij} - n^{-1} \sigma^{-4} \sigma_{1}^{2} N_{d} E_{p} N'_{d} \\ &+ \sigma^{-2} \sigma_{1}^{2} a n^{-1} N_{d} E_{p} \tilde{N}'_{d} - \sigma^{-2} n^{-1} N_{d} N'_{d} + n^{-1} a N_{d} \tilde{N}'_{d} \\ &+ \sigma^{-2} a \sigma_{1}^{2} n^{-1} \tilde{N}_{d} E_{p} N'_{d} - a^{2} \sigma_{1}^{2} n^{-1} \tilde{N}_{d} E_{p} \tilde{N}'_{d} + a n^{-1} \tilde{N}_{d} N'_{d} \end{split}$$

$$-a^2\sigma^2n^{-1}\tilde{N}_d\tilde{N}_d', (5.7.2)$$

where N_d , ℓ_{ij} are as in (5.3.2), (5.3.3) and (5.3.4), $\tilde{N}_d^{(v \times p)} = \begin{pmatrix} \sum_{i=0}^{p-1} \sum_{j=1}^{n} \ell_{ij}, \dots, \sum_{i=0}^{p-1} \sum_{j=1}^{n} \ell_{ij} \end{pmatrix}$ and $a = \sigma_1^2 \sigma^{-2} (\sigma^2 + p\sigma_1^2)^{-1}$.

The following two theorems can be proved along the line of proofs of Theorems 5.4.1 and 5.4.2 respectively.

Theorem 5.6.1. Under a non-additive mixed effects non-circular model, d^* is universally optimal over $\Omega_{t,n,p}$ for the estimation of direct effects.

Theorem 5.6.2. Under a non-additive mixed effects non-circular model, d^* is universally optimal over $\Omega_{t,n,p}$ for the residual effects if the conditions (i) and (ii) of Theorem 5.4.2 hold.

It can be also shown that results corresponding to those in Theorems 5.5.1 and 5.5.2 hold under the mixed effects model.

Appendix:

<u>Proof of Theorem 5.4.2.</u> By (5.3.2), (5.4.1), (5.4.2) and the definition of a SBURMD, it can be seen that for every SBURMD d^* the matrix G_2 commutes with V_{d^*} , $N_{d^*}N'_{d^*}$ and $(N_{d^*}\mathbf{1}_p)(N_{d^*}\mathbf{1}_p)'$. Hence by (5.3.1), Lemma 5.3.1, and Remark 1 following Theorem 5.4.1, it now remains to show that $G_2M_{d^*}M'_{d^*}$ is symmetric when d^* satisfies the conditions of Theorem 5.4.2.

From (5.3.2) it follows that

$$M_{d^*}M'_{d^*} = \sum_{j=1}^n \binom{p-1}{\sum_{i=0}^n \ell_{ij}} \binom{p-1}{\sum_{i=0}^n \ell_{ij}} \binom{p-1}{i=0} \ell_{ij}.$$
 (5A.1)

Since d^* is a SBURMD(t, n, p), by (5.3.4) and the definition of G_2 , for each $j(1 \le n)$

 $j \leq n$),

$$G_{2}\begin{pmatrix} \sum_{i=0}^{p-1} \ell_{ij} \end{pmatrix} = \mathbf{1}_{t} \otimes \left[t^{-1} \mathbf{1}_{t} + \sum_{i=1}^{p-1} \mathbf{e}_{d^{*}(i-1,j)} \right]$$
$$= \mathbf{1}_{t} \otimes \left[(p+1)t^{-1} \mathbf{1}_{t} - \mathbf{e}_{d^{*}(p-1,j)} \right].$$

This, together with (5A.1) yields

$$G_2 M_{d^*} M'_{d^*} = (p+1)t^{-1} \left(\mathbf{1}_t \otimes \mathbf{1}_t \right) \left(\sum_{j=1}^n \sum_{i=0}^{p-1} \ell_{ij} \right)'$$
$$- \sum_{j=1}^n \left(\mathbf{1}_t \otimes \mathbf{e}_{d^*(p-1,j)} \right) \left(\sum_{i=0}^{p-1} \ell_{ij} \right)'.$$

