FUNDAMENTAL CONCEPTS OF FRACTIONAL REPLICATION

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ABSTRACT

An overall and rigorous perspective of the subject of fractional replication in its most general form was needed. It was necessary to lay the groundwork for understanding the concepts and for developing new results. This monograph is an attempt at achieving these objectives. It is not a literature review of published research in this area but it is comprehensive and self-contained from the viewpoint of basic definitions, ideas, and procedures.

Chapter one is an introductory one. The second chapter contains preliminary definitions and notations. The polynomial model for observations in terms of the factorial effects is developed in Chapter 3; the least squares method of estimation is utilized. In Chapter 4, mathematical constraints and criteria are discussed leading to eight criteria for selecting a design. In the fifth chapter we classify the class of unbiased designs with and without negligibility assumptions on the total parametric vector and obtain search rules for minimal unbiased designs. Chapter 6 specifically deals with designs of arbitrary resolution where the partitioning of the total parametric vector is from the experimenter's viewpoint; this approach contains the designs for even and for odd resolution. Additional properties such as orthogonality and balancedness are introduced in Chapter 7 and are related to previously introduced designs. Chapter 8 lists twenty-three methods of constructing fractional factorial designs and presents the details of three of them, viz. Hadamard matrix methods, composition methods, and orthogonal latin square methods. Finally Chapter 9 gives a very selected list of references on the topics; we list 41 references selected from the approximately 1000 references available.

From the above it should be noted that our concept of fractional replications involves the following ideas:

(i) Fractional replication is discussed in its most general and unrestricted form from the linear model viewpoint.

(ii) Arbitrary replications of treatments of the factorial are permitted.

(iii) The total parametric vector is partitioned into sets of single degree of freedom contrasts which are meaningful to the experimenter. (This approach departs from the traditional resolution III, IV, and V plans.)

(iv) We attempt to characterize and then to construct a class of minimal unbiased designs so that the experimenter will have designs with a minimal number of points providing estimates for the specified parameters.

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PREFACE

This monograph was prepared during the 1972 Spring Term at Cornell University. The material herein is a result of preparing lectures for an advanced class in the design of experiments.

We wish to express our gratitude to the three graduate students, (J. Eccleston, P. Farquhar, and J. Joiner) for participating in the class. In particular, their queries, remarks during the discussions, and lectures on resolution III, IV, and V plans were helpful in preparing the final copy of the manuscript. Finally, we wish to thank Mrs. Anne White for her efforts in the typing of this monograph.

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CHAPTER 1

INTRODUCTION

The purpose of this monograph is to fill a void that currently exists in published literature regarding fractional replication. The literature, though voluminous, does not contain a comprehensive treatise on the various aspects of fractional replication. This monograph provides a place, then, where the interested person may direct his attention in the pursuit of knowledge about the theory of fractional replication; it also unifies the fundamental concepts of the theory in an organized manner for persons with sufficient mathematical and statistical background. This monograph is also a place to which a mathematician may turn in order to become acquainted with the subject. Finally, teachers of experiment and treatment designs will find in this monograph the necessary concepts and definitions for a course on fractional replication.

In presenting a comprehensive treatise on the subject of fractional replication, we have departed from the traditional approaches, notations, and definitions. We did this for several reasons. The first being that it is necessary to be *precise* and *rigorously* define all concepts involved. This is essential for the mathematician and for the statistician as they cannot work with fuzzily and vaguely defined concepts. The use of the term "factor" in factorial experiments is incomprehensible to a mathematician. Because of this situation, it is necessary to define terms in an unambiguous way.

Other reasons for departing from the traditional approach are:

(a) We wish the reader to be unencumbered by previous notions about fractional replication, i.e., we wish to make a fresh start.

(b) Traditional notation usually breaks down in a more general setting.

(c) Current concepts of fractional replication for the majority of statisticians relate solely to "so-called" and vaguely defined regular fractions.

(d) Current concepts of factorial experiments for the majority of statisticians pertain to n-way classifications with an equal number of observations per combination.

(e) The new notation used allows for generality and mathematical preciseness and rigor.

The traditional approach in experiment and treatment design work has been to construct classes of designs and then to describe the properties pertaining to the designs. We shall not use this approach; instead we shall first precisely define the concepts involved in fractional replication in combinatorial and statistical terms. Then, we shall discuss restraints and objectives as related to criteria for "goodness". We then present some characterizations and constructions using the developed concepts.

Specifically in Chapter 2 we present the preliminary concepts and definitions which are then used in the following chapters as a basis for developing the theory of fractional replication. Chapter 3 develops the orthogonal polynomial model together with the least squares estimation of the underlying parameters. Chapter 4 brings out mathematical and other constraints and criteria from the experimenter's point of view so that an optimal design can be selected in a rational manner. In Chapter 5 we develop the concept of minimal unbiased design for any linear parametric function. This leads to a characterization of such designs. Chapter 6 provides typical assumptions on the whole parametric vector, resulting in resolution type of plans as a special case. In Chapter 7 the properties of orthogonality and balancedness are introduced leading to further conditions on the selection of a design. Chapter 8 provides a list of construction methods and illustrates three of them. Finally, in Chapter 9 a fairly comprehensive literature list is given so that the reader may find further details on fractional replication. Whenever there was a need to clarify introduced concepts and definitions, examples are given.

CHAPTER 2

PRELIMINARIES AND NOTATIONS

In the first section of this chapter we present the concepts and definitions associated with fractional replication in a form suitable for those working in combinatorial and statistical theory. These then will serve as a basis for posing the resulting mathematical problems. The second section is mostly concerned with some statistical concepts and definitions which are required for the ensuing mathematical and statistical developments.

2.1. COMBINATORIAL ASPECTS AND DEFINITIONS

Definition 2.1. Consider t non-empty, not necessarily distinct sets* $G_1, G_2, \dots, G_t$ with cardinalities $k_1, k_2, \dots, k_t$ respectively. With each set G_i, we shall associate a formal symbol F_i, which will be denoted as the i-th factor.

The reader may question the reason for using two symbols F_i and G_i. The usefulness for this is especially apparent in the cases where the elements of the G_i's are labeled with the same names. Example 2.2 below is a case in point.

Definition 2.2. The elements of G_i when associated with the formal symbol F_i will be called the levels of the i-th factor.

Note that the levels of a factor are the possible levels specified by the experimenter at which an experiment can be conducted. This does not mean that all of them are used in a particular experiment.

Let G be the Cartesian product of the G_i's, that is, $G = \times_{i=1}^{t} G_i$, where the symbol $\times$ denotes the Cartesian product. Let $|G| = \prod_{i=1}^{t} k_i$ be the cardinality of G. The set G together with the F_i's is often referred to as the factor space.

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* A set will be defined to be a collection of distinct elements, i.e. a listing without repetitions. If repetitions are allowed we shall always use the term collection.

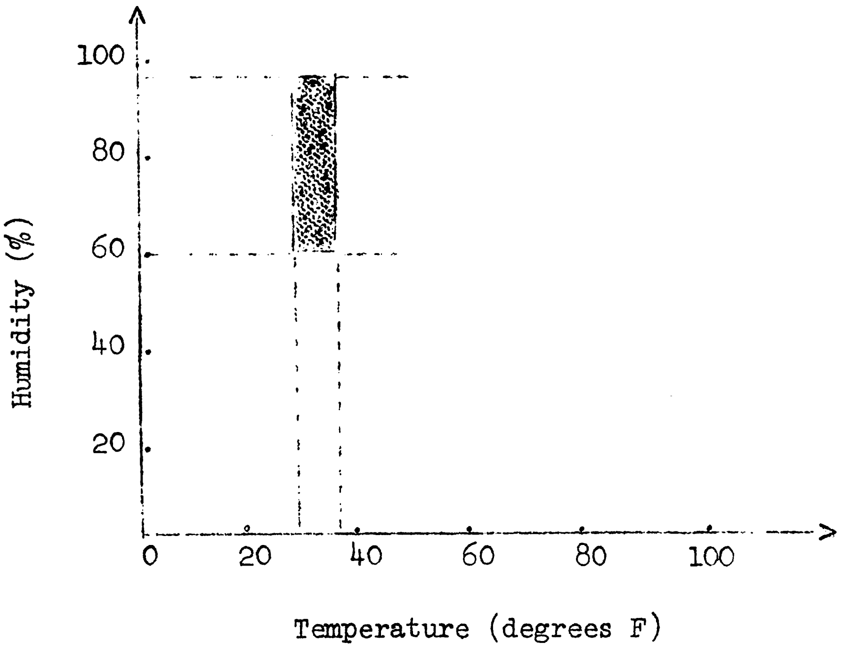
Hereafter, whenever we discuss G, it is to be understood that we mean the set G together with the associated factors $F_1, F_2, \ldots, F_t$.

Definition 2.3. An element of G is defined to be a treatment.

Note that the terms "combinations", "treatment combinations", "runs", and "assemblies" also appear in the literature as names for the elements of G; also note that in this setting, we allow $t = 1$.

Before proceeding further we present two examples to illustrate the concepts developed thus far.

Example 2.1. Consider an experiment where the effects of temperature and humidity on the keeping quality of potatoes held in storage are being studied. The range of experimentation for temperature is from 29°F to 38°F while that for humidity is from 60% to 95%. Represent temperature as the horizontal axis and humidity as the vertical axis in the Cartesian plane. The shaded area in the figure below represents the combinations of temperature and humidity which are of experimental interest:



Identifying temperature with F_1 and humidity with F_2, we see that $G_1 = [29^\circ F, 38^\circ F]$ and $G_2 = [60\%, 95\%]$. For example, a level of F_1 is $36^\circ F$ and a level of F_2 is 72.3%. Finally, the shaded area is G, and hence a treatment is a point in G, for instance, $(37^\circ F, 90\%)$.

Remark. From the above example it is clear that we will find it convenient sometimes not merely to let the elements of a G_i be numbers but rather numbers with units.

Example 2.2. A sociologist was interested in studying the influence of religious affiliation and income on attitude of individuals within a certain city toward extra-marital sexual relations. The three denominations which could be studied were Protestant (P), Catholic (C), and Jewish (J) and the income levels specified were low (L), medium (M) and high (H) as defined by the experimenter. The factors in this example are religion (F_1) and income (F_2) and the levels of the factors are given by $G_1 = \{P, C, J\}$ and $G_2 = \{L, M, H\}$.

Note that often levels in such an experiment are coded by $\{1,2,3\}$ for each G_i. With such nomenclature, it is clear why "level one of F_2" is a useful designation; that is why it was useful to introduce the symbol F_i.

In what follows we assume G to be finite of cardinality N unless otherwise stated and to be indexed by a suitable index set.

Definition 2.4. A factorial arrangement with parameters $k_1, k_2, \ldots, k_t$, m, n, $r_1, \ldots, r_N$ is defined to be a collection of n treatments of G such that the j-th treatment in G has multiplicity $r_j \geq 0$, with at least one nonzero r_j, and m is the number of nonzero r_j's. We denote such a factorial arrangement by the symbol $FA(k_1, \ldots, k_t; m; n; r_1, \ldots, r_N)$.

Note that in a statistical setting the multiplicity r_j is referred to as replication number of the j-th treatment. The statistician should observe that this definition is in agreement with the definition of a general t-way classification as used in statistical literature.

Definition 2.5. A factorial arrangement is said to be a complete factorial arrangement if $r_j > 0$ for all j.

Definition 2.6. A complete factorial arrangement is said to be minimal if $r_j = 1$ for all j. A minimal complete factorial arrangement will be denoted by $\mathrm{MFA}(k_1,\ldots,k_t)$ or simply MFA if there is no ambiguity.

There are many interesting and non-trivial combinatorial and statistical problems associated with factorial arrangements for which not all $r_j > 0$. Since this monograph is mainly devoted to this family of factorial arrangements a formal definition of a fractional replicate is required.

Definition 2.7. A factorial arrangement is said to be a fractional factorial arrangement, or more simply a fractional replicate, if some but not all $r_j > 0$. We denote a fractional replicate by $\mathrm{FFA}(k_1,\ldots,k_t;\ m;\ n;\ r_1,\ldots,r_N)$.

We now illustrate the above definitions in the following two examples.

Example 2.3. Let $G_1 = \{0,1\}$ and $G_2 = \{0,1,2\}$. Associate G_1 with the factor F_1 and G_2 with the factor F_2. The set G of treatments consists of $G = G_1 \times G_2 = \{(x_1,x_2),\ x_i \in G_i\} = \{(0,0),\ (0,1),\ (0,2),\ (1,0),\ (1,1),\ (1,2)\}$. Note that G is a minimal complete factorial arrangement. An example of a complete factorial arrangement that is not minimal is $\{(0,0),\ (0,0),\ (0,1),\ (0,2),\ (0,2),\ (0,2),\ (1,0),\ (1,1),\ (1,2)\} = \mathrm{FA}\ (2,3;\ 6;\ 9;\ 2,1,3,1,1,1)$. An example of a fractional replicate is $\{(0,0),\ (0,0),\ (1,2),\ (1,2),\ (1,2),\ (1,2)\} = \mathrm{FFA}(2,3;\ 2;\ 6;\ 2,0,0,0,0,4)$.

