Equivalences in Design of Experiments

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Equivalences in Design of Experiments

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Chapter 1

Introduction

In this chapter we first give a brief historical overview of the statistical theory of experimental designs. Thereafter, the structure and scope of the thesis is given. In our historical overview we focus on factorial designs, an important subclass of experimental designs. Factorial designs are nowadays probably the most widely used type of experimental designs in industry. The underlying theory, however, was largely developed in the context of agricultural experiments in the first half of the twentieth century.

1.1 Historical overview

The statistical theory of experimental designs was initiated by Fisher in the 1920s in the context of agricultural experiments performed at the Rothamsted Experimental Station. Although Fisher is rightly regarded as the founder of modern methods of experimental design, it would be wrong to assume that there were no earlier developments in experimental design (Yates (1964)). Already in the 19th century various types of layouts for field experiments at the Rothamsted Experimental Station had been devised on the basis of common sense. What was lacking, however, was a coherent theory on how to estimate the errors from the observed data. Only for the simple case of a comparison of two treatments a formal test had been introduced in 'Student' (1908). Fisher (1926) explained the basic principles of experimental design and advocated the ideas of replication, blocking and randomization. Of these three only the idea of randomization was new (Yates (1964)). However, what Fisher developed was an experimental strategy in which the three concepts together formed the basis for the analysis of an experiment (Street (1990)). Moreover, Fisher was the first to provide a concise argument for why full factorial experiments[1] were much more efficient than simple experiments where questions are investigated one at a time. Fisher explained that besides their efficiency factorial experiments had the advantage

[1] Full factorial designs are called complex experiments in the earlier works of Fisher and Yates.

that single-factor comparisons were given a much wider inductive basis than in single question methods, without extensive repetitions of the experiment.

Around 1930 it was formally recognized at the Rothamsted Experimental Station that the errors could be estimated from negligible higher order interactions (Yates (1975), p. 589). According to Yates (1964) the earliest statistical analysis of a factorial experiment in which negligible interactions are used in the estimation of the error appeared in Eden and Fisher (1929). Moreover, it was then realized that replications were not always necessary in order to estimate the error and that for experiments involving several variables a single replicate factorial design was often sufficient.

A major disadvantage of factorial experiments is that the size of blocks that they require rapidly becomes extremely large, because ideally all responses of a single replicate should be made in the same block. The block size may, however, be kept small at the cost of introducing non-orthogonality into the experimental design. The concept of confounding as it is introduced in Fisher (1926) and more extensively explained in Yates (1933) (reprinted in Yates (1970)) refers to such a deliberate introduction of non-orthogonality. Yates (1933) gives the following definition for orthogonality: "*Orthogonality is that property of the design which ensures that different classes of effects to which the material is subject shall be capable of direct and separate estimation without any entanglement*". If, in order to keep the block size small, complete replication within each block is sacrificed, then certain treatment effects will be confounded with block effects. In cases in which it is required to subdivide a complete replication into blocks, then it is best to do so in in such a way that only information on unimportant interactions is lost. This problem was solved in Fisher (1942) for factorial designs in which all variables are set at two levels and in Fisher (1945) for symmetric factorial designs with a prime power number of levels[2]. So confounding allows us to use smaller blocks at the cost of losing some information about higher-order interactions.

During the mid 1940s it was first realized that if certain treatment interactions may be assumed negligible, then only a selection of all possible treatment combinations needs to be considered in the experiment. The device of fractional replication was developed by Finney (1945). Finney studied the confounding of treatment effects on fractional replicates (or simply fractions) using the theory of finite Abelian groups. The fractions that Finney considered were subgroups of the Abelian group that coded the full factorial design. The fractional factorial designs provided an efficient alternative to the (replicated) full factorial designs and are nowadays widely used.

Independent of the British school of Fisher and Yates a theory of factorial

[2]In particular, Fisher (1942) used the theory of finite Abelian groups to show that using blocks of size 2^r it is possible to test all combinations of as many as $2^r - 1$ variables in such a way that all interactions confounded with block effects shall involve not less than three variables each. In Fisher (1945) it is shown that blocks of size p^{rs} suffice for use with $(p^{rs} - 1) / (p^r - 1)$ variables, each at p^r levels. These results anticipated the sphere-packing bound and construction of Hamming codes (see Cameron (1998) and Calderbank (1998)). The interconnection between experimental design and coding theory was first brought out in Bose (1964).

designs using finite geometry was developed by Bose and Kishen (see Bose and Kishen (1940) and Bose (1947)). In the approach of Bose and Kishen the runs in the factorial experiment are coded with the elements of a finite geometry of a Galois field. The confounding patterns are explained in geometric terms of lines, hyperplanes, etc. This geometric description of factorial designs proved very successful. Its application is, however, restricted by the facts that the number of elements in a Galois field must be a prime power and that a geometry must use the same field for every dimension (Bailey (1990)). This makes the generalization of results to asymmetrical factorial designs in which factors may have different numbers of levels very difficult. Despite these limitations, the geometric approach is still widely used.

Nowadays factorial designs are probably the most widely used type of experimental designs in industry. The first industrial application of experimental design is reported in Tippett (1935) where a fractional factorial design is used to discover the cause of difficulties in a cotton spinning machine. During the 1940s experimental design was used in the textile, electrical and mechanical industries. Current applications of experimental design can also be found in a wide range of other manufacturing industries such as the electronic, food, chemical, paper, automotive, and rubber industries (Bisgaard (1992)).

The large increase in applications of experimental designs that started late 1940s raised interest in finding experimental designs which are "good" in some well-defined sense. The related mathematical theory, which is now known as the theory of optimal design, was initiated by Kiefer in the 1950s.

In the 1970s Taguchi emphasized the importance of variation reduction for improving the quality of products and processes in industrial engineering. His work inspired researchers in experimental design to also consider how variables affect the variance (and not only the mean) of a quality measure. An important paper on this topic is Box and Meyer (1986), in which the identification of dispersion effects from unreplicated factorial designs is proposed.

More recent technological developments in biology (DNA microarrays) and chemical engineering (high-throughput reactors) generated new challenges in experimental design. So experimental designs is a lively subject with a rich history from both an applied and theoretical point of view.

1.2 Scope and structure of this thesis

This thesis is mainly an exploration of the mathematical framework underlying factorial designs. Most of the literature on experimental designs is either example-based with lack of general statements and clear definitions or so abstract that the link to real applications is lost. With this thesis we hope to contribute to closing this gap. By restricting ourselves to factorial designs it is possible to provide a framework which is mathematically rigorous yet applicable in practice. This framework is presented in Chapter 2.

In Chapter 3 we study the coding of factorial designs by finite Abelian groups. Finney used this coding to study confounding on the fractions that

are subgroups of the finite Abelian group. Recently, Diaconis and Viana have shown that the well-known sums of squares decomposition in analysis of variance for full factorial designs naturally arises from harmonic analysis on the finite Abelian group. Their theories cannot be directly applied to find the sums of squares decomposition for fractional factorial designs. We give an extension of the setups of Diaconis and Viana by developing the theoretical aspects of harmonic analysis of data structured on fractions that are cosets of finite Abelian groups. These cosets play a special role in experimental design and are referred to as regular fractions. Several other definitions for regular fractions have appeared in literature recently. We use the character theory of the finite Abelian group to show that these definitions are all equivalent. We moreover use character theory to prove that any regular fraction when interpreted as a coset is an orthogonal array of a certain strength related to the resolution of the fraction. This generalizes results by Rao and Bose for regular fractions of symmetric factorial designs with a prime power as the number of levels. This chapter is joint work with A. Di Bucchianico (Eindhoven University of Technology and EURANDOM). Part of the results in this chapter have appeared in Van de Ven and Di Bucchianico (2006).

In Chapter 4 we study the estimation of the dispersion parameters in a mixed linear model. This is the common model behind modern engineering approaches to experimental design like the Taguchi approach. Several estimators for the dispersion effects in unreplicated factorial designs are considered. In particular, we consider the estimation of dispersion effects using unreplicated fractional factorial designs as it was initiated by Box and Meyer in the 1980s. Under a linear model for the variance estimators for the dispersion effects are given in Wiklander (1998) (see also Wiklander and Holm (2003)), Liao and Iyer (2000) and Brenneman and Nair (2001). The proposed estimators all look very different at first sight. However, we prove that these estimators coincide for two-level full factorial designs and their regular fractions. The results of this chapter have appeared in Van de Ven (2005). A slightly modified version of this technical report has been accepted for publication in the Journal of Statistical Planning and Inference.

In Chapter 5 we study a problem arising in two-step production processes. In this problem an intermediate product processed in the first step is split into several parts in order to allow further processing in the second step. This type of situation is typically handled by using a split-plot design. However, in this specific example running a full factorial split-plot design was not feasible for economic reasons. We show how to apply recently developed analysis methods for fractional factorial split-plot designs developed by Bisgaard, Bingham and Sitter. We modify an algorithm by Franklin and Bailey to generate fractional factorial split-plot designs that identify a given set of effects while minimizing the number of required intermediate products. This chapter is joint work with E.E.M. van Berkum (Eindhoven University of Technology), E.J. Habers (Avery Dennison) and J.T.M. Wijnen (Eindhoven University of Technology). The results have appeared in Van Berkum et al. (2005).

Chapter 2

Factorial Designs

Factorial experiments have proven an efficient and economic means to determine the influence of several input variables on a response variable of interest. This type of experiments is nowadays used in a wide range of fields including industry, economics, biology and chemistry. Textbooks on design of experiments usually emphasize the practical side and hardly touch upon the underlying mathematical theory. Purely mathematical discussions of the underlying theory can be found in Bailey (1996), Tjur (1984) and Tjur (1991). These papers discuss factorial designs in a very abstract way and the connections to the practical aspects that the experimenter and statistical analyst face are not always clear. In this chapter we give the underlying mathematical theory and point out its connections with the more practically oriented discussions of factorial designs that are found in textbooks. The outline of this chapter is as follows. In Section 2.1 we present the mathematical theory that involves the definitions of partitions and interaction spaces as introduced in Bailey (1996), Tjur (1984) and Tjur (1991). The notions of identifiability, factorial effects and confounding are defined within the context of this theory. A formulation of the factorial effects in terms of Kronecker products is discussed in Section 2.2. The theory of partitions and interaction spaces is in Section 2.3 and 2.4 connected to the ANOVA and linear regression models, respectively. The estimability of factorial effects is defined in Section 2.5.

2.1 Preliminaries and notation

By k we denote the number of variables or experimental conditions considered in the experiment. The variables are denoted by $x_1, x_2, \ldots, x_k$. With each variable x_j we associate a finite set L_j of n_j level indicators where $n_j \geq 2$. The n_j elements in the set L_j represent the levels of the variable x_j that are considered in the experiment. If the variable x_j is continuous, then the values in the set L_j may correspond to real settings of the variable. In that case we refer to the levels as *actual* levels. In all other cases we refer to the elements in

L_j as *formal* levels.

Definition 2.1 (Factorial design) A factorial design is defined as any subset D of the Cartesian product $\prod_{j=1}^{k} L_j = L_1 \times L_2 \times \ldots \times L_k$ of the sets $L_1, L_2, \ldots L_k$.

The factorial design is a *full factorial design* if $D = \prod_{j=1}^{k} L_j$. In all other cases, D is called a *fractional factorial design* or, simply, *fraction*. A factorial design is symmetric if $n_1 = n_2 = \ldots = n_k$. If $p_1, p_2, \ldots, p_m$ (where $m \leq p$) denote the distinct number of levels for the variables in a factorial design, then the full factorial design in which q_j of the k variables are set at p_j levels is also referred to as a $p_1^{q_1} p_2^{q_2} \ldots p_m^{q_m}$ factorial design (where $\sum_{j=1}^{m} q_j = k$). From the definition of factorial design it is clear that the elements of factorial designs are vectors of length k. These elements are usually referred to as *treatments* or *runs*. We use d_j to refer to the jth element of the vector $d \in D$ and let N denote the number of runs in the design D. The most familiar factorial designs are those that have two levels for every variable in the experiment. An example of such a design is given in the following example.

Example 2.2 Consider the full factorial design with two variables x_1 and x_2 both at two levels, that is, the 2^2 factorial design. If the levels of the variables are coded by elements in the set $L_1 = L_2 = \{0, 1\}$, then the design is given by $D = \{(0,0), (1,0), (0,1), (1,1)\}$.

The single-observation data obtained in the experiment is a point y in the vector space $\mathbb{R}^D$ of real-valued functions defined on D. It evaluates as y_d or $y(d)$. The vector space $\mathbb{R}^D$ is an inner-product space with the inner product defined by

$$\langle f, g \rangle_D = \frac{1}{\mid D \mid} \sum_{d \in D} f(d)\, g(d) \tag{2.1}$$

for $f, g \in \mathbb{R}^D$. In some cases we prefer to have the data as a vector instead of a function. In order to have a unique way to represent each function $y \in \mathbb{R}^D$ as a vector, we assume a specific ordering of the runs in the design D. Assume that for each of the sets $L_j, 1 \leq j \leq k$, we have an ordering of the elements. The lexicographic order is a natural ordering for the elements in Cartesian products such as $\prod_{j=1}^{k} L_j$. Let d and t be elements of $\prod_{j=1}^{k} L_j$. The element d precedes t in the lexicographic ordering if for the smallest j for which $d_j \neq t_j$ we have that d_j precedes t_j in L_j. This is denoted by $d \prec_{\text{lex}} t$. Another way of ordering the treatments in a full factorial design is by the Yates order. In this order the element d precedes t if for the largest j for which $d_j \neq t_j$ we have that d_j precedes t_j in L_j.

Example 2.3 Consider the factorial design D in Example 2.2. If the ordering of elements in L_1 (and L_2) is given by $0 \prec 1$ (that is, 0 precedes 1) then the elements in D are ordered in lexicographic order according to

$$(0,0) \prec_{\text{lex}} (0,1) \prec_{\text{lex}} (1,0) \prec_{\text{lex}} (1,1).$$

The treatments in D are given in Yates order by

$$(0,0) \prec_{\text{Yates}} (1,0) \prec_{\text{Yates}} (0,1) \prec_{\text{Yates}} (1,1).$$

For each run $d \in D$ and subset $J \subseteq \{1,2,\ldots,k\}$ we define the restriction d_J of d to J by $d_J = (d_{j_1}, d_{j_2}, \ldots, d_{j_\ell})$ where $j_1, j_2, \ldots, j_\ell$ are the elements of J indexed to satisfy $j_1 < j_2 < \ldots < j_\ell$. We let D_J denote the set of all $\prod_{j\in J} n_j$ distinct restrictions d_J of runs $d \in D$ to J. Following Tjur (1984) we define a factor X_J as a function from the set of runs D into the restriction D_J.

Definition 2.4 (Factor) The factor $X_J, J \subseteq \{1,2,\ldots,k\}$, is the function from D into D_J defined by $X_J(d) = d_J$. The trivial factor is the function $X_\emptyset = 1$ defined on D.

Factors X_J with $\mid J \mid \geq 2$ are also referred to as *interactions*. In the literature fixed and random factors are distinguished. If the levels in L_j have been specifically chosen by the experimenter, we say that the factor $X_{\{j\}}$ is *fixed*. Alternatively, the levels in L_j may be randomly selected from the population of factor levels. In this case we say that the factor $X_{\{j\}}$ is *random*. A factor X_J with $\mid J \mid \geq 2$ is considered fixed if all factors $X_{\{j\}}, j \in J$, are fixed. The factor X_J is considered random if at least one of the factors $X_{\{j\}}, j \in J$, is random. The trivial factor $X_\emptyset$ is considered fixed. The factors each induce a partition on the set D of treatments.

Definition 2.5 (Partition) The partition π_J is the equivalence relation that X_J induces on D. The equivalence classes for π_J are the subsets $\{d \in D \mid X_J(d) = \text{constant}\}$.

Note that the trivial partition $\pi_\emptyset$ is the partition of D into a single equivalence class. We define $\Pi = \{\pi_J \mid J \subseteq \{1,2,\ldots,k\}\}$. The set Π is usually referred to as the complete factorial structure. The concepts of partition and complete factorial structure are illustrated in the next example.

Example 2.6 Consider the full factorial design in Example 2.2. The complete factorial structure is the set $\Pi = \{\pi_\emptyset, \pi_{\{1\}}, \pi_{\{2\}}, \pi_{\{1,2\}}\}$. The equivalence classes induced by the partitions that make up the complete factorial structure are illustrated in the next table.

Partition	Equivalence classes
$\pi_\emptyset$	$\{(0,0),(1,0),(0,1),(1,1)\}$
$\pi_{\{1\}}$	$\{(0,0),(0,1)\},\{(1,0),(1,1)\}$
$\pi_{\{2\}}$	$\{(0,0),(1,0)\},\{(0,1),(1,1)\}$
$\pi_{\{1,2\}}$	$\{(0,0)\},\{(1,0)\},\{(0,1)\},\{(1,1)\}$

An extensive treatment of partitions in the context of factorial designs can be found in Bailey (1996). The next properties of partitions are relevant for this work. Let J_1 and J_2 be two distinct subsets of $\{1,2,\ldots,k\}$. We say that π_{J_1} is coarser than π_{J_2} (or, equivalently, π_{J_1} nests π_{J_2} or π_{J_2} is finer than π_{J_1}) if every π_{J_2}-class is contained in a π_{J_1}-class. From Definition 2.5 we find that the

partition π_{J_2} is finer than π_{J_1} if and only if $J_1 \subset J_2$. The infimum $\pi_{J_1} \wedge \pi_{J_2}$ is the coarsest partition finer than both π_{J_1} and π_{J_2}. The supremum $\pi_{J_1} \vee \pi_{J_2}$ is the finest partition that is coarser than both π_{J_1} and π_{J_2}. Again from Definition 2.5, it is easily derived that $\pi_{J_1} \wedge \pi_{J_2} = \pi_{J_1 \cup J_2}$ and $\pi_{J_1} \vee \pi_{J_2} = \pi_{J_1 \cap J_2}$.

To each partition $\pi_J, J \subseteq \{1, 2, \ldots, k\}$, we associate a linear subspace V_J of $\mathbb{R}^D$ in the following way.

Definition 2.7 (Factor space) The factor space $V_J, J \subseteq \{1, 2, \ldots, k\}$, is the set of functions in the vector space $\mathbb{R}^D$ that are constant on each of the equivalence classes that the partition π_J induces on D.

It is easy to see that for all distinct sets J_1 and $J_2 \subseteq \{1, 2, \ldots, k\}$ we have that V_{J_1} is strictly contained in V_{J_2} if and only if $J_1 \subset J_2$. The definition is illustrated in the next example.

Example 2.8 Consider again the factorial design from Example 2.2. The factor space $V_J, J \subseteq \{1, 2, \ldots, k\}$, consists of all functions of the form y_J given in the next table

$d \in D$	$y_\emptyset(d)$	$y_{\{1\}}(d)$	$y_{\{2\}}(d)$	$y_{\{1,2\}}(d)$
$(0,0)$	$\tau_\emptyset$	$\tau_1(0)$	$\tau_2(0)$	$\tau_{12}(0,0)$
$(1,0)$	$\tau_\emptyset$	$\tau_1(1)$	$\tau_2(0)$	$\tau_{12}(1,0)$
$(0,1)$	$\tau_\emptyset$	$\tau_1(0)$	$\tau_2(1)$	$\tau_{12}(0,1)$
$(1,1)$	$\tau_\emptyset$	$\tau_1(1)$	$\tau_2(1)$	$\tau_{12}(1,1)$

where $\tau_\emptyset \in \mathbb{R}$ and τ_1, τ_2 and τ_{12} are functions from L_1, L_2 and $L_1 \times L_2$, respectively, into $\mathbb{R}$.

Note that if D is a full factorial design, then the dimension of the factor spaces are $\dim(V_\emptyset) = 1$ and $\dim(V_J) = \prod_{j \in J} n_j$ for $J \subseteq \{1, 2, \ldots, k\}$ and $J \neq \emptyset$.

The crucial step in analyzing the data obtained on factorial designs is determining the part of the response function $y \in \mathbb{R}^D$ that relates to each factor. That is, finding a decomposition of the response function $y \in \mathbb{R}^D$ of the form

$$y = \sum_{J \subseteq \{1,2,\ldots,k\}} y_J \quad \text{with } y_J \in V_J, \tag{2.2}$$

where y_J is the contribution of the factor X_J to the response[1]. The function $y_J \in V_J$ takes constant values on the equivalence classes induced by π_J. From $V_{J_1} \subset V_{J_2}$ for $J_1 \subset J_2$ we find that the decomposition of y given in (2.2) is not unique. A unique decomposition can be obtained by restricting the factor spaces V_J in such a way that identifiability of the decomposition is obtained.

Definition 2.9 (Identifiability) Let $H_1, H_2, \ldots, H_w$ denote a spanning set of linear subspaces for $\mathbb{R}^D$. A decomposition of a function $y \in \mathbb{R}^D$ of the form

$$y = \sum_{j=1}^{w} y_j \quad \text{with } y_j \in H_j, \tag{2.3}$$

[1]The problem of decomposing y is in fact more complicated because usually the measured response is assumed to be distorted by random noise. We have chosen to first discuss the noise-free case.

is identifiable if $y = \sum_{j=1}^{w} y_j = \sum_{j=1}^{w} f_j$ with $y_j, f_j \in H_j$ implies that $f_j = y_j$ for all $j, 1 \leq j \leq w$.

Equivalently, a decomposition is identifiable if the vector space $\mathbb{R}^D$ is the direct sum of the subspaces $H_j, 1 \leq j \leq w$. Identifiability of the decomposition of $y \in \mathbb{R}^D$ in (2.2) is usually obtained by restricting the choice for each function $y_J, J \subseteq \{1, 2, \ldots, k\}$, to a linear subspace H_J of V_J in such a way that these subspaces satisfy $\mathbb{R}^D = \bigoplus_{J \subseteq \{1,2,\ldots,k\}} H_J$

Remark 2.10 A different approach is taken in Terbeck and Davies (1998). For two-way analysis of variance (that is, $k = 2$) Terbeck and Davies (1998) propose a decomposition of $y \in \mathbb{R}^D$ of the form $y = y' + y_{\{1,2\}}$ where $y' \in V_\emptyset + V_{\{1\}} + V_{\{2\}}$ is chosen to minimize the number of runs $d \in D$ for which $y_{\{1,2\}}(d) \neq 0$. An interaction effect between the row and column variables is judged present when $y_{\{1,2\}} \neq 0$. Note that in this approach the decomposition of $\mathbb{R}^D$ depends on y, whereas in standard approaches the decomposition of the vector space $\mathbb{R}^D$ is chosen independently of y.

For D a full factorial design, the $H_J, J \subseteq \{1, 2, \ldots, k\}$, are often chosen to be the linear subspaces defined by

$$H_\emptyset = V_\emptyset \text{ and } H_J = V_J \cap \left(\bigcup_{j \in J} V_{J \setminus \{j\}} \right)^\perp \text{ for } J \subseteq \{1, 2, \ldots, k\} \text{ and } J \neq \emptyset. \tag{2.4}$$

The linear subspaces H_J are usually called interaction spaces.

Definition 2.11 (Interaction space) Let the factor spaces V_J be defined as in Definition 2.7. The interaction space associated with factor X_J is the subspace H_J of $\mathbb{R}^D$ defined by (2.4).

The interaction space H_{J_1} contains exactly those functions that are constant on the equivalence classes induced by the partition π_{J_1}, but not constant on the equivalence classes induced by the partitions π_{J_2} with $J_2 \subset J_1$. The definition for interaction space is illustrated in the next example.

Example 2.12 Consider again the factorial design from Example 2.2. The interaction spaces $H_J, J \subseteq \{1, 2, \ldots, k\}$, consist of all functions of the form y_J given in the next table

$d \in D$	$y_\emptyset(d)$	$y_{\{1\}}(d)$	$y_{\{2\}}(d)$	$y_{\{1,2\}}(d)$
$(0,0)$	$\tau_\emptyset$	$-\tau_1$	$-\tau_2$	τ_{12}
$(1,0)$	$\tau_\emptyset$	τ_1	$-\tau_2$	$-\tau_{12}$
$(0,1)$	$\tau_\emptyset$	$-\tau_1$	τ_2	$-\tau_{12}$
$(1,1)$	$\tau_\emptyset$	τ_1	τ_2	τ_{12}

where $\tau_\emptyset, \tau_1, \tau_2, \tau_{12} \in \mathbb{R}$.

In the decomposition of y given by

$$y = \sum_{J \subseteq \{1,2,\ldots,k\}} y_J \quad \text{where } y_J \in H_J, \tag{2.5}$$

with H_J the interaction space defined in Definition 2.11 the contribution of the factor X_J is restricted to the part that cannot be explained by factors $X_{J'}$ with $J' \subset J$. Moreover, from (2.4) it follows that $H_{J_1} \cap H_{J_2} = \{0\}$ for $J_1 \neq J_2$ and, hence,

$$\mathbb{R}^D = \bigoplus_{J \subseteq \{1,2,\ldots,k\}} H_J$$

is a decomposition of $\mathbb{R}^D$ as a direct sum of orthogonal subspaces. For the special case where D is a full factorial design Theorem 1 in Tjur (1984) tells us that (2.5) is the unique decomposition of the vector space $\mathbb{R}^D$ as an orthogonal direct sum of the linear subspaces $H_J \subseteq V_J, J \subseteq \{1, 2, \ldots, k\}$, that satisfies $V_J = \bigoplus_{J' \subseteq J} H_{J'}$ for all $J \subseteq \{1, 2, \ldots, k\}$. The dimension of the interaction space H_J is $\prod_{j \in J} (n_j - 1)$.

The decomposition of the vector space $\mathbb{R}^D$ as an orthogonal direct sum of the interaction spaces is commonly used in analysis of variance (ANOVA). The ANOVA models associated with this set of techniques are usually given by a full parametrization of the factor spaces $V_J, J \subseteq \{1, 2, \ldots, k\}$, together with a set of constraints on the parameters to obtain identifiability. In some cases a set of identifiability constraints is chosen that results in a direct sum decomposition of $\mathbb{R}^D$ that is different from the orthogonal direct sum of interaction spaces. We will discuss ANOVA models in detail in Section 2.3.

Other decompositions of $\mathbb{R}^D$ as a direct sum of subspaces (not necessarily orthogonal) are also often used. Another well-known example is the linear regression model. The use of linear regression models for data obtained in factorial experiments is discussed in Section 2.4. In linear regression the vector space $\mathbb{R}^D$ is decomposed as a direct sum of $N - r$ one-dimensional subspaces (corresponding to the regression) and one r-dimensional subspace (corresponding to the residual part). In this case identifiability of the decomposition is obtained if and only if the design matrix is full rank.

The experimenter may be interested in specific comparisons of the observations for the different levels of a specific factor. The notions of factorial effect and factorial contrast are introduced for this purpose. Let the function $\mu \in \mathbb{R}^D$ be defined by $\mu(d) = \mathrm{E}[y(d)]$ for all $d \in D$. The function value $\mu(d), d \in D$, is called the effect of the treatment combination d. The function μ is unknown and the treatment effects $\mu(d), d \in D$, are unknown parameters in the context of factorial designs.

Definition 2.13 (Effect/Factorial effect) For $v \in \mathbb{R}^D$, the linear combination

$$\sum_{d \in D} v(d)\, \mu(d) \tag{2.6}$$

is called an effect. The effect is said to belong to a factor X_J if $v \in H_J$. A *factorial effect* is an effect belonging to a factor .

Remark 2.14 A larger class of factorial effects belonging to the factor X_J is obtained when the restriction $v \in H_J$ is replaced by the restriction that $v \in V_J$ and $v \notin \sum_{J' \subset J} V_{J'}$. This way *each* effect $\sum_{d \in D} v(d)\,\mu(d)$ belongs to a unique factor X_J. This less rigid definition is, for instance, used in Terbeck and Davies (1998).

The order of a factorial effect belonging to a factor X_J is defined to be the number of elements in J. A factorial effect of order 1 is a *main effect*. A factorial effect is an *interaction effect* if it has order at least 2. Note that for $v \in H_J$ with $J \neq \emptyset$ the orthogonality of H_J and $H_\emptyset$ implies $\sum_{d \in D} v(d) = 0$. For this reason we will also refer to factorial effects that belong to an interaction space H_J with $J \neq \emptyset$ as *factorial contrasts*.

Example 2.15 Consider the full factorial design $D = L_1 \times L_2$ where $L_1 = L_2 = \{0, 1\}$. A possible set of effects is $\sum_{d \in D} v_J(d)\,\mu(d)$ with v_J given in the next table.

$d \in D$	$v_\emptyset(d)$	$v_{\{1\}}(d)$	$v_{\{2\}}(d)$	$v_{\{1,2\}}(d)$
$(0,0)$	1	-1	-1	1
$(0,1)$	1	-1	1	-1
$(1,0)$	1	1	-1	-1
$(1,1)$	1	1	1	1

For each function v_J in this table we have that $v_J \in H_J$, which implies that $\sum_{d \in D} v_J(d)\,\mu(d)$ is a factorial effect belonging to the factor X_J.

Note that on a full factorial design D there exists an unbiased estimator for every effect defined on D. This follows from

$$\mathrm{E}\left[\sum_{d \in D} v_J(d)\, y(d)\right] = \sum_{d \in D} v_J(d)\,\mathrm{E}\left[y(d)\right] = \sum_{d \in D} v_J(d)\,\mu(d). \tag{2.7}$$

Note that we do not need to assume a specific model for the data in order to make this statement. That is, it is true under any model.

If the number k of variables that need to be considered in the experiment is large, then full factorial designs may become quite expensive. In those cases, typically, only a fraction $F \subset D$ of the full factorial design $D = \prod_{i=1}^{k} L_i$ is run. Because data is only observed on a subset of D, the unbiased estimator given in (2.7) can no longer be used. However, depending on the exact form of the function μ (that is, the model for the data) it might still be possible to find unbiased estimators for factorial effects defined on D using only the observations made on the fraction F. We will consider this estimation issue for fractional factorial designs in Section 2.5 after we have discussed the most widely used models for the data. We first explain the notion of confounding which plays an important role in the theory of fractional factorial designs.

A straightforward way to deal with fractions of factorial designs is to restrict the interactions spaces H_J to the fraction F. The restriction $H_{J|F}$ of the interaction space H_J to F is simply obtained by restricting all functions in H_J to F.

An effect $\tau = \sum_{d \in D} v(d)\,\mu(d)$ can be restricted to F by restricting the summation to F, that is, $\tau_{|F} = \sum_{d \in F} v(d)\,\mu(d)$. As pointed out by Beder (2004), restrictions may destroy the orthogonality of interaction spaces. Moreover, the restriction of a factorial contrast defined on D to the fraction F may not be a factorial contrast on F. The restriction of a set of functions to a subset F of their domain D results in confounding (also referred to as aliasing) of functions. We now present a formal definition of confounding.

Definition 2.16 (Confounding and orthogonality) Let $F \subseteq D$ be a fraction of a full factorial design D. The two functions v_1 and $v_2 \in \mathbb{R}^D$ are said to be completely confounded on F if there exists an $r \in \mathbb{R}$ for which $v_1(d) = r\,v_2(d)$ for all $d \in F$. The functions are orthogonal on F if we have that

$$\langle v_1, v_2 \rangle_F := \frac{1}{\mid F \mid} \sum_{d \in F} v_1(d)\,v_2(d) = 0.$$

The functions v_1 and v_2 are partially confounded on F if they are neither completely confounded nor orthogonal on F.

Two factorial effects $\sum_{d \in D} v_1(d)\,\mu(d)$ and $\sum_{d \in D} v_2(d)\,\mu(d)$ defined on the full factorial design D are said to be completely confounded (or orthogonal or partially confounded) on the fraction F if the functions v_1 and v_2 are completely confounded (or orthogonal or partially confounded) on F. Two interaction spaces H_{J_1} and H_{J_2} are completely confounded on the fraction F if $H_{J_1|F} = H_{J_2|F}$. The interaction spaces are orthogonal if $H_{J_1|F}$ and $H_{J_2|F}$ are orthogonal. Two interaction spaces are partially confounded if they are neither orthogonal nor completely confounded. The notion of confounding is illustrated in the next example.