By (5.4.1), the first term in $G_2M_{d^*}M'_{d^*}$ is symmetric. By (5.3.4) the second term equals

$$t^{-1} \sum_{j=1}^{n} \left(\mathbf{1}_{t} \mathbf{e}_{d^{*}(0,j)}^{\prime} \right) \otimes \left(\mathbf{e}_{d^{*}(p-1,j)} \mathbf{1}_{t}^{\prime} \right)$$

$$+ \sum_{j=1}^{n} \left(\mathbf{1}_{t} \otimes \mathbf{e}_{d^{*}(p-1,j)} \right) \left(\sum_{j=1}^{p-1} \mathbf{e}_{d^{*}(i,j)}^{\prime} \otimes \mathbf{e}_{d^{*}(i-1,j)}^{\prime} \right)$$

$$= nt^{-3} \left(E_{t} \otimes E_{t} \right) + \sum_{h=0}^{t-1} \left(\mathbf{1}_{t} \otimes \mathbf{e}_{h} \right) \left(\sum_{j \in S_{d^{*}h}} \sum_{i=1}^{p-1} \mathbf{e}_{d^{*}(i,j)}^{\prime} \otimes \mathbf{e}_{d^{*}(i-1,j)}^{\prime} \right)$$

$$= nt^{-3} \left(E_{t} \otimes E_{t} \right) + \sum_{h=0}^{t-1} \left(\mathbf{1}_{t} \otimes \mathbf{e}_{h} \right) \left[\mathbf{1}_{t}^{\prime} \otimes \left\{ \nu_{2} \mathbf{1}_{t}^{\prime} - (\nu_{2} - \nu_{1}) \mathbf{e}_{h}^{\prime} \right\} \right]$$

$$= \left(nt^{-3} + \nu_{2} \right) \left(E_{t} \otimes E_{t} \right) - \left(\nu_{2} - \nu_{1} \right) \left(E_{t} \otimes I_{t} \right), \tag{5A.2}$$

by applying the conditions (i) and (ii) of Theorem 5.4.2. Since (5A.2) is symmetric the result follows.

Q.E.D.

Chapter 6

SOME RESULTS ON SERIALLY BALANCED SEQUENCES

6.1 <u>Introduction</u>

A class of designs very closely related to the R.M.D.'s, which were discussed in chapter 5, is the class of serially balanced sequences. As in the case of R.M.D.'s, in these designs also, the 'residual effect' of a treatment is an important source of variation along with the usual 'direct effect'.

Williams (1949) gave designs balanced for the estimation of residual effects. Finney and Outhwaite (1955), Finney (1956) introduced serially balanced sequences of types 1 and 2, to study experiments where there is only one experimental unit which is exposed to a sequence of treatments in succession. Such experiments are common in the field of biological assay and for the practical applications of such designs we refer to Finney (1956).

Sampford (1957) gave methods of construction of type 1 and type 2 sequences and gave the analysis of a particular subclass of type 1 sequences. This subclass of sequences was called "standard" by Sinha (1975) and he was the first to study the optimality properties of these sequences. Sinha (1975) proved the A-, D-, and E-optimality properties of standard type 1 sequences under the usual fixed effects additive model.

In this chapter we have studied serially balanced sequences under two different relevant models and investigated their optimality properties.

Section 6.2 consists of various definitions and notations which have been used

in the subsequent sections of this chapter. Throughout the chapter, the symbols $0, 1, 2, \ldots$ represent the different treatments and the sequences are written with rows as blocks.

In Section 6.3, the universal optimality of a particular class of serially balanced sequences has been proved; universal optimality results have also been obtained for more general types of sequences. In the next section a general method of constructing such optimal sequences has been presented. These two sections consider the usual fixed effects additive model that has been used by Sampford (1957) and Sinha (1975).

As in the case of R.M.D.'s, in the case of serially balanced designs also, the interaction between direct and residual effects may be an important source of variation, since the same experimental unit is subjected to a sequence of treatments repeatedly. So, in Section 6.5 a non-additive model, analogous to that in Chapter 5, is considered, by introducing the interaction due to direct and residual effects in the usual model. In Section 6.5, the calculus for factorial experiments is used to prove a number of optimality results. It is shown that under the non-additive model, the type 1 sequences are universally optimal for the estimation of direct effects among the class of all sequences of the same length. For the estimation of residual effects, a similar result holds for a class of sequences which are modified versions of type 1 sequences.