Example 2.4. In order to design an effective breakwater to protect a harbor from the forces of waves, an engineer measured the heights of the waves in the harbor area using a small scale model. The three specified lengths of breakwater were designated as d_1, d_2, and d_3, the two specified heights of breakwater were designated as h_1 and h_2, and the four feasible angles of the direction of force of the waves to the breakwater were designated as a_1, a_2, a_3 and a_4. Setting $G_1 = \{d_1, d_2, d_3\}$, $G_2 = \{h_1, h_2\}$ and $G_3 = \{a_1, a_2, a_3, a_4\}$ results in the following set of possible treatment combinations $G = G_1 \times G_2 \times G_3 = \{(d_1,h_1,a_1), (d_1,h_1,a_2), (d_1,h_1,a_3), (d_1,h_1,a_4), (d_1,h_2,a_1), (d_1,h_2,a_2), \ldots, (d_3,h_2,a_3), (d_3,h_2,a_4)\}$. These treatments may be reordered using the natural numbers 1,2,3,...,24 consecutively. Suppose now, that the engineer could not conduct an experiment using the minimal factorial arrangement but due to cost limitations he was forced to use the fractional replicate FFA(3,2,4; 8; 9; 2,0,0,0,1,0,1,1,1,0,0,0,0,1,0,0,0,0,0,0,0,0,1,1). In the original ordering this fractional replicate is $\{(d_1,h_1,a_1), (d_1,h_1,a_1), (d_1,h_2,a_1), (d_1,h_2,a_3), (d_1,h_2,a_4), (d_2,h_1,a_1), (d_2,h_2,a_2), (d_3,h_2,a_3), (d_3,h_2,a_4)\}$.

From the above example the necessity for a more compact notation becomes apparent. For this purpose the ordered elements of G, i.e., the g's themselves, can be used as subscripts so that after deleting all r_g's which are equal to zero from the notation we get a notation which is compact and informative. This might become cumbersome in the case where there are a large number of factors. Thus in the preceding fractional replicate we have FFA(3,2,4; 8; 9; $r_{(d_1,h_1,a_1)} = 2$, $r_{(d_1,h_2,a_1)} = 1$, $r_{(d_1,h_2,a_3)} = 1$, $r_{(d_1,h_2,a_4)} = 1$, $r_{(d_2,h_1,a_1)} = 1$, $r_{(d_2,h_2,a_2)} = 1$, $r_{(d_3,h_2,a_3)} = 1$, $r_{(d_3,h_2,a_4)} = 1$). Finally, note that if this notation is adopted there will appear exactly m such subscripts in the notation of a fractional factorial arrangement, which then reflect the m distinct treatments appearing in the fractional factorial arrangement.

With each treatment g in a factorial arrangement we associate a random variable y_g, which is called an observation or response or measurement. We omit the details of the customary measure-theoretic structure used in defining a random variable. For our purposes a random variable will always take on values in a finite-dimensional Euclidean set. This is so because each y_g will be finite dimensional and $n < \infty$ for any factorial arrangement. Let Γ be an arbitrary factorial arrangement, then with Γ we associate the $n \times 1$ observation vector Y_Γ, whose g-th ordered element is y_g. Let F_{Y_Γ} be the probability distribution of Y_Γ which is a (possibly) unknown) member of a specified class F^* of distributions.

Although various other models can be postulated in certain situations the one we will consider throughout this monograph is the following:

Definition 2.8. By a linear model associated with each treatment in a factorial arrangement Γ we mean a relationship of the form $E[y_g] = \theta' f(g)$, where $\theta' = (\theta_1, \theta_2, \ldots, \theta_k)$ is a vector of k unknown parameters; $f = (f_1, \ldots, f_k)$ is a vector of k continuous real-valued known functions on the collection of g's in Γ. The expectation of y_g is taken with respect to the distribution of y_g, i.e.,
$$E[y_g] = \int_{-\infty}^{\infty} y_g dF(y_g) = \theta' f(g).$$

Example 2.5. An engineer working in material sciences experimented on the conductivity of electricity using two types of materials and using direct and alternating currents in a cold chamber. For this example material type is factor F_1 and current type is factor F_2. Let $G_1 = \{0,1\} = G_2$. Then $G = G_1 \times G_2 = \{(0,0), (0,1), (1,0), (1,1)\}$. Suppose that $E(y_{(0,0)}, y_{(0,1)}, y_{(1,0)}, y_{(1,1)})$ $= (\mu_{(0,0)}, \mu_{(0,1)}, \mu_{(1,0)}, \mu_{(1,1)})$ where y_g is a one-dimensional random variable. Assume that the experimenter postulated the following relations between $E[y_g]$ and the parameters θ_1, θ_2, θ_3, and θ_4:

$$\begin{bmatrix} \mu(0,0) \\ \mu(0,1) \\ \mu(1,0) \\ \mu(1,1) \end{bmatrix} = \begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{bmatrix} .$$

Note that the assumed model relates to the minimal complete factorial arrangement and that $f_1(g) = f_1((x,y)) = 1$, $f_2(g) = f_2((x,y)) = (2x-1)$, $f_3(g) = f_3((x,y)) = (2y-1)$, and $f_4(g) = f_4((x,y)) = (2x-1)(2y-1)$.

Example 2.6. If in the previous example it was assumed that $\theta_4 = 0$ and the experimenter had considered the fractional factorial arrangement $\{(0,0), (0,1), (1,1)\}$, then the implied model for this arrangement would have been:

$$\begin{bmatrix} \mu(0,0) \\ \mu(0,1) \\ \mu(1,1) \end{bmatrix} = \begin{bmatrix} 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix} .$$

Remark. It is clear that we could have started with stating more general models and pointing out our model as a special case. More specifically we could have considered functional relationships of the form $E[y_g^p] = h(g, \theta_1, \theta_2, \ldots, \theta_k)$, where for each $g \in \Gamma$, the function h in certain settings could be quite complicated. Our linear model corresponds to the case $p = 1$ and the fact that h is linear in the parameters. The case $p = 1$ with the assumption that h is a non-linear in the parameters is known in the literature as a non-linear model.

2.2. STATISTICAL ESTIMATION UNDER THE LINEAR MODEL

Up to this point we have considered a theoretical model which may be written out on paper or on the blackboard. This is sufficient to describe many of the combinatorial problems and some statistical problems associated with factorial arrangements and with fractional replication in particular. However, in the real world of practical applications an experimenter specifies his model from both theoretical and experimental considerations of the phenomenon under study. He conducts an experiment and makes observations in order to obtain estimates of the parameters in the model and to obtain evidence of the appropriateness of the proposed model. In experimentation, a treatment g is applied to an entity, which is called an experimental unit. A response y_g is observed, estimates of the parameters of the model are obtained using the y_g's and inferences are made from these concerning the appropriateness of the specified model. The entire process of formulating and stating a model, taking observations, fitting the proposed model to the observations, and possibly conjecturing a new model until a model sufficiently describes the phenomenon under study is called "model building".

We will not be concerned with all the aspects of model building in this monograph since we are going to limit ourselves to the linear model. In this model $E[y_g] = \theta' f(g)$, where the set of parameters $\theta_1, \theta_2, \ldots, \theta_k$ will be referred to as the set of "factorial effects". Essentially, the vector θ reflects the behaviour of $E[Y_\Gamma]$ with respect to changes in the levels of the factors. Note that our designation of effects also includes the classical definition of effects in factorial experiments.

In matrix notation the linear model for any factorial arrangement Γ can be written as:

$$E[Y_\Gamma] = W_\Gamma \theta$$

where the element in the g-th row and the j-th column of W_Γ is equal to $f_j(g)$, where f_j is an explicitly known function; W_Γ is an $n \times k$ matrix and is known as a design matrix in the literature; θ is a $k \times 1$ vector of unknown factorial effects. Of course the functions $f_j(g)$'s must have meaning from the experimenter's viewpoint. This type of model is popular in practice. A celebrated one is the "orthogonal polynomial model", which may be written out similarly and which will be described in the next chapter in detail.

Suppose now that the experimenter's interest lies in obtaining information on θ using a factorial arrangement Γ. In typical applications the number of treatments in Γ depends upon the cardinality k of θ and might also be dictated by economical and physical constraints. For given θ and m, typically there will be many choices for the treatments in Γ such that information can be obtained on the parameters. Clearly, the procedures to obtain information on θ and the selection of the factorial arrangement should have certain desirable properties such that a choice can be made utilizing suitable and desired criteria.

More explicitly, we are dealing with a family of c competing factorial arrangements $\Gamma_1, \Gamma_2, \ldots, \Gamma_c$. The matrix equations for these are:

$$\begin{aligned} E\left[Y_{\Gamma_1}\right] &= W_{\Gamma_1}\theta \\ E\left[Y_{\Gamma_2}\right] &= W_{\Gamma_2}\theta \\ &\vdots \\ E\left[Y_{\Gamma_c}\right] &= W_{\Gamma_c}\theta \, . \end{aligned}$$

In actual experimentation we will be dealing with the observational vector Y_Γ rather than $E[Y_\Gamma]$ if the factorial arrangement Γ is used. Denote by $Y_\Gamma - E[Y_\Gamma]$ the deviation or error vector ϵ_Γ. The previous equations can be written out as:

$$Y_{\Gamma_1} = W_{\Gamma_1}\theta + \epsilon_{\Gamma_1}$$

$$Y_{\Gamma_2} = W_{\Gamma_2}\theta + \epsilon_{\Gamma_2}$$

$$\vdots$$

$$Y_{\Gamma_c} = W_{\Gamma_c}\theta + \epsilon_{\Gamma_c} \quad .$$

Note that each equation is capable of providing some information on θ. This information depends upon the treatments on which measurements have been made and the methods of estimating θ. Selecting the treatments in Γ_i underlying the Y_{Γ_i} is the treatment design problem, while selecting a method of estimating θ is a statistical estimation problem. Since the experimenter is usually confronted with classes of these two aspects we clearly need criteria for selecting a particular treatment design and a particular method of estimation. In the following chapters we delve into these aspects further.

CHAPTER 3

POLYNOMIAL MODEL AND ESTIMATION OF ITS PARAMETERS

The many mathematical and statistical problems related to fractional replication are best understood if we consider the minimal complete factorial arrangement ρ and its associated design matrix X_ρ along with the parametric vector β_ρ. This is so because the model associated with ρ is the base for any related factorial arrangement. In this chapter we develop an orthogonal polynomial model and provide the least squares estimates for a set of parametric functions $L\beta_\rho$ from a factorial arrangement with and without negligibility assumptions on some components of β_ρ.

3.1. THE POLYNOMIAL MODEL

We shall assume throughout that the levels of all factors are quantified. In order to understand the polynomial model for t-factor factorial we first introduce this for the case t = 1, that is for the single factor experiment. Denote the levels of this single factor by $\{z_1, z_2, \ldots, z_v\}$. Next, denote the observation related to the z_j-th level by y_{z_j}; then, we adopt the polynomial model for the expected value of the observation y_{z_j}, i.e.,

$$(3.1) \qquad E\left[y_{z_j}\right] = \theta_0 f_0(z_j) + \theta_1 f_1(z_j) + \ldots + \theta_{v-1} f_{v-1}(z_j), \qquad j = 1,2,\ldots,v.$$

In regression theory θ_0 is called the mean, θ_1 is the partial linear regression coefficient, θ_2 is the partial quadratic regression coefficient, etc.. The matrix representation of the above equation is

$$(3.2) \qquad E[Y] = P\theta,$$

where P is a v x v matrix with the (j,w)-th entry being equal to

$$(3.3) \qquad f_w(z_j) = z_j^w, \qquad \begin{array}{l} w = 0,1,\ldots,v-1 \\ j = 1,2,\ldots,v \end{array}$$

Remark. The reader should be warned of two things: (i) In $E\left[y_{z_j}\right]$ one may have fewer than v terms depending on the particular phenomenon at hand. However, the generality of the theory which we are going to discuss will not be affected by this. (ii) One could start with different functions not necessarily monomials in z's as long as they are independent on $\{z_1, z_2, \ldots, z_v\}$. A similar theory can be carried through for other than monomial settings.