Example 2.17 Consider the full factorial design D given in Example 2.2. As a first example we consider the interaction spaces given in Example 2.12. The restrictions of $y_\emptyset, y_{\{1\}}, y_{\{2\}}$ and $y_{\{1,2\}}$ to the fraction $F = \{(0,0),(1,1)\} \subset D$ are given in the next table.

$d \in F$	$y_\emptyset(d)$	$y_{\{1\}}(d)$	$y_{\{2\}}(d)$	$y_{\{1,2\}}(d)$
$(0,0)$	$\tau_\emptyset$	$-\tau_1$	$-\tau_2$	τ_{12}
$(1,1)$	$\tau_\emptyset$	τ_1	τ_2	τ_{12}

From this table we see that $H_{\{1\}}$ and $H_{\{2\}}$ are completely confounded on F. Moreover, $H_\emptyset$ and $H_{\{1,2\}}$ are completely confounded on F. All other pairs of interaction spaces $H_\emptyset, H_{\{1\}}, H_{\{2\}}$ and $H_{\{1,2\}}$ are orthogonal on F.

As a second example we consider the same full factorial design D and fraction F but now together with the factorial effects from Example 2.15. The restrictions of the functions v_J to the fraction $F \subset D$ are given by

$d \in D$	$v_\emptyset(d)$	$v_{\{1\}}(d)$	$v_{\{2\}}(d)$	$v_{\{1,2\}}(d)$
$(0,0)$	1	-1	-1	1
$(1,1)$	1	1	1	1

Note that the functions $v_{\{1\}}$ and $v_{\{2\}}$ are completely confounded. Equivalently, the factorial effects $\sum_{d\in D} v_{\{1\}}(d)\,\mu(d)$ and $\sum_{d\in D} v_{\{2\}}(d)\,\mu(d)$ are completely confounded on F. The functions $v_{\emptyset}$ and $v_{\{1\}}$ are orthogonal on F. As a result, the corresponding factorial effects $\sum_{d\in D} v_{\emptyset}(d)\,\mu(d)$ and $\sum_{d\in D} v_{\{1\}}(d)\,\mu(d)$ are also orthogonal on F.

As a final example we consider the fraction $F' = \{(0,0),(0,1),(1,0)\} \subset D$. The factorial effects defined in Example 2.15 when restricted to the fraction are given by

$d \in D$	$v_{\emptyset}(d)$	$v_{\{1\}}(d)$	$v_{\{2\}}(d)$	$v_{\{1,2\}}(d)$
$(0,0)$	1	-1	-1	1
$(0,1)$	1	-1	1	-1
$(1,0)$	1	1	-1	-1

The functions $v_{\{1\}}$ and $v_{\{2\}}$ are neither orthogonal nor completely confounded on the fraction F'. Hence, the corresponding factorial effects $\sum_{d\in D} v_{\{1\}}(d)\,\mu(d)$ and $\sum_{d\in D} v_{\{2\}}(d)\,\mu(d)$ are partially confounded on F'.

2.2 Factorial effects and Kronecker products

In this section we take a closer look at the factorial effects. We use the formulation involving Kronecker products of matrices. The Kronecker product formulation for factorial effects was introduced by Good (1958). A more formal and complete treatment is given in Kurkjian and Zelen (1962). The Kronecker product of two matrices is defined in the following way. For A and B matrices of size $r_A \times c_A$ and $r_B \times c_B$ respectively, the Kronecker product $A \otimes B$ is the $(r_A r_B) \times (c_A c_B)$ matrix

$$A \otimes B = \begin{pmatrix} a_{1,1}B & a_{1,2}B & \dots & a_{1,c_A}B \\ a_{2,1}B & a_{2,2}B & \dots & a_{2,c_A}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{r_A,1}B & a_{r_A,2}B & \dots & a_{r_A,c_A}B \end{pmatrix},$$

An equivalent definition of the Kronecker product for square matrices given by Madelung (1943) (p.85) is the following. Let $M_1, M_2, \dots, M_k$ denote a set of matrices where M_j has size $n_j \times n_j$ and assume that the elements in the set $L_j = \{1, 2, \dots, n_j\}$ are used to label both the rows and columns of the matrix M_j. The Kronecker product $M = M_1 \otimes M_2 \otimes \dots \otimes M_k$ is the matrix that has as its entries the values

$$(M)_{r,c} = \prod_{j=1}^{k} (M_j)_{r_j,c_j}, \tag{2.8}$$

where the rows and columns of M are indexed by the elements in the set $\prod_{j=1}^{k} L_j$. The Kronecker product M is taken to be the matrix containing these entries $(M)_{r,c}$ where rows and columns are ordered lexicographically with respect the indices r and c, respectively. The Kronecker product has the following

properties:

$$\left(\bigotimes_{j=1}^{k} M_j\right)^T = \bigotimes_{j=1}^{k} M_j^T, \tag{2.9}$$

$$\left(\bigotimes_{j=1}^{k} M_j\right)^{-1} = \bigotimes_{j=1}^{k} M_j^{-1} \tag{2.10}$$

and

$$\left(\bigotimes_{j=1}^{k} M_j\right)\left(\bigotimes_{j=1}^{k} B_j\right) = \bigotimes_{j=1}^{k} M_j\, B_j, \tag{2.11}$$

provided that all products $M_j B_j, 1 \leq j \leq k$, are well-defined. The Kronecker product gives the following easy method for constructing orthogonal bases for the interaction spaces. Let $D = \prod_{j=1}^{k} L_j$ be a full factorial design. We construct a basis for $\mathbb{R}^D$ that has the special property that for each interaction space H_J it has a subset that is a basis for H_J. This basis is constructed by first choosing a set of matrices $M_j, 1 \leq j \leq k$, that have all entries in the first row equal to 1. In addition, the matrices need to satisfy $M_j M_j^T = n_j\, I_{n_j}$. We index the rows of the matrix M_j by the elements in the set $E_j = \{0, 1, \ldots, n_j - 1\}$. The rows of the matrix $\bigotimes_{j=1}^{k} M_j$ are labeled by elements in the set $E = \prod_{j=1}^{k} E_j$. The columns of each matrix M_j are indexed by the elements of L_j. This implies that the columns of the matrix $\bigotimes_{j=1}^{k} M_j$ can be indexed by the elements of D and makes that we can see each row as a function from the D into $\mathbb{R}$. For each $e \in E$ we define a function $v_e \in \mathbb{R}^D$ by

$$v_e\,(d) = (M)_{e,d} \quad \text{where } M = \bigotimes_{i=1}^{k} M_i. \tag{2.12}$$

To each $e = (e_1, e_2, \ldots, e_k) \in E$ we associate a set $J\,(e)$ that contains exactly those indices $j \in \{1, 2, \ldots, k\}$ that satisfy $e_j \neq 0$. The next theorem states that each v_e defines a factorial effect.

Theorem 2.18 *The effects $\sum_{d \in D} v_e\,(d)\,\mu\,(d)\,, e \in E$, with $v_e \in \mathbb{R}^D$ as defined in (2.12) form a set of orthogonal factorial effects. The effect $\sum_{d \in D} v_e\,(d)\,\mu\,(d)$ is a factorial effect that belongs to the factor $X_{J(e)}$.*

Proof First we show that the functions $v_e, e \in E$, are orthogonal on D. The orthogonality follows using property (2.11) of the Kronecker product. More precisely, the orthogonality of the rows of each of the matrices M_j implies that

$$MM^T = \left(\bigotimes_{j=1}^{k} M_j\right)\left(\bigotimes_{j=1}^{k} M_j^T\right) = \bigotimes_{j=1}^{k} M_j M_j^T = \bigotimes_{j=1}^{k} n_j\, I_{n_j} = N\, I_N, \tag{2.13}$$

Hence, the rows in the matrix M are orthogonal. From this it follows directly that all functions $v_e, e \in E$, as defined in (2.12) are orthogonal on D. The next

step in the proof is showing that for each $e \in E$ we have that $v_e \in V_{J(e)}$ where $V_{J(e)}$ is the factor space for X_J. Using the definition for Kronecker product given in (2.8) we find that

$$v_e(d) = (M)_{e,d} = \left(\bigotimes_{j=1}^{k} M_j \right)_{e,d} = \prod_{j=1}^{k} (M_j)_{e_j,d_j} = \prod_{j \in J(e)} (M_j)_{e_j,d_j}, \quad (2.14)$$

where for the last equality we have used that $(M_j)_{e_j,d_j} = 1$ for $e_j = 0$. In (2.14) we see that the function $v_e(d)$ does not depend on the elements d_j of d for which $j \notin J(e)$. That is, the function v_e is constant on the equivalence classes in D induced by the partition $\pi_{J(e)}$. As a consequence, we have that $v_e \in V_{J(e)}$. Note that since we have that $V_{J_1} \subseteq V_{J_2}$ for $J_1 \subseteq J_2$ we have that $v_{e'} \in V_{J(e)}$ for all $e' \in E$ that satisfy $J(e') \subseteq J(e)$. It easy to see that the elements $e' = (e'_1, e'_2, \ldots, e'_k) \in E$ that satisfy this condition are exactly those that satisfy $e'_j = 0$ for all $j \in J(e)$. From this we find that for each $J \subseteq \{1, 2, \ldots, k\}$ exactly $\prod_{j \in J} n_j = \dim(V_J)$ of the functions $v_e, e \in E$, defined in (2.12) are elements of the factor space V_J. This together with the orthogonality of the functions $v_e, e \in E$, implies that the functions $v_e, e \in E$, that are in V_J form an orthogonal basis for V_J. Following the same line of reasoning we find that for each $j \in J$ a set of $\dim\left(V_{J\setminus\{j\}}\right)$ functions $v_e, e \in E$, forms an orthogonal basis for $V_{J\setminus\{j\}}$. The functions v_e that are in V_J but not in any of the factor spaces $V_{J\setminus\{j\}}$ for $j \in J$ form a basis for the interaction space H_J given in (2.4). Note that the functions v_e that satisfy this requirement are the functions in the set $\{v_e \mid e_j = 0 \text{ if and only if } j \notin J\}$. As a consequence, the effects $\sum_{d \in D} v_e(d)\, \mu(d)$ with $e \in E$ satisfying $e_j = 0$ if and only if $j \notin J$ are orthogonal and all belong to X_J. This completes the proof. □

Note that Theorem 2.18 gives us a set of $\prod_{j \in J}(n_j - 1) = \dim(H_J)$ orthogonal effects $\sum_{d \in D} v_e(d)\, \mu(d)$ that belong to the factor X_J. In other words, it gives us a basis for the set of all factorial effects that belong to the factor X_J. The functions $v_e, e \in E$, defined in (2.12) form an orthonormal basis for the inner product space $\mathbb{R}^D$. The orthonormality follows using (2.13) and observing that the diagonal elements of MM^T equal $N = \sum_{d \in D} v_e(d)\, v_e(d) = N\langle v_e, v_e \rangle$. We will find an unique expression for the expectation function $\mu \in \mathbb{R}^D$ as a linear combination of the factorial effects in $\{v_e \mid e \in E\}$ using the following lemma.

Lemma 2.19 *Consider a finite orthonormal set $\{v_1, v_2, \ldots, v_w\}$ in an inner product space with the inner product denoted by $\langle \cdot, \cdot \rangle$. Then $\{v_1, v_2, \ldots, v_w\}$ is a basis for $\mathcal{V} = span\{v_1, v_2, \ldots, v_w\}$ and every $v \in \mathcal{V}$ has a unique representation of the form*

$$v = \sum_{j=1}^{w} \langle v, v_j \rangle v_j. \quad (2.15)$$

Proof Let $v \in \mathcal{V}$. There exist $\beta_1, \beta_2, \ldots, \beta_w$ such that $v = \beta_1 v_1 + \beta_2 v_2 + \ldots + \beta_w v_w$. Using orthonormality of $\{v_1, v_2, \ldots, v_w\}$ we find that $\langle v, v_j \rangle = \beta_j$ for all j. As a result $\{v_1, v_2, \ldots, v_w\}$ is linearly independent and a basis for $\mathcal{V}$. □

The expansion given in (2.15) is called the Fourier-Bessel expansion. The unique Fourier-Bessel expansion of the expectation function $\mu \in \mathbb{R}^D$ with respect to the orthonormal basis $\{v_e \mid e \in E\}$ is given by

$$\mu = \sum_{e \in E} \langle v_e, \mu \rangle \, v_e, \tag{2.16}$$

where each coefficient $\langle v_e, \mu \rangle = \frac{1}{N} \sum_{d \in D} v_e(d) \, \mu(d)$ is a factorial effect. The decomposition in (2.16) uses a decomposition of each interaction space H_J as an orthogonal direct sum of the one-dimensional subspaces span $(\{v_e\})$ for e satisfying $J(e) = J$.

In cases where the variables in the experiment are quantitative a decomposition of the functions in $H_{\{j\}}$ into a linear, quadratic, cubic, ... component is sometimes preferred. Using orthogonal polynomials one can construct a decomposition of the interaction spaces $H_{\{j\}}, j \in \{1, 2, \ldots, k\}$, that has this property. For this we need for each $j, 1 \leq j \leq k$, a set of n_j polynomials $v_{j,0}, v_{j,1}, \ldots, v_{j,n_j-1}$ that are orthogonal on the levels in $L_j = \{\ell_{j,1}, \ell_{j,2}, \ldots, \ell_{j,n_j}\}$ and satisfy $\deg(v_{j,i}) = j$. Tables of orthogonal polynomials for the special case in which the levels are equally spaced are included in most textbooks on design of experiments. In cases where the levels are not equally spaced one can for instance use the Gramm-Schmidt orthonormalization procedure to construct a set of orthogonal polynomials. If we assume that the polynomials $v_{j,0} = 1, v_{j,1}, \ldots, v_{j,n_j-1}$ are normalized then a matrix M_j that satisfies $M_j M_j^T = n_j \, I_{n_j}$ is

$$M_j = \begin{pmatrix} 1 & 1 & \ldots & 1 \\ v_{j,1}(\ell_{j,1}) & v_{j,1}(\ell_{j,2}) & \ldots & v_{j,1}(\ell_{j,n_j}) \\ v_{j,2}(\ell_{j,1}) & v_{j,2}(\ell_{j,2}) & \ldots & v_{j,2}(\ell_{j,n_j}) \\ \vdots & \vdots & \ddots & \vdots \\ v_{j,n_j-1}(\ell_{j,1}) & v_{j,n_j-1}(\ell_{j,2}) & \ldots & v_{j,n_j-1}(\ell_{j,n_j}) \end{pmatrix}.$$

In the next example the use of orthogonal polynomials is illustrated for a 3^2 factorial experiment.

Example 2.20 Consider a full factorial design in two continuous variables x_1 and x_2 that in the experiment are set at three different levels. Let $D = L_1 \times L_2$ with the levels of the variables are coded by $L_1 = L_2 = \{0, 1, 2\}$. In this example we assume that the levels in each L_j represent three equidistant actual levels for the variables x_j. The levels are coded in such a way that the 0 in L_j corresponds to the lowest of these actual levels and the 2 to the highest. A special set of orthogonal factorial effects can be constructed using the following matrix M_j.

$$M_j = \begin{pmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \\ 1 & -2 & 1 \end{pmatrix}. \tag{2.17}$$

The rows of the matrix M_j contain the polynomials

$$\begin{aligned} v_0(x_j) &= 1 \\ v_1(x_j) &= x_j - 1 \\ v_2(x_j) &= 3x_j^2 - 6x_j + 1 \end{aligned}$$

evaluated at the levels in L_j. The rows of the matrix $M_1 \otimes M_2$ contain the polynomials $v_{(e_1,e_2)}(x_1, x_2) = v_{e_1}(x_1) v_{e_2}(x_2)$ where $(e_1, e_2) \in E$. By Theorem 2.18 each of the functions $v_e, e \in E$, (when restricted to D) defines a factorial effect $\sum_{d \in D} v_e(d) \mu(d)$. The functions $v_{(1,0)}$ and $v_{(2,0)}$ form an orthogonal basis for the interaction space $H_{\{1\}}$. The main effect defined by $v_{(1,0)}$ is called the linear effect of X_1. The function $v_{(2,0)}$ defines the quadratic effect of X_1. An orthogonal basis for the interaction space $H_{\{1,2\}}$ is formed by the functions $v_{(1,1)}, v_{(2,1)}, v_{(1,2)}$ and $v_{(2,2)}$. The function $v_{(1,1)}$ defines the linear-linear component of the interaction of X_1 and X_2. The quadratic-linear, linear-quadratic and quadratic-quadratic component of this interaction are defined by the functions $v_{(2,1)}, v_{(1,2)}$ and $v_{(2,2)}$, respectively.

The system of factorial effects for 3^k factorial designs based on the orthogonal polynomials on equally spaced levels is known as the linear-quadratic system. This system is discussed in detail in Section 5.6 of Wu and Hamada (2000). Another decomposition for 3^k factorial designs is the orthogonal components system introduced by Kempthorne (1947). We will illustrate this decomposition in Section 3.2.2.

2.3 ANOVA models

Analysis of variance (ANOVA) is the name for the set of techniques that is most frequently used for analyzing the data observed in factorial experiments. In this section we will consider the related ANOVA model and its connection with the interaction spaces defined in Section 2.1. Let $\mathcal{M}$ denote a set containing the sets of indices $J \subseteq \{1, 2, \ldots, k\}$ for which the factors X_J are included in the model. These correspond to the variables and combinations of variables that are hypothesized to have an influence on the measured response. If for $d \in D = \prod_{j=1}^{k} L_j$ and $J = (j_1, j_2, \ldots, j_m) \subseteq \{1, 2, \ldots, k\}$ we denote by d_J the vector $(d_{j_1}, d_{j_2}, \ldots, d_{j_m})$, then the ANOVA model is given by

$$y(d) = \sum_{J \in \mathcal{M}} \tau_J(d_J) + \varepsilon(d), \tag{2.18}$$

where $\varepsilon(d)$ denotes random noise. It is usually assumed that the $\varepsilon(d), d \in D$, are independent[2] normally distributed random variables with mean 0 and equal (but unknown) variance $\sigma^2 < \infty$. The ANOVA model is called *hierarchical* if

[2]We will abandon the assumptions of independent observations and constant variance in Chapters 4 and 5 in which we discuss the identification of dispersion effects and experiments with a restricted randomization, respectively.

$J \in \mathcal{M}$ implies that $J' \in \mathcal{M}$ for all $J' \subset J$. For each $J \in \mathcal{M}$ the $\tau_J(d_J), d_J \in \bigoplus_{j\in J} L_j$, form a set of unknown parameters that model the influence of the factor X_J. Note that the functions $y_J \in V_J$ are exactly those of the form $y_J(d) = \tau_J(d_J)$ with $\tau_J(d_J) \in \mathbb{R}$ and that the model in (2.18) is just a parameterized version of

$$y(d) = \sum_{J\in\mathcal{M}} y_J(d) + \varepsilon(d), \quad \text{where } y_J \in V_J. \tag{2.19}$$

The property $V_{J_1} \subset V_{J_2}$ for $J_1 \subset J_2$ that is satisfied by the factor spaces implies that the decomposition of y given in (2.18) is not identifiable. To obtain identifiability of the decomposition constraints are usually imposed on the parameters $\tau_J(d_J)$. The most widely used constraints are the linear constraints that the sum of the parameters $\tau_J(d_J)$ over the levels of any element d_j $(j \in J)$ of d_J is zero for any combination of levels for the other elements of d_J, *e.g.*,

$$\sum_{d_i\in L_i} \tau_{\{i\}}(d_j) = 0, \quad \sum_{d_i\in L_i} \tau_{\{i,j\}}(d_i, d_j) = \sum_{d_j\in L_j} \tau_{\{i,j\}}(d_i, d_j) = 0, \quad \ldots \tag{2.20}$$

These constraints force the function $y_J(d) = \tau_J(d_J)$ to be either zero on D or not to be constant on the equivalence classes induced by any of the partitions $\pi_{J\setminus\{j\}}$ for $j \in J$. That is, the function y_J is forced not to be in any of the factor spaces $V_{J\setminus\{j\}}$ for $j \in J$. Hence, for all $J \in \mathcal{M}$ the parametrization together with the constraints in (2.20) restrict the choice for the function $y_J(d) = \tau_J(d_J)$ to functions in the interaction space H_J. An additional constraint that is needed for the identifiability of the decomposition of y given in (2.18) is the restriction of the noise ε to the residual space H_{res} given by

$$H_{\text{res}} = \left(\bigcup_{J\in\mathcal{M}} H_J \right)^{\perp}.$$

In the ANOVA model (2.18) no distinction is made between fixed and random factors. The parametrization $y_J(d) = \tau_J(d_J)$ in (2.18) is used together with the identifiability constraints in (2.20) irrespective whether the factor X_J is fixed or random. A distinction between fixed and random factors is made because the hypotheses that are of interest differ for the two types of factors. If the factor X_J is fixed then interest is in estimating the parameters $\tau_J(d_J), d_J \in \prod_{j\in J} L_i$, and testing the hypothesis

$$\begin{array}{lll} H_0: & \tau_J(d_J) = 0 & \text{for all } d_J \in \prod_{j\in J} L_j \\ H_1: & \tau_J(d_J) \neq 0 & \text{for at least one } d_J \in \prod_{j\in J} L_j \end{array}.$$

Hence, for X_J a fixed factor the hypothesis concerns only the levels considered in the full factorial experiment. Alternatively, if the factor X_J is random then the parameters $\tau_J(d_J), d_J \in \bigoplus_{j\in J} L_j$, are usually assumed to be independent normally distributed random variables that are independent of the noise ε and have mean 0 and common variance σ_J^2. The hypothesis of interest for random

factors is

$$\begin{array}{ll} H_0: & \sigma_J^2 = 0 \\ H_1: & \sigma_J^2 > 0 \end{array}.$$

Let $\mathcal{M}_R$ denote the set consisting of all $J \in \mathcal{M}$ that correspond to a random factor X_J. Using the independence of all random variables $\tau_J(d_J), J \subset \mathcal{M}_R$, and $\varepsilon(d)$ we find that for all $d \in D$ the variance of the response $y(d)$ is

$$\text{Var}\left[y(d)\right] = \sigma^2 + \sum_{J \in \mathcal{M}_R} \sigma_J^2.$$

The variance of the observation $y(d)$ is the sum of error variance σ^2 and the variances $\sigma_J^2, J \subset \mathcal{M}_R$. For this reason the variances $\sigma_J^2, J \subset \mathcal{M}_R$, are called *variance components* . The estimation of variance components is considered in Section 4.3.

2.4 Linear regression models

In situations where $x_1, x_2, \ldots x_k$ are continuous variables linear regression models are usually preferred over ANOVA models because they allow for interpolation. Let $x = (x_1, x_2, \ldots, x_k)$ be a vector containing the variables considered in the experiment. The linear regression model for the case in which all factors are fixed is a model of the form

$$y(x) = \sum_{j=1}^{p} \theta_j f_j(x) + \varepsilon, \tag{2.21}$$

where $f_j, 1 \leq j \leq p$, are known functions, $\theta_j, 1 \leq j \leq p$, are unknown parameters and ε denotes the random noise. The functions $f_j(x)$ in the linear regression model (2.21) can be arbitrary and are often taken to be monomials in the variables $x_1, x_2, \ldots, x_k$. Usually ε is assumed to be a normally distributed random variable with zero mean and unknown variance $\sigma^2 < \infty$. If data is obtained on a design D, then the model is given in matrix notation by

$$y = Z\theta + \varepsilon, \tag{2.22}$$

where $\theta = (\theta_1, \theta_2, \ldots, \theta_p)$. Each row in (2.22) corresponds to a run $d \in D$. More precisely, the row in Z that corresponds to run d is $(f_1(d), f_2(d), \ldots, f_p(d))$. The matrix Z is usually referred to by *design matrix*. The elements in the vector ε are assumed to be independently distributed random variables with zero mean and equal variance $\sigma^2 < \infty$.

Note that the linear regression model (2.21) associates to each function $y \in \mathbb{R}^D$ a decomposition of the form

$$y = \sum_{j=1}^{p} y_j + y_{\text{res}} \text{ where } y_j = \text{span}\{f_{j|D}\}. \tag{2.23}$$

The part y_{res} is the contribution of the noise ε to the function y. In the linear regression model (2.21) the part y_{res} is not restricted to a linear subspace of $\mathbb{R}^D$. However, in order to obtain identifiability of the decomposition of y given in (2.23) we need to restrict y_{res} to some linear subspace H_{res} of $\mathbb{R}^D$. We will call a decomposition of the form given in (2.23) identifiable if there exists a linear subspace H_{res} of $\mathbb{R}^D$ for which the restriction of $y_{\text{res}} \in H_{\text{res}}$ results in a decomposition of y that is identifiable in the sense of Definition 2.9. The identifiability is directly related to the rank of the design matrix Z.

Lemma 2.21 *The decomposition of $y \in \mathbb{R}^D$ given in (2.23) is identifiable if and only if the matrix Z is full rank.*

Proof Clearly, the linear subspaces $\text{span}\{f_{j|D}\}, 1 \leq j \leq p$, of $\mathbb{R}^D$ are linearly independent if and only if the columns of Z are linearly independent. Hence, the decomposition of y in (2.23) is not identifiable if Z is not full rank. Next we assume that the columns of Z are linearly independent. We will show that for Z full rank and $p < N$ we can define a linear subspace H_{res} of $\mathbb{R}^D$ for which the decomposition in (2.23) with $y_{\text{res}} \in H_{\text{res}}$ is identifiable in the sense of Definition 2.9. Note that for the decomposition to be identifiable we need to restrict y_{res} to a linear subspace H_{res} of $\mathbb{R}^D$ that satisfies the requirements that $H_1, H_2, \ldots, H_p, H_{\text{res}}$ span $\mathbb{R}^D$ and that $\text{span}\{H_1, H_2, \ldots H_p\} \cup H_{\text{res}} = \{0\}$. A linear subspace of $\mathbb{R}^D$ that satisfies these two requirements is

$$H_{\text{res}} = \left(\bigcup_{j=1}^{p} H_j \right)^{\perp}, \tag{2.24}$$

which is a non-trivial linear subspace of $\mathbb{R}^D$ for p satisfying $1 < p < N$. Hence, if we restrict y_{res} to the subspace H_{res} as defined in (2.24) then the decomposition of y given in (2.23) is identifiable. □

For each full rank matrix Z we have that $Z\theta_1 = Z\theta_2$ implies that $\theta_1 = \theta_2$. In cases where Z is not full rank there exist $\theta_1 \neq \theta_2$ for which $Z\theta_1 = Z\theta_2$. Hence, the decomposition of y in (2.23) is identifiable if and only if $Z\theta_1 = Z\theta_2$ implies that $\theta_1 = \theta_2$. The last condition is commonly used to define identifiability of a parametrization for linear models (see, for instance, Section 2.1 of Christensen (2002)). The identifiability of a parametrization is closely connected to the notion of estimability which we now define.

Definition 2.22 (Estimability of a parameter) A parameter θ_j is said to be estimable on a design D under the linear regression model (2.21) if there exists a function $c \in \mathbb{R}^D$ for which

$$\text{E}\left(\sum_{d \in D} c(d)\, y(d) \right) = \theta_j.$$

In order to state a necessary and sufficient condition for the estimability of all parameters in the linear model (2.21) we need to following two lemmas.

Lemma 2.23 *For all matrices A and B we have that*

$$rank\,(AB) \leq \min\left(rank\,(A), rank\,(B)\right),$$

provided that AB exists.

Proof See Corollary 4.4.5 in Harville (1997). □

Lemma 2.24 *For any matrix Z of full column rank, the matrix Z^TZ is non-singular.*

Proof See Corollary 7.4.6 in Harville (1997). □

A necessary and sufficient condition for the estimability of all parameters in a linear regression model is given in the next theorem.

Lemma 2.25 *All parameters $\theta_1, \theta_2, \ldots, \theta_p$ in the linear regression model (2.21) are estimable if and only if the design matrix Z is full rank.*

Proof If Z is full rank then we find using Lemma 2.24 that Z^TZ is also full rank. This implies that the inverse Z^TZ exists. Unbiased estimators for all parameters can be found using

$$\mathrm{E}\left(\left(Z^TZ\right)^{-1}Z^Ty\right) = \left(Z^TZ\right)^{-1}Z^T\mathrm{E}\,(y) = \left(Z^TZ\right)^{-1}Z^TZ\theta = \theta.$$

Now assume that all parameters θ_j are estimable. In that case there exist vectors $a_1, a_2, \ldots, a_p \in \mathbb{R}^N$ that satisfy $\mathrm{E}\left(a_j^TY\right) = \theta_j$. Define the $N \times p$ matrix $A = (a_1 : a_2 : \ldots : a_p)$ and observe that $\mathrm{E}\left(A^TY\right) = \theta$. Note that $\theta = \mathrm{E}\left(A^TY\right) = A^T\mathrm{E}\,(Y) = A^TZ\theta$ implies that we must have $A^TZ = I_p$. By Lemma 2.23 we must have that

$$p = \mathrm{rank}\,(I_p) = \mathrm{rank}\left(A^TX\right) \leq \min\left(\mathrm{rank}\left(A^T\right), \mathrm{rank}\,(Z)\right).$$

Hence, we find that for all parameters to be estimable we need rank $(Z) \geq p$, which, since Z is of size $N \times p$, implies that Z is full rank. We have shown that the full rank property of the matrix Z is a necessary and sufficient condition for the estimability of all the parameters $\theta_1, \theta_2, \ldots, \theta_p$ in model (2.21). □

The relation between estimability and identifiability is the following. All parameters $\theta_j, 1 \leq j \leq p$, in a linear regression model are estimable if and only if the decomposition of y is identifiable. This follows from combining Lemmas 2.21 and 2.25.

2.5 Estimability of factorial effects

The notion of estimability is typically defined for parameters in a model. A parameter is said to be estimable under a particular model if an unbiased linear estimator for the parameter exists. It is less straightforward to give a definition for estimability of an effect on a fraction F of the full factorial design D on which it is defined. Hedayat et al. (1999) given the following definition.

Definition 2.26 (Estimability of an effect) Let $D = \prod_{i=1}^{k} L_i$ be a full factorial design and $F \subset D$ a fraction of D. An effect $\sum_{d \in D} v(d)\, \mu(d)$ is estimable on a fraction F under a particular model if there exists a $c \in \mathbb{R}^F$ for which

$$\mathrm{E}\left[\sum_{d \in F} c(d)\, y(d)\right] = \sum_{d \in D} v(d)\, \mu(d).$$

The estimability of factorial effects on a fraction is closely connected to the notion of confounding defined in Definition 2.16. In Section 3.4.4 we will illustrate this connection for regular fractions which form a special class of fractional factorial designs.

Chapter 3

Factorial Designs as Abelian Groups

Many important results in the literature on factorial designs were first derived using a group-theoretic approach. Fisher (1942) and Finney (1945) were the first to express the theory of symmetric factorial designs in terms of finite Abelian groups by labeling the runs in a symmetric full factorial design by the elements of an abstract group. The labeling proposed by Fisher (1942) and Finney (1945) can be easily extended to mixed factorial designs. If $n_1, n_2, \ldots, n_k$ denote the number of levels for the k factors in the experiment, then the runs in the mixed factorial design are labeled with the elements in the abstract Abelian group generated by k elements $a_1, a_2, \ldots, a_k$ and relations $a_1^{n_1} = a_2^{n_2} = \ldots = a_k^{n_k} = 1$. A realization of this abstract group was introduced in experimental design theory by Kempthorne (1947), who coded the runs in a full factorial design by the elements of the additive Abelian group $\mathbb{Z}/n_1\mathbb{Z} \times \mathbb{Z}/n_2\mathbb{Z} \times \ldots \times \mathbb{Z}/n_k\mathbb{Z}$. More recently, the coding introduced in Kempthorne (1947) was used by Dean and John (1975), John and Dean (1975), Lewis (1979), Bailey (1985), Kobilinsky (1985) and Collombier (1996). Bailey (1982a), Collombier (1996) and Pistone and Rogantin (2005) suggested to use $L_i = \Omega_{n_i}$ where Ω_{n_i} is the set of complex n_ith roots of unity to code the levels of for the variable x_i. When this coding is used the runs of a full factorial experiment form a multiplicative Abelian group under the operation of element-wise multiplication. The complex coding can be seen as a generalization of the frequently used coding $L_i = \{-1, 1\}$ for a variable x_i at two levels. The abstract group labeling, the integer coding and the complex coding are illustrated for a 3^2 factorial design in Table 3.1. Each of these ways of representing the treatments has been shown to be useful in the construction of factorial designs and the analysis of the data. However, some aspects of factorial designs are explained more easily using the coding as an additive Abelian group, while other aspects become more clear when the runs are coded by the elements of a multiplicative Abelian group. In this chapter we take a general approach and only assume that the each set L_i of levels is a finite Abelian group. The

Table 3.1: Different ways of representing the treatments in a 3^2 factorial design.