In Section 6.6 we again return to the usual fixed effects additive model of Section 6.2 and study the optimality properties of type 1 sequences under this model. The result of Sinha (1975) follow as a corollary of one of the results in this section.

6.2 Definitions and Notations

Definition 6.2.1 A serially balanced type 1 sequence of order v and index m is a closed chain of symbols such that (i) each of the v distinct symbols occurs mv times in the sequence; (ii) the sequence falls into mv blocks, each containing the v different symbols once each; and (iii) the v^2 possible different pairs of symbols occur m times each among the mv^2 pairs of consecutive symbols in the sequence (Sampford (1957)). Definitions 6.2.2. A serially balanced type 2 sequence of order v and index m is a closed chain of symbols such that (i) each of the v distinct symbols occurs m(v-1) times in the sequence; (ii) the sequence falls into m(v-1) blocks each containing the v symbols once each; and (iii) the v(v-1) possible ordered pairs of distinct symbols occur exactly m times each, no symbol following itself (Sampford (1957)).

It is assumed (cf. Sampford (1957)) that the last treatment in the last block is also applied as a conditioning treatment right in the beginning of the sequence, any observation arising out of this conditioning treatment being excluded from the analysis.

Two sequences are shown below. The first one is a type 1 sequence and the second one is a type 2 sequence.

Example 6.2.1
$$v = 4, m = 1$$
 $v = 4, m = 1$ (i) $0 5 1 4 2 3 (ii) 1 2 3 0 3 5 2 4 0 1 2 1 0 3 1 3 2 0 4 1 5 0 3 2 1 3 0 4 5 4 3 1 2 0$

<u>Definition 6.2.3.</u> A standard sequence of order v and index m is a closed chain of

symbols such that (i) each of the v distinct symbols occurs mv times in the sequence; (ii) the sequence falls into mv blocks, each containing the v symbols once each and (iii) on dividing the mv blocks into m sets of v each and numbering the v blocks in the j^{th} set as (j_1, j_2, \ldots, j_v) ; for every $j, 1 \leq j \leq m$, the blocks j_1, j_2, \ldots, j_v begin with the symbols $0, 1, \ldots, v-1$ (or $0, v-1, v-2, \ldots, 2, 1$) in the order and end with $1, 2, \ldots, v-1, 0$ (or $v-1, v-2, \ldots, 1, 0$) in the order. (Sinha (1975))

Clearly, standard sequences are not necessarily serially balanced and again, every serially balanced sequence is not standard. The following is an example of a standard type 1 sequence.

Example 6.2.2.

We now introduce one more sequence whose optimality properties will be investigated in Section 6.5.

Definition 6.2.4. A type 1* sequence of order v and index m is a closed chain of symbols such that (i) each symbol occurs mv times in the sequence, (ii) the sequence falls into mv blocks each containing the residual effect of each symbol once each; and (iii) the v^2 possible different pairs of symbols occurs m times each among the mv^2 pairs of consecutive symbols in the sequence.

The following is an example of a type 1* sequence.

The remaining definitions all relate to type 2 sequences.

<u>Definition 6.2.5.</u> A type 2 sequence is called completely reversible if each block ends or begins with the same symbol. (Sampford (1957)).

We now introduce two more sequences whose optimality properties will be investigated in Section 6.3.

<u>Definition 6.2.6.</u> A serially balanced completely reversible type 2 sequence will be called a type 2* sequence if (i) the sequence is of index 1 and (ii) each block ends with the same symbol.