Let H be a Gram-Schmidt transformation matrix which orthonormalizes the columns of P. It follows that system (3.2) can be rewritten as:

$$(3.4) \qquad E[Y] = PHH^{-1}\theta = M\phi ,$$

where M = PH and $\phi = H^{-1}\theta$. If we adopt the left-to-right orthonormalization of P, then the (j,h) entry in M is equal to

$$(3.5) \qquad m_{jh} = p_h(z_j) = \frac{1}{c_h}\left[z_j^h - \sum_{a=0}^{h-1} p_a(z_j) \sum_{b=1}^{v} z_b^h p_a(z_b)\right], \qquad \begin{array}{l} j = 1,2,\ldots,v \\ h = 1,2,\ldots,v-1 \end{array}$$

where c_h is the normalization constant

$$c_h = \left\{ \sum_{j=1}^{v} \left[z_j^h - \sum_{a=0}^{h-1} p_a(z_j) \sum_{b=1}^{v} z_b^h p_a(z_b) \right]^2 \right\}^{\frac{1}{2}}$$

and the (j,o) entry in $M = (1/\sqrt{v})$. If we denote the elements of ϕ by $\phi^0, \phi^1, \ldots, \phi^{v-1}$, then in regression theory ϕ^0 is called the intercept or mean, ϕ^1 is the linear regression coefficient eliminating the intercept ignoring all higher degree terms, ϕ^2 is the quadratic regression coefficient eliminating the intercept and the linear regression coefficient and ignoring all higher degree terms, etc. This order of eliminating and ignoring regression coefficients is due to the left-to-right orthonormalization of the matrix P.

<u>Remark</u>. In the case when the coded levels are 0,1,2,...,v-1, tables have been prepared which provide the matrix M up to a particular order.

We now generalize the orthogonal polynomial model to the case $t \geq 2$. Let ρ be the minimal complete factorial arrangement and Y_ρ be the corresponding observation vector. The following model is adopted throughout:

$$E\left[Y_\rho\right] = X_\rho \beta_\rho \ , \tag{3.6}$$

where the subscript of Y_ρ are lexicographically[*] ordered,

$$X_\rho = M_1 \otimes M_2 \otimes \ldots \otimes M_t$$

and

$$\beta_\rho = \phi_1 \circledast \phi_2 \circledast \ldots \circledast \phi_t$$

Here M_i and ϕ_i are the design matrix and the parametric vector for the i-th factor after left-to-right orthogonalization as described in (3.4) and (3.5). The symbols $\otimes$ and $\circledast$ indicate the usual Kronecker product and symbolic Kronecker product, respectively. The operations in both cases are carried from left to right. The

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[*] A real n-tuple $x = (x_1, x_2, \ldots, x_n)$ is said to be less than a real n-tuple $y = (y_1, y_2, \ldots, y_n)$ if and only if for the first ℓ such that $x_\ell \neq y_\ell$ we have $x_\ell < y_\ell$, $1 \leq \ell \leq n$.

operation $\circledast$ is defined as

$$\phi_1 \circledast \phi_2 \circledast \cdots \circledast \phi_t = \left(\left(\phi_1^0, \phi_1^1, \ldots, \phi_1^{v_1-1}\right) \circledast \left(\phi_2^0, \phi_2^1, \ldots, \phi_2^{v_2-2}\right) \circledast \cdots \circledast \left(\phi_t^0, \phi_t^1, \ldots, \phi_t^{v_t-1}\right)\right)'$$

$$= \left(\phi_1^0\phi_2^0 \cdots \phi_t^0,\ \phi_1^0\phi_2^0 \cdots \phi_t^1, \ldots, \phi_1^0\phi_2^0 \cdots \phi_t^{v_t-1}, \ldots, \phi_1^{v_1-1}\phi_2^{v_2-2} \cdots \phi_t^{v_t-1}\right)' .$$

The elements of β_ρ, also called factorial effects, have been traditionally named in the following manner: $\phi_1^0\phi_2^0 \cdots \phi_t^0$ is called the mean, $\phi_1^0\phi_2^0 \cdots \phi_q^p \cdots \phi_t^0$ is called the p-th main effect of the q-th factor $\phi_1^{v_1}\phi_2^{v_2}\phi_3^0 \cdots \phi_t^0$ is called the v_1-th degree of factor F_1 by v_2-th degree of factor F_2 interaction effect, etc. Also, an effect $\phi_1^{i_1}\phi_2^{i_2} \cdots \phi_t^{i_t}$ is said to be of degree or order k if k of the exponents $i_1, i_2, \ldots, i_t$ are non-zero.

As stated before there is an error vector associated with the observation vector Y_ρ, i.e., we may rewrite the model as

(3.7) $$Y_\rho = X_\rho \beta_\rho + \epsilon_\rho \text{ , and ,}$$

where

(3.8) $$E[\epsilon_\rho] = 0$$ $$\mathrm{Cov}\left(\epsilon_\rho\right) = \sigma^2 I .$$

We illustrate the above concepts with the following example.

Example 3.1. Consider a 3 x 4 factorial experiment with the following factor space:

$$\left\{G = G_1 \times G_2,\ F_1, F_2\right\} \text{ with } G_1 = \left\{0,2,5\right\},\ G_2 = \left\{0,1,3,6\right\} .$$

Then

$$P_1 = \begin{bmatrix} 1 & z_{11} & z_{11}^2 \\ 1 & z_{12} & z_{12}^2 \\ 1 & z_{13} & z_{13}^2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 2 & 4 \\ 1 & 5 & 25 \end{bmatrix}$$

and

$$P_2 = \begin{bmatrix} 1 & z_{21} & z_{21}^2 & z_{21}^3 \\ 1 & z_{22} & z_{22}^2 & z_{22}^3 \\ 1 & z_{23} & z_{23}^2 & z_{23}^3 \\ 1 & z_{24} & z_{24}^2 & z_{24}^3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 1 & 3 & 9 & 27 \\ 1 & 6 & 36 & 216 \end{bmatrix} .$$

Upon orthonormalizing the columns of P_1 and P_2 as described above, we obtain:

$$M_1 = \begin{bmatrix} \frac{+1}{\sqrt{3}} & \frac{-7}{\sqrt{114}} & \frac{+3}{\sqrt{38}} \\ \frac{+1}{\sqrt{3}} & \frac{-1}{\sqrt{114}} & \frac{-5}{\sqrt{38}} \\ \frac{+1}{\sqrt{3}} & \frac{+8}{\sqrt{114}} & \frac{+2}{\sqrt{38}} \end{bmatrix} \quad \text{and } M_2 = \begin{bmatrix} \frac{+1}{\sqrt{4}} & \frac{-5}{\sqrt{84}} & \frac{+9}{\sqrt{308}} & \frac{-5}{\sqrt{132}} \\ \frac{+1}{\sqrt{4}} & \frac{-3}{\sqrt{84}} & \frac{-3}{\sqrt{308}} & \frac{+9}{\sqrt{132}} \\ \frac{+1}{\sqrt{4}} & \frac{+1}{\sqrt{84}} & \frac{-13}{\sqrt{308}} & \frac{-5}{\sqrt{132}} \\ \frac{+1}{\sqrt{4}} & \frac{+7}{\sqrt{84}} & \frac{+7}{\sqrt{308}} & \frac{+1}{\sqrt{132}} \end{bmatrix} .$$

The parametric vectors for this example are

$$\phi_1' = \left(\phi_1^0, \phi_1^1, \phi_1^2\right) \text{ and } \phi_2' = \left(\phi_2^0, \phi_2^1, \phi_2^2, \phi_2^3\right) .$$

Then X_ρ and β_ρ are

$$X_\rho = M_1 \otimes M_2 = \begin{bmatrix} \frac{+1}{\sqrt{3}} M_2 & \frac{-7}{\sqrt{114}} M_2 & \frac{+3}{\sqrt{38}} M_2 \\ \frac{+1}{\sqrt{3}} M_2 & \frac{-1}{\sqrt{114}} M_2 & \frac{-5}{\sqrt{38}} M_2 \\ \frac{+1}{\sqrt{3}} M_2 & \frac{+8}{\sqrt{114}} M_2 & \frac{+2}{\sqrt{38}} M_2 \end{bmatrix}$$

and

$$\beta_\rho' = \left(\phi_1 \circledast \phi_2\right)' = \left(\phi_1^0\phi_2^0,\ \phi_1^0\phi_2^1,\ \phi_1^0\phi_2^2,\ \phi_1^0\phi_2^3,\ \phi_1^1\phi_2^0,\ \phi_1^1\phi_2^1,\ \phi_1^1\phi_2^2,\ \phi_1^1\phi_2^3,\ \phi_1^2\phi_2^0,\ \phi_1^2\phi_2^1,\ \phi_1^2\phi_2^2,\ \phi_1^2\phi_2^3\right).$$

In the model $E[Y_\rho] = X_\rho\beta_\rho$ the corresponding observation vector Y_ρ appears in the lexicographic order compatible with the order in β_ρ, i.e.

$$Y_\rho' = \left(y_{00},\ y_{01},\ y_{02},\ y_{03},\ y_{10},\ y_{11},\ y_{12},\ y_{13},\ y_{20},\ y_{21},\ y_{22},\ y_{23}\right) .$$

3.2. LEAST SQUARES ESTIMATION OF β_ρ FROM THE MINIMAL COMPLETE FACTORIAL ARRANGEMENT

Applying the least squares procedure to equation (3.7) we obtain the following estimator for β_ρ:

(3.9) $$\hat{\beta}_\rho = \left(X_\rho'X_\rho\right)^{-1}X_\rho'Y_\rho = X_\rho'Y_\rho$$

since $X_\rho'X_\rho = I$. The covariance matrix for this estimator is

(3.10) $$\mathrm{Cov}\left(\hat{\beta}_\rho\right) = \left(X_\rho'X_\rho\right)^{-1}\sigma^2 = \sigma^2 I .$$

From the minimal complete factorial arrangement one cannot obtain an unbiased estimator of σ^2 and hence of $\mathrm{Cov}(\hat{\beta}_\rho)$. It is clear that if one or more treatments are replicated the resulting design is capable of providing unbiased estimators for both β_ρ and σ^2.

<u>Remark</u>. If the $\mathrm{Cov}(\epsilon_\rho) = \sigma^2 V$ where V is a known matrix then the least squares estimator of β_ρ is equal to

$$\hat{\beta}_\rho = \left(X_\rho' V^{-1} X_\rho\right)^{-1} X_\rho V^{-1} Y_\rho$$

(3.11) with

$$\mathrm{Cov}\left(\hat{\beta}_\rho\right) = \left(X_\rho' V^{-1} X_\rho\right)^{-1} \sigma^2 \ .$$

3.3. LEAST SQUARES ESTIMATION OF LINEAR PARAMETRIC FUNCTIONS USING AN ARBITRARY FACTORIAL ARRANGEMENT UNDER A POLYNOMIAL MODEL

Let Γ be the factorial arrangement $FA(k_1, k_2, \ldots, k_t;\ m;\ n;\ r_1, r_2, \ldots, r_N)$. We associate a polynomial model with Γ in the following manner:

$$E\left[Y_\Gamma\right] = X_\Gamma \beta_\rho \ , \tag{3.12}$$

where $Y_\Gamma' = \left(y_{g_1}^{(1)}, y_{g_1}^{(2)}, \ldots, y_{g_1}^{(r_1)}, y_{g_2}^{(1)}, y_{g_2}^{(2)}, \ldots, y_{g_2}^{(r_2)}, \ldots, y_{g_n}^{(1)}, y_{g_n}^{(2)}, \ldots, y_{g_N}^{(r_N)}\right)$.

Here $y_{g_i}^{(h)}$ refers to the observation associated with the h-th repetition of the treatment g_i. The $n \times N$ matrix X_Γ is obtained from the matrix X_ρ of the related minimal complete factorial arrangement ρ, taking repetitions into account. Explicitly, the design matrix X_Γ can be written as

$$(3.13) \qquad X_\Gamma = \begin{bmatrix} 1_{r_1} & z_{g_1} \\ 1_{r_2} & z_{g_2} \\ \vdots & \\ 1_{r_N} & z_{g_N} \end{bmatrix}$$

where z_{g_i} is the i-th row of X_ρ in the previous section and 1_{r_i} is the column vector of ones of order r_i. It is understood that whenever $r_i = 0$, then the corresponding $1_{r_i} z_{g_i}$ is not present. Finally β_ρ is the vector of parameters as in (3.6).

Remark. The reader should note that he can associate with the minimal complete factorial arrangement an $X^*_\rho \beta^*_\rho$ where X^*_ρ is any arbitrary orthonormal matrix of order N and he will obtain similar results for the minimal complete factorial arrangement and for the results that follow. This departure is especially applicable in the case where the levels of the factors are qualitative.