Abstract group labeling $(a^3 = b^3 = 1)$	Integer coding		Complex coding $(\omega = e^{2\pi i/3})$	
	A	B	A	B
1	0	0	1	1
b	0	1	1	ω
b^2	0	2	1	ω^2
a	1	0	ω	1
ab	1	1	ω	ω
ab^2	1	2	ω	ω^2
a^2	2	0	ω^2	1
a^2b	2	1	ω^2	ω
a^2b^2	2	2	ω^2	ω^2

full factorial design $D = \prod_{i=1}^{k} L_i$ is seen as a finite Abelian group on which statistical data $y \in \mathbb{R}^D$ is gathered. Results from harmonic analysis can then be used for the purpose of statistical analysis. More precisely, the character theory of the finite Abelian group gives a set of orthogonal contrasts, which leads to a canonical decomposition of the total sum of squares. In the context of harmonic analysis, a regular fraction can be defined as a coset of a finite Abelian group. This definition can be shown to be equivalent to other definitions for regular fractions using the character theory of finite Abelian groups. The confounding relations for regular fractions are easily obtained using the Poisson summation formula. The character theory of finite Abelian groups has proven to be useful in the search and construction of factorial designs and as a means to study the confounding of effects in fractional factorial designs (see Bailey (1982b), Bailey (1985), Kobilinsky (1985), El Mossadeq et al. (1985), Bailey (1990), Kobilinsky (1990), Kobilinsky and Monod (1995) and Collombier (1996)). In this chapter we study both the confounding of effects and the analysis of statistical data structured on finite Abelian groups and cosets of such groups using character theory and harmonic analysis. The results presented in this chapter apply to designs that have the structure of a finite Abelian group. Some of the results are also valid for non-Abelian groups. References for the analysis of statistical data structured on non-Abelian groups are Diaconis (1988) and Viana (2005).

When discussing finite groups we assume that the group is multiplicative, except for some cases where an additive group is explicitly stated. An important role is played by the cosets of a group. Let H be a subgroup of the Abelian group G. The cosets of the subgroup H in G are the sets $aH = \{ah \mid h \in H\}$ where $a \in G$. Each element of G is contained in exactly one coset of H. Note that aH and bH for different $a, b \in G$ may refer to the same coset. In some cases it is useful to have a unique representation for each coset. A transversal

of H in G is defined as a set containing exactly one element from each coset of H in G.

The outline of this chapter is as follows. The basics of harmonic analysis on finite groups are explained in Section 3.1. In Section 3.2 we present the link between the characters and the interaction spaces. Also in that section, the theory of harmonic analysis is applied to data obtained in a full factorial experiment. Different algorithms for computing the effects in full factorial designs are discussed in Section 3.3. The equivalence of these algorithms is shown for the case of 2^k factorial designs. In Section 3.4 an overview of the different definitions for regular fractions is given. The main result of this chapter is a proof for the equivalence of these definitions given in Section 3.4.3. The proof uses the character theory of finite Abelian groups. The concepts of confounding and defining equations are considered within the algebraic framework of harmonic analysis. In Theorem 3.58 each regular fraction is shown to be an orthogonal array of a strength related to the resolution of the fraction. Finally, the use of pseudofactors is considered. The statistical inference for normally distributed data structured on finite groups and cosets of finite Abelian groups is discussed in Section 3.6.

3.1 Harmonic analysis on finite groups

In this section we give a short overview of harmonic analysis on finite groups. Serre (1977) and Terras (1999) give readable algebraic introductions to this topic. Statistical introductions can be found in Diaconis (1988) and Viana (2005). Both Diaconis (1988) and Viana (2005) consider the analysis of statistical data structured on groups. In this chapter we extend their results to the case where the statistical data is structured on a coset of a finite Abelian group. In Section 3.1.1 we first consider harmonic analysis on finite groups in general. The special case of harmonic analysis on finite Abelian groups is considered in Section 3.1.2. Fast algorithms exist for the computation of the Fourier transforms of functions defined on a finite Abelian group. One of the first versions of the Fast Fourier Transform was introduced by Good (1958) as a means to streamline the computation of effects in factorial designs. This Fast Fourier Transform algorithm is described in Section 3.1.3. Within the framework of harmonic analysis the confounding relations on a regular fraction are easily obtained using the Poisson summation formula. This formula is derived in Section 3.1.4.

3.1.1 The general case

In harmonic analysis (Serre (1977)) a group is studied through its linear representations in a vector space $\mathcal{V}$. An exact definition of a linear representation will be given shortly, but first we introduce the general linear group $GL(\mathcal{V})$ of a vector space $\mathcal{V}$. Unless stated otherwise, we assume that $\mathcal{V}$ is a vector space over the field of complex numbers. The general linear group $GL(\mathcal{V})$ is the set

of all isomorphisms of $\mathcal{V}$ onto itself. The elements of $GL(\mathcal{V})$ are, by definition, linear mappings of $\mathcal{V}$ into $\mathcal{V}$ which have an inverse. A linear representation is defined as follows.

Definition 3.1 A linear representation ρ of a group G in a vector space $\mathcal{V}$ is a group homomorphism from G into $GL(\mathcal{V})$.

Hence, a mapping $\rho : G \to GL(\mathcal{V})$ of a multiplicative group G is a representation if it satisfies $\rho(g_1 g_2) = \rho(g_1)\rho(g_2)$ for all $g_1, g_2 \in G$. The dimension of the representation ρ is defined to be the dimension of the vector space $\mathcal{V}$. For $\varphi : \mathcal{V} \to \mathcal{V}$ a linear map, we let $\operatorname{tr}\varphi$ denote the trace of the matrix representation of φ. The character of a representation is defined as follows.

Definition 3.2 Given a linear representation $\rho : G \to GL(\mathcal{V})$ of a group G, the function $\chi_\rho \in \mathbb{C}^G$ defined by $\chi_\rho(g) = \operatorname{tr}\rho(g)$ is called the character of the representation.

Note that because the trace is basis free, the character does not depend on the basis that is chosen for $\mathcal{V}$. Next we define the notion of irreducibility of a representation, but first we need to define the notion of a stable subspace.

Definition 3.3 Let ρ be a representation of G in $GL(\mathcal{V})$. A linear subspace $\mathcal{W}$ of $\mathcal{V}$ is stable under ρ if for all $w \in \mathcal{W}$ and all $g \in G$ we have that that $\rho(g)w \in \mathcal{W}$.

The irreducibility of a representation is defined as follows.

Definition 3.4 A representation ρ of G in $GL(\mathcal{V})$ is irreducible if the only proper linear subspace of $\mathcal{V}$ that is stable under ρ is the null space.

We refer to the character of an irreducible representation as an irreducible character. All characters have the following nice property.

Lemma 3.5 *The character χ_ρ of a linear representation ρ of a group G satisfies $\chi_\rho(g^{-1}) = \overline{\chi_\rho}(g)$ for all $g \in G$.*

Proof See Proposition 1 (ii) in Serre (1977). □

We now define equivalence for the linear representations of a group.

Definition 3.6 Two linear representations $\rho_1 : G \to GL(\mathcal{V}_1)$ and $\rho_2 : G \to GL(\mathcal{V}_2)$ of a group G are equivalent if there exists an invertible linear map $f : \mathcal{V}_1 \to \mathcal{V}_2$ for which $f\rho_1(g)f^{-1} = \rho_2(g)$ for all $g \in G$.

The characters of a group give us a very convenient equivalence criterion.

Lemma 3.7 *Two linear representations of a group G are equivalent if and only if they have the same character.*

Proof See Corollary 2 in Serre (1977). □

By $\mathbb{C}^G$ we denote the inner product space of all complex functions defined on G with the inner product

$$\langle f_1, f_2 \rangle_G = \frac{1}{|G|} \sum_{g \in G} f_1(g) \overline{f_2}(g).$$

In cases where there is no ambiguity about the finite group on which the inner product is defined, the inner product is simply denoted by $\langle f_1, f_2 \rangle$. Functions $f_1, f_2 \in \mathbb{C}^G$ are said to be orthogonal on G if $\langle f_1, f_2 \rangle_G = 0$. The characters of non-equivalent irreducible representations are orthogonal on the group G. This is summarized in the next theorem.

Theorem 3.8 *If χ_1 and χ_2 are the characters of two non-equivalent irreducible representations of G, then $\langle \chi_1, \chi_2 \rangle_G = 0$.*

Proof See Theorem 3 in Serre (1977). □

The characters also provide us with a very simple irreducibility criterion.

Lemma 3.9 *If χ_ρ is the character of a representation ρ of G, then $\langle \chi_\rho, \chi_\rho \rangle$ is a positive integer and $\langle \chi_\rho, \chi_\rho \rangle = 1$ if and only if ρ is irreducible.*

Proof See Theorem 5 in Serre (1977).

Two elements g' and $g \in G$ are called conjugate if there exists an element $h \in G$ such that $g' = hgh^{-1}$. Because conjugacy is an equivalence relation, it partitions the group G into equivalence classes $\{hgh^{-1} : h \in G\}$. A function $f \in \mathbb{C}^G$ satisfying $f\left(hgh^{-1}\right) = f(g)$ for all $h, g \in G$ is called a class function. By $\mathcal{C}(G)$ we denote the linear space of all class functions defined on a group G. The next lemma states that all characters are class functions.

Lemma 3.10 *For each linear representation ρ of a group G we have that its character $\chi_\rho \in \mathcal{C}(G)$.*

Proof Because ρ is a linear representation of G we have for all $g, h \in G$ that $\rho\left(hgh^{-1}\right) = \rho(h)\,\rho(g)\,\rho\left(h^{-1}\right)$. Hence, for all $h, g \in G$ we have

$$\begin{aligned} \chi_\rho\left(hgh^{-1}\right) &= \operatorname{tr}\left(\rho\left(hgh^{-1}\right)\right) = \operatorname{tr}\left(\rho(h)\,\rho(g)\,\rho\left(h^{-1}\right)\right) \\ &= \operatorname{tr}\left(\rho\left(h^{-1}\right)\rho(h)\,\rho(g)\right) = \operatorname{tr}\left(\left(\rho\left(h^{-1}h\right)\right)\rho(g)\right) \\ &= \operatorname{tr}\left(\rho(1)\,\rho(g)\right) = \operatorname{tr}\left(\rho(g)\right) = \chi_\rho(g), \end{aligned}$$

from which we conclude that χ_ρ is constant on the conjugacy classes of G. □

The next lemma states that the distinct irreducible characters of a group G form an orthonormal basis for $\mathcal{C}(G)$.

Lemma 3.11 *The non-equivalent irreducible characters form an orthonormal basis for* $\mathcal{C}(G)$.

Proof See Theorem 6 in Serre (1977) or Theorem 2.7 in Viana (2005). □

Let ρ be a linear representation of G into $GL(\mathcal{V})$ and $\rho_1, \rho_2, \ldots, \rho_w$ be the distinct non-equivalent irreducible representations of G, with corresponding characters $\chi_1, \chi_2, \ldots, \chi_w$. From Lemma 3.11 we know that $\{\chi_1, \chi_2, \ldots, \chi_w\}$ is an orthonormal basis for $\mathcal{C}(G)$. The Fourier-Bessel expansion of $f \in \mathcal{C}(G)$ with respect to this basis is

$$f = \sum_{j=1}^{w} \langle f, \chi_j \rangle \chi_j.$$

We let $\widehat{G}$ denote the set containing the characters for the distinct non-equivalent irreducible representations of G, that is, $\widehat{G} = \{\chi_1, \chi_2, \ldots, \chi_w\}$. The function $\widehat{f} : \widehat{G} \to \mathbb{C}$ defined by $\widehat{f}(\chi_j) = \langle f, \chi_j \rangle$ is called the Fourier transform of f.

It can be shown that for all j we have that $m_j = \langle \chi_j, \chi_\rho \rangle$ is the number of irreducible representations equivalent to ρ_j in any decomposition of ρ. That is, the representation ρ is isomorphic to the direct sum

$$\rho = m_1\rho_1 \oplus m_2\rho_2 \oplus \ldots \oplus m_w\rho_w.$$

The next theorem gives the projection matrices associated with this decomposition.

Theorem 3.12 *Let* ρ *be a linear representation of the group* G *into* $GL(\mathcal{V})$. *Let* $\rho_1, \rho_2, \ldots, \rho_w$ *be the distinct non-equivalent irreducible representations and let* $\chi_1, \chi_2, \ldots, \chi_w$ *and* $d_1, d_2, \ldots, d_w$ *be the corresponding characters and dimensions, respectively. Then*

$$P_j = \frac{d_j}{|G|} \sum_{g \in G} \overline{\chi_j}(g)\, \rho(g)$$

is a projection of $\mathcal{V}$ *onto a subspace* $\mathcal{V}_j$ *that is the sum of* m_j *isomorphic copies of the stable subspace associated with* $\rho_j, j = 1, 2, \ldots, w$. *Moreover,* $P_j P_k = 0$ *for all* $j \neq k$, $P_j^2 = P_j$ *for all* j *and* $\sum_{1 \leq j \leq w} P_j = I_v$, *where* $v = \dim \mathcal{V}$.

Proof See Theorem 8 in Serre (1977) and Theorem 2.8 in Viana (2005). □

The canonical decomposition given in the previous theorem does not depend on the initially chosen decomposition of ρ into irreducible representations. This follows from observing that the matrices P_j depend on the irreducible representations only through the irreducible characters which are equal for equivalent irreducible representations. In Section 3.6 we will use the decomposition of the identity matrix to find a decomposition of the total sum of squares into statistically independent parts. Because our data are indexed by the elements of a finite group (the runs of a factorial design) we take ρ to be the regular representation. The left regular representation is defined in the following way.

Definition 3.13 (Left regular representation) Let $\mathcal{V}$ be a vector space of dimension N with a basis $\{e_g \mid g \in G\}$. For each $h \in G$ let $\rho(h)$ be the linear map of $\mathcal{V}$ into $\mathcal{V}$ defined by $\rho(h)\, e_g = e_{hg}$. Then ρ is a representation of G, which is called the regular representation.

The right regular representation of a group G is the linear map ρ defined by $\rho(h)\, e_g = e_{gh}$ for all $h, g \in G$. Note that the right and left regular representation coincide when the group G is Abelian. In that case we simply refer to the linear representation ρ defined in Definition 3.13 as the regular representation.

3.1.2 The Abelian case

The irreducible representations of finite Abelian groups have several nice properties that we present in this section. However, we first we need some definitions.

Definition 3.14 (Cyclic group) A group is cyclic if it can be generated by a single element.

For example, if $G = \{1, a, a^2\}$ with $a \cdot a^2 = 1$ then G is cyclic. The group G is isomorphic to the additive group $\mathbb{Z}/3\mathbb{Z}$.

Definition 3.15 (Product of groups) The product $G \times H$ of the two groups $(G, \cdot_G)$ and $(H, \cdot_H)$ is the group with elements (g, h) with $g \in G$ and $h \in H$ and the product defined by

$$(g, h) \cdot (g', h') = (g \cdot_G g', h \cdot_H h')$$

for all $(g, h), (g', h') \in G \times H$.

The product of groups defined this way is commonly referred to as the direct product of groups. The following theorem shows that when studying representations and characters of a finite Abelian group we may without loss of generality assume that the group under study is a direct product of cyclic groups.

Theorem 3.16 (Fundamental Theorem of Abelian Groups) *Every finite Abelian group G is isomorphic to a direct product of cyclic groups, that is, there exist integers $k, n_1, n_2, \ldots, n_k$ for which*

$$G \cong \prod_{i=1}^{k} \mathbb{Z}/n_i\mathbb{Z}.$$

Proof See Terras (1999), p. 163. □

The set of all irreducible representations for the group $G = \prod_{i=1}^{k} \mathbb{Z}/n_i\mathbb{Z}$ is $\{\rho_z \mid z \in G\}$ with ρ_z given by

$$\rho_z(g) = (\omega_{n_1})^{z_1 g_1} (\omega_{n_2})^{z_2 g_2} \ldots (\omega_{n_k})^{z_k g_k}, \tag{3.1}$$

Table 3.2: The character table of $G = \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$.

$g \in G$	$\chi_{(0,0)}$	$\chi_{(1,0)}$	$\chi_{(0,1)}$	$\chi_{(1,1)}$
$(0,0)$	1	1	1	1
$(1,0)$	1	-1	1	-1
$(0,1)$	1	1	-1	-1
$(1,1)$	1	-1	-1	1

where $\omega_{n_j} = e^{\frac{2\pi i}{n_j}}$. All irreducible representations of G are one-dimensional, which implies that the irreducible characters equal the irreducible representations. The set of irreducible characters of the group G is $\widehat{G} = \{\chi_z \mid z \in G\}$ with χ_z given by

$$\chi_z(g) = (\omega_{n_1})^{z_1 g_1} (\omega_{n_2})^{z_2 g_2} \dots (\omega_{n_k})^{z_k g_k}. \tag{3.2}$$

Note that the irreducible characters and representations are indexed by the elements in the Abelian group G. In addition, all irreducible characters are functions from G to the complex unit circle, which we will denote by $\mathbb{T}$. The characters of a group can be represented in the form of a character table. This is a table in which each column corresponds to a unique character in $\widehat{G}$ and each row corresponds to an element in G. The character table has the value $\chi(g)$ in the position in the column for $\chi \in \widehat{G}$ and the row for $g \in G$. Table 3.2 is the character table for the group $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$. For a specific ordering of the rows and columns, the character table of a finite Abelian group can be shown to have the special structure of a Kronecker product.

Lemma 3.17 *Let $G = \prod_{i=1}^{k} \mathbb{Z}/n_i\mathbb{Z}$. The rows and the columns of the character table G can be arranged in such a way that the table has the structure of a Kronecker product.*

Proof For each $i, 1 \leq i \leq k$, define the $n_i \times n_i$ matrix M_i with rows and columns indexed by the elements of $\mathbb{Z}/n_i\mathbb{Z}$ as follows

$$(M_i)_{r_i,c_i} = (\omega_{n_i})^{r_i c_i} \text{ where } r_i, c_i \in \mathbb{Z}/n_i\mathbb{Z}. \tag{3.3}$$

Let A denote the following Kronecker product of the matrices $M_i, 1 \leq i \leq k$, given by

$$A = M_1 \otimes M_2 \otimes \dots \otimes M_k.$$

Using (2.8) we find that

$$(A)_{r,c} = \prod_{i=1}^{k} (M_i)_{r_i,c_i} = \prod_{i=1}^{k} (\omega_{n_i})^{r_i c_i} = \chi_c(r) \text{ where } r, c \in G.$$

Note that the column of A that is indexed by $c \in G$ contains the character χ_c evaluated in the different elements of G. The row indexed by $r \in G$ contains the

characters $\chi_c, c \in G$, all evaluated in r. Hence, the matrix A can be considered a character table for the group G. This concludes the proof. □

The multidimensional Fast Fourier Transform algorithm described by Good (1958) is based on the special property of the characters of finite Abelian groups shown in the last Lemma 3.17.

Lemma 3.18 *A function $\chi \in \mathbb{T}^G$ is an irreducible character of the finite Abelian group G if and only if it is a homomorphism.*

Proof This follows directly from Definition 3.2 and observing that all irreducible representations of finite Abelian groups are one-dimensional. □

The set of the irreducible characters of a finite Abelian group has the structure of an Abelian group.

Lemma 3.19 *The irreducible characters of any finite Abelian group form a multiplicative Abelian group under the operation of pointwise multiplication.*

Proof Using Lemma 3.18 it is sufficient to show that the set of all homomorphisms from a finite Abelian group G into $\mathbb{T}$ is a group. The function $\chi : G \to \mathbb{T}$ given by $\chi(g) = 1$ is a homomorphism, since for all g, h in G we have $\chi(gh) = \chi(g)\chi(h) = 1$. This function is the identity element in the group. Assume that χ_1 and χ_2 are two homomorphisms from G into $\mathbb{T}$ then for all $g, h \in G$ we have that $\chi_1\chi_2(gh) = \chi_1(gh)\chi_2(gh) = \chi_1(g)\chi_1(h)\chi_2(g)\chi_2(h) = \chi_1\chi_2(g)\chi_1\chi_2(h)$ which proves that also $\chi_1\chi_2$ is a homomorphism from G into $\mathbb{T}$. Note that $\chi : G \to \mathbb{T}$ implies that $\chi(g)\overline{\chi(g)} = 1$ for all g. The inverse $\chi^{-1} = \overline{\chi}$ is a homomorphism from G into $\mathbb{T}$ because $\chi(gh) = \chi(g)\chi(h)$ for all $g, h \in G$ implies that $\overline{\chi}(gh) = \overline{\chi}(g)\overline{\chi}(h)$ for all $g, h \in G$. □

The group $\widehat{G}$ for G an Abelian group is called the *dual* of G. The dual $\widehat{G}$ is isomorphic to G. For the group $G = \mathbb{Z}/n_1\mathbb{Z} \times \mathbb{Z}/n_2\mathbb{Z} \times \ldots \times \mathbb{Z}/n_k\mathbb{Z}$ the isomorphism $\varphi : G \to \widehat{G}$ is given by $\varphi(r) = \chi_r$ with χ_r defined as in (3.2). When $G \cong \widehat{G}$ we say that G is self-dual. We conclude this section by giving a lemma that helps finding an orthonormal basis for $\mathbb{C}^G$ when G is a finite Abelian group.

Lemma 3.20 *Every function defined on an Abelian group is a class function.*

Proof If G is an Abelian group we have that $hgh^{-1} = g$ for all $h, g \in G$. Hence, for all $g \in G$ the conjugacy class containing g is the set $\{g\}$. As a result any function defined on G is constant on the conjugacy classes. □

Combining Lemmas 3.11 and 3.20 we find that the irreducible characters of any finite Abelian group G form an orthonormal basis for $\mathbb{C}^G$.

3.1.3 The Fast Fourier Transform algorithm

For the remainder of this section we assume that the group G is finite and Abelian. We consider the computational aspects of determining the Fourier coefficients $\widehat{f}(\chi)$ in the expansion

$$f = \sum_{\chi \in \widehat{G}} \widehat{f}(\chi)\, \chi,$$

for some function $f \in \mathbb{C}^G$. Fast Fourier Transform algorithms provide efficient ways of computing the Fourier coefficients. The first Fast Fourier Transform (FFT) algorithm was proposed by Good (1958) as a means to streamline the computation of effects in factorial designs. In addition, Good (1958) illustrated that the same algorithm can be used to efficiently calculate multidimensional Fourier transforms[1]. Later, Cooley and Tukey (1965) showed how this FFT algorithm can be applied for efficiently calculating the one-dimensional Fourier transform when the number of data points is a highly composite number.

From Theorem 3.16 we know that we may, without loss of generality, assume that the Abelian group G is of the form $\prod_{j=1}^{k} \mathbb{Z}/n_j\mathbb{Z}$. The characters for G are given in (3.2). The Fourier coefficients are

$$\widehat{f}(\chi_z) = \frac{1}{|G|} \sum_{g \in G} f(g)\, \overline{\chi_z}(g), \tag{3.4}$$

where $z \in G$. Note that the computation of the part $\sum_{g \in G} f(g)\, \overline{\chi_z}(g)$ in (3.4) for a specific $z \in G$ requires N operations, where an operation is defined as the multiplication of two complex numbers followed by an addition of two complex numbers. Hence, when (3.4) is used to separately calculate each of the Fourier coefficients then a total number of N^2 operations is required. This number of operations can be reduced using the algorithm proposed by Good (1958). In Good (1958) the set of observations is given in the form of a vector. However, so far we have considered the data to be a function on the design rather than a vector. For this reason we present the algorithm using a notation that is different from that used in Good (1958). First observe that

$$\sum_{g \in G} f(g)\, \overline{\chi_z}(g) = \sum_{g \in G} f(g)\, \overline{(\omega_{n_1})^{z_1 g_1} (\omega_{n_2})^{z_2 g_2} \dots (\omega_{n_k})^{z_k g_k}}$$

is equal to

$$\sum_{g_1 \in \mathbb{Z}/n_1\mathbb{Z}} \cdots \sum_{g_{k-1} \in \mathbb{Z}/n_{k-1}\mathbb{Z}} \overline{(\omega_{n_1})^{z_1 g_1} \dots \left(\omega_{n_{k-1}}\right)^{z_{k-1} g_{k-1}}} \sum_{g_k \in \mathbb{Z}/n_k\mathbb{Z}} f(g)\, \overline{(\omega_{n_k})^{z_k g_k}}.$$

The algorithm consists of k steps. The output of each step is a function from G to the complex numbers. The output $\widehat{f}_i$ of the ith step forms the input for the

[1]The algorithm is based on a more widely applicable theorem in Good (1958) that we will present in Section 3.3. The theorem states how any Kronecker product of square matrices can be expressed as an ordinary product of sparse matrices.

$(i+1)$th step of the algorithm. The first step consists of computing for each $(g_1, \ldots, g_{k-1}, z_k) \in G$ the function values

$$\widehat{f_1}(g_1, \ldots, g_{k-1}, z_k) = \sum_{g_k \in \mathbb{Z}/n_k\mathbb{Z}} f(g) \overline{(\omega_{n_k})^{z_k g_k}}. \tag{3.5}$$

Each of these N computations requires n_k operations. Hence, the total number of operations needed in this first step is $n_k N$. The following steps can be described as follows. In the $(i+1)$th step $(1 \leq i \leq k-2)$ for all elements $(g_1, \ldots, g_{k-i-1}, z_{k-i}, \ldots, z_k) \in G$ values for $\widehat{f_{i+1}} \in \mathbb{C}^G$ are computed using

$$\widehat{f_{i+1}}(g_1, \ldots, g_{k-i-1}, z_{k-i}, \ldots, z_k) =$$
$$\textstyle\sum_{g_{k-i} \in (\mathbb{Z}/n_{k-i}\mathbb{Z})} \widehat{f_i}(g_1, \ldots, g_{k-i}, z_{k-i+1}, \ldots, z_k) \overline{(\omega_{n_{k-i}})^{z_{k-i} g_{k-i}}}.$$

The computation of each of these N values for $\widehat{f_{i+1}}$ requires n_{k-i} operations. The total number of operations needed in this step is $n_{k-i}N$. Finally, in the kth step one computes for all $(z_1, \ldots, z_k) \in G$ the values for

$$\widehat{f_k}(z_1, \ldots, z_k) = \sum_{g_1 \in (\mathbb{Z}/n_1\mathbb{Z})} \widehat{f_{k-1}}(g_1, z_2, \ldots, z_k) \overline{(\omega_{n_1})^{z_1 g_1}}.$$

This step requires $n_1 N$ operations. The Fourier coefficients are now given by

$$\widehat{f}(\chi_z) = \frac{1}{|G|} \widehat{f_k}(z_1, \ldots, z_k)$$

The total number of operations that were needed to find the values for all $\widehat{f}(\chi_z), z \in G$, using the described algorithm is $N \sum_{j=1}^{k} n_j$, which (except for the cases where $k = 1$ or $k = n_1 = n_2 = 2$) is smaller than the N^2 operations that are required when the Fourier coefficients are computed one at a time.

If some of the factors have a number of levels that is not a prime number, then the efficiency can be further improved using the ideas of Cooley and Tukey (1965). Suppose that for some $i, 1 \leq i \leq k$, we have that $n_i = r_1 r_2$ for some $r_1, r_2 \in \mathbb{N}$, then each element $g_i \in \mathbb{Z}/n_i\mathbb{Z}$ can be uniquely expressed as $g_i = a_1 + a_2$ where $a_1 \in A_1$ and $a_2 \in A_2$ with $A_1 = \{0, 1, 2, \ldots, r_1 - 1\}$ and $A_2 = \{0, r_1, r_1 + r_1, \ldots, n_i - r_1\}$. In the $(k-i+1)$th step of the FFT algorithm the values for $\widehat{f_{k-i+1}}$ are computed using

$$\widehat{f_{k-i+1}}(g_1, \ldots, g_{i-1}, z_i, \ldots, z_k) =$$
$$\textstyle\sum_{g_i \in (\mathbb{Z}/n_i\mathbb{Z})} \widehat{f_{k-i}}(g_1, \ldots, g_i, z_{i+1}, \ldots, z_k) \overline{(\omega_{n_i})^{z_i g_i}} =$$
$$\textstyle\sum_{a_1 \in A_1} \sum_{a_2 \in A_2} \widehat{f_{k-i}}(g_1, \ldots, g_{i-1}, a_1 + a_2, z_{i+1}, \ldots, z_k) \overline{(\omega_{n_i})^{z_i (a_1 + a_2)}} =$$
$$\textstyle\sum_{a_1 \in A_1} \overline{(\omega_{n_i})^{z_i a_1}} \sum_{a_2 \in A_2} \widehat{f_{k-i}}(g_1, \ldots, g_{i-1}, a_1 + a_2, z_{i+1}, \ldots, z_k) \overline{(\omega_{n_i})^{z_i a_2}}.$$

The values of $\widehat{f_{k-i+1}}$ can be computed by first determining the values for

$$\sum_{a_2 \in A_2} \widehat{f_{k-i}}(g_1, \ldots, g_{i-1}, a_1 + a_2, z_{i+1}, \ldots, z_k) \overline{(\omega_{n_i})^{z_i a_2}},$$

requiring a_2 operations each. These values can then be used to determine the values for $\widehat{f}_{k-i+1}$. The total number of operations needed in this step is reduced from $n_i N$ to $(r_1 + r_2) N$. It is easy to see that if $n_i = \prod_{j=1}^{m} r_{ij}$ for $r_{ij} \in \mathbb{N} \backslash \{0, 1\}$, then successive application of this procedure gives for each $i, 1 \leq i \leq k$, a method to compute the complete function $\widehat{f}_{k-i+1}$ requiring only $N \sum_{j=1}^{m} r_{ij}$ operations (instead of $N n_i$). The most efficient algorithm is obtained when all of the r_{ij} are prime, since in that case the number of operations cannot be further reduced by writing one of the r_{ij} as a product of two integers in $\mathbb{N} \setminus \{0, 1\}$.

3.1.4 Poisson summation formula

Good (1958) shows that the effects in a full factorial design can be efficiently calculated using a generalization of the algorithm of Yates (1937). In addition, he illustrates how the proposed algorithm can be used to speed up the computation of the discrete Fourier transform. In Good (1960), which is an addendum to Good (1958), the Poisson summation formula is introduced as a means to study the confounding of effects in factorial designs. Although Good (1960) presents the Poisson summation formula for the group $\mathbb{Z}/n_1\mathbb{Z} \times \mathbb{Z}/n_2\mathbb{Z} \times \ldots \times \mathbb{Z}/n_k\mathbb{Z}$ for arbitrary integers $n_1, n_2, \ldots, n_k$, its usefulness for the study of the confounding is only illustrated for the case where $n_1 = n_2 = \ldots = n_k = 2$. The Poisson summation formula is of great value when the data is obtained on a coset of a finite Abelian group and harmonic analysis is used for analyzing the data. The formula relates a sum of the function values f over a coset in a finite Abelian group G to a sum of the Fourier transforms $\widehat{f}$ over a coset in the dual $\widehat{G}$. Before we present the Poisson summation formula we introduce the quotient space and its dual. Let H be a subgroup of a group G. The quotient space G/H consists of the different cosets $gH = \{gh \mid h \in H\}$ of H in G.