Example 6.2.4. The following is a type 2* sequence where every ordered pair of distinct symbols occur exactly once.

$$v = 5, m = 1$$
 $1 \quad 2 \quad 3 \quad 4 \quad 0$
 $2 \quad 4 \quad 1 \quad 3 \quad 0$
 $3 \quad 1 \quad 4 \quad 2 \quad 0$
 $4 \quad 3 \quad 2 \quad 1 \quad 0$

Let $E_{mm'}$ be an $m \times m'$ matrix with all elements unity and I_m be the $m \times m$ identity matrix. Interpreting symbols as treatments, it is clear that in a type 2^* sequence the direct effect versus residual effect incidence matrix is $E_{vv} - I_v$, which is, in fact, the incidence matrix of a symmetric balanced incomplete block (SBIB) design. So, Definition 6.2.6 may be extended to

Definition 6.2.7. A type $2^*(u)$ sequence of order v and length $vu(u \le v - 1)$ is a closed chain of symbols such that (i) each of the v distinct symbols occurs u times in the sequence, (ii) the sequence falls into u blocks each containing the v symbols once each (iii) the direct effect versus first order residual effect incidence matrix is that of an SBIB design and (iv) each block ends with the same treatment.

Clearly, type $2^*(u)$ sequences constitute a much larger class than type 2^* sequences. For practical applications, a type $2^*(u)$ sequence is usually more economic than a type 2^* sequence (since the former is of a shorter length) and it reduces to a type 2^* sequence if u = v - 1.

Example 6.2.5. With v = 7, the following is a type $2^*(3)$ sequence.

$$v = 7, u = 3$$
1 2 3 4 5 6 0
2 4 6 1 3 5 0
4 1 5 2 6 3 0

6.3 Optimality Results Under Additive Model

Let C(n) be the class of all sequences with v symbols and length n. Consider an arrangement of v symbols (treatments) $0, 1, \ldots, v-1$ according to any sequence in C(n). Suppose the sequence consists of b blocks and the conditioning treatment has been applied as usual. The following fixed-effects additive linear model has been used by Sampford (1957) and Sinha (1975)

$$y_{ij} = \mu + \beta_i + \delta_{g_{ij}} + \xi_{h_{ij}} + e_{ij}$$
 (6.3.1)

where g_{ij}, h_{ij} are the treatments whose direct and residual effects occur in y_{ij} , the j^{th} observation from the i^{th} block, μ is the general mean, β_i is the i^{th} block effect and $\delta_{\omega}, \xi_{\omega}$ are respectively the direct and first order residual effects due to the ω -th

treatment ($\omega = 0, 1, ..., v-1$), $\beta_i, \delta_\omega, \xi_\omega$ being measured from the general mean. The random disturbances e_{ij} are uncorrelated with means zero and a constant variance σ^2 .

Let $N^{(v \times b)}(N^{*(v \times b)})$ be the incidence matrix considering direct (first order residual) effects of treatments with respect to blocks. Let r_{ω} be the number of replications of the ω -th treatment ($\omega = 0, 1, \ldots, v-1$) and k_i be the i-th block size ($i = 1, 2, \ldots, b$). Let $\mathbf{r}^{\delta} = \mathrm{Diag}(r_0, \ldots, r_{v-1}), \mathbf{k}^{\delta} = \mathrm{Diag}(k_1, \ldots, k_b)$.

Let $Z^{(v \times v)} = ((z_{\omega\omega'}))$, where $z_{\omega\omega'}$ is the number of times the direct effect of the ω -th treatment occurs with the first order residual effect of the ω' -th treatment.

For any sequence in C(n), under the model (6.3.1), it can be easily seen that the coefficient matrices of the reduced normal equations for direct and first order residual effects are respectively given by

$$G_{1} = \mathbf{r}^{\delta} - (Z N) \begin{bmatrix} \mathbf{r}^{\delta} & N^{*} \\ N^{*'} & \mathbf{k}^{\delta} \end{bmatrix}^{-} \begin{bmatrix} Z' \\ N' \end{bmatrix}$$

$$G_{2} = \mathbf{r}^{\delta} - (Z' N^{*}) \begin{bmatrix} \mathbf{r}^{\delta} & N \\ N' & \mathbf{k}^{\delta} \end{bmatrix}^{-} \begin{bmatrix} Z \\ N^{*'} \end{bmatrix}$$
(6.3.2)

The optimality result in this section is based on a result due to Kiefer (1975). The following three lemmas will be required in the proof. The proof of the first lemma is trivial and hence omitted.