Suppose that the experimenter is interested in estimating a set of linear parametric functions specified by $L\beta_\rho$ where L is a matrix of order $v \times N$ of rank $v \le N$. We shall distinguish between the following two cases which are treated successively.

Case 1. No specific a priori assumptions on the components of β_ρ. Let Γ be such that $L\beta_\rho$ is estimable, i.e., there exists a matrix K_Γ such that

$$(3.14) \qquad L = K_\Gamma X_\Gamma .$$

It can be shown that the least squares estimator of $L\beta_\rho$, denoted by $\widehat{L\beta_\rho}$, is given by

(3.15) $$\widehat{L\beta_\rho} = L\left(X_\Gamma' X_\Gamma\right)^- X_\Gamma' Y_\Gamma ,$$

where $(A)^-$ denotes a generalized inverse of A. The expected value and the covariance matrix of this estimator are respectively:

(3.16) $$E\left[\widehat{L\beta_\rho}\right] = K_\Gamma X_\Gamma\left(X_\Gamma' X_\Gamma\right)^- X_\Gamma' X_\Gamma \beta_\rho = K_\Gamma X_\Gamma \beta_\rho = L\beta_\rho ;$$

(3.17) $$\mathrm{Cov}\left(\widehat{L\beta_\rho}\right) = L\left(X_\Gamma' X_\Gamma\right)^- L'\sigma^2 = K_\Gamma X_\Gamma\left(X_\Gamma' X_\Gamma\right)^- X_\Gamma' K_\Gamma' \sigma^2 .$$

It is well known that $X_\Gamma\left(X_\Gamma' X_\Gamma\right)^- X_\Gamma'$ is invariant under any choice of a generalized inverse for $X_\Gamma' X_\Gamma$.

Remark. Case one includes the response surface estimation by setting $L = X_\Gamma$. In this special case one also uses the term prediction. Since here $E\left[\widehat{L\beta_\rho}\right] = E\left[\widehat{X_\Gamma\beta_\rho}\right] = X_\Gamma\beta_\rho = E\left[Y_\Gamma\right]$, the estimator $\widehat{L\beta_\rho}$ is written as $\widehat{E\left[Y_\Gamma\right]}$ which provides a justification for the preceding terminology.

Case 2. The experimenter has a priori knowledge of the exact values of some components of β_ρ. We may assume without loss of generality that these values are zero and $\beta_\rho' = \left[\beta_1' \,\vdots\, \beta_2'\right] = \left[\beta_1' \,\vdots\, 0\right]$. Note that in this case the model (3.12) reduces to the following:

(3.18) $$E\left[Y_\Gamma\right] = \left[X_{\Gamma_1} \,\vdots\, X_{\Gamma_2}\right]\begin{bmatrix}\beta_1\\ \cdots\\ 0\end{bmatrix} = X_{\Gamma_1}\beta_1 .$$

Let Γ be such that $L_1\beta_1$ is estimable, i.e., as in equation (3.14) we have the condition that there exists a K_{Γ_1} such that

(3.19) $$L_1 = K_{\Gamma_1} X_{\Gamma_1} .$$

The least squares estimator of $L_1\beta_1$ together with its covariance matrix are given by the following equations:

$$\widehat{L_1\beta_1} = L_1\left(X'_{\Gamma_1} X_{\Gamma_1}\right)^{-} X'_{\Gamma_1} Y_{\Gamma} \quad , \tag{3.20}$$

$$\mathrm{Cov}\left(\widehat{L_1\beta_1}\right) = L_1\left(X'_{\Gamma_1} X'_{\Gamma_1}\right)^{-} L_1'\sigma^2 \quad . \tag{3.21}$$

Note that $\widehat{L_1\beta_1}$ is unbiased.

Remark. If in reality $\beta_2 \neq 0$, then $\widehat{L_1\beta_1}$ is no longer unbiased since

$$E\left[\widehat{L_1\beta_1}\right] = L_1\beta_1 + A_{\Gamma}\beta_2 \tag{3.22}$$

where

$$A_{\Gamma} = L_1\left(X'_{\Gamma_1} X_{\Gamma_1}\right)^{-} X'_{\Gamma_1} X_{\Gamma_2} \quad . \tag{3.23}$$

The covariance of this biased estimator is clearly equal to (3.21). In this case the covariance matrix is not informative enough since it does take into account the bias. A better quantity is the mean square of $\widehat{L_1\beta_1}$ which is defined and given by

$$\mathrm{MSE}\left(\widehat{L_1\beta_1}\right) = \mathrm{Cov}\left(\widehat{L_1\beta_1}\right) + A_{\Gamma}\beta_2\beta_2'A_{\Gamma}' \quad . \tag{3.24}$$

CHAPTER 4

MATHEMATICAL AND STATISTICAL CONSTRAINTS AND CRITERIA

In this chapter we shall formulate the problem of factorial experimentation from what we consider to be the experimenter's point of view. To do this we assume that the following has already been established:

(i) the factor-space $\{G, F_i, i = 1,\dots,t\}$ has been explicitly defined,

(ii) a model has been postulated for $E[Y_\rho]$,

and

(iii) specified functions of the parameters which are of interest to the experimenter are indicated.

In this monograph, we limit ourselves to the case where the model in (ii) is the polynomial model and to linear parametric functions $L\beta_\rho$ in (iii). In selecting a design it is realistic to impose the condition that the design is capable of providing an unbiased estimator of $L\beta_\rho$, i.e., $L\beta_\rho$ is estimable. The class of all such designs is denoted by $\Delta(L)$, and will be referred to as the class of unbiased designs. In most situations, if not all, the experimenter is not free to choose the treatments or design points in an arbitrary fashion. There may be economical, social, political, environmental, and/or other constraints which confine the experimenter to a certain class of designs, $\Delta(L,C) = \left\{\Gamma_1,\dots,\Gamma_s\right\}$. Of course, any design in $\Delta(L,C)$ provides an unbiased estimator for $L\beta_\rho$. However, in many situations the experimenter will need to introduce some reasonable and meaningful quantity associated with a $\Gamma \in \Delta(L,C)$, say $Q(\Gamma)$; he will then need to select a Γ^* in $\Delta(L,C)$ such that $Q(\Gamma^*)$ is minimum. The quantity $Q(\Gamma)$ is called the objective function in many areas of mathematics. In summary, the problem can be stated as follows:

Given $\{G, F_i, i = 1,\dots,t\}$, $E[Y_\rho] = X_\rho\beta_\rho$, and a desirable quantity Q associated with every design Γ, then select a Γ^* such that:

(i) $L\beta_\rho$ is estimable,

(ii) Γ^* satisfies all the constraints of the experiment,

and

(iii) $Q(\Gamma^*) \quad Q(\Gamma)$ for every Γ which satisfies (i) and (ii).

The resulting Γ^* is called an <u>optimal design</u> with respect to Q.

4.1. SOME CONSIDERATIONS ON CONSTRAINTS IN SELECTING A FACTORIAL ARRANGEMENT

Hereafter by a design we mean any arbitrary factorial arrangement. We also define a design to be <u>feasible</u> for $L\beta_\rho$ if it can provide an unbiased estimator of $L\beta_\rho$. Let $\Delta(L)$ be the collection of all feasible designs for $L\beta_\rho$. Typically in any experiment the experimenter is not at liberty to select any design Γ in $\Delta(L)$. He will be confronted with many considerations such as physical, economical, environmental, political, etc., which constrain him to a subclass of designs in $\Delta(L)$. Let C denote the set of all constraints and let $\Delta(L,C)$ be the constrained class of feasible designs. Now, three cases can occur: (i) $\Delta(L,C)$ is empty. In this case the experimenter must modify his class of constraints in C. (ii) $\Delta(L,C)$ contains a single design, so that this will be the selected design. (iii) $\Delta(L,C)$ has cardinality greater than one. Here he will be better off by imposing one statistical criterion (or more such criteria if possible) for selecting a design in $\Delta(L,C)$. We shall study this latter aspect in some detail in section 4.2.

Not all constraints (for instance, social and political) are mathematically treatable, because these might not easily be stated in a quantitative form. However, the economic aspect of designs can be put in a suitable mathematical form as will be explained next.

In carrying out any experiment the experimenter has a budget assigned to him to cover the total cost of experimentation. Suppose that his budget equals B dollars. Taking account of the two types of costs, namely the fixed (or overhead) cost K_o and the variable cost K_v, we may write

$$B = K_o + K_v \ . \tag{4.1}$$

For each design Γ in $\Delta(L)$ we may calculate this variable cost and indicate it by $K_v^*(\Gamma)$. Those designs in $\Delta(L)$ for which $K_v^*(\Gamma) \le K_v$ form the constrained class $\Delta(L,B)$ of designs constrained by the budget B. If a treatment g in Γ is denoted by $(i_1 i_2 \ldots i_t)$, where i_j is the i_j-th level of the j-th factor, then the cost $K_v^*(\Gamma)$ can be written as

$$K_v^*(\Gamma) = \text{Purchase Cost} + \text{Application Cost} + \text{Maintenance Cost} + \text{Response Cost} \tag{4.2}$$

$$= \sum_{(i_1 i_2 \ldots i_t) \in \Gamma} \left[P(i_1 i_2 \ldots i_t) + A(i_1 i_2 \ldots i_t) + M(i_1 i_2 \ldots i_t) + R(i_1 i_2 \ldots i_t) \right] .$$

The costs in equation (4.2) may be decomposed into sums of costs associated with the levels appearing in a treatment. For example, if it makes sense we can write:

$$P(i_1 i_2 \ldots i_t) = \sum_j P_j(i_j) \ , \tag{4.3}$$

where $P_j(i_j)$ is the purchase cost of the i_j-th level of the j-th factor.

The approach which is taken above and which we adopt throughout is known as the fixed budget approach in contrast to the variable budget approach. In this last case we start out with a class of designs constrained by estimability of $L\beta_\rho$, and, possibly other constraints (see next section) and then select a design which minimizes the budget.

4.2. CRITERIA FOR SELECTING AN OPTIMAL FACTORIAL ARRANGEMENT

In this section we assume the polynomial model $E[Y_\rho] = X_\rho\beta_\rho$ such that for an arbitrary factorial arrangement Γ the induced model is $E[Y_\Gamma] = X_\Gamma\beta_\rho$. A difficult problem is to characterize the set of all unbiased designs in easily usable terms of the treatments for a fixed $L\beta_\rho$. Let C be a set of constraints on the designs. If an unbiased design with respect to $L\beta_\rho$ satisfies the constraints in C, it will be termed a feasible design. The class of all feasible designs to estimate $L\beta_\rho$ was earlier denoted as $\Delta(L,C)$. We assume $\Delta(L,C)$ to be nonempty (In practice if it is empty, then the experimenter will need to modify the constraints and/or L so as to make it nonempty.). Whenever $\Delta(L,C)$ contains more than one design, there will be a choice, so that a suitable criterion is needed for selecting a design. This is usually formulated in terms of a real objective function Q on $\Delta(L,C)$, which Γ is chosen to minimize; if several Γ achieve the minimum, a second objective function may be used to choose among them, etc. A design which minimizes $Q(\Gamma)$ over Δ will be called a Q-optimal design.

We will now introduce notation $Q_1,Q_2,\ldots,Q_8$ for some of the objective functions which are often used in statistical and mathematical literature and which may be classified as:

(i) Quantities which reflect variances and covariances of $\widehat{L\beta_\rho}$.

(ii) Quantities which reflect the combinatorial nature of the design.

(iii) Quantities which measure departure from the initial assumptions on β_ρ.

4.2.1. SELECTING OPTIMAL DESIGNS WITH RESPECT TO CRITERIA BASED ON THE SPECTRUM OF THE INFORMATION MATRIX

Let $\lambda_j(\Gamma)$ be the j-th nonzero eigenvalue of the information matrix $(L(X_\Gamma'X_\Gamma)^- L')^{-1}$ of $\widehat{L\beta_\rho}$ using design Γ, $j = 1,2,\ldots,s$ = rank of L such that $\lambda_j(\Gamma) \geq \lambda_{j+1}(\Gamma)$. The following Q_i's are useful quantities under (i) above:

$Q_1(\Gamma) = 1/\prod_{j=1}^{s} \lambda_j(\Gamma)$ which is proportional to the generalized variance. The optimal design obtained is usually called "determinant optimal" or in short a"d-optimal" design.

$Q_2(\Gamma) = \sum_{j=1}^{s} 1/\lambda_j(\Gamma)$ which is proportional to the average variance. Here the optimal design is referred to in the literature as "average variance optimal" or simply "a-optimal" design.

$Q_3(\Gamma) = 1/\lambda_s(\Gamma)$. The corresponding optimal design is called, in the literature, an "eigenvalue optimal" or "e-optimal".