Lemma 3.21 *Let H be a subgroup of a finite Abelian group G. The quotient space G/H is a finite Abelian group.*

Proof The group operation in G/H is the product given by

$$\begin{aligned} (aH)(bH) &= \{ah_1bh_2 \mid h_1, h_2 \in H\} = \{abh_1h_2 \mid h_1, h_2 \in H\} \\ &= \{abh \mid h \in H\} = (ab)H. \end{aligned}$$

From this we find that H is an identity element in G/H, that G/H is closed under multiplication and that $a^{-1}H$ is the inverse of aH. The associativity of the group operation follows by using that G is Abelian. This completes the proof. □

A concept that is related to the quotient space is that of the annihilator $\widehat{G}_H$ of a subgroup H of G (the hat in the notation for the annihilator will be justified by Lemma 3.25). The annihilator is defined in the following way.

Definition 3.22 (Annihilator) Let G be a finite Abelian group and H a subgroup of G. The annihilator of H in G is the set

$$\{\chi \in \widehat{G} \mid \chi(h) = 1 \text{ for all } h \in H\}.$$

Note that the annihilator contains exactly those characters in $\widehat{G}$ that are constant on H and its cosets.

Example 3.23 Consider the finite Abelian group $G = \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$ and the subgroup $H = \{(0,0),(1,1)\}$ of G. The character table of G is given in Table 3.2. From this table it is easily seen that $\widehat{G}_H = \{\chi_{(0,0)}, \chi_{(1,1)}\}$.

The annihilator was introduced in design of experiments by Bailey (1977) as a means to study confounding. The use of the annihilator to study the confounding in regular fractional factorial designs is discussed in Section 3.4. We now show that the annihilator of a finite Abelian group is a subgroup of the dual $\widehat{G}$.

Lemma 3.24 *The annihilator $\widehat{G}_H$ of a subgroup H of a finite Abelian group G is a subgroup of $\widehat{G}$.*

Proof It is trivial to see that $1 \in \widehat{G}_H$. The set $\widehat{G}_H$ is closed under multiplication, since for all χ_1 and $\chi_2 \in \widehat{G}_H$ we have that $\chi_1\chi_2(h) = \chi_1(h)\chi_2(h) = 1$ for all $h \in H$. Let $\chi \in \widehat{G}_H$ and denote by χ^{-1} its inverse in $\widehat{G}$ then $\chi(h) = 1$ for all $h \in H$. From $\chi^{-1}(h)\chi(h) = 1$ for all $h \in G$ we find that $\chi^{-1}(h) = 1$ on H and $\chi^{-1} \in \widehat{G}_H$. Hence, we have shown that each annihilator $\widehat{G}_H$ is a subgroup in $\widehat{G}$. □

Combining Lemmas 3.21 and 3.19 we find that the dual of the quotient space is a multiplicative Abelian group. The dual of the quotient space G/H can be shown to be isomorphic to the annihilator $\widehat{G}_H$.

Lemma 3.25 *Let H be a subgroup of a finite Abelian group G. The dual of the quotient space G/H is isomorphic to $\widehat{G}_H$, that is, $\widehat{G/H} \cong \widehat{G}_H$.*

Proof Let T denote a transversal of H in G. We define the function $\varphi : \widehat{G}_H \to \widehat{G/H}$ by $(\varphi(\chi))(aH) = \chi(a)$ for all $a \in T$. We first show that the function φ is a homomorphism. This follows from observing that for all χ_1 and $\chi_2 \in \widehat{G}_H$ we have that $(\varphi(\chi_1\chi_2))(aH) = \chi_1\chi_2(a) = \chi_1(a)\chi_2(a) = (\varphi(\chi_1))(aH)(\varphi(\chi_2))(aH)$. Define the function $\psi : \widehat{G/H} \to \widehat{G}_H$ by $(\psi(\alpha))(g) = \alpha(aH)$ for all $g \in G$ where a is the unique element in T that satisfies $g \in aH$. Since $(\varphi(\psi(\alpha)))(aH) = (\psi(\alpha))(a) = \alpha(aH)$ for all $a \in T$ and $\alpha \in \widehat{G/H}$ it follows that φ is surjective. Injectivity follows from the fact that $(\psi(\varphi(\chi)))(g) = (\psi(\chi))(aH) = \chi(a) = \chi(a)\chi(h) = \chi(ah) = \chi(g)$ holds for all $a \in T$ and all $g \in aH$. Hence, the group homomorphism φ is an isomorphism. □

In the proof for the Poisson summation formula we need the following lemma.

Lemma 3.26 *Let H be a subgroup of an Abelian group G. Then for $\chi \in \widehat{G}$ we have that*

$$\sum_{h \in H} \chi(h) = \begin{cases} |H| & \text{for } \chi \in \widehat{G}_H \\ 0 & \text{for } \chi \notin \widehat{G}_H \end{cases}.$$

Proof Let the function $\chi_{|H} : H \to \mathbb{T}$ be defined by $\chi_{|H}(h) = \chi(h)$ for all $h \in H$. For $\chi \in \widehat{G}_H$ we have by definition that $\chi_{|H} = 1$ on H, which implies that $\sum_{h\in H} \chi(h) = |H|$. The result for $\chi \notin \widehat{G}_H$ is obtained by first observing that $\chi_{|H}$ is a character on H. Since $\chi_{|H} \neq 1$ on H we must have that characters $\chi_{|H}$ and 1 are orthogonal on H. From this we find that $\sum_{h\in H} \chi(h) = 0$, which completes the proof. □

We are now ready to present the Poisson summation formula.

Theorem 3.27 *Let H be a subgroup of a finite Abelian group G and $f \in \mathbb{C}^G$. Then for $a \in G$, $g \in G$ and $\alpha \in \widehat{G}$ we have*

$$\frac{1}{|H|} \sum_{h\in H} \overline{\alpha}(agh) f(agh) = \sum_{\chi\in\widehat{G}_H} \widehat{f}(\alpha\chi) \chi\left(ag^{-1}\right) \tag{3.6}$$

with important special cases

$$\frac{1}{|H|} \sum_{h\in H} \overline{\alpha}(ah) f(ah) = \sum_{\chi\in\widehat{G}_H} \widehat{f}(\alpha\chi) \chi(a) \tag{3.7}$$

and

$$\frac{1}{|H|} \sum_{h\in H} f(h) = \sum_{\chi\in\widehat{G}_H} \widehat{f}(\chi). \tag{3.8}$$

Proof Define the function $s \in \mathbb{C}^G$ by $s(g) = \sum_{h\in H} \overline{\alpha}(agh) f(agh)$. The Fourier transform $\widehat{s}(\chi)$ is

$$\widehat{s}(\chi) = \frac{1}{|G|} \sum_{g\in G} s(g) \overline{\chi}(g) = \frac{1}{|G|} \sum_{g\in G} \sum_{h\in H} \overline{\alpha}(agh) f(agh) \overline{\chi}(g).$$

Since any character of the Abelian group G is also a representation of G we have that

$$\widehat{s}(\chi) = \frac{\overline{\chi}\left(a^{-1}\right)}{|G|} \sum_{g\in G} \sum_{h\in H} \overline{\alpha}(agh) f(agh) \overline{\chi}(agh) \overline{\chi}\left(h^{-1}\right).$$

After changing the order of summation we can rewrite $\widehat{s}(\chi)$ as

$$\begin{aligned} \widehat{s}(\chi) &= \chi(a) \textstyle\sum_{h\in H} \frac{\chi(h)}{|G|} \sum_{g\in G} f(agh) \overline{\alpha\chi}(agh) \\ &= \chi(a) \textstyle\sum_{h\in H} \chi(h) \widehat{f}(\alpha\chi) \\ &= \widehat{f}(\alpha\chi) \chi(a) \textstyle\sum_{h\in H} \chi(h). \end{aligned}$$

Using Lemma 3.26 we find that $\widehat{s}(\chi) = |H| \widehat{f}(\alpha\chi) \chi(a)$ for $\chi \in \widehat{G}_H$ and $\widehat{s}(\chi) = 0$ for $\chi \notin \widehat{G}_H$. The Fourier-Bessel expansion of s is

$$\begin{aligned} s(g) &= \textstyle\sum_{\chi\in\widehat{G}} \widehat{s}(\chi) \overline{\chi}(g) \\ &= \textstyle\sum_{\chi\in\widehat{G}_H} |H| \widehat{f}(\alpha\chi) \chi(a) \overline{\chi(g)} \\ &= |H| \textstyle\sum_{\chi\in\widehat{G}_H} \widehat{f}(\alpha\chi) \chi\left(ag^{-1}\right). \end{aligned}$$

From this we find (3.6) by substitution of $\sum_{h\in H}\overline{\alpha}\,(agh)\,f\,(agh)$ for $s\,(g)$. The form given in (3.7) follows by setting g equal to 1 in (3.6). Finally, if in (3.7) we set $\alpha = 1$ and $a = 1$ we find (3.8). □

Note that another special case of (3.6) is the formula for the Fourier transform

$$\frac{1}{|G|}\sum_{h\in G}\overline{\alpha}\,(h)\,f\,(h) = \widehat{f}\,(\alpha)\,,$$

which is found by choosing $H = G$ and $a = g = 1$. The Fourier inverse formula

$$f\,(a) = \sum_{\chi\in\widehat{G}}\widehat{f}\,(\chi)\,\chi\,(a)$$

follows from (3.6) by choosing $H = \{\mathrm{id}_G\}$, $\alpha = 1$ and $g = 1$. The use of the Poisson summation formula to study confounding is illustrated in Section 3.4.4.

3.2 Harmonic analysis and full factorial designs

In this section we consider full factorial designs $\prod_{j=1}^{k} L_j$ where the n_j elements of L_j form a finite Abelian group. We first illustrate the relationship between interaction spaces, factorial contrasts and the Fourier transform of the expectation function on the group. More precisely, it is shown that each character of the finite Abelian group can uniquely be linked to an interaction space H_J. The Fourier transform of a character that is linked to H_J can be seen as a complex contrast that belongs the factor X_J. In addition, the characters that are linked to the interaction space H_J form an orthonormal basis for H_J. In Section 3.2.2 we determine a canonical decomposition for the sums of squares in a practical example.

3.2.1 Interaction spaces and factorial effects

Consider a full factorial design with treatments coded by a finite Abelian group $G = \prod_{j=1}^{k} L_j$ where each set L_j of levels is a finite Abelian group consisting of n_j elements. If by $\times_j$ we denote the group operation of L_j then G forms a group with a group operation $\times$ defined by

$$(g_1, g_2, \ldots, g_k)\times(z_1, z_2, \ldots, z_k) = (g_1\times_1 z_1, g_2\times_2 z_2, \ldots, g_k\times_k z_k)\,.$$

Note that the group G is also Abelian. The identity element of G is $\mathrm{id}_G = (\mathrm{id}_{L_1}, \mathrm{id}_{L_2}, \ldots, \mathrm{id}_{L_k})$ where id_{L_j} is used to denote the identity element of the group L_j. Because the groups L_j are Abelian we have that for all these groups $L_j \cong \widehat{L_j}$. The isomorphism between L_j and $\widehat{L}_j$ is denoted by $\varphi_j : L_j \to \widehat{L}_j$. The set $\widehat{L}_j$ is given by $\{\varphi_j\,(z_j) \mid z_j \in L_j\}$. In particular, $\mathrm{id}_{\widehat{L}_j} = \varphi_j\left(\mathrm{id}_{L_j}\right)$.

The set of characters of the group G is $\widehat{G} = \{\chi_z \mid z \in G\}$ where the character $\chi_z : G \to \mathbb{T}$ is defined by

$$\chi_z(g) = \prod_{j=1}^{k} (\varphi_j(z_j))(g_j). \tag{3.9}$$

The mapping $\psi : G \to \widehat{G}$ with $\psi(z) = \chi_z$ is an isomorphism of groups. Hence, we have that $\chi_{\mathrm{id}_G} = \mathrm{id}_{\widehat{G}}$ and $\chi_z \chi_g = \chi_{zg}$ for all $z, g \in G$. In Section 3.1.2 we showed that the characters of any finite Abelian group G form an orthonormal basis for the inner product space $\mathbb{C}^G$. We expand the expectation function $\mu \in \mathbb{R}^G$ with respect to this basis. The Fourier transforms of the expectation function $\mu = \mathrm{E}[y]$ are

$$\widehat{\mu}(\chi_z) = \frac{1}{|G|} \sum_{g \in G} \overline{\chi_z}(g)\, \mu(g), \quad z \in G. \tag{3.10}$$

The Fourier transform $\widehat{y}(\chi_z)$ is an unbiased estimator for $\widehat{\mu}(\chi_z)$. This follows by observing that

$$\begin{aligned} \mathrm{E}[\widehat{y}(\chi_z)] &= \mathrm{E}\left[\tfrac{1}{|G|} \textstyle\sum_{g \in G} y(g)\, \overline{\chi_z}(g)\right] = \tfrac{1}{|G|} \textstyle\sum_{g \in G} \mathrm{E}[y(g)]\, \overline{\chi_z}(g) \\ &= \tfrac{1}{|G|} \textstyle\sum_{g \in G} \mu(g)\, \overline{\chi_z}(g) = \widehat{\mu}(\chi_z). \end{aligned} \tag{3.11}$$

This implies that all Fourier transforms $\widehat{\mu}(\chi_z), z \in G$, are estimable on G. Note that if in Definition 2.13 we allow the function v to be a complex-valued function, then the Fourier transforms in (3.10) form a set of factorial effects for the full factorial design G. Since $1 \in \widehat{G}$ for any Abelian group G, the orthonormality of the characters implies that the Fourier transforms $\widehat{\mu}(\chi_z)$ for $z \neq \mathrm{id}_G$ are factorial contrasts. The set of factorial effects formed by the characters of G has a special property that we illustrate now. Using that $\varphi_j(z_j) = 1$ if and only if $z_j = \mathrm{id}_{L_j}$ we find that the character χ_z depends on the jth coordinate z_j of z if and only if $z_j \neq \mathrm{id}_{L_j}$. The set of characters that depend on all the coordinates indexed by the elements in J, but not on the other coordinates, is given by

$$B_J = \{\chi_z \mid z \in G \text{ that satisfy } z_j = \mathrm{id}_{L_j} \text{ if and only if } j \notin J\}. \tag{3.12}$$

Note that the characters in B_{J_1} are exactly those characters that are constant on the equivalence classes of G induced by π_{J_1}, but not constant on those induced by π_{J_2}, for $J_2 \subset J_1$. If the factor spaces and interaction spaces are defined as subsets of $\mathbb{C}^G$ instead of $\mathbb{R}^G$, then the characters in B_J form an orthonormal basis for the interaction space H_J. The orthogonality of the characters of the group was shown in Lemma 3.11. In addition, we have that $|B_J| = \prod_{j \in J}(n_j - 1) = \dim(H_J)$ (where H_J is seen as a vector space over $\mathbb{C}$ not $\mathbb{R}$). Note that this implies that a (complex) factorial effect $\sum_{g \in G} v(g)\, \mu(g)$ belongs to a factor X_J if and only if the function v lies in the linear space spanned by the characters in B_J.

3.2.2 Example: a 3^3 factorial design

As an example of an application of harmonic analysis to factorial designs we consider the simplified seat-belt experiment that is analyzed in Section 5.1 of Wu and Hamada (2000). The goal of this experiment was to identify the variables that have an effect on the pull strength of truck seat belts following a crimping operation which joins an anchor and cable. The three variables considered are the hydraulic pressure of the crimping machine (X_1), die flat middle setting (X_2) and length of crimp (X_3). The investigation was done by three times running a 3^3 full factorial experiment. The observed strengths are given in Table 3.3. We analyze the data using harmonic analysis on the group $G = (\mathbb{Z}/3\mathbb{Z})^4$, where the fourth dimension corresponds to the replication. The set of irreducible representations for this group is $\{\rho_z \mid z \in G\}$ with ρ_z given in (3.1). The decomposition of the total sum of squares that was found using Theorem 3.12 and taking for ρ the regular representation is given in Table 3.4. The residual sum of squares is obtained by summing the sum of squares for the 54 irreducible representations $\rho_{(z_1,z_2,z_3,z_4)}$ with $z_4 \in \{1,2\}$. Note that the sums of squares associated with an irreducible representation ρ_z and its complex-conjugate $\overline{\rho_z}$ are equal. This has some consequences for statistical inference that we discuss in Section 3.6.

From the decomposition given in Table 3.4 two other decompositions of the total sum of squares can be computed directly. The finest of these two is the decomposition into orthogonal components. The corresponding system of parametrization is called the orthogonal components system. This system was introduced by Kempthorne (1947) and it is discussed in Section 5.3 of Wu and Hamada (2000). We mention it here only briefly. For a symmetric factorial design with k factors at n levels the component $X_1^{z_1}X_2^{z_2}\ldots X_k^{z_k}$ for $z \in (\mathbb{Z}/n\mathbb{Z})^k$ in this system represents the contrasts among the average response values observed on sets $C_0, \ldots, C_{n-2}, C_{n-1}$ where

$$C_j = \left\{(g_1, g_2, \ldots, g_k) \in (\mathbb{Z}/n\mathbb{Z})^k \mid z_1g_1 + z_2g_2 + \ldots + z_kg_k = j \mod n\right\}.$$

From Table 3.4 we find that the sum of squares for the components X_1X_2 and $X_1X_2^2$ are $2 \times 1.36373 \times 10^6 = 2.72746 \times 10^6$ and $2 \times 285397 = 570794$, respectively.

The other decomposition of the total sums of squares that we can compute directly from Table 3.4 is the standard ANOVA decomposition for a multi-way layout as discussed in Section 2.4 of Wu and Hamada (2000). For instance, in the seat-belt experiment the sum of squares for the interaction $X_{\{1,2\}}$, which is more commonly denoted by $X_1 \times X_2$, is $2 \times 1.36373 \times 10^6 + 2 \times 285397 = 3.29825 \times 10^6$. The standard ANOVA decomposition for a full factorial design may also be obtained using a method proposed in Ledermann (1968). This method, which uses the representation theory of symmetric groups, is illustrated in Section 3.7.

Table 3.3: Design matrix and response data of the Seat-Belt Experiment.

	Factor					
Run	X_1	X_2	X_3	Strength		
1	0	0	0	5164	6615	5959
2	0	0	1	5356	6117	5224
3	0	0	2	3070	3773	4257
4	0	1	0	5547	6566	6320
5	0	1	1	4754	4401	5436
6	0	1	2	5524	4050	4526
7	0	2	0	5684	6251	6214
8	0	2	1	5735	6271	5843
9	0	2	2	5744	4797	5416
10	1	0	0	6843	6895	6957
11	1	0	1	6538	6328	4784
12	1	0	2	6152	5819	5963
13	1	1	0	6854	6804	6907
14	1	1	1	6799	6703	6792
15	1	1	2	6513	6503	6568
16	1	2	0	6473	6974	6712
17	1	2	1	6832	7034	5057
18	1	2	2	4968	5684	5761
19	2	0	0	7148	6920	6220
20	2	0	1	6905	7068	7156
21	2	0	2	6933	7194	6667
22	2	1	0	7227	7170	7015
23	2	1	1	7014	7040	7200
24	2	1	2	6215	6260	6488
25	2	2	0	7145	6868	6964
26	2	2	1	7161	7263	6937
27	2	2	2	7060	7050	6950

Table 3.4: Sum of squares decompostion for the Seat-Belt Experiment.

Factor	Orthogonal component	Irreducible representation	Sum of Squares
X_1	X_1	$\rho_{(1,0,0,0)}$	1.73109×10^7
		$\rho_{(2,0,0,0)}$	1.73109×10^7
X_2	X_2	$\rho_{(0,1,0,0)}$	469270
		$\rho_{(0,2,0,0)}$	469270
X_3	X_3	$\rho_{(0,0,1,0)}$	4.77474×10^6
		$\rho_{(0,0,2,0)}$	4.77474×10^6
$X_{\{1,2\}}$	X_1X_2	$\rho_{(1,1,0,0)}$	1.36373×10^6
		$\rho_{(2,2,0,0)}$	1.36373×10^6
	$X_1X_2^2$	$\rho_{(1,2,0,0)}$	285397
		$\rho_{(2,1,0,0)}$	285397
$X_{\{1,3\}}$	X_1X_3	$\rho_{(1,0,1,0)}$	1.4928×10^6
		$\rho_{(2,0,2,0)}$	1.4928×10^6
	$X_1X_3^2$	$\rho_{(1,0,2,0)}$	443294
		$\rho_{(2,0,1,0)}$	443294
$X_{\{2,3\}}$	X_2X_3	$\rho_{(0,1,1,0)}$	213607
		$\rho_{(0,2,2,0)}$	213607
	$X_2X_3^2$	$\rho_{(0,1,2,0)}$	10567
		$\rho_{(0,2,1,0)}$	10567
$X_{\{1,2,3\}}$	$X_1X_2X_3$	$\rho_{(1,1,1,0)}$	2.24646×10^6
		$\rho_{(2,2,2,0)}$	2.24646×10^6
	$X_1X_2X_3^2$	$\rho_{(1,1,2,0)}$	131508
		$\rho_{(2,2,1,0)}$	131508
	$X_1X_2^2X_3$	$\rho_{(1,2,1,0)}$	102768
		$\rho_{(2,1,2,0)}$	102768
	$X_1X_2^2X_3^2$	$\rho_{(1,2,2,0)}$	122720
		$\rho_{(2,1,1,0)}$	122720
residual			1.09226×10^7
total			6.88581×10^7

3.3 Algorithms for computing the effects

Different algorithms for computing effect estimates in full factorial designs have been proposed over the years. The most well-known algorithms are the Yates algorithm (Yates (1937)), the interaction algorithm (Good (1958)), the symbolic algorithm (Cochran and Cox (1957), p.158; Kempthorne (1952), p.240) and Ordinary Least Squares estimation. It is folklore that these algorithms all give the same results. Rigorous proofs of the equivalence of these algorithms do not seem to be available in literature except for the Yates and the interaction algorithm (see Good (1958) and Good (1960)). In this section we present a rigorous proof for the equivalence of all these algorithms.

3.3.1 The Yates algorithm

Yates (1937) described a simple adding-and-subtracting algorithm to compute the effect estimates in 2^k factorial experiments. The algorithm is an early example of a Fast Fourier Transform algorithm. Although Yates (1937) used the abstract group labeling for the treatments in the full factorial experiment, we choose to present the algorithm in the notation introduced in Chapter 2. We let $L_1 = L_2 = \ldots = L_k = \{0, 1\}$ and assume that 0 codes the lower level of a quantitative variable or the reference setting for a qualitative variable. The input of the algorithm is a column vector y_{yates} containing the observations $y(d), d \in D$, in Yates order of d. The output of the algorithm is a column vector τ_{yates} containing the effect estimates $\tau(d), d \in D$, in Yates order of d. The effect estimates are computed by setting $v_0 = y_{\text{yates}}$ and successively computing for $i = 0, 1, \ldots, k$ the column vectors v_{i+1} whose elements $(v_i + 1)_j, 1 \leq j \leq N$, are recursively defined by

$$(v_{i+1})_j = \begin{cases} (v_i)_{2j} + (v_i)_{2j-1} & \text{for } j = 1, 2, \ldots, \frac{N}{2}; \\ (v_i)_{2(j-\frac{N}{2})} - (v_i)_{2(j-\frac{N}{2})-1} & \text{for } j = \frac{N}{2}+1, \frac{N}{2}+2, \ldots, N, \end{cases}$$

where $(v_i)_j$ denotes the jth element of v_i. The output of the algorithm is the vector $\tau_{\text{yates}} = \frac{1}{2^{k-1}} v_k$.

3.3.2 The interaction algorithm

The interaction algorithm was introduced in Good (1958). The algorithm is an extension of the Yates algorithm to the general class of asymmetrical factorial designs. The algorithm includes the multidimensional Fast Fourier Transform as a special case. The algorithm follows from expressing the Kronecker product of a set of square matrices as an ordinary product of sparse matrices.

Theorem 3.28 (Good, 1958) *Let k square matrices $M_i, 1 \leq i \leq k$, be given. Assume that matrix M_i is of size $n_i \times n_i$ and let $N = \prod_{j=1}^{k} n_j$. Then*

$$M_1 \otimes M_2 \otimes \ldots \otimes M_k = C_1 C_2 \ldots C_k,$$

where

$$\begin{array}{lcccccccc} C_1 & = & M_1 & \otimes & I_{n_2} & \otimes & \ldots & \otimes & I_{n_k}; \\ C_2 & = & I_{n_1} & \otimes & M_2 & \otimes & \ldots & \otimes & I_{n_k}; \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ C_k & = & I_{n_1} & \otimes & I_{n_2} & \otimes & \ldots & \otimes & M_k. \end{array}$$

Each matrix C_i, $1 \leq i \leq k$, has at most $n_i N$ non-zero elements.

When presenting the interaction algorithm we assume that the levels of the variable x_i are coded by $L_i = \{0, 1, \ldots, n_i - 1\}$ for all $i, 1 \leq i \leq k$. The column vector y_{lex} contains the observations $y(d), d \in D$, in lexicographic order of d. The computation of the effect estimates is given in matrix notation by $\tau_{\text{lex}} = \Delta Z y_{\text{lex}}$ with Δ a diagonal matrix. Following Section 2.2 we assume that the matrix Z is of the form $\bigotimes_{i=1}^{k} M_i$, where each M_i is a square matrix of size $n_i \times n_i$ satisfying $M_i M_i^T = I_{n_i}$ and with all elements in the first row equal to 1. The interaction algorithm determines the vector τ_{lex} containing the effects estimates $\tau(d), d \in D$, in lexicographic order. This vector is computed efficiently (in the sense of Section 3.1.3) by first setting $v_0 = y$ and recursively determining the vectors $v_{i+1} = C_{k-i} v_i$ for $i = 0, 1, \ldots k-1$. The vector τ_{lex} is found using $\tau_{\text{lex}} = \Delta v_k$. Obtaining $v_{i+1}, 0 \leq i \leq k-1$, from v_i requires at most $n_{k-i} N$ operations, where an operation is defined as a multiplication of two real numbers followed by an addition of two real numbers. The computation of v_k takes a total of $N \sum_{i=1}^{k} n_i$ operations, whereas directly evaluating the product $Z y_{\text{lex}}$ requires N^2 operations.

In the case of a 2^k factorial design Good (1960) suggests to code lower level of quantitative variables with 1 and the higher level with 0. In case of qualitative variables 1 should be used for the reference treatment. The effects can be computed using the interaction algorithm with

$$M_1 = M_2 = \ldots = M_k = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{3.13}$$

and $\Delta = \frac{1}{N} I_N$. The coding suggested in Good (1960) differs from the standard way of coding. This coding makes that the interaction algorithm has two positive features that the Yates algorithm does not have. First, it has the historical advantage of providing an easy check of arithmetic. Since the matrices $M_i, 1 \leq i \leq k$, are equal to their own inverses we have that if all computations are done correctly, then the algorithm applied to the vector of effect estimates should return to original observations. A second positive feature is that the algorithm enables the original data to be smoothed by equating higher-order effect estimates to zero and applying the algorithm to the vector of effect estimates.

The interaction algorithm can be used to compute estimates for recursively defined effects in general factorial designs. Let for $i, 1 \leq i \leq k$, the functions $v_{i,0}, v_{i,1}, v_{i,2}, \ldots, v_{i,n_i-1} : L_i \to \mathbb{C}$ with $v_{i,0} = 1$ form an orthogonal basis for the vector space containing all functions from L_i into $\mathbb{C}$. We assume that this orthogonal basis is chosen in such a way that for (averaged) data $y_i : L_i \to \mathbb{C}$

observed on L_i the inner products $\langle v_{i,j}, y_i \rangle_{L_i}$ for $j, 1 \leq j \leq k-1$ are contrasts of interest. Define the matrices $M_i, 1 \leq i \leq k$, by

$$M_i = \begin{pmatrix} 1 & 1 & \dots & 1 \\ v_{i,1}(0) & v_{i,1}(1) & \dots & v_{i,1}(n_i - 1) \\ v_{i,2}(0) & v_{i,2}(1) & \dots & v_{i,2}(n_i - 1) \\ \vdots & \vdots & \ddots & \vdots \\ v_{i,n_i-1}(0) & v_{i,n_i-1}(1) & \dots & v_{i,n_i-1}(n_i - 1) \end{pmatrix} \tag{3.14}$$

The vector $(M_1 \otimes M_2 \otimes \ldots \otimes M_k)\, \mu_{\text{lex}}$ contains a complete set of recursively defined effects. As outlined in Section 2.2, a common choice for the functions $v_{i,j}, 0 \leq j \leq n_i - 1$, for x_i a quantitative variable is the set of orthogonal polynomials of degree j on the n_i (equally spaced) points in L_i. The vector $Zy_{\text{lex}} = (M_1 \otimes M_2 \otimes \ldots \otimes M_k)\, y_{\text{lex}}$ of effect estimates can be computed efficiently using Theorem 3.28.

The multidimensional Fast Fourier Transform algorithm that we described in Section 3.1.3 is a special instance of the interaction algorithm. To see this, assume that the rows and columns of the matrix A that is defined in the proof of Lemma 3.17 are ordered lexicographically. Then a vector $\widehat{f}_{\text{lex}}$ containing the Fourier coefficients $\widehat{f}(\chi_g), g \in G$, in lexicographic order of g is given by

$$\widehat{f}_{\text{lex}} = \frac{1}{|G|} A\, f_{\text{lex}},$$

where f_{lex} contains the observations $f(g), g \in G$, in lexicographic order of g. The matrix A is a Kronecker product of k matrices $M_i, 1 \leq i \leq k$, as defined in (3.3), which makes that the vector $\widehat{f}_{\text{lex}}$ of Fourier coefficients can efficiently be computed using Theorem 3.28 and the interaction algorithm.

3.3.3 The symbolic algorithm

The symbolic algorithm for computing the effect estimates in a 2^k factorial design is explained in Cochran and Cox (1957) (p. 158) and Kempthorne (1952) (p. 240). We assume that $L_1 = L_2 = \ldots = L_k = \{0, 1\}$, with the assumption that 0 codes the lower level of a quantitative variable or the reference setting for a qualitative variable. The effect estimate $\tau_{\text{symbolic}}(d), d \in D$, is found by first symbolically expanding the product

$$\frac{1}{2^{k-1}} \prod_{i=1}^{k} \left(x_i + (-1)^{d_i} \right) \tag{3.15}$$

and then substituting each monomial $\prod_{i=1}^{k} x_i^{r_i}, r \in D$, in this expansion of (3.15) by the observed response $y(r)$.

3.3.4 Ordinary Least Squares estimation

The general linear regression model is given by

$$Y = Z\theta + \varepsilon, \tag{3.16}$$

where Z is a known full-rank $N \times p$ matrix and θ an unknown column vector of length p. The elements of the random vector ε are assumed to be uncorrelated random variables with zero mean and identical (but unknown) variance $\sigma^2 < \infty$. Interest is in estimating the unknown parameters in the vector θ as good as possible. The Ordinary Least Squares (OLS) estimator[2] for θ is defined as

$$\widehat{\theta} = \underset{\theta \in \mathbb{R}^N}{\operatorname{argmin}} \left|\left|Y - Z\theta\right|\right|^2, \tag{3.17}$$

where $||\cdot||$ denotes the L_2 norm in $\mathbb{R}^N$. The OLS estimator minimizes the sum of the squared residuals (within the class of linear estimators). The OLS estimator for θ as defined in (3.17) is given by

$$\widehat{\theta} = \left(Z^T Z\right)^{-1} Z^T Y. \tag{3.18}$$

The Best Linear Unbiased Estimator (BLUE) for θ is defined as the unbiased estimator $\widehat{\theta} = b^T y, b \in \mathbb{R}^N$, that has minimum variance. That is, the unbiased estimator $b^T Y$ for θ is a BLUE if for every other unbiased estimator $c^T y, c \in \mathbb{R}^N$, for θ we have that the matrix $\operatorname{Var}[b^T y] - \operatorname{Var}[c^T y]$ is positive definite. The Gauss-Markov theorem (see for instance Stapleton (1995)) states that in a linear model with uncorrelated errors having zero mean and equal variance, the Ordinary Least Squares estimator is a Best Linear Unbiased Estimator. Under the additional assumption that the errors are normally distributed, the Ordinary Least Squares estimator is easily shown to be equal to the Maximum Likelihood (ML) estimator.