<u>Lemma 6.3.1.</u> Let $X = \{X_1, X_2, X_3\}$. Then $\{X_1'X_1 - X_1'X_2(X_2'X_2)^{-}X_2'X_1\}$

$$-\left[X_1'X_1-\left(X_1'X_2 & X_1'X_3\right)\left(\begin{array}{cc}X_2'X_2 & X_2'X_3 \\ X_3'X_2 & X_3'X_3\end{array}\right)^{\top}\left(\begin{array}{cc}X_2'X_1 \\ X_3'X_1\end{array}\right)\right]$$

is nonnegative definite.

Lemma 6.3.2. Let n = vu ($u \le v - 1$). Then, for any sequence in C(vu),

(i)
$$tr(G_1) \le v(u-1)$$
, (ii) $tr(G_2) \le v(u-1)$.

Proof: Since, by Lemma 6.3.1,

$$\mathbf{r}^{\delta} - Z\mathbf{r}^{-\delta}Z' - \left[\mathbf{r}^{\delta} - (Z\ N) \begin{pmatrix} \mathbf{r}^{\delta} & N^* \\ N^{*'} & \mathbf{k}^{\delta} \end{pmatrix}^{-} \begin{pmatrix} Z' \\ N' \end{pmatrix}\right]$$

is nonnegative definite, it follows by (6.3.2) that

$$tr(G_{1}) \leq tr(\mathbf{r}^{\delta} - Z\mathbf{r}^{-\delta}Z') = n - \sum_{\omega=0}^{v-1} \sum_{\omega'=0}^{v-1} \left(z_{\omega\omega'}^{2}/r_{\omega'}\right)$$

$$\leq n - \sum_{\omega=0}^{v-1} \sum_{\omega'=0}^{v-1} \left(z_{\omega\omega'}/r_{\omega'}\right) = v(u-1)$$

since n = vu and $\sum_{\omega=0}^{v-1} z_{\omega\omega'} = r_{\omega'}$ for each ω' . This proves (i). (ii) can be proved similarly.

Lemma 6.3.3. Let n = vu $(u \le v - 1)$. Then for a type $2^*(u)$ sequence (if it exists) $tr(G_1) = tr(G_2) = v(u - 1).$

<u>Proof:</u> By Definition 6.2.7, for a type $2^*(u)$ sequence the direct effect versus block and first order residual effect versus block incidence matrices are those of a randomized block design.

Hence $N=N^*=E_{vu}$ and $\mathbf{r}^\delta=u\;I_v,\;\mathbf{k}^\delta=v\;I_u$. Further, the direct effect versus first order residual effect incidence matrix Z is that of an SBIB design and hence

$$ZZ' = (u - \lambda)I_v + \lambda E_{vv} , \qquad (6.3.3)$$

 λ being the usual λ parameter of the SBIB design given by Z. Hence by (6.3.2), for such a sequence

$$G_1 = u I_v - \begin{bmatrix} Z E_{vu} \end{bmatrix} \begin{bmatrix} u I_v & E_{vu} \\ E_{uv} & v I_u \end{bmatrix} \begin{bmatrix} Z' \\ E_{uv} \end{bmatrix}.$$
 (6.3.4)

It can be shown that

$$\begin{bmatrix} u & I_v & E_{vu} \\ E_{uv} & v & I_u \end{bmatrix}^- = \begin{bmatrix} u^{-1} & I_v & -(vu)^{-1} & E_{vu} \\ -(uv)^{-1} & E_{uv} & v^{-1}I_u + (vu)^{-1} & E_{uu} \end{bmatrix}$$

and hence applying (6.3.3), after some simplication it follows from (6.3.4) that

$$G_1 = (\lambda/u)(vI_v - E_{vv}).$$
 (6.3.5)

Hence, remembering that $\lambda(v-1) = u(u-1)$, it follows that

$$tr(G_1)=v(u-1).$$

Similarly it can be shown that $tr(G_2) = v(u-1)$.

Note that if v = 2, then the relation $v > u > \lambda$ makes G_1 as in 6.3.5 a null matrix. Similarly, G_2 will also be a null matrix if v = 2. To avoid such trivialities, consider hereafter v > 2.

Then, by (6.3.5) the matrix $G_i(i=1,2)$ for a type $2^*(u)$ sequence is completely symmetric. It has also maximum trace in C(vu) (by Lemmas 6.3.2 and 6.3.3). Therefore by Proposition 1 in Kiefer (1975), the following universal optimality result holds.