$Q_4(\Gamma) = \max_{g\epsilon\Gamma} \mathrm{Var}[\widehat{E(Y_g)}]$. The optimal design in this case is called "global optimal" or in short "g-optimal" design.

A few words are in order about the intuitive meaning of the above criteria. In principle, statistical decision theory, including design construction, is based on a structure which includes specification of a "loss", or "disutility" function W, which in the present setting expresses the cost to the experimenter (or society) as a function of the chosen design Γ, the chosen value of the estimate of $L\beta_\rho$, and the "true state of nature" (distribution of Y_Γ). The estimate is a chance variable which depends on the value taken on by Y_Γ and on the estimator of $L\beta_\rho$ which we use (a function from the reals to the reals).

For a given design and estimator, the expectation of this loss is called the risk function, a function of the state of nature. No design and estimator will yield a uniformly smallest risk function, so some real functional Q^* of this risk function is minimized instead. The choice of W and Q^* is often discussed in terms of axioms of rational behavior which will not be treated here. For simplicity, let us suppose here that n is fixed and all factorial arrangements cost the same amount, and that we are using the least squares estimator of $L\beta_\rho$ computed under the assumption that $\beta_2 = 0$ (see also Box and Draper [1959, 1963] and Karson, Manson, and Hader [1969] for a different treatment of the problem). The Q_i's listed above then reflect various functionals of expected loss due to misestimation by this estimator. Q_1, Q_2, and Q_3 are, respectively, proportional to the determinant, trace, and maximum eigenvalue of the covariance matrix of $\widehat{L\beta_\rho} = \widehat{L_1\beta_1}$. Each of these has intuitively the right "shape": roughly, it is small for designs that tend to estimate $L\beta_\rho$ with small error.

In practice, an experimenter will be unlikely to know his Q exactly. Fortunately, there is usually a kind of insensitivity to using a slightly incorrect Q: if Q' is the one he "should" use and Q'' is a slightly different one, then a Q''-optimal design Γ'' will have $Q'(\Gamma'')$ close to the minimum of Q'. This being so, in the absence of exact knowledge of this Q', design theorists often compute Q''-optimal designs for Q'' which makes computation simple; Q_1, Q_2, Q_3 are of that nature, and there are computational algorithms associated with each of them. A slight variation of Q_2 is

$$(4.4) \qquad Q^{(H)}(\Gamma) = \text{trace}\left[H \, \text{Cov}(\widehat{L\beta_\rho})\right]/\sigma^2$$

where H is a specified non-negative definite matrix. It can be shown that any design which is Q-optimal for a Q which depends only on the matrix $\mathrm{Cov}(\widehat{L\beta_\rho})/\sigma^2$ in a reasonable way, is $Q^{(H)}$-optimal for some H. Thus, the class of $Q^{(H)}$-optimal designs for all H is of considerable interest. Computationally, the determination of a $Q^{(H)}$-optimal design can be reduced to that of a Q_2-optimal (= $Q^{(I)}$-optimal) design for a slightly different model. In addition, certain intuitive features of the various criteria may determine the choice among them. For example, Q_1-optimality yields set-estimators (statements of the type "$L\beta_\rho$ is in the set obtained from the value of Y_Γ") of small volume and good performance, in a commonly employed sense, of a test of hypothesis such as "$L\beta_\rho = 0$".

If one is perhaps interested not just in $L\beta_\rho$, where L was chosen merely to give a convenient basis for the whole space of linear functions, one is really interested in, then one might consider σ^{-2} Var(estimator of $c'L\beta_\rho$) = $c'\,\mathrm{Cov}(\widehat{L\beta_\rho})c/\sigma^2$ for arbitrary vector c. Normalizing by restricting c to $c'c = 1$ and averaging over that sphere, one is led to consideration of Q_2-optimality. Similarly, if instead of averaging we consider

$$\max_{c'c = 1} \mathrm{Var}(\text{estimator of } c'L\beta_\rho) ,$$

we are lead to Q_3-optimality. Q_4-optimality obviously refers to the accuracy of our estimate of the entire "response-surface" $E[y_g]$.

If one changes the levels in G_i by a linear transformation, Q_2- and Q_3-optimality are not invariant. For example, if t = 1 and one changes the scale of measurement by replacing the levels $\{z_1, z_2, \ldots, z_v\}$ by $\{bz_1, bz_2, \ldots, bz_v\}$, then

$$\sum_{i=0}^{v-1} \theta_i x^i = \sum_{i=0}^{v-1} (\theta_i/b^i)(bz)^i = \sum_{i=0}^{v-1} \bar{\theta}_i (bz)^i$$

(say), and the $\bar{\theta}_i = (\theta_i/b^i)$ are the "new regression coefficients". The Q_2-optimal design that minimizes $\sum_{i=0}^{v-1} \mathrm{Var}(\hat{\theta}_i)$ does not minimize $\sum_{i=0}^{v-1} \mathrm{Var}(\hat{\bar{\theta}}_i)$, but rather minimizes $\sum_{i=0}^{v-1} b^{2i}\mathrm{Var}(\hat{\bar{\theta}}_i)$. Thus, for equally spaced levels $(z_1,z_2,\dots,z_v) = (b, 2b,\dots,vb)$ one would obtain a different design for each b if one were really interested in Q_2-optimality for each b, as one should (but a single design if one were interested in $\sum_{i=0}^{v-1} \mathrm{Var}(\hat{\theta}_i)b^{2i}$). Q_1-optimality has the practical invariant advantage that a single design is optimum for all b, so that less tabling is required. Q_4-optimality is even invariant under non-linear transformations on G.

4.2.2. SELECTING OPTIMAL DESIGNS
BASED ON OTHER CRITERIA

Let ℓ_j' be the j-th normalized row of L and let $a_j(\Gamma)\sigma^2$ be the variance of $\widehat{\ell_j'\beta_\rho}$. A design Γ is said to be *variance balanced* if $a_j(\Gamma)\sigma^2$ is independent of j . If the experimenter is interested in variance balanced designs, then

$$\sum_{j=1}^{s}(a_j(\Gamma)-\bar{a}(\Gamma))^2, \text{ for } \bar{a}(\Gamma) = \sum_{j=1}^{s} a_j(\Gamma)/s \tag{4.5}$$

is a quantity which measures departure from variance balancedness. This motivates the defining quantity

$$Q_5(\Gamma) = \sum_{j=1}^{s}(a_j(\Gamma)-\bar{a}(\Gamma))^2 \quad .$$

A similar quantity reflecting the variability among the covariance of $\widehat{\ell_j'\beta_\rho}$ could be added to $Q_5(\Gamma)$. The resulting quantity measures departure from *covariance balancedness*. Of course it is possible to write many of these measures (i.e., the orthogonally invariant ones) in terms of the characteristic roots of the information matrix $\widehat{L\beta}_\rho$. A shortcoming of Q_5 (or its extension) is that $Q_5(\Gamma)$ can be zero for a design with relatively large $\bar{a}(\Gamma)$.

Under the assumption that $\beta_2 = 0$ the model using design Γ is equal to $E[Y_\Gamma] = X_{\Gamma_1}\beta_1$. If this assumption is violated the least squares estimator of $L_1\beta_1$ is biased and from equation (3.24) we know that

$$(4.6) \qquad MSE\left(\widehat{L_1\beta_1}\right) = Cov\left(\widehat{L_1\beta_1}\right) + A_\Gamma\beta_2\beta_2'A_\Gamma' = V(\Gamma) + B(\Gamma).$$

One can introduce a measure to reflect a magnitude of $MSE(\widehat{L_1\beta_1})$ or in general a convex combination of $V(\Gamma)$ and $B(\Gamma)$. However, this is not an easy problem because $MSE(\widehat{L_1\beta_1})$ is a function of the unknown parameters σ^2 and β_2 and thus one would have to deal with an objective function such as $Q_6 = \max_{\beta\,\sigma\,\Lambda} trace(V(\Gamma) + B(\Gamma))$, where Λ is some specified set of parameter values. In certain situations where the experimenter can say something about the relative magnitudes of σ^2 and $\beta_2'\beta_2$ and the measure is the trace of $MSE(\widehat{L_1\beta_1})$, some progress is possible. For example, if $\sigma^2/\beta_2'\beta_2$ is "large" (the usual case in the "philosophy" of this section, viz., of primarily worrying about $\beta_2 = 0$), then the quantity to be minimized is approximately the trace of $V(\Gamma)$. On the other hand, if $\sigma^2/\beta_2'\beta_2$ is "small", then the trace of $B(\Gamma)$ should be minimized. Note that these are approximate statements based on a priori knowledge concerning σ^2 and $\beta_2'\beta_2$. These difficulties can be partially overcome or circumvented if the experimenter limits his concern to $V(\Gamma)$ and to $B(\Gamma)$ separately. This means that two quantities should be introduced for measuring the magnitudes of $V(\Gamma)$ and $B(\Gamma)$. Quantities such as Q_1, Q_2, and Q_3 as introduced previously can be associated with $V(\Gamma)$. The trace and similar quantities can be associated with the bias measure $B(\Gamma)$(see Box and Draper [1959,1963] and Karsen, Manson,and Hader [1969] for a slightly different approach to this problem).

A somewhat different approach utilizes the expected value of $\widehat{L_1\beta_1}$, which from equation (3.22) is equal to:

$$E\left[\widehat{L_1\beta_1}\right] = L_1\beta_1 + A_\Gamma\beta_2$$

where

$$A_\Gamma = L_1\left(X'_{\Gamma 1}X_{\Gamma 1}\right)X'_{\Gamma 1}X_{\Gamma 2} \text{ .}$$

Of the various measures which can be introduced, those which take into account all the entries of A_Γ and their magnitudes are the appealing ones. The following measures are of this nature and are also norms of A_Γ in the mathematical sense:

$$m_1(A_\Gamma) = \left(\sum_i \sum_j a^2_{ij}(\Gamma)\right)^{\frac{1}{2}}$$

$$m_2(A_\Gamma) = \operatorname*{Max}_i \sum_j \mid a_{ij}(\Gamma) \mid$$

$$m_3(A_\Gamma) = \operatorname*{Max}_{i,j} \mid a_{ij}(\Gamma) \mid$$

$$m_4(A_\Gamma) = \sum_i \sum_j \mid a_{ij}(\Gamma) \mid$$

where $|a_{ij}(\Gamma)|$ indicates the absolute value of $a_{ij}(\Gamma)$. All these measures are indeed matrix norms, because they satisfy the following properties:

(a) $m_i(A_\Gamma) \geq 0$

(b) $m_i(\alpha A_\Gamma) = |\alpha| m_i(A_\Gamma)$

(c) $m_i(A_\Gamma + B_\Gamma) \leq m_i(A_\Gamma) + m_i(B_\Gamma)$ if $A_\Gamma + B_\Gamma$ is defined.

(d) $m_i(A_\Gamma B_\Gamma) \leq m_i(A_\Gamma) \cdot m_i(B_\Gamma)$ if $A_\Gamma B_\Gamma$ is defined.

(e) $m_i(A_\Gamma) = 1$ if A_Γ has 1 in cell (r,s) and zero elsewhere.

There are no non-trivial relations between these measures. The first measure $m_1(A_\Gamma)$ enjoys some desirable properties which the others do not possess, namely:

(i) $m_1(A_\Gamma)$ is orthogonally invariant, i.e., $m_1(P_1A_\Gamma) = m_1(A_\Gamma P_2) = m_1(A_\Gamma)$ if P_1 and P_2 are orthogonal matrices.

(ii) $m_1(A_\Gamma) = (\text{trace } A_\Gamma' A_\Gamma)^{\frac{1}{2}}$, which implies that $m_1(A_\Gamma)$ is the positive square root of the sum of the eigenvalues of $A_\Gamma' A_\Gamma$. In particular, if A_Γ is a square matrix, then $m_1(A_\Gamma) = (\text{trace } A_\Gamma' A_\Gamma)^{\frac{1}{2}} = (\text{trace } A_\Gamma A_\Gamma')^{\frac{1}{2}} = (\Sigma\lambda_i^2(\Gamma))^{\frac{1}{2}}$, where the λ_i's are the eigenvalues of A_Γ.

If one is interested in $\mathrm{MSE}(\widehat{L_1\beta_1})$, then only $m_1(A_\Gamma)$ is relevant and $m_2(A_\Gamma)$, $m_3(A_\Gamma)$, $m_4(A_\Gamma)$ would not be used; if $A_\Gamma\beta_2$ is to be considered in a different light, then all these measures might be studied.