For factorial designs and a saturated model the matrix Z has the special structure of a Kronecker product. Let $L_i = \{\ell_{i,0}, \ell_{i,1}, \ldots, \ell_{i,n_i-1}\}$ denote the set of levels for the variable x_i. For each $i, 1 \leq i \leq n_i$ we define the $n_i \times n_i$ matrix M_i by

$$M_i = \begin{pmatrix} 1 & \ell_{i,0} & (\ell_{i,0})^2 & \ldots & (\ell_{i,0})^{n_i-1} \\ 1 & \ell_{i,1} & (\ell_{i,1})^2 & \ldots & (\ell_{i,1})^{n_i-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \ell_{i,n_i-1} & (\ell_{i,n_i-1})^2 & \ldots & (\ell_{i,n_i-1})^{n_i-1} \end{pmatrix}. \tag{3.19}$$

The design matrix Z for the saturated model is given by $Z = \bigotimes_{i=1}^{k} M_i$.

When Ordinary Least Squares estimation is used for analyzing the data obtained in 2^k factorial experiments, then typically the levels of each variable $x_i, 1 \leq i \leq k$, are coded by the elements in $L_i = \{-1, 1\}$. By convention the level -1 is used for the lower level and 1 for the higher level. This choice of levels results in orthogonality of the matrices $M_i, 1 \leq i \leq k$. The matrices

[2]The term ordinary is used to distinguish this estimator from the Weighted Least Squares estimator (WLS) in which a weighted L_2 norm is used instead of the ordinary L_2 norm. The WLS estimator is usually preferred when the assumption of equal variance of the errors in ε is not satisfied. In such a case the weights are chosen to be inversely proportional to the variance, giving points with a lower variance a greater statistical weight.

$M_i, 1 \leq i \leq k$, are given by

$$M_i = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}. \tag{3.20}$$

These matrices satisfy $M_i^T M_i = 2I_2$. Using properties (2.9) and (2.11) of the Kronecker product we find that

$$Z^T Z = \left(\bigotimes_{i=1}^{k} M_i^T \right) \left(\bigotimes_{i=1}^{k} M_i \right) = \bigotimes_{i=1}^{k} \left(M_i^T M_i \right) = \bigotimes_{i=1}^{k} (2I_2) = 2^k I_N.$$

The Ordinary Least Squares estimator for θ is given by

$$\widehat{\theta} = \frac{1}{2^k} Z^T Y. \tag{3.21}$$

3.3.5 Equivalence of algorithms

We are now ready to a rigorous proof for the equivalence of the four algorithms for computing the effect estimates in 2^k factorial experiments that were discussed. In this section we use the following definition for equivalence. Two algorithms from the Yates algorithm, interaction algorithm and symbolic algorithm are equivalent if the effects computed by the algorithms are proportional. Least Squares estimation and one of the algorithms for computing the effects are defined to be equivalent if the parameter estimates in Ordinary Least Squares estimation are proportional to the effects computed using this other algorithm.

Theorem 3.29 *The following algorithms for computing the effect estimates in 2^k factorial designs are equivalent:*

- *the Yates algorithm (Section 3.3.1);*
- *the interaction algorithm (Section 3.3.2);*
- *the symbolic algorithm (Section 3.3.3);*
- *Ordinary Least Squares estimation using $L_i = \{-1, 1\}$ (Section 3.3.4).*

Proof The equivalence of the Yates and interaction algorithm is shown in Good (1958) and Good (1960). We show the equivalence of the interaction algorithm, the symbolic algorithm and Ordinary Least Squares estimation by showing that the computed effect estimates and parameter estimates are proportional to the Fourier coefficients of the response function on the design coded by $D = (\mathbb{Z}/2\mathbb{Z})^k$.

Firstly, the effect estimates computed using the interaction algorithm are given by

$$\tau_{\text{interaction}}(d) = \frac{1}{2^k} \sum_{z \in D} (M_1 \otimes M_2 \otimes \ldots \otimes M_k)_{d,z} \, y(z)$$

Using the definition of Kronecker product given in (2.8) we find that

$$(M_1 \otimes M_2 \otimes \ldots \otimes M_k)_{d,z} = \prod_{i=1}^{k} (M_i)_{d_i,z_i}$$

Note that the elements of the matrices $M_i, 1 \leq i \leq k$, defined in (3.13) can be expressed as $(M_i)_{d_i,z_i} = (-1)^{d_i z_i}$. From this we find that

$$(M_1 \otimes M_2 \otimes \ldots \otimes M_k)_{d,z} = \prod_{i=1}^{k} (-1)^{d_i z_i} = \chi_d(z),$$

with $\chi_d, d \in \{0,1\}^k$, the character of the Abelian group $(\mathbb{Z}/2\mathbb{Z})^k$ defined in (3.2). As a result we find that

$$\tau_{\text{interaction}}(d) = \frac{1}{2^k} \sum_{z \in D} \chi_d(z)\, y(z) = \langle \chi_d, y \rangle_D = \widehat{y}(\chi_d).$$

Secondly, we consider the effect estimates computed using the symbolic algorithm. We determine the coefficients $a_z(d), z \in D$, in the expansion

$$\frac{1}{2^{k-1}} \sum_{z \in D} \left(a_d(z) \prod_{i=1}^{k} x_i^{z_i} \right)$$

of (3.15). Note that

$$a_d(z) = \prod_{1 \leq i \leq k \,\wedge\, z_i = 0} (-1)^{d_i} = \prod_{i=1}^{k} (-1)^{d_i(1-z_i)}.$$

When we equip the set $D = \{0,1\}^k$ with the operation of element-wise addition modulo 2, then we obtain the Abelian group $D = (\mathbb{Z}/2\mathbb{Z})^k$. Observe that

$$a_d(z) = \chi_d(1-z) = \chi_d(1)\,\chi_d(-z) = \chi_d(-z) = \chi_d(z),$$

where $\chi_d, d \in D$, is the character of the Abelian group $(\mathbb{Z}/2\mathbb{Z})^k$ defined in (3.2). The effect estimates $\tau_{\text{sym}}(d), d \in D$, computed using the symbolic algorithm are

$$\tau_{\text{symbolic}}(d) = \frac{1}{2^{k-1}} \sum_{z \in D} \chi_d(z)\, y(z) = 2\langle \chi_d, y \rangle_D = 2\widehat{y}(\chi_d).$$

Finally, the Ordinary Least Squares estimate $\widehat{\theta}$ for the vector θ for a 2^k factorial experiment is

$$\widehat{\theta} = \frac{1}{2^k} Z^T y = \frac{1}{2^k} (M_1 \otimes M_2 \otimes \ldots M_k)^T y,$$

with $M_i, 1 \leq i \leq k$, as defined in (3.20). The estimator for $\theta_d, d \in D$, is

$$\widehat{\theta}_d = \frac{1}{2^k} \sum_{z \in D} \left(M_1 \otimes M_2 \otimes \ldots \otimes M_k\right)_{d,z} y\left(z\right).$$

Note that the elements of the matrices $M_i, 1 \leq i \leq k$, in (3.20) are $\left(M_i\right)_{d_i,z_i} = \left(-1\right)^{\left(1-d_i\right)z_i}$. Using the definition of Kronecker product given in (2.8) we find that

$$\begin{aligned} \left(M_1 \otimes M_2 \otimes \ldots \otimes M_k\right)_{d,z} &= \prod_{i=1}^{k} \left(M_i\right)_{d_i,z_i} = \prod_{i=1}^{k} \left(-1\right)^{\left(1-d_i\right)z_i} \\ &= \chi_z\left(1-d\right) = \chi_z\left(d\right) = \chi_d\left(z\right). \end{aligned}$$

Hence, we have found that

$$\widehat{\theta}_d = \frac{1}{2^k} \sum_{z \in D} \chi_d\left(z\right) y\left(z\right) = \left\langle \chi_d, y \right\rangle = \widehat{y}\left(\chi_d\right).$$

To summarize, we have shown that for each $d \in D$,

$$\tau_{\text{symbolic}}\left(d\right) = 2\,\tau_{\text{interaction}}\left(d\right) = 2\,\widehat{\theta}_d = 2\widehat{y}\left(\chi_d\right),$$

which proves the equivalence of the symbolic algorithm, the interaction algorithm and Ordinary Least Squares estimation. □

The interaction algorithm and Ordinary Least Squares estimation can be used to analyze the data obtained in any asymmetric full factorial experiment. If the design matrix Z is of the form $Z = M_1 \otimes M_2 \otimes \ldots \otimes M_k$ where the matrices $M_i, 1 \leq i \leq k$, are orthogonal, then using (2.9) and (2.10) we find that $Z^T Z = I$. The Ordinary Least Squares estimator for the model (3.16) is

$$\widehat{\theta} = Z^T Y.$$

It is easily seen that any matrix M_i of the form given in (3.19) with $n_i > 2$ cannot be orthogonal, because the orthogonality of the first and third column of M_i implies that $\ell_{i,j} = 0$ for all $j, 1 \leq j \leq n_i - 1$. However, if the orthogonal polynomial basis introduced in Section 2.4 is used, then the matrix Z has the form of a Kronecker product of orthogonal matrices. In that case, the matrices $M_i, 1 \leq i \leq k$, are of the more general form given in (3.14). The functions $c_{i,j} : L_i \to \mathbb{R}$ for $j, 1 \leq j \leq n_i - 1$, are the n_i orthogonal polynomials on L_i where $c_{i,j}$ is of degree j. From this we find that if the function values of the orthogonal polynomials are used as independent variables in a regression model, then the interaction algorithm can be used to efficiently compute the Ordinary Least Squares estimates for the parameters in full factorial designs.

3.4 Regular fractions

When the number of variables is large then full factorial designs require a large number of runs. In such cases typically fractional factorial designs are preferred

over full factorial designs. These designs have the advantage that they require a fewer number of runs. However, a disadvantage of fractional factorial designs is that there is confounding of effects. Due to this confounding only a subset of the effects can be unbiasedly estimated and in order to do this it is necessary to assume that some of the other effects are zero. A special class of fractional factorial designs is formed by the regular fractions. Regular fractions typically have an easy confounding structure. These fractions can be thought of as being full factorial designs restricted by a set of defining equations of a simple form.

Remark 3.30 A further specification of the form of the defining equations is important because for any fraction $F \subseteq D$ of the full factorial design D we can find a set of equations defined on D that has the fraction F as its solution. In the algebraic framework of Pistone et al. (2001) defining equations are used to describe any design (regular or non-regular). The defining equations are used to study confounding in designs which lack an easy confounding structure. More precisely, Pistone et al. (2001) define a design as a finite set of points $D \in Q^k$, where Q denotes an arbitrary field. Each design can be described by its ideal $\text{Ideal}(D)$. The ideal $\text{Ideal}(D)$ of D is the set of polynomials $Q[x_1, x_2, \ldots, x_k]$ whose zeros include the design points in D. The design D is the variety of the $\text{Ideal}(D)$, that is, $D = \{(x_1, x_2, \ldots, x_k) \in Q^k \mid p(x_1, x_2, \ldots, x_k) = 0 \text{ for all } p \in \text{Ideal}(D)\}$. Hence, the design D is given as the set of solutions of a set of polynomial defining equations.

A classical example of a regular fraction is the following.

Example 3.31 Two examples of regular fractions of a 2^3 design using different notation are the following. The design F_1 has the levels of the factors coded by the elements in $L_i = \Omega_2 = \{-1, 1\}$. The design F_2 uses the elements of $L_i = \mathbb{Z}/2\mathbb{Z} = \{0, 1\}$ to code the levels. The defining equations for the regular fractions F_1 and F_2 are $X_1X_2X_3 = 1$ and $X_1+X_2+X_3 = 0 \mod 2$, respectively. That is, the fraction F_1 consists of those treatments $(d_1, d_2, d_3) \in \Omega_2 \times \Omega_2 \times \Omega_2$ from the full factorial design that satisfy $d_1d_2d_3 = 1$.

D_1		
X_1	X_2	X_3
1	1	1
−1	−1	1
−1	1	−1
1	−1	−1

D_2		
X_1	X_2	X_3
0	0	0
1	1	0
1	0	1
0	1	1

Note that the two designs D_1 and D_2 are group-isomorphic. The isomorphism between the two groups $\mathbb{Z}/2\mathbb{Z}$ and Ω_2 is given by $\varphi : \mathbb{Z}/2\mathbb{Z} \to \Omega_2$ by $\varphi(0) = 1$ (that is, the identity in $\mathbb{Z}/2\mathbb{Z}$ is mapped to the identity in Ω_2) and $\varphi(1) = -1$. That is, if in D_2 we let the level 1 correspond to the higher level of a variable, then in order for D_1 to the exactly the same design we must let the level -1 correspond to the higher level of a variable. Coding the higher level of a variable with -1 and the lower level with 1 may seem a bit counterintuitive.

Different definitions for regular fractions are given in the literature. In Section 3.4.1 we give an overview of these definitions. We adopt the definition of regular fraction as the coset of an Abelian group. This definition is the most convenient when studying factorial designs using the character theory of finite Abelian groups and has the advantage that it also applies to the case of asymmetrical factorial designs. In Section 3.4.2 we show how using the character theory each regular fraction can be characterized by a set of defining equations. The different definitions for regular fraction are shown te be equivalent in Section 3.4.3. In Section 3.4.4 confounding is discussed using the annihilator. The relationship with orthogonal arrays is discussed in Section 3.4.5. In that section it is shown that all regular fractions are orthogonal arrays. Several advantages of the use of pseudofactors are discussed in Section 3.4.6.

3.4.1 Definitions for regular fractions

In this section we discuss several definitions for regular fractions. Regular fractions of 2^k factorial designs have been widely studied. However, formal definitions of regular fractions for general (symmetric) factorial designs have appeared in literature only recently. Different definitions of regular fraction are given in Collombier (1996), Wu and Hamada (2000), Pistone and Rogantin (2005) and Dey and Mukerjee (1999). Each of these definitions is briefly discussed here.

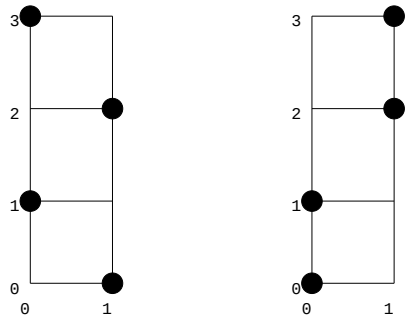
The first definition of regularity that we present was first based on the finite field approach introduced in Bose (1947). This approach is restricted to symmetric factorials where the number of levels n is a prime power. Only for these values of n there exists a field $GF(n)$ with n elements. The field $GF(n)$ is called the Galois field of order n and is unique up to isomorphism. If n is prime, then $GF(n) \cong \mathbb{Z}/n\mathbb{Z}$. If $n = p^q$ for some prime number p and integer $q > 1$, then $GF(n)$ can be represented by p-ary polynomials modulo an irreducible polynomial of degree q. Raktoe et al. (1981) define a fraction as regular if it is a subspace or coset of the vector space $(GF(n))^k$. In Chapter 5 of Collombier (1996) this definition is extended to the case of asymmetrical factorial designs where the number of levels are not necessarily a prime power. In the work of Collombier (1996) the runs of a full factorial design are identified with the elements of a finite Abelian group G. The corresponding definition of a regular fraction is as follows.

Definition 3.32 (Collombier) Let the runs of a full factorial design be coded by the elements of the finite Abelian group G. A fraction $F \subseteq G$ is regular if it is a coset in the full factorial design G.

This definition is illustrated in the next example.

Example 3.33 Two fractions F_1 and F_2 of the $2^1 4^1$ factorial design are given in Figure 3.1. The fraction F_1 is coded by the subset $\{(1,0),(0,1),(1,2),(0,3)\}$ of the Abelian group $G = \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$. The fraction F_2 is coded by the subset $\{(0,0),(0,1),(1,2),(1,3)\}$ of G. The fraction F_1 that is a coset in $G =$

Figure 3.1: A regular fraction F_1 (left) and a non-regular fraction F_2 (right) of a $2^1 4^1$ experiment.



$\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$. The fraction F_2 not a coset in G. Hence, according to Definition 3.32 F_1 is a regular fraction of G and F_2 is a non-regular fraction.

Definition 3.32 appears to be the most convenient definition for regular fraction when considering factorial designs within the framework of harmonic analysis. It is considered in detail in the following sections.

The definition given in the introduction of Section 5 of Wu and Hamada (2000) has to be associated with a specific set of factorial effects.

Definition 3.34 (Wu and Hamada) Let the runs of a full factorial design be coded by the elements in $D = L_1 \times L_2 \times \ldots \times L_k$. Assume that the set of factorial effects that are of interest are given by $\sum_{d \in D} v_j(d)\,\mu(d), 1 \leq j \leq r$, with $v_j \in \mathbb{C}^D$. A fraction $F \subseteq D$ is regular if for all i and j, $1 \leq i, j \leq r$, the factorial effects $\sum_{d \in D} v_i(d)\,\mu(d)$ and $\sum_{d \in D} v_j(d)\,\mu(d)$, are either orthogonal or completely confounded on F.

Equivalently, a fraction is regular if there is no partial confounding of the factorial effects $\sum_{d \in D} v_j(d)\,\mu(d), 1 \leq j \leq r$. Note that in Definition 3.34 we allow the functions v_j to take complex values, rather than just real values. For these complex factorial effects the confounding is defined as given in Definition 2.16, but with

$$\langle v_1, v_2 \rangle_F := \frac{1}{|F|} \sum_{d \in F} v_1(d)\,\overline{v_2}(d).$$

Moreover, in the case of complete confounding we allow $r \in \mathbb{C}$. The reason for allowing complex factorial effects is our special interest in the factorial effects $\widehat{\mu}(\chi) = \sum_{g \in G} \chi(g)\,\mu(g)$ where $\chi \in \widehat{G}$.

Example 3.35 Consider again the fractions F_1 and F_2 of the $2^1 4^1$ factorial design given in Example 3.35. The characters of the Abelian group $G = \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$ are given by

$$\chi_z(g) = (-1)^{z_1 g_1}\, i^{z_2 g_2} \text{ for } z \in G.$$

The following two tables show the characters $\chi_z, z \in G$, evaluated on the fraction F_1.

$g \in F_1$	$\chi_{(0,0)}(g)$	$\chi_{(0,1)}(g)$	$\chi_{(0,2)}(g)$	$\chi_{(0,3)}(g)$
$(1,0)$	1	1	1	1
$(0,1)$	1	i	-1	$-i$
$(1,2)$	1	-1	1	1
$(0,3)$	1	$-i$	-1	i

$g \in F_1$	$\chi_{(1,0)}(g)$	$\chi_{(1,1)}(g)$	$\chi_{(1,2)}(g)$	$\chi_{(1,3)}(g)$
$(1,0)$	-1	-1	-1	-1
$(0,1)$	1	i	-1	$-i$
$(1,2)$	-1	-1	-1	1
$(0,3)$	1	$-i$	-1	i

On the fraction F_1 we have that $\chi_{(1,2)} = -\chi_{(0,0)}$, which means that $\widehat{\mu}\left(\chi_{(1,2)}\right)$ is completely confounded with $\widehat{\mu}\left(\chi_{(0,0)}\right)$ on F_1. In addition we have that $\chi_{(1,3)} = -\chi_{(0,1)}, \chi_{(1,0)} = -\chi_{(0,2)}$ and $\chi_{(0,3)} = -\chi_{(1,1)}$. The factorial effects that are not completely confounded on F_1 can be shown to be orthogonal on F_1. Now let us consider the fraction F_2. The characters $\chi_r, r \in G$, evaluated on F_2 are given in the next two tables.

$g \in F_2$	$\chi_{(0,0)}(g)$	$\chi_{(0,1)}(g)$	$\chi_{(0,2)}(g)$	$\chi_{(0,3)}(g)$
$(0,0)$	1	1	1	1
$(0,1)$	1	i	-1	$-i$
$(1,2)$	1	1	1	1
$(1,3)$	1	$-i$	-1	i

$g \in F_2$	$\chi_{(1,0)}(g)$	$\chi_{(1,1)}(g)$	$\chi_{(1,2)}(g)$	$\chi_{(1,3)}(r)$
$(0,0)$	1	1	1	1
$(0,1)$	1	i	-1	$-i$
$(1,2)$	-1	1	-1	-1
$(1,3)$	-1	i	1	$-i$

Observe that $\langle \chi_{(0,0)}, \chi_{(1,1)} \rangle_{F_2} = 2 - 2i$ and that there does not exist an element $c \in \mathbb{C}$ for which $\chi_{(0,0)} = c\chi_{(1,1)}$. This means that the factorial effects $\widehat{\mu}\left(\chi_{(0,0)}\right)$ and $\widehat{\mu}\left(\chi_{(1,1)}\right)$ are partially confounded on F_2.

Note that in this example the factorial effects are not partially confounded on F_1, but on F_2 they are. Hence, when the set of factorial effects under consideration is the set of Fourier transforms $\mu(\chi), \chi \in \widehat{G}$, then fraction F_1 is regular and fraction F_2 is non-regular.

Pistone and Rogantin (2005) consider regular fractions of symmetric factorial designs. In presenting their definition we assume that all k factors are set at n levels. Pistone and Rogantin (2005) code the runs in the full factorial design by the elements in the multiplicative Abelian group $D = (\Omega_n)^k$. Their definition for a regular fractions is the following.

Definition 3.36 (Pistone and Rogantin) Let the runs of a full factorial design be coded by the elements of the finite Abelian group $D = (\Omega_n)^k$. A fraction $F \subseteq D$ is regular if there exists a subgroup L of $(\mathbb{Z}/n\mathbb{Z})^k$ and a homorphism $\psi : L \to \Omega_n$ for which

$$F = \{(d_1, d_2, \ldots, d_k) \in D \mid d_1^{\ell_1} d_2^{\ell_2} \ldots d_k^{\ell_k} = \psi(\ell) \text{ for all } \ell \in L\}.$$

An equivalent definition of a regular fraction is given in terms of the indicator function. The indicator function was first introduced in the literature on experimental design in Fontana et al. (2000) as a means to characterize fractions of two-level factorial designs. The coefficients of its polynomial expansion provide useful information regarding orthogonality of effects and design properties as regularity and resolution. The representation of the fraction by its indicator function was generalized to two-level factorial designs with replications by Ye (2003) and multilevel factorial experiments using orthogonal polynomials and integer coding of levels by Cheng and Ye (2004). Pistone and Rogantin (2005) use the indicator function for multilevel factorial experiments with the factor levels coded by the complex roots of unity. In this paper we only consider the case in which there are no replications. We apply the indicator function to the case where G is a finite Abelian group and use its expansion with respect to the orthogonal basis for $\mathbb{C}^G$ formed by the characters in $\widehat{G}$. For G a full factorial design coded as a finite Abelian group, the indicator function G of a fraction $F \subseteq G$ is the function $\mathcal{I}_F : G \to \{0, 1\}$ defined by

$$\mathcal{I}_F(g) = \begin{cases} 1 & \text{if } g \in F \\ 0 & \text{if } g \notin F \end{cases}.$$

The indicator function is expressed in a unique way as a linear combination of the characters in $\widehat{G}$ using the Fourier-Bessel expansion,

$$\mathcal{I}_F = \sum_{\chi \in \widehat{G}} \widehat{\mathcal{I}_F}(\chi)\, \chi \text{ where } \widehat{\mathcal{I}_F}(\chi) = \langle \mathcal{I}_F, \chi \rangle_G = \frac{|F|}{|G|} \langle 1, \chi \rangle_F. \tag{3.22}$$

Let for $g \in (\mathbb{Z}/n\mathbb{Z})^k$ the function $\chi_g : D \to \Omega_n$ be defined as $\chi_g(d) = d_1^{g_1} d_2^{g_2} \ldots d_k^{g_k}$. The functions in the set $\{\chi_g \mid g \in (\mathbb{Z}/n\mathbb{Z})^k\}$ form an orthonormal basis for $L^2(D)$. This follows from observing that the functions in $\{\chi_g \mid g \in (\mathbb{Z}/n\mathbb{Z})^k\}$ are exactly the irreducible characters of the Abelian group D. A fraction F of D is regular if its indicator function $\mathcal{I}_F : D \to \{0, 1\}$ expressed in terms of the orthonormal basis $\{\chi_g \mid g \in (\mathbb{Z}/n\mathbb{Z})^k\}$ has the form

$$\mathcal{I}_F = \frac{1}{|L|} \sum_{\ell \in L} \overline{\psi(\ell)} \chi_\ell,$$

for L a subgroup of $(\mathbb{Z}/n\mathbb{Z})^k$ and $\psi : L \to \Omega_n$ a homomorphism. A similar result was obtained independently by Ye (2004). He also used the multiplicative Abelian group $D = (\Omega_n)^k$ to code the runs in a symmetric full factorial design.

Ye (2004) shows that a fraction $F \subseteq D$ is regular if and only if for all coefficients $\widehat{\mathcal{I}_F}(\chi_g)$ in the expansion

$$\mathcal{I}_F = \sum_{g \in (\mathbb{Z}/n\mathbb{Z})^k} \widehat{\mathcal{I}_F}(\chi_g)\, \chi_g$$

we have that $\left(\widehat{\mathcal{I}_F}(\chi_g) / \widehat{\mathcal{I}_F}(\chi_0)\right)^n = 1$ or $\widehat{\mathcal{I}_F}(\chi_g) = 0$.

The definition of Dey and Mukerjee (1999) is another definition which is based on the finite field approach introduced in Bose (1947). Hence, the definition is restricted to symmetric factorials where the number of levels n is a prime power. If the full factorial design is coded by the elements in $D = (GF(n))^k$, then a regular fraction is defined as follows.

Definition 3.37 (Dey and Mukerjee) Let the runs of a full factorial design be coded by the vectors in $D = (GF(n))^k$. A fraction $F \subseteq D$ is regular if there exist a $c \in (GF(n))^k$ and a $p \times k$ matrix A $(p \leq k)$ with entries in $GF(n)$ for which

$$F = \{z \in (GF(n))^k \mid Az = c\}$$

Pistone and Rogantin (2005) showed that for n^k factorial designs with n a prime power, Definitions 3.36 and 3.37 are equivalent.

3.4.2 Defining equations

In this section we adopt Definition 3.32 for regular fraction. We show how any regular fraction can be defined as the solution of a set of equations. In particular, the defining equations for regular fractions are shown to have the special and very simple form given by $\chi(g) = \chi(a)$, where $\chi \in \widehat{G}$ and $a \in G$.

Lemma 3.38 *Given an Abelian group G, a non-empty subset $S \subseteq \widehat{G}$ and an element $a \in G$. The set defined by $\{g \in G \mid \chi(g) = \chi(a)$ for all $\chi \in S\}$ is a coset in G. In particular, the set defined by $\{h \in G \mid \chi(h) = 1$ for all $\chi \in S\}$ is a subgroup of G.*

Proof Let $C = \{g \in G \mid \chi(g) = \chi(a)$ for all $\chi \in S\}$. Define H by $H := a^{-1}C$. We will show that H is a subgroup of G. Note that

$$\begin{array}{rcll} H = a^{-1}C & = & \{a^{-1}g \in G \mid \chi(g) = \chi(a) \text{ for all } \chi \in S\} \\ & = & \{a^{-1}g \in G \mid \chi\left(a^{-1}\right)\chi(g) = \chi\left(a^{-1}\right)\chi(a) \text{ for all } \chi \in S\} \\ & = & \{a^{-1}g \in G \mid \chi\left(a^{-1}g\right) = 1 \text{ for all } \chi \in S\} \\ & = & \{h \in G \mid \chi(h) = 1 \text{ for all } \chi \in S\}. \end{array}$$

We show that the set H is a subgroup of G. First because $\chi(1) = 1$ for all $\chi \in \widehat{G}$ we have that $1 \in H$. In addition for $h_1, h_2 \in H$ and $\chi \in S$ we have that $\chi(h_1 h_2) = \chi(h_1)\chi(h_2) = 1$. This implies that for h_1 and $h_2 \in H$ we have that $h_1 h_2 \in H$. Now it remains to show that every element $h \in H$ has its inverse in

H. Clearly, $h^{-1} \in G$ and for all $\chi \in S$ we have that $\chi\left(h^{-1}\right) = \chi\left(h^{-1}\right)\chi(h) = \chi\left(h^{-1}h\right) = \chi(1) = 1$. This implies that $h^{-1} \in H$ and, hence, we have shown that H is a subgroup of G. The result that C is a coset follows from observing that $C = aH$. □

Lemma 3.38 gives a way of defining subgroups of the Abelian group G and their cosets. The set S can in terms of experimental design be thought of as a set of contrasts that are chosen to be completely confounded with the mean.

Lemma 3.39 *Let H be a subgroup of an Abelian group G and $a \in G$. Then $aH = \{g \in G \mid \chi(g) = \chi(a)$ for all $\chi \in \widehat{G}_H\}$. In particular, $H = \{h \in G \mid \chi(h) = 1$ for all $\chi \in \widehat{G}_H\}$.*

Proof By the definition of $\widehat{G}_H$ we have for all $\chi \in \widehat{G}_H$ that $\chi(h) = 1$ for each $h \in H$. Then for any $a \in G$ we have that $\chi(ah) = \chi(a)$. From this $aH \subseteq \{h \in G \mid \chi(h) = \chi(a)$ for all $\chi \in \widehat{G}_H\}$. For the converse, recall from Lemma 3.25 that $\widehat{G}_H$ is isomorphic to the dual of the quotient space. From this we find that the elements in $\widehat{G}_H$ form an orthonormal basis for the linear space of all complex-valued functions that are constant on the cosets of H in G. Now assume that there exists an element $gh \notin aH$ where $h \in H$ for which $\chi(gh) = \chi(a)$ for all $\chi \in \widehat{G}_H$. Then using $\chi(a) = \chi(gh) = \chi(g)\chi(h) = \chi(g)$ we find that for all $\chi \in \widehat{G}_H$ and all $h \in aH \cup gH$ (where aH and gH are different cosets) we have that $\chi(h) = \chi(a)$. This contradicts that $\widehat{G}_H$ is an orthogonal basis for the linear space of complex-valued functions defined on G that are constant on the cosets of H. Hence, $\{h \in G \mid \chi(h) = \chi(a)$ for all $\chi \in \widehat{G}_H\} \subseteq aH$. This completes the proof for $aH = \{g \in G \mid \chi(g) = \chi(a)$ for all $\chi \in \widehat{G}_H\}$. The statement $H = \{h \in G \mid \chi(h) = 1$ for all $\chi \in \widehat{G}_H\}$ follows directly by choosing $a = 1$. □

Lemma 3.39 shows how any coset aH of an Abelian group G can be described as the solution of a set of equations. In the literature on experimental design the subgroup $\widehat{G}_H$ is usually referred to as the defining contrasts subgroup. The coset aH is the the fraction defined by the equation. When $a = 1$ the fraction is called principal fraction. The theory is illustrated in the next example. We use an example from the well-studied class of two-level factorial designs to illustrate how the multiplicative defining equations arise within the proposed algebraic framework.