Theorem 6.3.1. Within the class C(vu) if a type $2^*(u)$ sequence exists then it is universally optimal for both direct and first order residual effects, under the model assumed, provided v > 2.

Noting that a type 2^* sequence is nothing but a type $2^*(u)$ sequence of length v(v-1), it follows that

Corollary 6.3.1. Within the class C(v(v-1)) if a type 2* sequence exists then it is universally optimal for both direct and first order residual effects, under the model assumed, provided v > 2.

Remarks:

- 1. These optimality results are fairly general since the competing designs are all possible designs of the same length.
- 2. As Definition 6.2.6 indicates, a type 2* sequence has index unity. A question naturally arises that if a type 2* sequence be repeated m(>1) times, then whether such a sequence will also be universally optimal, both for direct and residual effects, within the class C(mv(v-1)) of sequences of length mv(v-1). The answer to this question will be in the negative as the following example illustrates.

Example 6.3.1. With v = 3, m = 3, consider the two sequences

 S_1 is obtained by repeating a type 2* sequence thrice, while S_2 is a type 1 sequence. Both S_1 and S_2 belong to C(18). By direct computation it can be shown that S_1 is inferior to S_2 from the point of view of D-optimality for estimating any complete set of orthonormal contrasts of direct effects. Hence S_1 cannot be universally optimal in C(18) for direct effects.

This above phenomenon is expected since if a type 2^* sequence be repeated m(>1) times then the direct effect versus residual effect incidence matrix no longer remains that of an SBIB design and so the technique of Lemma 6.3.3 fails.

3. The universal optimality results proved in this section hold even if in the model

- (6.3.1) the random disturbances e_{ij} have a (known) intraclass correlation structure, instead of being uncorrelated. It may be pointed out that "class" in the intraclass correlation structure refers to a block. Since in this kind of experimentation all the observations relate to the same experimental unit, the study of optimality properties in the presence of correlation of this kind sometimes becomes relevant. The proof of this robustness property of the optimality results is lengthy but straightforward. The details may be found in Mukerjee and Sen (1983).
- 4. For some further results on the universal optimality of type 2* sequences under a different kind of model, where a certain fraction of the direct effect of a treatment wears off leaving only a fraction of the direct effect as the residual effect of the treatment, we refer to Sen and Sinha (1986).

6.4 A Method of Constructing Type 2* (u) Sequences

This section considers the problem of constructing the sequences which were shown to be optimal in the previous section.

Sampford (1957) gave methods of constructing completely reversible type 2 sequences. Since a type 2^* sequence is nothing but a completely reversible type 2 sequence of index unity, where each block ends with the same treatment, such sequences in v symbols, can be constructed following Sampford (1957). This can be always done for every odd $v(v \geq 3)$ and also for some even v.

As for type $2^*(u)$ sequences, which are generalizations of type 2^* sequences, the constructional aspects pose more stringent combinatorial problems. The following

method of construction is obtained by suitably modifying the method of differences for the construction of balanced incomplete block designs (Raghavarao (1971, Ch. 5)). This method has a fairly wide coverage and is described below.

Suppose v is a prime and let M be a module $\{0, 1, \ldots, v-1\}$ and $S = \{a_1, \ldots, a_u\}$ be a set of u distinct nonzero elements M such that among the ordered differences arising out of S, each non-zero element of M is repeated a constant number (say, λ) of times. Then

$$a_1 \quad 2a_1 \quad \dots \quad (v-1)a_1 \quad 0$$
 $a_2 \quad 2a_2 \quad \dots \quad (v-1)a_2 \quad 0$
 $\vdots \quad \vdots \quad \vdots \quad \vdots$
 $a_u \quad 2a_u \quad \dots \quad (v-1)a_u \quad 0$

$$(6.4.1)$$

where each entry is reduced mod v, can be seen to be a type $2^*(u)$ sequence (with blocks, as usual, given by rows) in v symbols and length vu. This is because, with notations as in Section 6.3, clearly $N=N^*=E_{vu}$. Further, for $0 \le \omega \le v-1$, in (6.4.1), the symbol ω is followed by the symbols $\omega + a_i(1 \le i \le u)$. Hence Z is the incidence matrix of the SBIB design generated by the method of differences from the initial set $\{a_1, \ldots, a_u\}$, proving our assertion.