Because of properties (a) through (e) together with (i) and (ii), we take $m_1(A_\Gamma)$ to be our measure of bias of $L_1\beta_1$ by $A_\Gamma\beta_2$ as indicated above. We define A_Γ to be the <u>bias matrix</u> for design $\Gamma \in \Delta(L)$. In the literature A_Γ is also referred to as the <u>alias</u> or <u>contamination matrix</u>. We formally introduce the following quantity for selecting an optimal design with respect to bias

$$Q_7(\Gamma) = m_1(A_\Gamma) \quad .$$

To complete this section, we define a design Γ to be <u>bias balanced</u> if $\left(\sum_j a_{hj}^2(\Gamma)\right)^{\frac{1}{2}}$ is a constant for all h, where $A_\Gamma = \left(a_{hj}(\Gamma)\right)$. The following measure can be used to select an optimal design $\Gamma \in \Delta(L)$ with respect to departure from bias balancedness:

$$Q_8(\Gamma) = \sum_h (b_h(\Gamma) - \bar{b}(\Gamma))^2$$

where

$$\Big(\sum_j a_{hj}^2(\Gamma)\Big)^{\frac{1}{2}} = b_h(\Gamma) \text{ and } \bar{b}(\Gamma) = \Big(\sum_h b_h(\Gamma)\Big)/s \quad .$$

Note that the use of $Q_8(\Gamma)$ carries the same danger as pointed out in connection with $Q_5(\Gamma)$.

4.3. APPROACHES, APPROXIMATIONS AND APPLICATIONS IN SELECTING FACTORIAL DESIGNS

It is important to be clear on three different aspects in the selection of a design.

(i) Nature of domain G of controlled variable in the application under consideration by the experimenter. One can have a continuum in the t dimensional Euclidean space or a finite (or countable) set, just as in the "continuous" and in the "discrete" case in probability theory. If G is infinite, regularity properties (like continuity), in the natural topology, of the regression functions $\theta'f(g)$, is assumed out of realism or the desire to get anywhere in computing designs. As in other optimization problems, characterization of an extremum is often easier over a continuum than over a large discrete space, but this has nothing to do with whether or not the experimenter is actually faced with a discrete G or a continuum.

(ii) Approaches. One can try to choose a design criterion (a) having to do with utility or loss, or (b) motivated by simplicity in equal spacing, simple matrices to invert, or other pleasing regularity which does not guarantee optimality in the sense of (a) without further proof in special settings where such "appealing" designs may indeed be optimum.

(iii) Approximations. It may be difficult to compute a design satisfying (ii)(a) or even (ii)(b) (for the latter, note settings where a design with equal variance of "elementary estimators" is difficult to characterize). So, as elsewhere in mathematics, one sometimes solves instead a closely related problem which is more tractable, and from that solution obtains an almost optimum solution to the original problem. This could take many forms; for example, in terms of (i), a large finite space G might be replaced by a continuum containing it and a solution over the continuum might then be implemented by using a "nearby" element of the original finite space (which will not necessarily be the optimum over the finite space). This last is not what is usually meant in the design literature by the "APPROXIMATE THEORY". Rather what is meant, which applies equally to either case of (i), is the solution one obtains if "fractional observations" are allowed (the "EXACT THEORY" referring to solving the original problem with integers for replication numbers). It turns out that this approximate theory problem is often easier to solve and can then be implemented by finding a "nearby" integer-valued set of replication numbers which will yield a design that is often close to the optimum for the exact problem.

CHAPTER 5

CHARACTERIZATION OF UNBIASED DESIGNS

In this chapter the concept of minimal unbiased designs for linear parametric functions is introduced. We provide a characterization of these designs in the case where no assumption is made on the total parametric vector and the case where some elements of this vector are assumed to be zero. These minimal unbiased designs then lead to a class of unbiased designs for the linear parametric function. Examples are given to illustrate the concepts and the developments.

5.1. THE PROBLEM OF CHARACTERIZING UNBIASED DESIGNS

The first problem in the study and use of factorial arrangements should be the characterization of the class of all unbiased designs $\Delta(L)$, with respect to the given $L\beta_\rho$. Let Γ be a design in $\Delta(L)$ and let X_Γ be the design matrix associated with Γ. The available theory in linear estimation states that $L\beta_\rho$ is estimable if and only if L is in the row space of X_Γ. Clearly, this tells us little of "immediate use" about which treatments should be in $\Delta(L)$. What researchers on linear models do is the following: they pick a design such that β_ρ is estimable which in turn guarantees estimability of $L\beta_\rho$ This means that Γ be at least a minimal complete factorial arrangement. Of course, all of these designs are contained in $\Delta(L)$, but they do not exhaust $\Delta(L)$, if L is not the identity matrix. For example, if L is a 1xN matrix then $\Delta(L)$ can contain designs of any number of distinct treatments from 1 to N inclusive. The lower bound is clearly achieved whenever $L_{1\times N}$ is a multiple of a row X_ρ for the minimal complete factorial arrangement ρ.

Consider now a general $L_{s\times N}$. A design containing treatments corresponding to rows of X_ρ having non-zero coefficients in the linear combinations clearly is unbiased. In other words if ℓ_i' is the i-th row of L of the form

$$\ell_i' = \sum_{j=1}^{N} \alpha_{ij}(R_j(\rho))$$

where $R_j(\rho)$ is the j-th row of X_ρ and if Γ_i is a design consisting of those treatments corresponding to the $R_j(\rho)$'s in ℓ_i' having non-zero α_{ij}'s, then the design containing the union of the Γ_i's is an unbiased design.

The following example illustrates the above concepts.

Example 5.1. Consider the 2x2 factorial with the model:

$$E\begin{bmatrix} y_{00} \\ y_{10} \\ y_{01} \\ y_{11} \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix}\begin{bmatrix} \phi_1^0 \phi_2^0 \\ \phi_1^1 \phi_2^0 \\ \phi_1^0 \phi_2^1 \\ \phi_1^1 \phi_2^1 \end{bmatrix} = X_\rho \beta_\rho .$$

Let $L = \begin{bmatrix} 1 & 0 & 0 & 1 \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \end{bmatrix}$ and suppose the experimenter is interested in estimating $L\beta_\rho$. The traditional linear model theory says that one needs an arrangement containing the minimal complete factorial arrangement ρ, i.e., a design containing all the above four treatments. But, clearly a design containing (00), (10), and (11) is unbiased and this has fewer treatments. The reason is that:

$$L = \begin{bmatrix} \ell_1' \\ \ell_2' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} R_1(\rho) \\ R_2(\rho) \\ R_3(\rho) \\ R_4(\rho) \end{bmatrix}$$

Here $\Gamma_1 = \{(00), (11)\}$, $\Gamma_2 = \{(10)\}$ and $\Gamma_1 \cup \Gamma_2 = \{(00), (10), (11)\}$. Any design containing $\Gamma_1 \cup \Gamma_2$ is an unbiased design.

It is clear that the general problem of characterizing unbiased designs in a useful way is not solved. We will next give results in some special cases. Before doing this we define an unbiased design for $L\beta_\rho$ to be minimal if the number of treatments in the design is minimal. Such a design will be referred to as a minimal unbiased design.

5.2. CHARACTERIZATION OF MINIMAL UNBIASED DESIGNS FOR $L\beta_\rho$ WITH NO ASSUMPTIONS ON β_ρ

Let L be an s×N matrix and suppose that the experimenter is interested in estimating $L\beta_\rho$. The following algorithm generates a unique minimal unbiased design for $L\beta_\rho$. Since L is in the row space of X_ρ we may write

$$L' = X_\rho' C \tag{5.1}$$

where C is an N×s matrix of coefficients. Since X_ρ is orthogonal the unique solution for C is

$$C = X_\rho L' \,. \tag{5.2}$$

Hence, the unique minimal design is given by those treatments i for which the i-th row of C is not all zeros. Clearly any design containing this minimal design will also be an unbiased design.

Example 5.2. Consider the 3x3 factorial such that the coded levels of the factors are $\{0,1,2\}$. Then under the orthogonal polynomial model the design matrix X_ρ is equal to

$$X_\rho = \begin{bmatrix} \frac{1}{3} & \frac{-1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & \frac{-1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & \frac{1}{2} & \frac{-1}{2\sqrt{3}} & \frac{-1}{2\sqrt{3}} & \frac{1}{6} \\ \frac{1}{3} & 0 & \frac{-\sqrt{2}}{3} & \frac{-1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{3}} & \frac{-1}{3} \\ \frac{1}{3} & \frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & \frac{-1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & \frac{-1}{2} & \frac{1}{2\sqrt{3}} & \frac{-1}{2\sqrt{3}} & \frac{1}{6} \\ \frac{1}{3} & \frac{-1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & 0 & \frac{-\sqrt{2}}{3} & 0 & \frac{1}{\sqrt{3}} & 0 & \frac{-1}{3} \\ \frac{1}{3} & 0 & \frac{-\sqrt{2}}{3} & 0 & \frac{-\sqrt{2}}{3} & 0 & 0 & 0 & \frac{2}{3} \\ \frac{1}{3} & \frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & 0 & \frac{-\sqrt{2}}{3} & 0 & \frac{-1}{\sqrt{3}} & 0 & \frac{-1}{3} \\ \frac{1}{3} & \frac{-1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & \frac{-1}{2} & \frac{-1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & \frac{1}{6} \\ \frac{1}{3} & 0 & \frac{-\sqrt{2}}{3} & \frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & 0 & 0 & \frac{-1}{\sqrt{3}} & \frac{-1}{3} \\ \frac{1}{3} & \frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & \frac{1}{2} & \frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & \frac{1}{6} \end{bmatrix} .$$

Let $L = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$, then from the above it follows that the minimal design for $L\beta_\rho$ is determined by the non-zero rows of C which are shown below:

$$C = X_{\rho}L' = \begin{bmatrix} \frac{-1}{\sqrt{6}} & \frac{1}{2} & \frac{-1}{2\sqrt{3}} \\ \frac{-1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\ \frac{-1}{\sqrt{6}} & \frac{-1}{2} & \frac{-1}{2\sqrt{3}} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{1}{\sqrt{6}} & \frac{-1}{2} & \frac{1}{2\sqrt{3}} \\ \frac{1}{\sqrt{6}} & 0 & \frac{-1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{2} & \frac{1}{2\sqrt{3}} \end{bmatrix} .$$

Hence the unique minimal design is

$$\Gamma = \{(00), (10), (20), (02), (12), (22)\} .$$

5.3. CHARACTERIZATION OF MINIMAL UNBIASED DESIGNS FOR $L\beta_1$ UNDER THE ASSUMPTION THAT $\beta_2 = 0$

We assume that $\beta_{\rho}' = \left(\beta_1' \vdots \beta_2' = 0\right)$ where β_1 is a pxl vector of parameters. The problem here is to find a minimal unbiased design for $L_1\beta_1$. Recall that the model in this case is equal to

$$E\left[Y_{\rho}\right] = X_{\rho 1}\beta_1 . \tag{5.3}$$

For L_1 to be in the row space of $X_{\rho 1}$ there must exist a matrix C_1 such that

$$(5.4) \qquad L_1' = X_{\rho 1}' C_1 \ .$$

Clearly a solution for C_1 is given by

$$(5.5) \qquad C_1 = X_{\rho 1} L_1', \text{ since } X_{\rho 1}' X_{\rho 1} = I \ .$$

Hence an unbiased design for $L_1\beta_1$ is given by those treatments i for which the i-th rows of C_1 are non-zero rows. Such a design is not necessarily minimal as the following example indicates.

Example 5.3. Consider the 2X2 factorial with coded levels $\{0,1\}$, and let $\beta_1' = \left(\phi_1^0\phi_2^0, \phi_1^1\phi_2^0\right)$. The induced model is then given by

$$E \begin{bmatrix} y_{00} \\ y_{10} \\ y_{01} \\ y_{11} \end{bmatrix} = \tfrac{1}{2} \begin{bmatrix} 1 & -1 \\ 1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \phi_1^0\phi_2^0 \\ \phi_1^1\phi_2^0 \end{bmatrix} = X_{\rho 1}\beta_1 \ .$$

If $L_1 = \frac{1}{2}(1 \ -1)$ then a solution for C_1 is given by

$$C_1 = X_{\rho 1} L_1' = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix} \ .$$

Thus an unbiased design determined by C_1 is $\{(00), (01)\}$. But clearly the designs $\{(00)\}$ and $\{(01)\}$ are two minimal unbiased designs for this problem. This clearly follows from the non-uniqueness of C_1 which in turn reflects the dependency of the rows of $X_{\rho 1}$. For these minimal designs the reader may verify that the solutions for the coefficient matrices are

$$C_1^* = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad C_1^{**} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}.$$

From the above it follows that the problem of determining unbiased designs in this setting is solved by finding those solutions to C_1 in the equation $X'_{\rho 1}C_1 = L'_1$ for which C_1 has maximum number of rows with all elements equal to zero. In the literature this problem is known as the <u>non-singularity problem</u> in fractional replication when $L_1 = I_p$. As of the present, all these problems are unresolved.