Example 3.40 Consider a full 2^4 factorial design coded as the additive Abelian group $G = (\mathbb{Z}/2\mathbb{Z})^4$. The set of irreducible characters for this group is given by $\{\chi_z \mid z \in G\}$ where

$$\chi_z(g) = (-1)^{z_1 g_1}(-1)^{z_2 g_2}(-1)^{z_3 g_3}(-1)^{z_4 g_4}.$$

Let $S = \{\chi_z \mid z \in \{(1,1,1,0),(0,1,1,1)\}\}$. The subgroup $H = \{g \in G \mid \chi(g) = 1$ for all $\chi \in S\} = \{(0,0,0,0),(0,1,1,0),(1,0,1,1),(1,1,0,1)\}$ is a

regular fraction of G. The subgroup H by definition contains exactly those elements $g \in G$ that satisfy the following equations

$$\begin{array}{rcl} \chi_{(1,1,1,0)}(g) & = & (-1)^{g_1}(-1)^{g_2}(-1)^{g_3} = 1, \\ \chi_{(0,1,1,1)}(g) & = & (-1)^{g_2}(-1)^{g_3}(-1)^{g_4} = 1. \end{array}$$

If we define factors $I : G \to \{1\}$ by $I' := \chi_{(0,0,0,0)}$ and $X_1', X_2', X_3', X_4' : G \to \Omega_2$ by $X_j' := \chi_{e_j}$, then the two equations can be written as $X_1'X_2'X_3' = I$ and $X_2'X_3'X_4' = I$. These equations are called multiplicative defining relations for the fraction H. Note that the fraction $H = \{g \in G \mid \chi(g) = 1 \text{ for all } \chi \in \widehat{G}_H\}$ where $\widehat{G}_H = \{\chi_z \mid z \in \{(0,0,0,0),(1,1,1,0),(0,1,1,1),(1,0,0,1)\}\}$. The fraction H is defined as the set of all elements $g \in G$ that satisfy $\chi_z(g) = 1$ for all $z \in \{(0,0,0,0),\{(1,1,1,0),(0,1,1,1),(1,0,0,1)\}$. More specifically, H consists of all $g \in G$ that satisfy the following equations

$$\begin{array}{rcl} \chi_{(0,0,0,0)}(g) & = & 1, \\ \chi_{(1,1,1,0)}(g) & = & (-1)^{g_1}(-1)^{g_2}(-1)^{g_3} = 1, \\ \chi_{(0,1,1,1)}(g) & = & (-1)^{g_2}(-1)^{g_3}(-1)^{g_4} = 1, \\ \chi_{(1,0,0,1)}(g) & = & (-1)^{g_1}(-1)^{g_4} = 1, \end{array}$$

which gives the relation

$$1 = (-1)^{g_1}(-1)^{g_2}(-1)^{g_3} = (-1)^{g_2}(-1)^{g_3}(-1)^{g_4} = (-1)^{g_1}(-1)^{g_4}.$$

Hence, H consists of all $g \in G$ on which functions $X_1'X_2'X_3'$, $X_2'X_3'X_4'$, $X_1'X_4'$ are equal to 1. That is, it is the set of consisting of all solutions in G for the system $I = X_1'X_2'X_3' = X_2'X_3'X_4' = X_1'X_4'$ of equations.

The cosets $a+H$ of H in G are regular fractions. On the fraction $F = a+H$ we have that $\chi(g) = \chi(a)$ for all $\chi \in \widehat{G}_H$, more specifically, for all $g \in F$ and $a = (a_1, a_2, a_3, a_4)$ we have

$$\begin{array}{rcl} \chi_{(0,0,0,0)}(g) & = & 1, \\ \chi_{(1,1,1,0)}(g) & = & (-1)^{g_1}(-1)^{g_2}(-1)^{g_3} = (-1)^{a_1}(-1)^{a_2}(-1)^{a_3}, \\ \chi_{(0,1,1,1)}(g) & = & (-1)^{g_2}(-1)^{g_3}(-1)^{g_4} = (-1)^{a_2}(-1)^{a_3}(-1)^{a_4}, \\ \chi_{(1,0,0,1)}(g) & = & (-1)^{g_1}(-1)^{g_4} = (-1)^{a_1}(-1)^{a_4}. \end{array}$$

For $a = (1,0,0,0)$ we find that for all $g \in F$,

$$\begin{array}{rcl} \chi_{(0,0,0,0)}(g) & = & 1, \\ \chi_{(1,1,1,0)}(g) & = & (-1)^{g_1}(-1)^{g_2}(-1)^{g_3} = -1, \\ \chi_{(0,1,1,1)}(g) & = & (-1)^{g_2}(-1)^{g_3}(-1)^{g_4} = 1, \\ \chi_{(1,0,0,1)}(g) & = & (-1)^{g_1}(-1)^{g_4} = -1. \end{array}$$

The fraction $(1,0,0,0)+H$ is the set of all solutions in G to the system $I = -X_1'X_2'X_3' = X_2'X_3'X_4' = -X_1'X_4'$ of equations. Note that the functions X_1', X_2', X_3', X_4' are factors when the runs in the design are coded by the elements in the multiplicative group $(\Omega_2)^4$.

Table 3.5: A regular fraction of a $4^2 2$ factorial design.

X_1	X_2	X_3
0	0	0
0	1	1
0	2	0
0	3	1
1	0	1
1	1	0
1	2	1
1	3	0
2	0	0
2	1	1
2	2	0
2	3	1
3	0	1
3	1	0
3	2	1
3	3	0

In the next example we illustrate the theory in the case of an asymmetrical design.

Example 3.41 In this example we consider a regular fraction of the $4^2 2$ factorial design. We code the runs in the full factorial designs with the elements in the group $G = \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$. A regular fraction H of G consisting of 16 runs is given in Table 3.5. The annihilator for this fraction is $\widehat{G}_H = \{\chi_{(0,0,0)}, \chi_{(2,2,1)}\}$. The corresponding defining equation is $I' = X_1'^2 X_2'^2 X_3'$.

3.4.3 Equivalence of definitions

We are now ready to present the main result of this section. We show that the Definitions 3.32 (Collombier (1996)), 3.34 (Wu and Hamada (2000)) and 3.36 (Pistone and Rogantin (2005)) are equivalent. The results are shown using the character theory of finite Abelian groups.

First we present a theorem that states an important property of the characters of a finite Abelian group. The theorem is a slight extension of the results stated as Propositions 1.4 and 1.5 in Chapter 5 of Collombier (1996).

Theorem 3.42 *Let H be a subgroup of an Abelian group G and $a \in G$. The irreducible characters $\chi_1, \chi_2 \in \widehat{G}$ are either orthogonal or completely confounded on the coset aH. More specifically, the irreducible characters χ_1 and χ_2 are orthogonal on aH if they belong to different cosets of $\widehat{G}_H$ and are completely confounded on aH if they belong to the same coset of $\widehat{G}_H$.*

Proof Choose an irreducible character $\alpha \in \widehat{G}$ and consider the coset $\alpha \widehat{G}_H$ in $\widehat{G}$. This is the set

$$\alpha \widehat{G}_H = \{\chi \in \widehat{G} \mid \chi(h) = \alpha(h) \text{ for all } h \in H\}.$$

Using that all characters $\chi \in \widehat{G}$ satisfy $\chi\left(g^{-1}\right) = \overline{\chi}(g)$ and $\chi(gh) = \chi(g)\chi(h)$ for all $g, h \in G$, we find that

$$\begin{aligned} \alpha \widehat{G}_H &= \{\chi \in \widehat{G} \mid \chi(ah) = \chi(a)\alpha(h) \text{ for all } h \in H\} \\ &= \{\chi \in \widehat{G} \mid \chi(ah) = \chi(a)\alpha\left(a^{-1}\right)\alpha(ah) \text{ for all } h \in H\} \\ &= \{\chi \in \widehat{G} \mid \chi(ah) = \chi(a)\overline{\alpha}(a)\alpha(ah) \text{ for all } h \in H\}. \end{aligned}$$

From this we find that $\chi(d) = c\alpha(d)$ for all $d \in aH$ where $c = \overline{\alpha}\chi(a)$. Hence, all characters in $\alpha \widehat{G}_H$ are completely confounded with the character $\alpha \in \widehat{G}$ on any coset aH.

In order to prove that the characters in different cosets of $\widehat{G}_H$ in $\widehat{G}$ are orthogonal on cosets of H in G, assume that α is chosen such that $\alpha \widehat{G}_H \neq \widehat{G}_H$. Then for $\chi_1, \chi_2 \in \widehat{G}_H$ the inner product $\langle \chi_1, \alpha\chi_2 \rangle_{aH}$ can be shown to equal zero in the following way

$$\begin{aligned} \langle \chi_1, \alpha\chi_2 \rangle_{aH} &= \tfrac{1}{|H|} \textstyle\sum_{h \in H} \chi_1(ah)\overline{\alpha\chi_2}(ah) \\ &= \tfrac{\chi_1(a)\overline{\alpha\chi_2}(a)}{|H|} \textstyle\sum_{h \in H} \chi_1(h)\overline{\alpha}(h)\,\overline{\chi_2}(h). \end{aligned}$$

Since $\chi_1, \chi_2 \in \widehat{G}_H$ we find that

$$\langle \chi_1, \alpha\chi_2 \rangle_{aH} = \frac{\chi_1(a)\overline{\alpha\chi_2}(a)}{|H|} \sum_{h \in H} \overline{\alpha}(h).$$

Using Lemma 3.26 and $\overline{\alpha} \notin \widehat{G}_H$ we find that $\sum_{h \in H} \overline{\alpha}(h) = 0$. Hence, we have shown that when α is chosen such that $\alpha \widehat{G}_H \neq \widehat{G}_H$ characters χ_1 and $\alpha\chi_2$ are orthogonal on any coset aH in G. The result generalizes to $\langle \chi_1, \chi_2 \rangle_{aH} = 0$ for χ_1 and χ_2 in different cosets of $\widehat{G}_H$. The inner product satisfies $\langle \alpha\chi_1, \alpha\chi_2 \rangle_{aH} = \langle \chi_1, \chi_2 \rangle_{aH}$ for all $\alpha \in G$. Hence, we can always multiply the characters χ_1 or χ_2 by some $\alpha \in \widehat{G}$ such that either $\alpha\chi_1$ or $\alpha\chi_2$ is an element of the annihilator $\widehat{G}_H$. This concludes the proof. □

From Theorem 3.42 we know that there is no partial confounding of the characters in $\widehat{G}$ on the cosets in G. The definition of regular fraction by Wu and Hamada (2000) (Definition 3.34) refers to the non-existence of partial confounding. This property has to be associated with a specific set of factorial effects. Here, we consider regularity with respect to set of factorial effects formed by the characters in $\widehat{G}$. In order to prove that for this specific basis the definition of regular fraction given by Collombier (1996) (Definition 3.32) is equal to the definition given by Wu and Hamada (2000) (Definition 3.34), it remains to be shown that the cosets in a finite Abelian group G are the only subsets of G on which there is no partial confounding of characters. Before we can state and prove this result, we first need a lemma.

Lemma 3.43 *Let G be a Abelian group and $F \subseteq G$ a fraction of G. Then for all $\chi_1, \chi_2 \in \widehat{G}$ and $a \in G$ the following statements hold.*

1. *χ_1 and χ_2 are completely confounded on aF if and only if they are completely confounded on F;*
2. *χ_1 and χ_2 are orthogonal on aF if and only if they are orthogonal on F;*
3. *χ_1 and χ_2 are partially confounded on aF if and only if they are partially confounded on F.*

Proof If characters χ_1 and $\chi_2 \in \widehat{G}$ satisfy $\chi_1(f) = c\chi_2(f)$ for all $f \in F$ and some non-zero $c \in \mathbb{C}$, then for all $f \in F$ we have that $\chi_1(af) = \chi_1(a)\chi_1(f) = c\chi_1(a)\chi_2(f) = c\chi_1(a)\chi_2\left(a^{-1}\right)\chi_2(af) = c\chi_1\overline{\chi_2}(a)\chi_2(af)$. Hence, if χ_1 and χ_2 are completely confounded on F then they are completely confounded on aF. Since this statement holds for any $a \in G$ the converse is also true. Secondly, if χ_1 and χ_2 are orthogonal on F then we have

$$\begin{aligned}\langle \chi_1, \chi_2 \rangle_{aF} &= \tfrac{1}{|F|}\textstyle\sum_{f\in F}\chi_1(af)\overline{\chi_2}(bf) \\ &= \tfrac{1}{|F|}\textstyle\sum_{f\in F}\chi_1(a)\chi_1(f)\overline{\chi_2}(a)\overline{\chi_2}(f) \\ &= \tfrac{\chi_1(a)\overline{\chi_2}(a)}{|F|}\textstyle\sum_{f\in F}\chi_1(f)\overline{\chi_2}(f) = \chi_1\overline{\chi_2}(a)\langle \chi_1, \chi_2\rangle_F = 0.\end{aligned}$$

Hence, orthogonality of χ_1 and χ_2 on F implies orthogonality of χ_1 and χ_2 on aF. This statement holds for any $a \in G$. Hence, its converse is also true. The third statement follows from parts 1 and 2 and Definition 2.16 of partial confounding. □

We will now show that the cosets in G are the only fractions on which there is no partial confounding of characters in $\widehat{G}$.

Theorem 3.44 *Let G be a finite Abelian group and $F \subseteq G$ a fraction of G. If there is no partial confounding of characters in $\widehat{G}$ on F, then F is a coset in G.*

Proof Let $a \in F$ and consider $H = a^{-1}F$. Then we have that $1 \in H$. Denote by $\widehat{G}_F$ the set of characters that are constant on F, that is, the characters that on F are completely confounded with 1. From Lemma 3.43 part 2 we know that $\widehat{G}_H = \widehat{G}_F$. Since there is no partial confounding of characters in $\widehat{G}$ on F, we know that all characters in $\widehat{G} \setminus \widehat{G}_F$ are orthogonal to 1 on F. From Lemma 3.43 we find that this can only be true if and only if all characters in $\widehat{G}\setminus\widehat{G}_F = \widehat{G}\setminus\widehat{G}_H$ are orthogonal to $1 \in \widehat{G}_H$ on H. We will show that H is a subgroup using the indicator function $\mathcal{I}_H$. Note that for all $\chi \in \widehat{G}_H$ we have that $\chi(h) = \chi(1) = 1$ for all $h \in H$. The characters $\chi \in \widehat{G} \setminus \widehat{G}_H$ are orthogonal to 1 on H. The Fourier coefficients of the indicator function $\mathcal{I}_H$ are given by

$$\langle \mathcal{I}_H, \chi \rangle = \begin{cases} \frac{|H|}{|G|} & \chi \in \widehat{G}_H \\ 0 & \chi \notin \widehat{G}_H \end{cases}.$$

Denote by $\langle H \rangle$ the subgroup in G generated by H. Since $\langle H \rangle$ is a subgroup of G we can use Theorem 3.42 to obtain the Fourier coefficients of the indicator function. These are

$$\langle \mathcal{I}_{\langle H \rangle}, \chi \rangle = \begin{cases} \frac{|\langle H \rangle|}{|G|} & \chi \in \widehat{G}_{\langle H \rangle} \\ 0 & \chi \notin \widehat{G}_{\langle H \rangle} \end{cases} .$$

The result now follows if we could prove that for any $H \subseteq G$ satisfying $1 \in H$ the equality $\widehat{G}_{\langle H \rangle} = \widehat{G}_H$ holds. The proof for this is as follows. If χ is constant on the set H then $\chi(h) = \chi(1) = 1$ for all $h \in H$. In that case we find that for all g and h in H we have that $\chi(gh) = \chi(g)\chi(h) = 1$. Hence, $\chi(h) = 1$ for all $h \in H$ implies that $\chi(h) = 1$ for all $h \in \langle H \rangle$. Clearly, any character $\chi \in \widehat{G}$ that is not constant on H is also not constant on $\langle H \rangle$. This proves that $\widehat{G}_{\langle H \rangle} = \widehat{G}_H$, which implies that

$$\mathcal{I}_H = \frac{|H|}{|\langle H \rangle|} \mathcal{I}_{\langle H \rangle}.$$

Both $\mathcal{I}_H$ and $\mathcal{I}_{\langle H \rangle}$ are indicator functions. This forces $\frac{|H|}{|\langle H \rangle|}$ to equal 1. Hence, we find that $\mathcal{I}_H = \mathcal{I}_{\langle H \rangle}$, which proves that H is a subgroup in G. As a result $F = aH$ is a coset in G. □

Theorems 3.42 and 3.44 show that the given for a regular fraction by Collombier (1996) (Definition 3.32) of regular fraction is equivalent to that given by Wu and Hamada (2000) (Definition 3.34) when the set of factorial effects that is under consideration is given by the characters $\widehat{G}$ of the group G.

We now show that definition of regular fractions given in Collombier (1996) (Definition 3.32) and Pistone and Rogantin (2005) (Definition 3.36) are equivalent. In the proof we need the following result.

Lemma 3.45 *Let H be a subgroup of a finite Abelian group G. If T is a transversal of $\widehat{G}_H$ in $\widehat{G}$, then $\widehat{H} = \{\chi_{|H} \mid \chi \in T\}$.*

Proof Let the representation ρ correspond to an irreducible character in T and denote by $\rho_{|H}$ its restriction to H. Then $\rho_{|H}$ is an irreducible representation of H. That $\rho_{|H}$ is a representation of H follows from

$$\rho_{|H}(h_1 h_2) = \rho(h_1 h_2) = \rho(h_1)\rho(h_2) = \rho_{|H}(h_1)\rho_{|H}(h_2) \text{ for all } h_1, h_2 \in H.$$

The representation $\rho_{|H}$ is irreducible since it is one-dimensional. Hence, the elements in the set $\{\chi_{|H} \mid \chi \in T\}$ are all irreducible characters of H. The representations that correspond to these irreducible characters are all non-equivalent. Let $\alpha_1, \alpha_2 \in T$ and assume that $\alpha_1(h) = \alpha_2(h)$ for all $h \in H$. Then $\alpha_1 \widehat{G}_H = \{\chi \in H \mid \chi(h) = \alpha_1(h) \text{ for all } h \in H\} = \{\chi \in H \mid \chi(h) = \alpha_2(h) \text{ for all } h \in H\} = \alpha_2 \widehat{G}_H$ which contradicts $\alpha_1, \alpha_2 \in T$. Hence, for different elements $\alpha_1, \alpha_2 \in T$ we have that $\alpha_1(h) \neq \alpha_2(h)$ for at least one $h \in H$. Using Lemma 3.7 we find that the set of irreducible representations for H obtained from the characters in T is a set of non-equivalent representations. Using

that $\widehat{G}_H$ is isomorphic to the dual of the quotient space G/H (see Lemma 3.25) and that G/H is Abelian we find that the number of elements of $\widehat{G}_H$ is given by

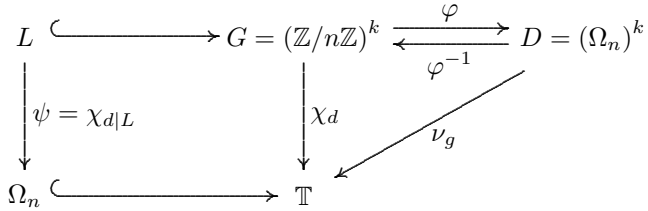
$$\left|\widehat{G}_H\right| = \left|\widehat{G/H}\right| = |G/H| = \frac{|G|}{|H|}.$$

Since $\left|\widehat{G}\right| = |G|$ the number of cosets of $\widehat{G}_H$ in $\widehat{G}$ equals $|H|$. From this we find that $|T| = \left|\widehat{H}\right|$ and that the elements in $\widehat{H} = \{\chi_{|H} \mid \chi \in T\}$ form a complete set of non-equivalent irreducible representations for H. □

The definition for a regular fraction given by Pistone and Rogantin (2005) (Definition 3.36) for symmetric factorial designs also defines a coset. We state the next lemma.

Lemma 3.46 *Let L be a subgroup of $(\mathbb{Z}/n\mathbb{Z})^k$ and $\psi : L \to \Omega_n$ a homomorphism. The set $\{(d_1, d_2, \ldots, d_k) \in (\Omega_n)^k \mid d_1^{\ell_1} d_2^{\ell_2} \ldots d_k^{\ell_k} = \psi(\ell)$ for all $\ell \in L\}$ is a coset in $(\Omega_n)^k$.*

Proof To simplify notation we let $G = (\mathbb{Z}/n\mathbb{Z})^k$ and $D = (\Omega_n)^k$. The morphisms between the relevant groups are given in the following commutative diagram.



From Lemma 3.45 we know that any homomorphism $\psi : L \to \mathbb{T}$ can be seen as the restriction to L of some homomorphism $\chi : G \to \mathbb{T}$. The set of all homomorphisms from G into $\mathbb{T}$ is given by $\widehat{G} = \{\chi_d \mid d \in D\}$ where $\chi_d(g) = d_1^{g_1} d_2^{g_2} \ldots d_k^{g_k}$. Hence, we have that $\psi = \chi_{a|L}$ for some $a \in D$. Consider the functions $\nu_g : D \to \mathbb{T}$ defined by $\nu_g(d) = \chi_d(g)$. For all $g \in G$ we have that ν_g is a character on D. As a result we find that

$$\begin{array}{ll} \{d \in D \mid d_1^{\ell_1} d_2^{\ell_2} \ldots d_k^{\ell_k} = \psi(\ell) \text{ for all } \ell \in L\} & = \\ \{d \in D \mid \nu_\ell(d) = \chi_a(\ell) \text{ for all } \ell \in L\} & = \\ \{d \in D \mid \nu_\ell(d) = \nu_\ell(a) \text{ for all } \ell \in L\} & = \\ \{d \in D \mid \nu(d) = \nu(a) \text{ for all } \nu \in S\}, & \end{array}$$

where $S = \{\nu_\ell \mid \ell \in L\} \subseteq \widehat{D}$. The result now follows from Lemma 3.38. □

The final lemma in this section states that any coset in $D = (\Omega_n)^k$ is regular according to the definition given by Pistone and Rogantin (2005) (Definition 3.36).

Lemma 3.47 *Let H be a subgroup of $(\Omega_n)^k$ and $a \in (\Omega_n)^k$. There exists a subgroup L of $(\mathbb{Z}/n\mathbb{Z})^k$ and a homomorphism $\psi : L \to \Omega_n$ such that $aH = \{(d_1, d_2, \ldots, d_k) \in (\Omega_n)^k \mid d_1^{\ell_1} d_2^{\ell_2} \ldots d_k^{\ell_k} = \psi(\ell) \text{ for all } \ell \in L\}$.*

Proof A commutative diagram containing the morphisms between the relevant groups is given in the proof of Lemma 3.46. Again we let $D = (\Omega_n)^k$ and $G = (\mathbb{Z}/n\mathbb{Z})^k$. Consider the subgroup L of G defined by $L = \{\ell \in G \mid h_1^{\ell_1} h_2^{\ell_2} \ldots h_k^{\ell_k} = 1 \text{ for all } h \in H\}$. Then $\widehat{G}_H = \{\nu_\ell \mid \ell \in L\}$ where $\nu_\ell : D \to \mathbb{T}$ is defined as $\nu_\ell(d) = d_1^{\ell_1} d_2^{\ell_2} \ldots d_k^{\ell_k}$ for all $d \in D$. The isomorphism $\varphi : G \to D$ is given by $\varphi(g) = (\omega_n^{g_1}, \omega_n^{g_2}, \ldots, \omega_n^{g_k})$. Let $\psi : L \to \Omega_n$ be defined as $\psi(\ell) = \nu_{\varphi^{-1}(a)}(\varphi(\ell))$. We show that ψ is a homomorphism of L. Using that both φ and $\nu_{\varphi^{-1}(a)}$ are homomorphisms we find that

$$\begin{aligned} \psi(\ell_1 + \ell_2) &= \nu_{\varphi^{-1}(a)}(\varphi(\ell_1 + \ell_2)) \\ &= \nu_{\varphi^{-1}(a)}(\varphi(\ell_1)\varphi(\ell_2)) \\ &= \nu_{\varphi^{-1}(a)}(\varphi(\ell_1))\nu_{\varphi^{-1}(a)}(\varphi(\ell_2)) \\ &= \psi(\ell_1)\psi(\ell_2). \end{aligned}$$

For arbitrary $a \in D$ and $\ell \in L$ let $b = \varphi^{-1}(a)$ and $m = \varphi(\ell)$. Then the following equality holds

$$\begin{aligned} \nu_\ell(a) &= {a_1}^{\ell_1} {a_2}^{\ell_2} \ldots {a_k}^{\ell_k} \\ &= \left(\omega_n^{b_1}\right)^{\ell_1} \left(\omega_n^{b_2}\right)^{\ell_2} \cdots \left(\omega_n^{b_k}\right)^{\ell_k} \\ &= \left(\omega_n^{\ell_1}\right)^{b_1} \left(\omega_n^{\ell_2}\right)^{b_2} \cdots \left(\omega_n^{\ell_k}\right)^{b_k} \\ &= {m_1}^{b_k} {m_2}^{b_2} \ldots {m_k}^{b_k} \\ &= \nu_b(m) \\ &= \nu_{\varphi^{-1}(a)}(\varphi(\ell)). \end{aligned}$$

Using this we find that

$$\begin{aligned} &\{d \in D \mid d_1^{\ell_1} d_2^{\ell_2} \ldots d_k^{\ell_k} = \psi(\ell) \text{ for all } \ell \in L\} &&= \\ &\{d \in D \mid \nu_\ell(d) = \nu_{\varphi^{-1}(a)}(\varphi(\ell)) \text{ for all } \ell \in L\} &&= \\ &\{d \in D \mid \nu_\ell(d) = \nu_\ell(a) \text{ for all } \ell \in L\} &&= \\ &\{d \in D \mid \nu(d) = \nu(a) \text{ for all } \nu \in \widehat{G}_H\} &&= aH, \end{aligned}$$

where the last equality follows from Lemma 3.39. □

From Lemmas 3.46 and 3.47 we find that the regular fractions that Pistone and Rogantin (2005) define are exactly the cosets of the multiplicative group $(\Omega_n)^k$.

3.4.4 Confounding relations and estimability of effects

In this section we consider the estimability of the Fourier coefficients of the expectation function given in (3.10) for the case where observations are made on a regular fraction F of the full factorial design G. The estimability is related to the confounding of the characters. The confounding of characters in $\widehat{G}$ on a regular fraction $F = aH$ of G was given in Theorem 3.42. Using the

Poisson summation formula derived in Section 3.1.4 we find a complete set of confounding relations on the regular fraction.

Recall that the expectation function $\mu \in \mathbb{R}^G$ is defined by $\mu(g) = \mathrm{E}[y(g)]$ for all $g \in G$. At this point no assumptions about the distribution of y are needed. The function μ has a Fourier expansion given by

$$\mu = \sum_{\chi \in \widehat{G}} \widehat{\mu}(\chi)\, \chi.$$

In the case where data is obtained for all treatments in the full factorial design G, each Fourier coefficient $\widehat{\mu}(\chi), \chi \in \widehat{G}$, can be unbiasedly estimated by the Fourier coefficient $\widehat{y}(\chi)$ of the response function $y \in \mathbb{R}^G$. This was shown in (3.11). However, since in this case we do not observe data on the full factorial design but only on a fraction we cannot determine the Fourier coefficients $\widehat{y}(\chi)$. The next lemma gives the confounding relations for the factorial effects $\mu(\chi), \chi \in \widehat{G}$, on a regular fraction aH of a full factorial design G. More precisely, it gives linear combinations of the Fourier coefficients $\widehat{\mu}(\chi), \chi \in \widehat{G}$, that can be estimated unbiasedly. It also tells us how each of these linear combinations can be estimated. The lemma is based on the analogue of the Poisson summation formula that is given in (3.7). Good (1960) was the first to use the Poisson summation formula to find the confounding relations on a regular fraction.

Lemma 3.48 *Let H be a subgroup of a finite Abelian group G, $a \in G$ and $\alpha \in \widehat{G}$. For all response functions $y \in \mathbb{R}^G$ and the expectation function μ defined by $\mu = E[y]$ we have that*

$$E\left[\frac{1}{|H|} \sum_{g \in aH} \overline{\alpha}(g)\, y(g)\right] = \sum_{\chi \in \alpha \widehat{G}_H} \overline{\alpha}\chi(a)\, \widehat{\mu}(\chi). \tag{3.23}$$

Proof The result follows from (3.7) by substituting y for f, taking the expected value at both sides of the equation and using $\mathrm{E}[\widehat{y}] = \widehat{\mu}$ obtained in (3.11) . □

The right-hand side of (3.23) gives linear combinations of effects $\widehat{\mu}(\chi), \chi \in \widehat{G}$, that are estimable on the regular fraction aH. These linear combinations can be shown to form a basis for the linear space of all effects that are estimable on the regular fraction aH. This is stated in the next lemma.

Lemma 3.49 *Let H be a subgroup of a finite Abelian group G and $a \in G$. Let T denote a transversal of $\widehat{G}$ in $\widehat{G}$. The functions*

$$\sum_{\chi \in \alpha \widehat{G}_H} \overline{\alpha}\chi(a)\, \widehat{\mu}(\chi), \quad \alpha \in T,$$

form a basis for the linear space of effects that are estimable on the regular fraction aH.

Proof Note that knowing (3.23) it suffices to show that the functions $\overline{\alpha_{|aH}}, \alpha \in T$, form an orthogonal basis for $\mathbb{C}^{aH}$. The orthogonality follows from Theorem 3.42 using that by the definition of the transversal each $\alpha \in T$ belongs to a different coset of $\widehat{G}_H$. In Lemma 3.45 we showed that $|T| = \left|\widehat{H}\right|$. The result follows by observing that

$$|T| = \left|\widehat{H}\right| = |H| = \dim\left(\mathbb{C}^{aH}\right).$$

This concludes the proof. □

The following corollary follows directly from the last lemma.

Corollary 3.50 *The assumption that $\widehat{\mu}(\chi) = 0$ for all $\chi \in \alpha\widehat{G}_H \setminus \{\alpha\}$ is a necessary and sufficient condition for the factorial effect $\widehat{\mu}(\alpha)$ to be estimable on a regular fraction aH of G.*

In the following example we determine the confounding relations for a regular fraction of the 2^3 full factorial design.

Example 3.51 We consider the full 2^3 factorial design coded as the additive Abelian group $G = (\mathbb{Z}/2\mathbb{Z})^3$. Consider the subgroup

$$H = \{(0,0,0), (1,1,0), (1,0,1), (0,1,1)\}.$$

From Lemma 3.39 we find that $H = \{g \in G \mid \chi(g) = 1 \text{ for all } \chi \in \widehat{G}_H\}$. The annihilator $\widehat{G}_H$ of H in G is

$$\widehat{G}_H = \{\chi_z \mid z \in \{(0,0,0), (1,1,1)\}\}$$

with χ_z as defined in (3.2). We are interested in the exact confounding relations on the regular fraction H. The cosets of $\widehat{G}_H$ in $\widehat{G}$ are

$$\begin{aligned}
\widehat{G}_H &= \{\chi_{(0,0,0)}, \chi_{(1,1,1)}\};\\
\chi_{(1,0,0)}\widehat{G}_H &= \{\chi_{(1,0,0)}, \chi_{(0,1,1)}\};\\
\chi_{(0,1,0)}\widehat{G}_H &= \{\chi_{(0,1,0)}, \chi_{(1,0,1)}\};\\
\chi_{(0,0,1)}\widehat{G}_H &= \{\chi_{(0,0,1)}, \chi_{(1,1,0)}\}.
\end{aligned}$$

Let $y \in \mathbb{R}^F$ be the function that maps each element of the fraction to the response value that is observed in the corresponding run. Using Lemma 3.48 we find that

$$\begin{aligned}
\mathrm{E}\left[\tfrac{1}{4}(y_{000} + y_{110} + y_{101} + y_{011})\right] &= \widehat{\mu}\left(\chi_{(0,0,0)}\right) - \widehat{\mu}\left(\chi_{(1,1,1)}\right);\\
\mathrm{E}\left[\tfrac{1}{4}(y_{000} - y_{110} - y_{101} + y_{011})\right] &= \widehat{\mu}\left(\chi_{(1,0,0)}\right) - \widehat{\mu}\left(\chi_{(0,1,1)}\right);\\
\mathrm{E}\left[\tfrac{1}{4}(y_{000} - y_{110} + y_{101} - y_{011})\right] &= \widehat{\mu}\left(\chi_{(0,1,0)}\right) - \widehat{\mu}\left(\chi_{(1,0,1)}\right);\\
\mathrm{E}\left[\tfrac{1}{4}(y_{000} + y_{110} - y_{101} - y_{011})\right] &= \widehat{\mu}\left(\chi_{(0,0,1)}\right) - \widehat{\mu}\left(\chi_{(1,1,0)}\right),
\end{aligned}$$

where we have used $y_{g_1g_2g_3}$ to denote $y(g_1, g_2, g_3)$. Note that if we assume that

$$\widehat{\mu}\left(\chi_{(1,1,1)}\right) = \widehat{\mu}\left(\chi_{(0,1,1)}\right) = \widehat{\mu}\left(\chi_{(1,0,1)}\right) = \widehat{\mu}\left(\chi_{(1,1,0)}\right) = 0,$$

then unbiased estimators for $\widehat{\mu}\left(\chi_{(0,0,0)}\right), \widehat{\mu}\left(\chi_{(1,0,0)}\right), \widehat{\mu}\left(\chi_{(0,1,0)}\right)$ and $\widehat{\mu}\left(\chi_{(0,0,1)}\right)$ can directly be read off from the previous equations.