In particular, if v = 4t + 3 be a prime, then S may be taken as any block (not containing the symbol zero) of the SBIB design, constructed by the method of differences, involving (4t + 3) symbols, with block size (2t + 1) and the usual parameter $\lambda = t$ (Raghavarao, (1971), p. 83). This gives a type $2^*(u)$ sequence with v = 4t + 3, u = 2t + 1. For example, if v = 7 or 11 one may take $S = \{1, 2, 4\}$ or $S = \{1, 3, 4, 5, 9\}$ respectively. The $2^*(u)$ sequence in Example 6.2.5 was constructed starting from such an S.

Apart from this series, other SBIB designs, obtained by the method of differences, can be reoriented to yield type $2^*(u)$ sequences. The following example serves as an illustration.

Example 6.4.1. Let v = 13. Then $M = \{0, 1, ..., 12\}$. Let $S = \{1, 2, 4, 10\}$. Then among the ordered differences arising out of S, each non-zero member of M is repeated $\lambda (=1)$ times. On developing S, as in (6.4.1) as

one gets a type $2^*(u)$ sequence with v = 13, u = 4. Incidentally, S is as well an initial block from which, by the method of differences, one can construct an SBIB design in 13 symbols with block size 4 and the usual parameter $\lambda = 1$.

Remark: The results in this section appear in Mukerjee and Sen (1985). It may be remarked that subsequently some similar results were independently obtained by Jimbo (1986).

6.5 Optimality Properties of a Type 1 Sequence Under a Non-additive Model

In this section, as in Chapter 5, the interaction between direct and residual effects is considered as a source of variation. So the following fixed effects non-additive model is used.

$$y_{ij} = \mu + \beta_i + \delta_{gij} + \xi_{hij} + \gamma_{hij,gij} + e_{ij}$$
 (6.5.1)

where $y_{ij}, \mu, \beta_i, \delta_{g_{ij}}, \xi_{h_{ij}}$ are as in 6.3.1 and $\gamma_{\omega,\omega'}$ represents the interaction effect due to treatments ω and ω' .

Using an interpretation similar to that in Section 5.3 of Chapter 5, a serially balanced sequence of type 1 may be looked upon as a v^2 factorial experiment with the direct and residual effects representing the main effects of the first and second factor respectively, while the direct-versus-residual interaction represents the usual 2-factor interaction.

The following result on factorial experiments will be used subsequently.

Lemma 6.5.1. Consider an equireplicate two-factor experiment d_{\circ} in a block design such that within each block, the levels of the first factor F_1 occur equally frequently. Let \mathcal{C} be the class of all designs with the same number of observations. Then, under

possible presence of interaction,

- (i) main effect F_1 is orthogonal to both main effect F_1 and interaction effect F_1F_2 and
- (ii) d_o is universally optimal for F_1 within C

The proof of this lemma is straightforward and hence omitted.

Consider any type 1 sequence. Then, remembering the analogy between such a sequence and a factorial experiment, from Definition 6.2.1 and Lemma 6.5.1 it follows that

Theorem 6.5.1. Under a non-additive model,

- (i) in a type 1 sequence, best linear unbiassed estimators of direct effect contrasts are orthogonal to best linear estimators of residual and interaction effects contrasts and
- (ii) within the class $C(mv^2)$, a type 1 sequence of order v and index m, if it

exists, is universally optimal for the estimation of direct effect contrasts.

Remarks:

- As in section 5.4 it may be seen that under a non-additive model not all contrasts belonging to the direct or the residual effects are estimable in a type 2* or a type 2*(u) sequence. Hence the optimality results on such sequences, as in section 6.3, do not remain robust under non-additivity.
- 2. It may be noted that, under the non-additive model, in a type 1 sequence, residual effect will not be in general orthogonal to the interaction effect. The following example illustrates this:

Example 6.5.1. Consider the type 1 sequence:

$$v = 3, m = 2$$
 $0 \quad 1 \quad 2$
 $2 \quad 0 \quad 1$
 $1 \quad 2 \quad 0$
 $0 \quad 2 \quad 1$
 $1 \quad 0 \quad 2$
 $2 \quad 1 \quad 0$