In the next chapter we delve deeper into the partioning of β_ρ and the resulting minimal unbiased design problem for the case wherein the experimenter is interested in the parameters themselves rather than linear functions.

<u>Remark</u>. So far, we have ignored the problem of estimating σ^2 if it is unknown. However, if the experimenter is interested in estimating this parameter, then the design should take repetitions and/or the addition of treatments into account.

CHAPTER 6

GENERALIZATION OF DESIGNS OF ARBITRARY RESOLUTION

In this chapter we introduce a general partioning of β_ρ in order to estimate some or all of its components with or without negligibility assumptions. We discuss the resulting four exhaustive cases. These general cases include the classical designs of arbitrary resolutions as special cases. In addition we point out search algorithms for finding minimal unbiased designs in each of the four cases.

6.1. THE PARTIONING OF β_ρ FROM THE EXPERIMENTER'S VIEWPOINT

In investigating a phenomenon the experimenter is interested in estimating all the elements of β_ρ if he has no advance knowledge concerning any of them. In other situations he knows some of the elements of β_ρ and he is interested in some specified subset of the remaining ones. More precisely, these two situations lead to the following formulation.

Without loss of generality the total parametric vector β_ρ can be partioned as

$$\beta_\rho' = \left(\beta_1' \vdots \beta_2' \vdots \beta_3'\right) \tag{6.1}$$

where β_1 is an n_1 vector to be estimated, β_2 is an n_2x1 vector not of interest and not assumed to be known, and β_3 is an n_3x1 vector of parameters assumed to be known, such that: $1 \leq n_1 \leq N$, $0 \leq n_2 \leq N-1$ and $0 \leq n_3 = N-n_1-n_2 \leq N-1$. Explicitly we then have the following four cases:

(i) $n_1 = N$, $n_2 = n_3 = 0$.

(ii) $n_2 = 0$, $n_3 \neq 0$.

(iii) $n_2 \neq 0$, $n_3 \neq 0$.

(iv) $n_2 \neq 0$, $n_3 = 0$.

Note that the cases in sections 5.2 and 5.3 are respectively cases (i) and (ii) above. Also the reader should not confuse the β_2 above with the β_2 in the previous chapters. We now connect the concept of "resolution" with the partioning (6.1).

Recalling the definition of an effect of order k from Chapter 3, a design is said to be of resolution R if it permits unbiased estimation of all effects up to order $k < R/2$ when all effects of order R-k and higher are assumed to be zero. The designs of resolution R have been traditionally divided into two types, namely:

(a) $R = 2r$, known as designs of even resolution.

(b) $R = 2r+1$, known as designs of odd resolution.

Thus an even-resolution design is such that all interaction effects (note that main effects = first order interaction effects) involving r-1 or fewer factors are estimable ignoring all interactions of r+1 or more factors. In this case the interactions of r factors are neither completely estimable nor completely ignored. On the other hand, an odd-resolution design is a design which allows unbiased estimation of all interaction effects involving r or fewer factors ignoring all interactions of r+1 or more factors.

Note that an even-resolution design is a special case of (iii) and an odd-resolution design is a special case of (ii) above.

We now study each of the four cases (i) to (iv) separately.

Case (i). Since we have to estimate all the N components of β_ρ, it is clear that the minimal unbiased design is the minimal complete factorial arrangement ρ Hence any design containing ρ will be an unbiased design for β_ρ. If Γ is any such design, then the least squares estimate of β_ρ is:

$$\hat{\beta}_\rho = \left(X_\Gamma' X_\Gamma\right)^{-1} X_\Gamma' Y_\Gamma \tag{6.2}$$

where the rows of X_Γ are the rows of X_ρ taking repetitions into account.

Case (ii). Here the results follow immediately from section 5.3. The basic model is written as:

$$E\left[Y_\rho\right] = X_\rho\beta_\rho = \left[X_{\rho1} \,\vdots\, X_{\rho3}\right]\begin{bmatrix}\beta_1\\ \cdots\\ \beta_3\end{bmatrix} = X_{\rho1}\beta_1 \quad . \tag{6.3}$$

It follows that the search for a minimal unbiased design reduces to finding n_1 independent rows of $X_{\rho1}$, which in general leads to many designs. Any design Γ containing a minimal unbiased design is then an unbiased design for β_1. The least squares estimator using design Γ is obtained as:

$$\hat{\beta}_1 = \left(X_\Gamma' X_\Gamma\right)^{-1} X_\Gamma' Y_\Gamma \quad . \tag{6.4}$$

Exhibiting the whole class of minimal unbiased designs is at present unresolved for a general setting. In some particular cases, such as designs of odd-resolution (e.g. resolution III and V), some work has been done and the interested reader is referred to the pertinent literature.

As an example, consider the 2x2x2 factorial with levels zero and one for each factor. Let $\beta_1' = \left(\phi_1^1\phi_2^0\phi_3^0,\ \phi_1^1\phi_2^1\phi_3^1\right)$ and let β_3 contain the remaining six parameters. It can be easily verified that the designs $\{(000),\ (101)\}$ and $\{(110),\ (111)\}$ are minimal unbiased designs. Of course, the reader may exhibit many more. In this same factorial if we are interested in a resolution III plan then it can be shown that there are 58 minimal unbiased designs for $\beta_1' = \left(\phi_1^0\phi_2^0\phi_3^0,\ \phi_1^1\phi_2^0\phi_3^0,\ \phi_1^0\phi_2^1\phi_3^0,\ \phi_1^0\phi_2^0\phi_3^1\right)$ One of these is $\{(000),\ (011),\ (101),\ (110)\}$. In this connection the reader may try to find the number of minimal unbiased designs of resolution III for the 2x2x2x2 factorial.

<u>Case (iii)</u>. The basic model for this particular case is conveniently written as:

$$(6.5)\qquad E\left[Y_\rho\right] = X_\rho \beta_\rho = \left[X_{\rho 1} \vdots X_{\rho 2} \vdots X_{\rho 3}\right]\begin{bmatrix}\beta_1\\ \cdots\\ \beta_2\\ \cdots\\ \beta_3\end{bmatrix}$$

$$= \left[X_{\rho 1} \vdots X_{\rho 2}\right]\begin{bmatrix}\beta_1\\ \cdots\\ \beta_2\end{bmatrix} .$$

For any arbitrary design Γ the model is

$$(6.6)\qquad E\left[Y_\Gamma\right] = \left[X_{\Gamma 1} \vdots X_{\Gamma 2}\right]\begin{bmatrix}\beta_1\\ \cdots\\ \beta_2\end{bmatrix} .$$

Applying the least-squares procedure to (6.6) we obtain the following normal equations:

$$(6.7)\qquad \begin{bmatrix} X'_{\Gamma 1} X_{\Gamma 1} & \vdots & X'_{\Gamma 1} X_{\Gamma 2}\\ \cdots\cdots & & \cdots\cdots\\ X'_{\Gamma 2} X_{\Gamma 1} & \vdots & X'_{\Gamma 2} X_{\Gamma 2}\end{bmatrix}\begin{bmatrix}\beta_1\\ \cdots\\ \beta_2\end{bmatrix} = \begin{bmatrix}X'_{\Gamma 1}\\ \cdots\\ X'_{\Gamma 2}\end{bmatrix} Y_\Gamma .$$

It is clear that there exists no unbiased estimator of β_1 unless $X'_{\Gamma 1}X_{\Gamma 2} = 0$ and $X_{\Gamma 1}$ is of full rank. If these conditions are satisfied then (6.7) reduces to

$$(6.8)\qquad \left[X'_{\Gamma 1} X_{\Gamma 1}\right]\beta_1 = X'_{\Gamma 1} Y_\Gamma$$

so that the least squares estimator is equal to:

$$(6.9)\qquad \hat{\beta}_1 = \left[X'_{\Gamma 1} X_{\Gamma 1}\right]^{-1} X'_{\Gamma 1} Y_\Gamma .$$

Hence, a search for a minimal unbiased design is equivalent to finding a set of treatments of cardinality greater than n_1 (this is obvious from the above conditions) such that the rank of $X_{\Gamma 1}$ is equal to n_1 and the columns of X_Γ are orthogonal to the columns of $X_{\Gamma 2}$.

The problem of finding unbiased designs (not of the trivial type, i.e., those which contain ρ) is an unsolved problem at present. In certain cases, such as resolution IV, certain classes of unbiased designs have been constructed.

As an illustration consider the previous 2x2x2 factorial. The design $\Gamma = \{(100), (010), (001), (011), (101), (110)\}$ is an unbiased design of resolution IV of the minimal type. The matrices $X_{\Gamma 1}$ and $X_{\Gamma 2}$ are as follows:

$$(6.10) \qquad X_{\Gamma 1} = \frac{1}{2\sqrt{2}} \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix}, \quad X_{\Gamma 2} = \frac{1}{2\sqrt{2}} \begin{bmatrix} 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 \end{bmatrix}$$

so that $X'_{\Gamma 1} X_{\Gamma 2} = 0$. Note that a design, such that $\phi_1^0\phi_2^0\phi_3^0$ is also estimable, requires at least the minimal complete factorial. The resulting design is not of resolution IV.

<u>Case (iv)</u>. The basic model for this case is:

$$(6.11) \qquad E\left[Y_\rho\right] = X_\rho \beta_\rho = \left[X_{\rho 1} \vdots X_{\rho 2}\right] \begin{bmatrix} \beta_1 \\ \cdots \\ \beta_2 \end{bmatrix}$$

so that for any unbiased design Γ with the model

$$(6.12) \qquad E\left[Y_\Gamma\right] = \left[X_{\Gamma 1} \vdots X_{\Gamma 2}\right] \begin{bmatrix} \beta_1 \\ \cdots \\ \beta_2 \end{bmatrix},$$

we have conditions similar to case (iii), i.e. rank $\left[X_{\Gamma 1}\right] = n_1$ and $X'_{\Gamma 1} X_{\Gamma 2} = 0$. Under these conditions the least squares estimator for β_1 is (as before) equal to:

$$\hat{\beta}_1 = \left[X'_{\Gamma 1} X_{\Gamma 1}\right]^{-1} X'_{\Gamma 1} Y_{\Gamma} \quad (6.13)$$

The search for unbiased designs in general is clearly an unsolved problem.

CHAPTER 7

ON ORTHOGONALITY AND BALANCEDNESS OF FRACTIONAL FACTORIAL DESIGNS

The purpose of imposing orthogonality and/or balancedness on factorial designs can be justified in several ways. (i) Many optimal designs in various settings turn out to be orthogonal and/or balanced. (ii) The problem of finding an optimal design with respect to a given optimality criterion Q (see Chapter 4) among all non-trivial unbiased designs is in general untractable. So one way to reduce the size of the class is to impose orthogonality and/or balancedness and search for an optimal design among the reduced class. (iii) Even though at present, with modern electronic computers, one can handle very complex analyses, the two concepts above will help in reducing the number of steps in any kind of computing and verification thereof. (iv) These two properties are desired by many experimenters for some reasons such as equal precision of the estimates, uncorrelated estimates, etc.

7.1. CONCEPTS OF ORTHOGONALITY AND BALANCEDNESS

Consider the partitioned parametric vector β_ρ as in (6.1) i.e.,

$$\beta_\rho' = \left(\beta_1' \vdots \beta_2' \vdots \beta_3'\right) .$$

We define an unbiased design Γ for β_1 to be orthogonal if

$$\text{(7.1)} \qquad \text{Cov}\left(\hat{\beta}_1\right) = \sigma^2 V ,$$

where V is a diagonal matrix. An unbiased design Γ for β_1 is said to be balanced if it is variance balanced (see Chapter 4). This implies that

$$\text{(7.2)} \qquad \text{Cov}\left(\hat{\beta}_1\right) = \left(uI + W\right)\sigma^2$$

where u is a scalar and W is a matrix with zeros in the main diagonal. The concept of balancedness can be generalized to the case where the covariance matrix of $\hat{\beta}_1$ is of the form

$$(7.3) \qquad \text{Cov}\left(\hat{\beta}_1\right) = (Z + W)\sigma^2$$

with

$$(7.4) \qquad Z = u_1 I_1 \oplus u_2 I_2 \oplus \cdots \oplus u_v I_v, \qquad v < n,$$

where $\oplus$ denotes the usual direct sum operation, i.e.

$$(7.5) \qquad Z = \begin{pmatrix} u_1 I_1 & & 0 \\ & \ddots u_2 I_2 & \\ 0 & & \ddots u_v I_v \end{pmatrix}.$$

Some authors have further restricted the concept of balancedness by imposing additional structures on the off-diagonal elements of $\text{Cov}\left(\hat{\beta}_1\right)$ in (7.3).