Another form of confounding occurs when there are factors that in the experiment are set at more than two levels. In that case some of the irreducible characters are complex. If χ is a complex irreducible character of a finite Abelian group G then $\overline{\chi}$ is an irreducible character of G that is not equivalent to χ. For such χ we have that $\widehat{\mu}(\overline{\chi}) = \overline{\widehat{\mu}(\chi)}$ when we assume μ to be real-valued. This type of confounding is discussed in more detail in Section 3.6 and is related to the equality of the sums of squares for conjugated pairs of irreducible representations that we found in the example considered in Section 3.2.2.

3.4.5 Connection with orthogonal arrays

In this section we assume that the full factorial design is coded by the Abelian group $G = \prod_{i=1}^{k} L_i$, where L_i is an Abelian group consisting of n_i elements. We use the character theory of the finite Abelian group to show that all regular fractions of G as defined in Definition 3.32 are orthogonal arrays. An orthogonal array is defined as follows.

Definition 3.52 An orthogonal array OA $(N, k, n_1 \times n_2 \times \ldots \times n_k, t)$ having N rows, $k\,(\geq 2)$ columns, $n_1, n_2, \ldots, n_k\,(\geq 2)$ symbols and strength $t\,(\leq k)$ is an $N \times k$ array, with elements in the jth column from a set of n_j distinct symbols $(1 \leq j \leq n)$, in which all possible combinations of symbols appear equally often as rows in every $N \times t$ subarray.

For an extensive treatment of orthogonal arrays (both from a combinatorial and statistical perspective) the reader is referred to the book by Hedayat et al. (1999). The main theorem in this section states that all regular fractions are orthogonal arrays of a strength related to the resolution of the fraction. The property that each regular fraction is an orthogonal array was first pointed out in Rao (1947) and Bose (1947) for symmetric factorial designs with a prime power as the number of levels. The same result is also stated in Theorem 8.2.2. in Raktoe et al. (1981). This theorem also explains how the strength of the orthogonal array is related to the resolution of the fraction. The term resolution was introduced by Box and Hunter (1961) as a means to classify regular fractions of 2^k factorial designs. It was generalized to non-regular fractions of 2^k factorial designs by Webb (1964). Raktoe et al. (1981) give the following definition for the resolution of a fraction which applies to any factorial design.

Definition 3.53 (Raktoe, Hedayat and Federer) A fractional factorial design is said to be of resolution R if all factorial effects up to order $\left\lfloor \frac{R-1}{2} \right\rfloor$ are estimable, under the assumption that all factorial effects of order $\left\lceil \frac{R+1}{2} \right\rceil$ and higher are zero, with the additional convention that if R is odd than the general

mean is also estimable and if R is even then the general mean is not of interest for estimation[3].

We illustrate this definition using the classical notation for two-level factorial designs. In the first example we consider a fraction of resolution $R = 3$.

Example 3.54 The 2^{3-1} design with defining relation $I = X_1X_2X_3$ has resolution $R = 3$. For the resolution we find that $\left\lfloor \frac{R-1}{2} \right\rfloor = 1$ and $\left\lceil \frac{R+1}{2} \right\rceil = 2$. That is, the main effects and mean are estimable under the assumption that all interactions are negligible.

Rao (1947) presented a lower bound for the number of runs in an orthogonal array of strength 3 with k columns with n symbols. Margolin (1969) showed that the number of runs in each fraction (regular or non-regular) of a n^k factorial design of resolution 4 satisfies the same lower bound. The following example illustrates the definition for resolution using a fraction of resolution $R = 4$.

Example 3.55 The 2^{4-1} design with defining relation $I = X_1X_2X_3X_4$ has resolution 4. For this resolution we find that $\left\lfloor \frac{R-1}{2} \right\rfloor = 1$ and $\left\lceil \frac{R+1}{2} \right\rceil = 3$. That is, the main effects and mean are estimable under the assumption that the effects of order 3 and higher are negligible.

We define the weight wt (g) of an element $g \in G$ as the number of coordinates g_i of g that satisfy $g_i \neq \mathrm{id}_{L_i}$. In the special case where $L_i = \mathbb{Z}/n_i\mathbb{Z}$ for all i this definition coincides with that of the Hamming weight (which is defined as the number of non-zero coordinates of a vector). For regular fractions aH of G the resolution can now be expressed in terms of the elements of the annihilator of H in G.

Lemma 3.56 *Let H be a subgroup of G and $a \in G$. The resolution of the regular fraction $F = aH$ is*

$$R = \min\left\{ wt\ (g) \mid \chi_g \in \widehat{G}_H \ \textit{and}\ g \neq id_G \right\}. \tag{3.24}$$

Proof We show that the resolution R given in (3.24) satisfies the conditions in Definition 3.53. Let h be an element of G that satisfies wt $(h) \leq j$ where $j = \left\lfloor \frac{R-1}{2} \right\rfloor$. This implies that $R = 2j + 1$ (for R odd) or $R = 2j + 2$ (for R even). The characters that on F are completely confounded with χ_h are the elements of the coset $\chi_h \widehat{G}_H = \{\chi_{hg} \mid \chi_g \in \widehat{G}_H\}$. For each $g \neq \mathrm{id}_G$ for which wt $(g) \geq R$ we have that wt $(hg) \geq R - j \geq j + 1$. This follows by observing that multiplying an element of $g \in G$ with an element of weight j changes at most j of its coordinates. Hence, a character χ_h that satisfies wt $(h) \leq j$ is only confounded with characters χ_g with wt $(g) \geq R - j$. Using Corollary 3.50 we

[3] Hedayat et al. (1999) impose the extra restriction that all effects up to order k are estimated with relative efficiency of 1 and that the corresponding ordinary least squares are uncorrelated, where the relative efficiency of an effect is defined as the normalized ratio of the variance of the least-squares estimate of the effect under the complete factorial and the least-squares estimate under the fraction.

find that all factorial effects $\widehat{\mu}(\chi_h)$ of order wt $(h) \leq j$ are estimable under the assumption that $\widehat{\mu}(\chi_g) = 0$ for all factorial effects $\widehat{\mu}(\chi_g)$ of order wt $(g) \geq R-j$. In Section 3.2.1 we explained that the factorial effects $\widehat{\mu}(\chi)$ with $\chi \in B_J$ as in (3.12) form a basis for the set of factorial effects that belong to X_J. From this we find that any factorial effect belonging to a factor X_J of order $|J| \leq j$ is estimable under the assumption that all factorial effects belonging to factors $X_{J'}$ of order $|J'| \geq R - j$ are zero. Since, we have used that $R = 2j + 1$ or $R = 2j+2$, we have that $R-j = j+1$ (for R odd) or $R-j = j+2$ (for R even). Note that $R-j \geq j$ in both cases. For R odd we find that under the assumption that effects of order $R - j = j + 1$ and higher are zero, all effects of order up to j are estimable. If R is even then all effects of order up to j are estimable under the assumption that effects of order $R - j = j + 2$ and higher are zero. From (3.24) is follows directly that the mean is only confounded with effects of order R and higher and is in also estimable under the stated assumptions. □

Proposition 6.4 in Pistone and Rogantin (2005) gives a necessary and sufficient condition for a fractional factorial design to be an orthogonal array of strength t. Pistone and Rogantin allow replicated runs in the fractional factorial design and use the complex coding ($L_j = \Omega_{n_j}$) for the factor levels. The condition is related to the Fourier coefficients of the indicator function of the fraction. This result can be generalized to cases in which each set L_j of levels is a finite Abelian group (not necessarily isomorphic to $\mathbb{Z}/n_j\mathbb{Z}$). The set of symbols appearing in the jth column are the elements of the group L_j. We prove the more general lemma for the case with no replications. We use the notation introduced in Section 3.2.1, in particular the characters of the group G are $\chi_z, z \in G$, with χ_z as in (3.9).

Lemma 3.57 *A fraction $F \subseteq G$ is an OA $(|F|, k, n_1 \times n_2 \times \ldots \times n_k, t)$ if and only if all the coefficients $\widehat{\mathcal{I}_F}(\chi_g)$ of the indicator function $\mathcal{I}_F$ for $g \in G \setminus \{id_G\}$ with weight wt $(g) \leq t$ are zero.*

Proof For each set $S \subseteq \{1, 2, \ldots, k\}$ we define the function $\mathcal{R}_S : G \to \mathbb{N}$ that for each $(g_1, g_2, \ldots, g_k) \in G$ returns the number of runs $(f_1, f_2, \ldots, f_k) \in F$ that have $g_j = f_j$ for all $j \in S$. For given S the Fourier expansion of R_S can be derived using the indicator function $\mathcal{I} : G \to \{0, 1\}$ of the fraction F. To this end, let $H_S = \{g \in G \mid g_j = \mathrm{id}_{L_j} \text{ for all } j \in S\}$ and ${H_S}^{\perp} = \{g \in G \mid g_j = \mathrm{id}_{L_j} \text{ for all } j \notin S\}$. Note that H_S is a subgroup of G and that its annihilator in G is given by $\widehat{G}_{H_S} = \{\chi_z \mid z \in {H_S}^{\perp}\}$. We find that

$$\begin{aligned} \mathcal{R}_S(g) &= \textstyle\sum_{h \in H_S} \mathcal{I}_F(g+h) \\ &= \textstyle\sum_{h \in H_S} \sum_{\chi \in \widehat{G}} \widehat{\mathcal{I}_F}(\chi)\, \chi(g+h) \\ &= \textstyle\sum_{\chi \in \widehat{G}} \widehat{\mathcal{I}_F}(\chi)\, \chi(g) \sum_{h \in H_S} \chi(h). \end{aligned}$$

Using Lemma 3.26 and $\widehat{G}_{H_S} = \{\chi_z \mid z \in {H_S}^{\perp}\}$ we find that

$$\sum_{h \in H_S} \chi_z(h) = \begin{cases} |H_S| & \text{for } z \in {H_S}^{\perp} \\ 0 & \text{for } z \notin {H_S}^{\perp} \end{cases}.$$

As a consequence, the function $\mathcal{R}_S$ can be expressed as

$$\mathcal{R}_S = |H_S| \sum_{z \in {H_S}^\perp} \widehat{\mathcal{I}_F}(\chi_z)\, \chi_z. \tag{3.25}$$

First assume that the $\widehat{\mathcal{I}_F}(\chi_z) = 0$ for all $z \in G \setminus \{\mathrm{id}_G\}$ that satisfy wt $(g) \leq t$. Since for all subsets $S \subseteq \{1, 2, \ldots, k\}$ with $|S| = t$ the elements in ${H_S}^\perp$ have a weight which is at most t, we find that for each of these subsets

$$\mathcal{R}_S = |H_S| \widehat{\mathcal{I}_F}(\chi_{\mathrm{id}_G})\, \chi_{\mathrm{id}_G}.$$

It follows from $\chi_{\mathrm{id}_G}(g) = 1$ for all $g \in G$ that the function $\mathcal{R}_S$ is constant on G. This implies that the possible combinations of levels for the t factors indexed by the elements in S each appear in an equal number of runs in the fraction F. Since this result holds for all $S \subseteq \{1, 2, \ldots, k\}$ with $|S| = t$ we find that the fraction F is an orthogonal array of strength t.

For the converse, assume that for all S with $|S| = t$ we have that the function $\mathcal{R}_S$ is constant on F. Then from the expansion (3.25) we find that $\widehat{\mathcal{I}_F}(\chi_r) = 0$ for all $r \in {H_S}^\perp \setminus \{\mathrm{id}_G\}$. Note that ${H_S}^\perp = \{g \in G \mid g_j = \mathrm{id}_{L_j} \text{ for all } j \notin S\}$. The result $\widehat{\mathcal{I}_F}(\chi_g) = 0$ for all $g \in G$ satisfying wt $(g) \leq t$ follows from observing that $z \in G \setminus \{\mathrm{id}_G\}$ with weight wt $(g) = p \leq t$ appears in the set ${H_S}^\perp \setminus \{\mathrm{id}_G\}$ when S is chosen to include the index i of each of the p coordinates of z that satisfy $z_i \neq \mathrm{id}_{L_i}$. □

This last lemma provides meaning to the word *orthogonal* in orthogonal arrays. All pairs of characters χ_z and χ_g that satisfy wt (z) + wt $(g) \leq t$ are orthogonal on F. This follows from observing that

$$\langle \chi_z, \chi_g \rangle_F = \langle 1, \chi_{zg^{-1}} \rangle_F = \langle \mathcal{I}_F, \chi_{zg^{-1}} \rangle_G = \widehat{\mathcal{I}_F}\left(\chi_{zg^{-1}}\right) = 0,$$

where the last equality is obtained using wt $\left(zg^{-1}\right) \leq$ wt (z) + wt $\left(g^{-1}\right)$ = wt (z) + wt $(g) \leq t$. Hence, a pair of factorial effects $\widehat{\mu}(\chi_z)$ and $\widehat{\mu}(\chi_g)$ is orthogonal if wt (z) + wt $(g) \leq t$. Any pair of interaction spaces H_{J_1} and H_{J_2} is orthogonal if we have that $|J_1| + |J_2| \leq t$ on F. The next theorem states that any regular fraction of resolution R is an orthogonal array of resolution $R - 1$. This result was shown in Raktoe et al. (1981) for the symmetric case with the number of levels equal to a prime power. We proof the result for the general case of an asymmetrical factorial design (with the n_j not necessarily a prime factor).

Theorem 3.58 *Let a full factorial design be coded by the Abelian group* $G = \prod_{i=1}^{k} L_i$ *with* L_i *an Abelian group of* n_i *elements. The runs in a regular fraction* $F = aH$ *of* G *of resolution* R *(when written as rows) represent an orthogonal array of strength* $R - 1$.

Proof The coefficients of the indicator function for a regular fraction aH of G are given by

$$\widehat{\mathcal{I}_F}(\chi_g) = \begin{cases} 0 & \text{if } \chi_g \notin \widehat{G}_H \\ \frac{|H|}{|G|}\chi_r(a) & \text{if } \chi_g \in \widehat{G}_H \end{cases}.$$

By Lemma 3.56 the elements $g \in G$ that correspond to coefficients $\widehat{\mathcal{I}_F}(\chi_g) \neq 0$ satisfy wt $(g) \geq R$. Hence, for all $g \leq R-1$ we have that $\widehat{\mathcal{I}_F}(\chi_g) = 0$. The result now follows by applying Lemma 3.57. Note that strength of the orthogonal array cannot be larger that $R-1$, because for the regular fraction to have resolution it is required that at least one h with $\chi_h \in \widehat{G}_H$ satisfies wt $(h) = R$. □

3.4.6 Pseudofactors

If n_i is not a prime number, then different Abelian groups exist that consist of n_i elements. Each of these groups can be used to code the n_i levels of the variable x_i. The cases $n_i = 4$ and $n_i = 6$ are illustrated in the following example.

Example 3.59 Two non-isomorphic Abelian groups that consist of 4 elements are the cyclic group $\mathbb{Z}/4\mathbb{Z}$ and $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$. Two isomorphic Abelian groups of 6 elements are $\mathbb{Z}/6\mathbb{Z}$ and $\mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$.

In cases where the levels of the variable x_i are not coded by the elements in $\mathbb{Z}/n_i\mathbb{Z}$, but by the elements of another (not necessarily non-isomorphic) Abelian group of n_i elements, we typically speak of *pseudofactors*. For instance, if the group $L_i = \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z} = \{(0,0), (0,1), (1,0), (1,1)\}$ is used to code the 4 levels of a variable, then we say that pseudofactors are used. In this example there are two pseudofactors that each have two levels. The name pseudofactors is appropriate because the functions that map each $d \in D$ to the the first coordinate and second coordinate, respectively, can be regarded as two separate factors. However, the values of both factors are needed to find the level at which the variable x_i is set in a specific run of the experiment. This explains the prefix pseudo. The use of pseudofactors has several advantages that we discuss in this section.

Bailey (1985) illustrates two different ways of using pseudofactors to find regular fractions. Firstly, pseudofactors can simplify the search for regular fractions using the Sylow theorem. Secondly, a design coded using pseudofactors may have more regular fractions than one coded without pseudofactors. We now shortly discuss these two applications of pseudofactors.

The Sylow theorem gives a sufficient condition on the order of a subgroup of a group G. The theorem states that if m divides $|G|$, then G has a subgroup of order m provided that m is a prime power (see Cohn (1974), p.247). A special class of subgroups of G are the Sylow p-subgroups where p is a prime divisor of $|G|$. The following definition of a Sylow p-subgroup is taken from Cohn (1974).

Definition 3.60 (Sylow p-subgroup) Let G be a group of order $n = p^s n'$ where p does not divide n'. Any subgroup of G of order p^s is a Sylow p-subgroup.

Let P denote the set of primes dividing $N = |G|$. By Proposition 9.7.4 in Cohn (1974) each finite Abelian group G has a unique Sylow p-subgroup W_p for each $p \in P$ and $G = \prod_{p \in P} W_p$. Moreover, for any subgroup H of G we have that $H = \prod_{p \in P} H_p$ where H_p is a subgroup of the Sylow p-subgroup W_p of G. We

illustrate how pseudofactors and the Sylow theorem can simplify the search for subgroups and, hence, for regular fractions. First we construct a group that is isomorphic to the full factorial design $\prod_{i=1}^{k} \mathbb{Z}/n_i\mathbb{Z}$ using pseudofactors in the following way. Each of the groups $\mathbb{Z}/n_i\mathbb{Z}$ is replaced by the group $L_i = \mathbb{Z}/n_{i1}\mathbb{Z} \times \mathbb{Z}/n_{i2} \times \ldots \times \mathbb{Z}/n_{iq_i}\mathbb{Z}$, where $n_{i1}, n_{i2}, \ldots, n_{iq_i}$ denote different prime powers (one for each prime divisor of n_i) that divide n_i. Since $n_{i1}, n_{i2}, \ldots, n_{iq_i}$ are powers of different primes they must be pairwise coprime. A consequence of this is that the groups $\mathbb{Z}/n_i\mathbb{Z}$ and L_i are isomorphic. The full factorial design using pseudofactors is $G = \prod_{i=1}^{k} L_i$. In the decomposition $G = \prod_{p \in P} W_p$ of G as a direct product Sylow p-subgroups W_p, each W_p is the direct sum of the $\mathbb{Z}/n_{ij}\mathbb{Z}$ (where $1 \leq i \leq k$ and $1 \leq j \leq q_i$) for which n_{ij} is equal to a prime power of p. Each subgroup H of G is of the form $H = \prod_{p \in P} H_p$ where H_p is a subgroup of W_p. Hence, the subgroups of the Sylow p-subgroups of G can serve as building blocks for the subgroups of G.

Example 3.61 Consider an experiment with 5 variables with the number of levels given by $n_1 = n_2 = 2$ and $n_3 = n_4 = 3$ and $n_5 = 6$. In this we have that

$$\left(\mathbb{Z}/2\mathbb{Z}\right)^2 \times \left(\mathbb{Z}/3\mathbb{Z}\right)^2 \times \mathbb{Z}/6\mathbb{Z} \cong \left(\mathbb{Z}/2\mathbb{Z}\right)^3 \times \left(\mathbb{Z}/3\mathbb{Z}\right)^3,$$

where the decomposition of Sylow p-subgroups is given on the right-hand side. The Sylow 2-subgroup in this decomposition is $W_2 = \left(\mathbb{Z}/2\mathbb{Z}\right)^3$. A subgroup H_2 of W_2 is

$$H_2 = \{(0,0,0), (1,1,0), (0,1,1), (1,0,1)\}.$$

The annihilator of H_2 in W_2 is $\{\chi_{(0,0,0)}, \chi_{(1,1,1)}\}$ where $\chi_w, w \in W_2$, is used to denote a character of W_2 as given in (3.2). The Sylow 3-subgroup in this decomposition is $W_3 = \left(\mathbb{Z}/3\mathbb{Z}\right)^3$. A subgroup H_3 of W_3 is

$$\begin{aligned} H_3 = \quad & \{(0,0,0), (1,1,1), (2,2,2), (1,2,0), (2,0,1), \\ & (0,1,2), (2,1,0), (0,2,1), (1,0,2)\} \end{aligned}$$

The annihilator of H_3 in W_3 is $\{\chi_{(0,0,0)}, \chi_{(1,1,1)}\}$ where $\chi_w, w \in W_3$, is used to denote a character of W_3 as given in (3.2). The subgroup $H = H_2 \times H_3$ of $G = \left(\mathbb{Z}/2\mathbb{Z}\right)^3 \times \left(\mathbb{Z}/3\mathbb{Z}\right)^3$ is a regular fraction of resolution 3 of the full factorial design G where pseudofactors are used to code the levels for x_5 (each combination of one of the first three coordinates and one of the last three coordinates can be chosen to represent the levels of this variable). The regular fraction H consists of 36 runs. The annihilator of H in G is

$$\widehat{G}_H = \{(0,0,0,0,0,0), (1,1,1,0,0,0), (0,0,0,1,1,1), (1,1,1,1,1,1)\},$$

which is the direct product of the annihilators of H_2 in W_2 and H_3 in W_3.

In the second application discussed in Bailey (1985) the use pseudofactors results in a group that is not isomorphic to $\prod_{i=1}^{k} \mathbb{Z}/n_i\mathbb{Z}$. Bailey (1985) gives the example of a $2^2 4^2$ factorial design. For this factorial design a fraction of resolution 3 can only be found using pseudofactors.

Table 3.6: A regular $\frac{1}{4}$ fraction of resolution 3 of a $2^2 4^2$ factorial design.

X_1	X_2	X_3	X_4
0	0	(0, 0)	(0, 0)
0	0	(0, 1)	(0, 1)
0	0	(1, 0)	(1, 0)
0	0	(1, 1)	(1, 1)
0	1	(0, 0)	(0, 1)
0	1	(0, 1)	(0, 0)
0	1	(1, 0)	(1, 1)
0	1	(1, 1)	(1, 0)
1	0	(0, 0)	(1, 0)
1	0	(0, 1)	(1, 1)
1	0	(1, 0)	(0, 0)
1	0	(1, 1)	(0, 1)
1	1	(0, 0)	(1, 1)
1	1	(0, 1)	(1, 0)
1	1	(1, 0)	(0, 1)
1	1	(1, 1)	(0, 0)

Example 3.62 Example 8 in Bailey (1985) shows the use of pseudofactors for constructing regular fractions. In the example a $2^2 4^2$ factorial design is considered. If the runs in the full factorial design are coded by the elements in the Abelian group $L_1 \times L_2 \times L_3 \times L_4$ with $L_1 = L_2 = \mathbb{Z}/2\mathbb{Z}$ and $L_3 = L_4 = \mathbb{Z}/4\mathbb{Z}$, then it can be shown that no regular $\frac{1}{4}$ fraction of resolution 3 exists. However, a regular $\frac{1}{4}$ fraction of resolution 3 can be constructed using pseudofactors. That is, if the runs are coded by elements in $G = L_1 \times L_2 \times L_2 \times L_4$ with $L_1 = L_2 = \mathbb{Z}/2\mathbb{Z}$ and $L_3 = L_4 = \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$, then a $\frac{1}{4}$ regular fraction $H \subset G$ of resolution 3 corresponds to the annihilator

$$\widehat{G}_H = \{\chi_{(0,0,0,0,0,0)}, \chi_{(1,0,1,0,1,0)}, \chi_{(0,1,0,1,0,1)}, \chi_{(1,1,1,1,1,1)}\}$$

Note that $\text{wt}\,[(1,0,1,0,1,0)] = \text{wt}\,[(0,1,0,1,0,1)] = 3$ and $\text{wt}\,[(1,1,1,1,1,1)] = 4$, which implies that the corresponding coset H has resolution 3. The design is given in Table 3.6 where X_1 and X_2 denote the two-level factors and (X_{31}, X_{32}) and (X_{41}, X_{42}) the four-level factors. Note that the treatments of the regular fraction H form an orthogonal array OA $(16, 4, 2 \times 2 \times 4 \times 4, 2)$ where the four columns correspond to the factors X_1, X_2, X_3 X_4 with $X_1, X_2 : G \to \mathbb{Z}/2\mathbb{Z}$ given by $X_1(g) = g_1$ and $X_2(g) = g_2$. The factors $X_3, X_4 : G \to \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$ are defined by $X_3(g) = g_3$ and $X_4(g) = g_4$. The symbols in the first two columns of the orthogonal array are the elements of $\mathbb{Z}/2\mathbb{Z}$. The symbols in the last two columns are the elements of $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$.

Note that in Example 3.62 the use of pseudofactors (all at two levels) results in a set of characters that are all real-valued. This is another possible advantage

of the use of pseudofactors. We know from the results in Section 3.4.5 that any regular fraction of resolution R is an orthogonal array of strength $R-1$. This result also applies when pseudofactors are used in the design.

3.5 Other designs related to groups

In this section we give an overview of experimental designs that are related to groups. First in Section 3.5.1 we discuss the Latin square designs and their relation with groups and orthogonal arrays. In Section 3.5.2 it is explained how the character theory can be used to assess the efficiency of cyclic designs. An application of the theory of harmonic analysis for the analysis of the data obtained in a microarray experiment is discussed in Section 3.5.3.

3.5.1 Latin squares

Latin squares were first applied as experimental designs in agricultural studies early in the 20th century. The classic example is the use of a Latin square configuration to test a variety of crops. If n varieties of crops are to be tested, then a field is laid out in a $n \times n$ array of plots. The Latin square design guarantees that each crop is planted in one plot in each row or column and is used to offset any possible systematic variation, for example in fertility, moving across or down the field. The definition of a Latin square is as follows.

Definition 3.63 (Latin square) A Latin square of order n ($n \geq 2$) is an $n \times n$ array with entries taken from an alphabet Σ of n symbols, with the property that each symbol occurs exactly once in each row and column.

A simple example of a Latin square is the following.

Example 3.64 Let $\Sigma = \{a, b, c\}$. The array

a	b	c
b	c	a
c	a	b

is a Latin square of order 3.

Latin square designs are directly related to orthogonal arrays. Each Latin square of order n corresponds to an orthogonal array OA $\left(n^2, 3, n, 2\right)$ [4]. The orthogonal array for a Latin square design A is obtained by indexing the rows and columns by elements in Σ. The array that has as its rows $(i, j, a_{i,j})$ with $i, j \in \Sigma$ is an orthogonal array of strength 2. Orthogonal arrays of strength 2 with more than three columns can be constructed using a set of orthogonal Latin squares, where the orthogonality is defined as follows.

[4] In cases in which the orthogonal array is symmetric, that is $n_1 = n_2 = \ldots = n_k = n$ for some $n \geq 2$, an orthogonal array OA $(N, k, n_1 \times n_2 \times \ldots \times n_k, t)$ is usually denoted by OA (N, k, n, t).

Definition 3.65 (Orthogonal Latin squares) Two Latin squares $A = (a_{i,j})$ and $B = (b_{i,j})$ of order n are orthogonal if for all $\ell, m \in \Sigma$ there are unique values for i and j such that $a_{i,j} = \ell$ and $b_{i,j} = m$.

Example 3.66 The Latin square

a	b	c
c	a	b
b	c	a

and the one given in Example 3.64 are orthogonal.

Two orthogonal Latin squares can be used to form an OA $\left(n^2, 4, n, 2\right)$ orthogonal array. This is done by correspondingly labeling the rows and columns of Latin squares A and B by the elements in Σ and constructing the array with rows $(i, j, a_{i,j}, b_{i,j})$ with $i, j \in \Sigma$. In general, an orthogonal array OA $\left(n^2, k, n, 2\right)$ exists if and only if $k - 2$ pairwise orthogonal Latin squares of order n exist. This is Theorem 8.28 in Hedayat et al. (1999).

The Cayley tables of groups give rise to a subclass of Latin squares. The Cayley table is the group-theoretic analogue of the addition and multiplication tables.

Definition 3.67 (Cayley table) A Cayley table A of a group $(G, \cdot)$ is an array with both the rows and columns indexed by the elements G and with the entry $a_{g,h}$ given by $g \cdot h$ for $g, h \in G$.

Typically the first row and column are taken to correspond to the identity element of G which makes that the first row and column act as headers. The Latin square in Example 3.64 is the Cayley table of the additive group $\mathbb{Z}/3\mathbb{Z}$. The Cayley table is symmetric if and only if the group is Abelian. An example of a Cayley table of a non-Abelian group is the following.

Example 3.68 The Cayley table for the symmetric group S_3 is given by

1	(12)	(13)	(23)	(123)	(132)
(12)	1	(123)	(132)	(13)	(23)
(13)	(132)	1	(123)	(23)	(12)
(23)	(123)	(132)	1	(12)	(13)
(123)	(23)	(12)	(13)	(132)	1
(132)	(13)	(23)	(12)	1	(123)

which is a Latin square of order 6.

The Cayley table of a group is always a Latin square. This is stated in the next lemma.

Lemma 3.69 *The Cayley table of any group G is a Latin square.*

Proof It suffices to show that the entries in each row and column of the Cayley table of a group G are distinct. First we show that for all $g \in G$ the entries in the row of the Cayley table that correspond to g are all distinct. This follows from observing that for the entries in the row that corresponds to $g \in G$ we have that $g \cdot h_1 = g \cdot h_2$ for $h_1, h_2 \in G$ implies that $g^{-1} \cdot g \cdot h_1 = g^{-1} \cdot g \cdot h_2$ and, hence, $h_1 = h_2$. Also the entries in the column that corresponds to $h \in G$ are all distinct, because $g_1 \cdot h = g_2 \cdot h$ for $g_1, g_2 \in G$ implies that $g_1 = g_2$. □

Each Latin square is the multiplication table of a quasigroup, which we define now.

Definition 3.70 A quasigroup is a set Σ together with a binary operation $\cdot$ that satisfies

- for all $a, b \in \Sigma$ there is a unique $c \in \Sigma$ such that $a \cdot c = b$;
- for all $a, b \in \Sigma$ there is a unique $c \in \Sigma$ such that $c \cdot a = b$.

From this definition it follows that each group is also a quasigroup (the unique elements c are given by $c = a^{-1} \cdot b$ and $c = b \cdot a^{-1}$, respectively). A quasigroup differs from a group in several ways. Firstly, a quasigroup is not required to have an identity element. Secondly, the binary operation does not have to be associative. A quasigroup that is not a group is given in the next example.

Example 3.71 An example of a quasigroup that is not a group is the set $\Sigma = \{\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5\}$ together with the binary operation $\cdot$ defined by the Cayley table

$\cdot$	σ_1	σ_2	σ_3	σ_4	σ_5
σ_1	σ_1	σ_2	σ_3	σ_4	σ_5
σ_2	σ_3	σ_5	σ_4	σ_2	σ_1
σ_3	σ_2	σ_4	σ_1	σ_5	σ_3
σ_4	σ_4	σ_1	σ_5	σ_3	σ_2
σ_5	σ_5	σ_3	σ_2	σ_1	σ_4

The operation $\cdot$ is not associative. For instance, $(\sigma_2 \cdot \sigma_2) \cdot \sigma_1 = \sigma_5 \cdot \sigma_1 = \sigma_5$ and $\sigma_2 \cdot (\sigma_2 \cdot \sigma_1) = \sigma_2 \cdot \sigma_3 = \sigma_4$. Moreover, there does not exist an element in $e \in \Sigma$ that satisfies $\sigma_j \cdot e = e \cdot \sigma_j = \sigma_j$ for all j.

3.5.2 Cyclic designs

In this section we assume that n different treatments are administered to N experimental units. It is assumed that the experimental units are divided into blocks in such a way that the units within each block are relatively homogeneous. Furthermore, each experimental unit receives exactly one treatment. The designs in this class are called block designs. Block designs in which only a subset of treatments appear in each block are usually referred to by incomplete block design. A special class of incomplete block designs is the class of cyclic designs that we consider in this section. The theory of cyclic designs is directly related

Table 3.7: Concurrence matrix for the cyclic design in Example 3.73.