Interpreting this sequence as a 2-factor design with the direct effect and the residual effect as the two factors respectively, the C-matrix of this design is

$$C = 2(I_1 \otimes I_2) - rac{1}{3} egin{bmatrix} 2 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 0 \ 0 & 2 & 0 & 0 & 1 & 1 & 1 & 0 & 1 \ 0 & 0 & 2 & 1 & 1 & 0 & 0 & 1 & 1 \ 1 & 0 & 1 & 2 & 0 & 0 & 0 & 1 & 1 \ 0 & 1 & 1 & 0 & 2 & 0 & 1 & 1 & 0 \ 1 & 1 & 0 & 0 & 0 & 2 & 1 & 0 & 1 \ 1 & 1 & 0 & 0 & 0 & 1 & 1 & 2 & 0 & 0 \ 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 2 \end{bmatrix}$$

It can be easily verified (cf. Chauhan and Dean (1986)) that for this design, the main

effect of the second factor (i.e., residual effect) is not orthogonal to the interaction effect. So under a non-additive model, a type 1 sequence will not be generally optimum for the estimation of residual effects. However, we can modify type 1 sequences to get type 1* sequences which are optimal for residual effects.

From Definition 6.2.4 and Lemma 6.5.1, the following theorem follows easily.

Theorem 6.5.2. Under a non-additive model,

- (i) in a type 1* sequence, the best linear unbiassed estimators of residual effect contrasts are orthogonal to best linear estimators of direct and interaction effect contrasts and
- (ii) within the class $C(mv^2)$, a type 1* sequence of order v and index m, if it exists, is universally optimal for the estimation of residual effect contrasts.

Remarks:

- 1. It can be shown through examples that type 1* sequences are not optimal for the direct effects.
- 2: The construction of type 1* sequences pose no new problem. From Definitions 6.2.1 and 6.2.4 it is clear that starting from a type 1 sequence, one can easily construct a type 1* sequence by applying the symbol i in 'period' p of the type 1* sequence provided the symbol i occurs in 'period' (p+1) of the type 1 sequence. In fact, the type 1* sequence in Example 6.2.3 has been constructed by this method starting from the type 1 sequence in Example 6.2.1.
- 6.6 Optimality Properties of a Type 1 Sequence Under an Additive Model

 In this section the underlying model is the usual fixed effects additive model

in (6.3.1). The following result follows in a straightforward manner using a lemma similar to Lemma 6.5.1 for an additive model.

Theorem 6.6.1. Under an additive model

- (i) in a type 1 sequence, the best linear unbiassed estimators of direct effect contrasts are orthogonal to those of the residual effect contrasts and
- (ii) within the class $C(mv^2)$, a type 1 sequence of order v and index m, if it exists, is universally optimal for the estimation of direct effects.

We here introduce a concept called "strong optimality". Consider a class of designs \mathcal{C} for estimating a parameter θ . For any design $d \in \mathcal{C}$, let Σ_d be the dispersion matrix of the BLUE of θ in d, provided θ is estimable in d. Let $\mathcal{C}_{\circ} = \{d | d \in \mathcal{C}, \theta \text{ is estimable in } d\}$. Then a design d_{\circ} is called "strongly optimal" in \mathcal{C} if $d_{\circ} \in \mathcal{C}_{\circ}$ and $\Sigma_d - \Sigma_{d_{\circ}}$ is n.n.d. $\forall d \in \mathcal{C}_{\circ}$

Turning our attention to the residual effects, from Theorem 6.6.1 (i) and Definition 6.2.1, the following result is immediate.

Theorem 6.6.2. Under an additive model, a type 1 sequence is strongly optimal for the estimation of residual effect contrasts within the class of all designs having the same 'residual-effect-versus-block' incidence matrix.

Remark: Theorem 6.6.2 covers, as a special case, the principal result in Sinha (1975). Sinha (1975) essentially proves Theorem 6.6.2 when the type 1 sequence is a standard sequence. (cf. Definition 6.2.3). Theorem 6.6.2 states that the observations of Sinha are valid even when a type 1 sequence is not a standard one. Examples of type 1 sequences may be given, which are not standard sequences.

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