Many results have been obtained concerning unbiased designs which possess either the orthogonality property or balancedness property or both. Here we shall only clarify mostly the orthogonality concept via examples for the four cases (i) to (iv) of the previous chapter.

7.2. ORTHOGONALITY IN VARIOUS SETTINGS

Case (i), $n_2 = n_3 = 0$. Any design Γ which contains ρ a fixed number of times and no parts of ρ is an unbiased orthogonal design for $\beta_1 = \beta_\rho$. Note that such a design is also balanced according to (7.1).

Case (ii), $n_2 = 0$, $n_3 \neq 0$. Any unbiased orthogonal design Γ should satisfy, in addition to unbiasedness, the following equation:

(7.6) $$\left(X'_{\Gamma} X_{\Gamma}\right)^{-1} = V \ .$$

As an illustration consider the 2x2x2 factorial with levels zero and one for each factor. Let $\beta'_1 = \left(\phi_1^0\phi_2^0\phi_3^0,\ \phi_1^1\phi_2^0\phi_3^0,\ \phi_1^0\phi_2^1\phi_3^0,\ \phi_1^0\phi_2^0\phi_3^1\right)$. It can be easily verified that the design $\{(100), (010), (001), (111)\}$ is a minimal unbiased orthogonal and balanced design.

Case (iii), $n_2 \neq 0$, $n_3 \neq 0$. An unbiased orthogonal design for this case should not only satisfy the unbiasedness condition but also

(7.7) $$\left(X'_{\Gamma 1} X_{\Gamma 1}\right)^{-1} = V \ .$$

As an example consider a 3x3 factorial with the levels of each factor being 0, 1, and 2. Let $\beta'_1 = \left(\phi_1^1\phi_2^0,\ \phi_1^2\phi_2^0\right)$, $\beta'_2 = \left(\phi_1^0\phi_2^0,\ \phi_1^0\phi_2^1,\ \phi_1^0\phi_2^2\right)$, and $\beta'_3 = \left(\phi_1^1\phi_2^1,\ \phi_1^1\phi_2^2,\ \phi_1^2\phi_2^1,\ \phi_1^2\phi_2^2\right)$. Then the design $\{(00), (10), (20)\}$ is a minimal unbiased orthogonal design. The matrices $X_{\Gamma 1}$ and $X_{\Gamma 2}$ are

$$X_{\Gamma 1} = \begin{bmatrix} \frac{-1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} \\ 0 & \frac{-2}{3\sqrt{2}} \\ \frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} \end{bmatrix} , \quad X_{\Gamma 2} = \begin{bmatrix} \frac{1}{3} & \frac{-1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} \\ \frac{1}{3} & \frac{-1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} \\ \frac{1}{3} & \frac{-1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} \end{bmatrix} ,$$

where $X'_{\Gamma 1} X_{\Gamma 1} = \frac{1}{3} I$ and $X'_{\Gamma 1} X_{\Gamma 2} = 0$.

Case (iv), $n_2 \neq 0$, $n_3 = 0$. A design Γ in this final case must satisfy the unbiased condition together with

$$(7.8) \qquad \left(X'_{\Gamma 1} \, X_{\Gamma 1}\right)^{-1} = V \, .$$

As an example the above 3X3 factorial with $\beta_1' = \left(\phi_1^1\phi_2^0, \, \phi_1^0\phi_2^1, \, \phi_1^1\phi_2^1, \, \phi_1^2\phi_2^1, \, \phi_1^1\phi_2^2\right)$ and $\beta_2' = \left(\phi_1^0\phi_2^0, \, \phi_1^2\phi_2^0, \, \phi_1^0\phi_2^2, \, \phi_1^2\phi_2^2\right)$, the reader can verify that the design {(00), (10), (20), (01), (21), (02), (12), (22)} is an unbiased orthogonal design.

As special cases of the above designs, the reader will find in the literature constructions of orthogonal resolution III, IV, and V type of designs.

CHAPTER 8

SOME KNOWN TECHNIQUES FOR CONSTRUCTING FRACTIONAL FACTORIAL DESIGNS

A detailed description of all the known techniques for the construction of fractional factorial designs would call for a book of at least a couple of hundred pages. The purpose of this monograph is not to do this. What we shall do is the following: list known techniques together with illustrations of some of them, and provide the reader with a large number of selected literature citations (next chapter). We believe this approach is not only compatible with the spirit of this monograph but also does not bias the reader with the techniques preferred by the authors.

The following construction techniques appear in the literature:

1. Trial and error and/or computer methods
2. Hadamard matrix methods.
3. Confounding techniques.
4. Group theory methods.
5. Finite geometrical methods.
6. Algebraic decomposition techniques.
7. Combinatorial-topological methods.
8. Fold-over techniques.
9. Collapsing of levels methods.
10. Composition (Direct product and direct sum) methods.
11. Permutation of levels and/or factors methods.
12. Coding theory methods.
13. Orthogonal array techniques.
14. Partially balanced array techniques.
15. Orthogonal latin square methods.

16. Block design techniques.
17. Weighing design techniques.
18. F-square techniques.
19. Lattice design methods.
20. Graph-theoretical methods.
21. One at a time methods.
22. Inspection methods (see Chapter 5).
23. Other methods.

We will discuss and illustrate techniques 2, 10 and 15.

Hadamard matrix methods. A matrix of order n is said to be a Hadamard-matrix H_n if its entries are ± 1 and $H'_n H_n = nI_n$. It is known that a necessary condition for H_n to exist is that $n = 2$ or $n = 0 (\text{mod } 4)$. Whether this condition is also sufficient has not yet been settled. Also it is known that in the class of matrices of order n with absolute value of the entries less than or equal to 1, a Hadamard matrix H_n has maximal absolute value determinant. Since a Hadamard matrix is still a Hadamard matrix if any row or any column is multiplied by -1, we may always write any H_n-matrix and that it's first column consists of all 1's. Such a matrix is called a semi-normalized Hadamard matrix and is denoted by $\tilde{H}_n$.

Consider a semi-normalized Hadamard matrix of order n. Replace all -1 entries by 0 and delete the first column. Denote this matrix by D_n. This will result in an $n \times (n-1)$ zero-one matrix, providing us a saturated d-optimal resolution III(or main effects) plan for the 2^{n-1} factorial by calling the rows of this matrix a treatment. Incidentally, by selecting any k columns of D_n, one obtains an unsaturated d-optimal plan for a 2^k factorial where $\log_2 n \leq k < n-1$.

As an example consider the semi-normalized Hadamard matrix of order 8.

$$\tilde{H}_8 = \begin{bmatrix} 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

The matrix D_8 below provides a saturated d-optimal resolution III design for the 2^7 factorial:

	Factors						
	F_1	F_2	F_3	F_4	F_5	F_6	F_7
	0	0	0	1	1	1	0
	1	0	0	0	0	1	1
	0	1	0	0	1	0	1
Treatment Combinations	0	0	1	1	0	0	1
	1	1	0	1	0	0	0
	1	0	1	0	1	0	0
	0	1	1	0	0	1	0
	1	1	1	1	1	1	1

Also, for example, the first 4 columns is an unsaturated d-optimal design for the 2^4 in 8 runs. Finally, physically different but still d-optimal designs can be obtained by level permutations of the factors in the given designs. For example, if the level 0 of F_1 is permuted to level 1 of F_1, then a d-optimal design for the 2^4 factorial consisting of the original first 4 columns is transformed into a physically different design which is also d-optimal.

Composition methods. In this category, for example, falls the direct product method of constructing fractional factorial designs. An application of this method consists in combining two orthogonal resolution III plans for the $k_1^{m_1}$ and $k_2^{m_2}$ factorials in n_1 and n_2 runs respectively into a fractional factorial plan for the $k_1^{m_1} \times k_2^{m_2}$ factorial in n_1n_2 runs such that all main effects and a subset of all two-factor interaction effects comprising interactions between one k_1- and one k_2-level factor are orthogonally estimable. Explicitly, the direct product composition method is as follows. Let D_1 and D_2 be the respective orthogonal main effect designs for the $k_1^{m_1}$ and $k_2^{m_2}$ factorials. The design $D_1 \otimes D_2$ consists of treatments $g = (g_1, g_2)$, where $g_1 \epsilon D_1$ and $g_2 \epsilon D_2$, and is called the direct product design. To illustrate this method, the orthogonal main effect plan for the 2^7 factorial is as given previously, so that together with the orthogonal main effect plan below for the 3^4 factorial

	Factors			
	F_8	F_9	F_{10}	F_{11}
Treatment Combinations	0	0	0	0
	0	1	1	2
	0	2	2	1
	1	0	1	1
	1	1	2	0
	1	2	0	2
	2	0	2	2
	2	1	0	1
	2	2	1	0

we obtain the plan $D_1 \otimes D_2$, which is equal to:

$$D_1 \otimes D_2 = \begin{array}{|ccccccccccc} F_1 & F_2 & F_3 & F_4 & F_5 & F_6 & F_7 & F_8 & F_9 & F_{10} & F_{11} \\ \hline 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 2 \\ - & - & - & - & - & - & - & - & - & - & - \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 2 & 2 & 1 & 0 \\ - & - & - & - & - & - & - & - & - & - & - \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 2 & 2 & 1 & 0 \end{array}$$

This design with 8x9 = 72 runs allows orthogonal estimation of main effects and the two-factor interactions of one of the factors $F_1, F_2, \ldots, F_7$ with one of the factors F_8, F_9, F_{10}, F_{11}.

This method can be generalized in several directions, i.e., we may drop the orthogonality condition and/or increase the factorial to more than two different levels of factors.

Orthogonal Latin squares method. Let S be a set of cardinality k. Then a Latin square of order k on S is a square matrix of order k with entries from S such that every element of S appears exactly once in each row and column. Two Latin squares L_1 and L_2 on S are said to be orthogonal if upon superposition of L_1 on L_2, the resulting k^2 entries are all distinct. By a set of t mutually orthogonal Latin squares of order k on S we mean a collection of t Latin squares of order k on S such that they are pairwise orthogonal. One can construct many different fractional factorial plans via orthogonal Latin squares. Here we describe a method to produce an orthogonal main effect plan for k^{k+1} factorial in k^2 runs by transforming a set of k-1 mutually orthogonal Latin squares of order k on S. This is achieved by identifying the rows and columns in each square by the elements of S and forming treatments of the form $g = (i_1, i_2, \ldots, i_{k-1})$, where i_r, $3 \le r \le k-1$ is the entry in the (i_1, i_2) cell of the r-th Latin square. For example, let $S = \{1,2,3\}$ and

$$L_1 = \begin{array}{c|ccc} & \multicolumn{3}{c}{\text{columns}} \\ \text{rows} & 1 & 2 & 3 \\ \hline 1 & 1 & 2 & 3 \\ 2 & 2 & 3 & 1 \\ 3 & 3 & 1 & 2 \end{array}\ , \qquad L_2 = \begin{array}{c|ccc} & \multicolumn{3}{c}{\text{columns}} \\ \text{rows} & 1 & 2 & 3 \\ \hline 1 & 1 & 2 & 3 \\ 2 & 3 & 1 & 2 \\ 3 & 2 & 3 & 1 \end{array}\ ,$$

then the following design with 9 runs is an orthogonal main effect plan for the 3^4 factorial.

Factors

	F_1	F_2	F_3	F_4
Treatment Combinations	1	1	1	1
	1	2	2	2
	1	3	3	3
	2	1	2	3
	2	2	3	1
	2	3	1	2
	3	1	3	2
	3	2	1	3
	3	3	2	1

where factor F_1 represents the rows in L_1, factor F_2 the columns in L_1, factor F_3 the treatments in L_1, and factor F_4 the treatments in L_2.

In a similar fashion, one can obtain fractional replication from a generalization of the Latin square, viz., the F-square.

CHAPTER 9

SELECTED LITERATURE

For an extensive coverage of literature citations on the various aspects of fractional replication and factorial experiments, the reader is directed to A Bibliography on Experiment and Treatment Designs, Pre-1968 by W. T. Federer and L. N. Balaam (Oliver and Boyd, in press), and specifically to the approximately 2000 references in the section on treatment design. We have selected a number of references to published results which cover some of the theory associated directly with fractional replication in factorials and have included papers through the present time, for inclusion in this monograph. They are listed in alphabetical-chronological order and follow starting on the next page. The reader should note that the references were selected to present a cross-section of ideas current in fractional replication; for further reading in this area, he is referred to literature citations in the following papers and to the detailed bibliography given above.

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