	1	2	3	4	5	6
1	3	1	1	2	1	1
2	1	3	1	1	2	1
3	1	1	3	1	1	2
4	2	1	1	3	1	1
5	1	2	1	1	3	1
6	1	1	2	1	1	3

to the theory of Abelian groups because in the construction of these designs the treatments are typically labelled by elements of a cyclic group. An overview of the theory is given in John (1987) (see also John and Williams (1995)). Bailey (1990) studies cyclic designs using the character theory of Abelian groups.

In order to give a precise definition of a cyclic design we introduce the notion of a translate. For each subset $H \subset G$ and element $a \in G$ we define the translate aH by $aH = \{ah \mid h \in H\}$. Note that in the special case that H is a subgroup, the distinct translates are the cosets of H in G. A cyclic design is defined as follows.

Definition 3.72 (Cyclic design) A cyclic design is an incomplete block design that consists of blocks that are translates of the same subset H of a cyclic group G containing the treatment labels that has the additional property that all distinct translates of H appear equally often as blocks.

The following example of a cyclic design is taken from Bailey (1990).

Example 3.73 Let the treatments be labeled by the elements of the additive cyclic group $G = \mathbb{Z}/6\mathbb{Z}$ and consider the design that consists of the blocks $\{0,1,3\}$, $\{1,2,4\}$, $\{2,3,5\}$, $\{3,4,0\}$, $\{4,5,1\}$, $\{5,0,2\}$. This design is a cyclic design because the blocks are the distinct translates of the subset $H = \{0,1,3\}$ of G. The concurrence matrix for this design is given in Table 3.7

Since blocks are chosen in such a way that the experimental units within blocks are relatively homogeneous, comparisons within blocks are usually more accurate than comparisons between blocks. The cyclic design in the Example 3.73 has the nice property that each pair of treatments appears together in at least one block which makes that all pairs of treatments can be compared within blocks. The next example illustrates that not all cyclic designs have this property.

Example 3.74 Let the treatments be labeled by the elements of the additive cyclic group $G = \mathbb{Z}/6\mathbb{Z}$ and consider the design that consists of the blocks $\{0,2,4\}$, $\{1,3,5\}$, $\{2,4,0\}$, $\{3,5,1\}$, $\{4,0,2\}$, $\{5,1,3\}$. This design is a cyclic design because each of the two distinct translate of the subset $H = \{0,2,4\}$ of G appears three times as a block. The concurrence matrix for this design is given in Table 3.8

Table 3.8: Concurrence matrix for the cyclic design in Example 3.74.

	1	2	3	4	5	6
1	3	0	3	0	3	0
2	0	3	0	3	0	3
3	3	0	3	0	3	0
4	0	3	0	3	0	3
5	3	0	3	0	3	0
6	0	3	0	3	0	3

The cyclic design in Example 3.74 is an example of disconnected block design. A block design is called disconnected if its concurrence graph is disconnected. The reader is referred to Section 1.6 of John (1987) for the details on connectedness of block designs.

A model that takes into account the between blocks variability is given in matrix notation by

$$y = \tau_0 + Z_t\tau_t + Z_b\tau_b + \varepsilon,$$

where the matrices Z_t and Z_b are of size $N \times n$ and $N \times b$, respectively. The rows of these matrices are indexed by the experimental units and their columns are indexed by the treatment labels and block labels, respectively. The entry $(Z_t)_{r,c}$ equals 1 if experimental unit r is assigned to treatment c and 0 otherwise. Moreover, $(Z_b)_{r,c} = 1$ if experimental unit r is in block c and $(Z_t)_{r,c} = 0$ otherwise. The vectors τ_t and τ_b are unknown vectors containing the treatment and block effects, respectively. In John (1987) it is shown that the least squares estimator $\widehat{\tau}_t$ for the vector τ_t of treatments effects can be found by solving the system of reduced normal equations given by

$$A\,\widehat{\tau}_t = q.$$

where the column vector q contains the n treatment totals. For a cyclic design the $n \times n$ matrix A is given by

$$A = rI_n - \frac{1}{b}M, \tag{3.26}$$

where M denotes the concurrence matrix of the design, r is the number of times that each treatment is replicated and b denotes the number of treatments per block. The eigenvectors and eigenvalues of the information matrix A are important for the study of the efficiency and optimality of the cyclic design. The non-zero eigenvalues of the matrix $\frac{1}{r}A$ are called the *canonical efficiency factors*. The reader is referred to Section 2.3 of John (1987) for a more detailed discussion of the properties of these efficiency factors. Bailey (1990) shows how the canonical efficiency factors can be directly obtained from the characters of the cyclic group G. A main theorem in Bailey (1990) states that the characters of G (viewed as vectors with coordinates indexed by the elements of G) form an

Table 3.9: Calculation of the canonical efficiency factors in Example 3.73.

j	Eigenvalue λ_j			Canonical efficiency factor λ'_j
1	$3+1+1+2+1+1$	$=$	9	0
2	$3+\omega_6+\omega_6^2+2\omega_6^3+\omega_6^4+\omega_6^5$	$=$	1	8/9
3	$3+\omega_6^2+\omega_6^4+2+\omega_6^2+\omega_6^4$	$=$	3	2/3
4	$3+\omega_6^3+1+2\omega_6^3+1+\omega_6^3$	$=$	1	8/9
5	$3+\omega_6^4+\omega_6^2+2+\omega_6^4+\omega_6^2$	$=$	3	2/3
6	$3+\omega_6^5+\omega_6^4+2\omega_6^3+\omega_6^2+\omega_6^1$	$=$	1	8/9

eigenvector basis for the concurrence matrix M of any cyclic design. From 3.26 it can be directly seen that the matrix $\frac{1}{r}A$ and the concurrence matrix M have the same eigenvectors. If the eigenvectors of M are denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, then the eigenvectors $\lambda'_1, \lambda'_2, \ldots, \lambda'_n$ of the matrix $\frac{1}{r}A$ are given by

$$\lambda'_j = 1 - \frac{\lambda_j}{rb}.$$

Knowledge of the eigenvectors of M makes it easy to calculate the eigenvalues λ_j and, hence, the canonical efficiency factors λ'_j. If we denote by $\chi_1, \chi_2, \ldots, \chi_n$ the characters of G and index the rows and columns of the concurrence matrix M by the elements of G, then the eigenvalues of M are given by

$$\lambda_j = \sum_{g \in G} M_{g,1}\, \chi_j(g), \quad j = 1, 2, \ldots, n.$$

In the next example we illustrate the computation of the canonical efficiency factors for the cyclic design in Example 3.73.

Example 3.75 Consider the cyclic design given in Example 3.73 with the treatments labeled by the elements of $G = \mathbb{Z}/6\mathbb{Z}$ and the concurrence matrix in Table 3.7. The characters $\chi_1, \chi_2, \ldots, \chi_6 : G \to \mathbb{C}$ of G are given by

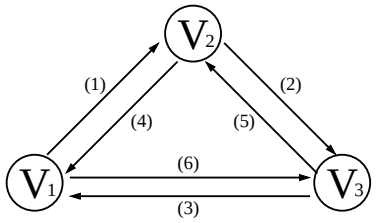
$$\chi_j(g) = \omega_6^{(j-1)g}$$

where $\omega_6 = \exp \frac{2\pi i}{6}$. The calculation of the canonical efficiency factors is given in Table 3.9.

3.5.3 Microarray experiments

cDNA microarray experiments are extensively used to study relative expression levels of genes across biological samples. Typically, cDNA microarrays consist of thousands of individual DNA sequences printed in a high-density array. The cDNA microarray experiments involve mixing two mRNA samples, each of which have been converted into cDNA and then labeled with its own fluorophore. Typically, a green Cyanine 3 (Cy3) dye is used for one sample and a

Figure 3.2: A loop design with dye swap for comparing three varieties.



red Cyanine 5 (Cy5) dye for the other. The mixture is then hybridized with the arrayed DNA probes. After the hybridization fluorescence measures are made separately for each dye at each spot on the microarray. The red and green fluorescence intensities at each spot are indicative of the relative abundance of the corresponding DNA probe in the two mRNA samples. It is important to note that the amount of a certain DNA probe in an mRNA sample can only be determined relative to the amount of this probe in a second mRNA sample. In other words we are dealing with paired comparisons. For this reason the standard ANOVA approach can not be applied directly. Yang and Speed (2002) and Churchill (2002) give reviews of the design issues for cDNA microarray experiments. In this section we one of the designs that is proposed in these review papers within the framework of harmonic analysis.

All cDNA microarray experiments can be represented as directed graphs. The nodes correspond to the different mRNA samples that are under study. The arrows connect the pairs of samples that are compared on a single microarray. By convention, the sample at the tail is labelled with the green Cy3 dye and the sample at the head with the red Cy5 dye. The design that we consider as an example is given in Figure 3.2. This design is used for comparing three different mRNA samples labelled V_1, V_2 and V_3 (because the term "variety" is commonly used for the samples under investigation).

The data analysis for a microarray experiment is usually done by comparing the observations made for the same gene on different slides. The observations for a single gene can be indexed by the elements in the set $L_A = \{1, 2, \ldots, 6\}$. We define two commuting actions that can be performed on the set L_A of labels. The first action is that of cyclically relabeling the samples under study. The corresponding group of actions is $G_V = \{1, (123)(456), (132)(465)\} \cong C_3$ which acts on L_A by $\psi_V : a \to \psi_V a$ for all $a \in L_A$ and $\psi_V \in G_V$. The second action that we define is that of a dye-swap. The group of actions is given by $G_D = \{1, (14)(25)(36)\} \cong C_2$. We let the group G_D act on the set L_A in the same way as G_V does. We let the group $G = G_V \times G_D$ act on the set L_A by $(\psi_V, \psi_D) : a \to \psi_V \psi_D a$. Note that each label in L_A can be obtained by letting a unique element in G act on $1 \in L_A$. We use this property to identify the labels with the elements of the group. By $\varphi : G \to L_A$ we denote the function that

Table 3.10: Character table for the group $C_3 \times C_2$ ($\omega_3 = \exp\left(\frac{2\pi i}{3}\right)$).

g	$\varphi(g)$	$\chi_{(0,0)}(g)$	$\chi_{(1,0)}(g)$	$\chi_{(2,0)}(g)$	$\chi_{(0,1)}(g)$	$\chi_{(1,1)}(g)$	$\chi_{(2,1)}(g)$
1	1	1	1	1	1	1	1
γ	2	1	ω_3	ω_3^2	1	ω_3	ω_3^2
γ^2	3	1	ω_3^2	ω_3	1	ω_3^2	ω_3
ψ	4	1	1	1	-1	-1	-1
$\psi\gamma$	5	1	ω_3	ω_3^2	-1	$-\omega_3$	$-\omega_3^2$
$\psi\gamma^2$	6	1	ω_3^2	ω_3	-1	$-\omega_3^2$	$-\omega_3$

Table 3.11: Orthogonal contrasts for the loop design in Figure 3.2.

Character	Effect/Contrast
$\chi_{(0,0)}$	$\mu_1 + \mu_2 + \mu_3 + \mu_4 + \mu_5 + \mu_6$
$\chi_{(1,0)}$	$(\mu_1 + \mu_4) + \omega_3(\mu_2 + \mu_5) + \omega_3^2(\mu_3 + \mu_6)$
$\chi_{(2,0)}$	$(\mu_1 + \mu_4) + \omega_3^2(\mu_2 + \mu_5) + \omega_3(\mu_3 + \mu_6)$
$\chi_{(0,1)}$	$(\mu_1 + \mu_2 + \mu_3) - (\mu_4 + \mu_5 + \mu_6)$
$\chi_{(1,1)}$	$(\mu_1 - \mu_4) + \omega_3(\mu_2 - \mu_5) + \omega_3^2(\mu_3 - \mu_6)$
$\chi_{(1,2)}$	$(\mu_1 - \mu_4) + \omega_3^2(\mu_2 - \mu_5) + \omega_3(\mu_3 - \mu_6)$

maps each element (ψ_V, ψ_D) of G to $\psi_V\psi_D 1$. The mapping φ and the irreducible characters of the group G are given in Table 3.10. The contrasts and effects that are obtained using harmonic analysis are given in Table 3.11. The contrasts that correspond to the characters $\chi_{(1,0)}$ and $\chi_{(2,0)}$ compare the relative expression for the different pairs averaged over the different ways of assigning the dyes to the samples. The character $\chi_{(0,1)}$ compares the average relative expression for the different loops (clockwise and anti-clockwise), that is, it measures the effect of a dye-swap. The characters $\chi_{(1,1)}$ and $\chi_{(2,1)}$ compare the effect of a dye-swap for the different sample pairs and measure the dye-sample pair interaction.

We like to conclude this section by stressing that the set of orthogonal contrasts that was obtained in the example is solely based on the symmetry of the design and that no specific model for the data was assumed.

3.6 Statistical inference

In this section we assume that the observations that are made on the finite group are independently distributed normal variables. In Section 3.6.1 a general finite group is considered. The general procedure in the case of independent random variables with equal variance is to decompose the total sums of squares using

the decomposition of the identity matrix given in Theorem 3.12 for the regular representation. We show that if some of the characters are not real-valued then the sums of squares that appear in the decomposition are not independent. A new decomposition that is based on the decomposition in Theorem 3.12 is proposed. The parts of this new decomposition are shown to be independent. In Section 3.6.2 we illustrate the analysis of statistical data structured on a coset of a finite Abelian group or, equivalently, data obtained in a regular fractional factorial design.

3.6.1 Statistical inference for normal data on finite groups

In this section we consider the set of observations made on a finite group G as a vector in $\mathbb{R}^{|G|}$. To this end we let $\{e_g \mid g \in G\}$ denote the standard basis for $\mathcal{V} = \mathbb{R}^{|G|}$ indexed by the elements in G. The vector of observations with respect to this basis is given by $y = \sum_{g \in G} y(g)\, e_g$. We assume that this vector has a multivariate normal distribution, more precisely $y \sim \mathcal{N}_N\left(\mu, \sigma^2 I_N\right)$, where $N = |G|$ and $\mu = \sum_{g \in G} \mu(g)\, e_g$. No assumptions are made on the expectation function $\mu \in \mathbb{R}^G$. The decomposition of $y^T y = \sum_{g \in G} (y(g))^2$ based on the canonical decomposition of the identity matrix I_N is given in Theorem 3.12 is

$$y^T y = \sum_{j=1}^{w} SS_j \text{ where } SS_j = y^T P_j y. \tag{3.27}$$

Let $\widetilde{y}$ denote the vector of length $|G|$ with each of its elements equal to the average of all observations made on G. The total sum of squares that is usually considered in analysis of variance is given by

$$SS_T = (y - \widetilde{y})^T (y - \widetilde{y}) = y^T y - |G|\, \widetilde{y}^T \widetilde{y}.$$

The decomposition (3.27) also gives us a decomposition for SS_T. To see this, assume without loss of generality that the irreducible representation ρ_1 in Theorem 3.12 is the trivial representation, that is, ρ_1 is the one-dimensional representation given by $\rho_1(g) = 1$ for all $g \in G$. The corresponding projection matrix is $P_1 = \frac{1}{|G|} \sum_{j=1}^{w} \rho(g)$. The matrices $\rho(g)$ for ρ the regular representation are permutation matrices with $\rho(g)_{hj} = 1$ if and only if $h = gj$. Since for each pair $h, j \in G$ there is a unique g for which $h = gj$ we find that P_1 is the all-one matrix. This implies that $y^T P_1 y = |G|\, \widetilde{y}^T \widetilde{y}$ and, hence, a decomposition of SS_T is simply $\sum_{j=2}^{w} SS_j$ with SS_j defined as in (3.27). For the purpose of statistical inference we are interested in the distribution of the sums of squares SS_j that appear in this decomposition for SS_T. The distribution of quadratic forms in normal random variables has been widely studied. Let A be a real symmetric matrix and assume that $y \sim \mathcal{N}_N(\mu, V)$ with V nonsingular. A theorem by Driscoll (1999) states that the quadratic form $y^T A y$ has a chi-square distribution if and only if AV is idempotent. The chi-square distribution has rank (A) degrees of freedom and non-centrality parameter $\mu^T A \mu$. This is an extension of an earlier result by Pearson. Another important theorem that is known as

Craig's theorem states a necessary and sufficient condition for the independence of two quadratic forms. If $y \sim \mathcal{N}_N(\mu, V)$ with V nonsingular and A_1 and A_2 are real symmetric matrices then the condition that is necessary and sufficient for $y^T A_1 y$ and $y^T A_2 y$ to be statistically independent is $A_1 V A_2 = 0$. A detailed proof can be found in Driscoll and Krasnicka (1995). However, because of the property $\sum_{j=1}^{w} P_j = I_N$ the most direct way to find the distribution of the SS_j is to use the Fisher-Cochran theorem.

Theorem 3.76 (Fisher-Cochran theorem) *Let $y \sim \mathcal{N}_N(\mu, I_N)$ and denote by $P_1, P_2, \ldots, P_w$ a set of w real symmetric $N \times N$ matrices, such that*

$$I_N = \sum_{j=1}^{w} P_j.$$

Then a necessary and sufficient condition for $y^T P_j y \sim \chi^2(\nu_j, \lambda_j)$ with $y^T P_j y$ and $y^T P_i y$ independent for $i \neq j$ is

$$N = \sum_{j=1}^{w} rank\,(P_j),$$

in which case $\nu_j = rank\,(P_j)$ and $\lambda_j = \mu P_j \mu$.

Proof See Rao (1973), p. 185. □

The condition that all matrices $P_1, P_2, \ldots, P_w$ are idempotent is sufficient for the requirement $N = \sum_{j=1}^{w} \text{rank}\,(P_j)$ to be satisfied. This follows easily using the next lemma.

Lemma 3.77 *The rank of an idempotent matrix is equal to its trace.*

Proof See Rao (1973), p. 28. □

Using Lemma 3.77 we find that if all matrices $P_1, P_2, \ldots, P_w$ in the decomposition $I_N = \sum_{j=1}^{w} P_j$ are idempotent we have that

$$N = \text{tr}\,(I_N) = \text{tr}\left(\sum_{j=1}^{w} P_j\right) = \sum_{j=1}^{w} \text{tr}\,(P_j) = \sum_{j=1}^{w} \text{rank}\,(P_j).$$

If the projection matrices P_j are complex, then Theorem 3.76 cannot be applied directly. Recall that in the example of the 3^3 factorial design that we discussed in Section 3.2.2 we encountered projection matrices with complex entries. In that example we found that the sum of squares associated with an irreducible representation ρ_z was equal to that associated with its complex-conjugate $\overline{\rho_z}$. This equality of sum of squares can be shown to occur for all possible realizations of the random vector y and, hence, the sums of squares appearing in the decomposition given in (3.27) cannot all be pairwise independent. We propose

a method for statistical inference where equal sums of squares are combined. The resulting decomposition consists of mutually independent sum of squares. Before we present these results we first need some lemmas that state some properties of the matrices P_j that appear in the canonical decomposition that were not mentioned in Theorem 3.12.

Lemma 3.78 *Each matrix P_j that appears in the canonical decomposition for the regular representation is Hermitian.*

Proof Using Lemma 3.5 we find that $\chi_j(g) = \overline{\chi_j}\left(g^{-1}\right)$ for all irreducible characters χ_j and elements $g \in G$. The matrices $\rho(g), g \in G$, are permutation matrices and satisfy $\rho\left(g^{-1}\right) = (\rho(g))^T$. Hence, we have

$$\begin{aligned} P_j^T &= \tfrac{d_j}{|G|}\sum_{g\in G}\overline{\chi_j}(g)\,\rho(g)^T = \tfrac{d_j}{|G|}\sum_{g\in G}\chi_j\left(g^{-1}\right)\left(\rho\left(g^{-1}\right)\right) \\ &= \tfrac{d_j}{|G|}\sum_{g\in G}\chi_j(g)\,(\rho(g)) = \overline{P_j}, \end{aligned}$$

which completes the proof. □

The next lemma guarantees that the decomposition of the total sum of squares given in (3.27) when applied to the regular representation is a decomposition into real parts that are all non-negative.

Lemma 3.79 *Each matrix P_j that appears in the canonical decomposition for the regular representation is positive semidefinite.*

Proof Using that P_j is idempotent and Hermitian we find that

$$y^T P_j y = y^T P_j^2 y = y^T \overline{P_j}^T P_j y = (P_j y, P_j y),$$

where $(P_j y, P_j y)$ denotes the standard inner product on $\mathbb{C}^N$. Note that we have that $(P_j y, P_j y) \geq 0$ and that $(P_j y, P_j y) = 0$ only if $P_j y = 0$. We find that P_j is positive semidefinite by observing that this implies that $y^T P_j y \in \mathbb{R}$ and $y^T P_j y \geq 0$ for all $y \in \mathbb{R}^N$. The matrix P_j is not positive definite because it need not be full rank and, hence, $P_j y = 0$ does not imply $y = 0$. □

We propose a decomposition of the $N \times N$ identity matrix into real symmetric matrices that is based on the canonical decomposition for the regular representation. To this end we use that for every complex matrix that appears in the canonical decomposition also its complex conjugate appears in the decomposition.

Lemma 3.80 *If P is a regular canonical projection, then so is $\overline{P}$.*

Proof If a character $\chi_j = \operatorname{tr}\rho_j$ is real-valued on G, then because all $\rho(g)$ of the regular representation are permutation matrices we have that all entries in P_j are real-valued. Hence, without loss of generality we assume that χ_j is not real-valued on G. We now show that if ρ_j is an irreducible representation of G then also $\rho_i = \overline{\rho_j}$ is an irreducible representation of G. Clearly $\rho_j(gh) =$

$\rho_j(g)\,\rho_j(h)$ for all $g,h \in G$ implies $\overline{\rho_j}(gh) = \overline{\rho_j}(g)\,\overline{\rho_j}(h)$ for all $g,h \in G$ from which we find that ρ_i is a representation of G. Let χ_j denote the character of ρ_j and χ_i the character of ρ_i. Because ρ_j is irreducible we have by Lemma 3.9 that $\langle \chi_j, \chi_j \rangle = 1$. The character χ_i satisfies $\chi_i = \overline{\chi_j}$ which implies that $\langle \chi_i, \chi_i \rangle = \langle \overline{\chi_j}, \overline{\chi_j} \rangle = \langle \chi_j, \chi_j \rangle = 1$. Using Lemma 3.9 we find that also ρ_i is irreducible. From the assumption that χ_j is not real-valued on G we have that $\chi_j(g) \neq \overline{\chi_j}(g) = \chi_i(g)$ for some $g \in G$. Lemma 3.7 now implies that the representations ρ_j and ρ_i are non-equivalent. From $\rho_i = \overline{\rho_j}$ it follows that the dimensions d_j and d_i are equal. The projection matrix P_i for the irreducible representation ρ_i in the canonical decomposition is

$$P_i = \frac{d_i}{|G|} \sum_{g \in G} \overline{\chi_i}(g)\,\rho(g) = \frac{d_j}{|G|} \sum_{g \in G} \chi_j(g)\,\rho(g) = \overline{P_j},$$

which concludes the proof. □

The last lemma tells us that if a matrix P_j in the canonical decomposition is complex, then its complex conjugate $\overline{P_j} = P_i$ is also in the decomposition. The corresponding sums of squares SS_j and SS_i are equal. This follows from

$$SS_j = y^T P_j y = \left(y^T P_j y\right)^T = y^T P_j^T y = y^T \overline{P_j} y = y^T P_i y = SS_i,$$

where we have used that P_j is Hermitian. Our strategy now is to replace each complex conjugate pair of matrices P_j and P_i in the decomposition by their sum $P_j + P_i$. This way we find a new decomposition $I_N = Q_1 + Q_2 + \ldots + Q_m$. The corresponding decomposition of $y^T y$ is

$$y^T y = \sum_{j=1}^{m} SS_j^\star \text{ where } SS_j^\star = y^T Q_j y. \tag{3.28}$$

Lemma 3.81 *The matrices Q_j in the decomposition given in (3.28) are real, symmetric and idempotent.*

Proof It is trivial to see that all entries in the matrix $Q_j = P_j + \overline{P_j}$ are real. The symmetry of the matrix $Q_j = P_j + \overline{P_j}$ is obtained from the fact that P_j is Hermitian in the following way

$$Q_j^T = \left(P_j + \overline{P_j}\right)^T = P_j^T + \overline{P_j}^T = \overline{P_j} + P_j = Q_j.$$

From Lemma 3.80 we have that $\overline{P_j} = P_i$ for some $i \neq j$. In addition, from Theorem 3.12 we know that $P_j^2 = P_j$, $P_i^2 = P_i$, $P_j P_i = 0$ and $P_i P_j = 0$. From these two results we find that

$$Q_j^2 = \left(P_j + \overline{P_j}\right)^2 = (P_j + P_i)^2 = P_j^2 + P_j P_i + P_i P_j + P_i^2 = P_j + P_i = P_j + \overline{P_j} = Q_j.$$

Hence, the matrices Q_j are real, symmetric and idempotent. □

Since all Q_j in decomposition (3.28) are idempotent we find using Lemma 3.77 that

$$N = \mathrm{tr}\,(I_N) = \mathrm{tr}\left(\sum_{j=1}^{m} Q_j\right) = \sum_{j=1}^{m} \mathrm{tr}\,(Q_j) = \sum_{j=1}^{m} \mathrm{rank}\,(Q_j)\,. \tag{3.29}$$

This result is used in the proof of the next theorem.

Theorem 3.82 *If $y \sim \mathcal{N}_N\left(\mu, \sigma^2 I_N\right)$ then we have that the random variables*

$$\frac{SS_j^\star}{\sigma^2} = \frac{y^T Q_j y}{\sigma^2}, \quad j = 1, 2, \ldots, m,$$

in (3.28) are independently distributed according to a $\chi^2\left(\nu_j^\star, \lambda_j^\star\right)$ distribution with $\nu_j^\star = \mathrm{rank}\,(Q_j)$ and $\lambda_j^\star = \mu^T Q_j \mu$.

Proof Define the random vector $x = \frac{y}{\sigma}$ and note that $x \sim \mathcal{N}_N\left(\frac{\mu}{\sigma}, I_N\right)$. Because the matrices $Q_1, Q_2, \ldots, Q_m$ are real and symmetric and satisfy $I_N = \sum_{j=1}^m Q_j$ and $N = \sum_{j=1}^m \mathrm{rank}\,(Q_j)$ we can apply Theorem 3.76 (the Fisher-Cochran theorem) and find that the random variables

$$x^T Q_j x = \frac{SS_j^\star}{\sigma^2}, \quad j = 1, 2, \ldots, m,$$

are independently distributed according to a $\chi^2\left(\nu_j^\star, \lambda_j^\star\right)$ distribution with $\nu_j^\star = \mathrm{rank}\,(Q_j)$ and $\lambda_j^\star = \frac{\mu^T Q_j \mu}{\sigma^2}$. □

If for some of the non-centrality parameters we can assume that $\lambda_k^\star = 0$ then the usual F-test can be applied to test the hypothesis $\lambda_j^\star = 0$ against $\lambda_j^\star \neq 0$ for all j of interest. The following lemma and corollary illustrate that if the representation ρ_j is one-dimensional with character χ_j then an equivalent hypothesis can be stated in terms of the Fourier coefficients $\widehat{\mu}\,(\chi_j)$ and $\widehat{\mu}\,(\overline{\chi_j})$.

Lemma 3.83 *Let the function $y \in \mathbb{C}^G$ be represented as a vector by $y = \sum_{g\in G} y\,(g)\,e_g$. If ρ is taken to be the regular representation, then for all one-dimensional irreducible representations ρ_j and the matrices P_j defined in Theorem 3.12 we have that*

$$y^T P_j y = d_j\,|G|\,\widehat{y}\,(\chi_j)\,\widehat{y}\,(\overline{\chi_j})\,.$$

Proof The product $\widehat{y}\,(\chi_j)\,\widehat{y}\,(\overline{\chi_j})$ can be expressed as

$$\begin{aligned}
\widehat{y}\,(\chi_j)\,\widehat{y}\,(\overline{\chi_j}) &= \tfrac{1}{|G|^2}\textstyle\sum_{g\in G}\sum_{h\in G}\overline{\chi_j}\,(g)\,y\,(g)\,\chi_j\,(h)\,y\,(h)\\
&= \tfrac{1}{|G|^2}\textstyle\sum_{g\in G}\sum_{h\in G}\overline{\chi_j}\,(g)\,y\,(g)\,\overline{\chi_j}\left(h^{-1}\right)y\,(h)\\
&= \tfrac{1}{|G|^2}\textstyle\sum_{g\in G}\sum_{h\in G}\overline{\chi_j}\left(gh^{-1}\right)y\,(g)\,y\,(h)\\
&= \tfrac{1}{|G|^2}\textstyle\sum_{g^\star\in G}\sum_{h\in G}\overline{\chi_j}\,(g^\star)\,y\,(g^\star h)\,y\,(h)\\
&= \tfrac{1}{|G|^2}\textstyle\sum_{g^\star\in G}\overline{\chi_j}\,(g^\star)\sum_{h\in G}y\,(g^\star h)\,y\,(h)
\end{aligned}$$

The matrix $\rho(g)$ satisfies $\rho(g)\, e_h = e_{gh}$ for all $h \in G$. With respect to the basis $\{e_g \mid g \in G\}$ the matrix $\rho(g^\star)$ has entries $(\rho(g^\star))_{rh} = 1$ if $g^\star h = r$ and $(\rho(g^\star))_{rh} = 0$ if $g^\star h \neq r$. This implies that

$$\begin{aligned} d_j\, |G|\, \widehat{y}(\chi_j)\, \widehat{y}(\overline{\chi_j}) &= \tfrac{d_j}{|G|} \textstyle\sum_{g^\star \in G} \overline{\chi_j}(g^\star)\, y^T \rho(g^\star)\, y \\ &= y^T \left(\tfrac{d_j}{|G|} \textstyle\sum_{g^\star \in G} \overline{\chi_j}(g^\star)\, \rho(g^\star) \right) y \\ &= y^T P_j y, \end{aligned}$$

which completes the proof. □

The next corollary follows directly from Theorem 3.82 using the previous lemma.

Corollary 3.84 *Let the function $\mu \in \mathbb{R}^G$ be represented as a vector by $\mu = \sum_{g \in G} \mu(g)\, e_g$. If ρ_j is a one-dimensional irreducible representation of G, then the non-centrality parameter of the distribution of the quadratic form $SS_j^\star = y^T Q_j y$ is*

$$\lambda_j^\star = \mu^T Q_j \mu = 2\, \frac{d_j\, |G|}{\sigma^2} \widehat{\mu}(\chi_j)\, \widehat{\mu}(\overline{\chi_j}).$$

Note that we have that $\lambda_j^\star = 0$ if and only if $\widehat{\mu}(\chi_j) = 0$ (which is equivalent to $\widehat{\mu}(\overline{\chi_j}) = 0$). Hence, testing the hypothesis $\lambda_j^\star = 0$ against $\lambda_j^\star \neq 0$ is equivalent to simultaneously testing whether $\widehat{\mu}(\chi_j) = 0$ and $\widehat{\mu}(\overline{\chi_j}) = 0$ against the alternative hypothesis that at least one of these Fourier coefficients is not equal to 0. If the alternative hypothesis is true then both Fourier coefficients are not equal to 0 because $\widehat{\mu}(\overline{\chi_j}) = \overline{\widehat{\mu}(\chi_j)}$.

In the special case where the finite group G on which the data is structured is Abelian, all irreducible representations are one-dimensional. In that case each hypothesis of the form $\lambda_j^\star = 0$ against $\lambda_j^\star \neq 0$ has an equivalent hypothesis in terms of the Fourier coefficient $\widehat{\mu}(\overline{\chi_j})$ if χ_j is real-valued or the Fourier coefficients $\widehat{\mu}(\chi_j)$ and $\widehat{\mu}(\overline{\chi_j})$ if χ_j is not real-valued.

Example 3.85 We continue the example of the simplified seat-belt experiment in Section 3.2.2. The statistical analysis is presented in Table 3.12. The sum of squares for complex conjugate pairs of irreducible representations are added to form a single sum of squares of two degrees of freedom. The results are similar to those obtained by Wu and Hamada (2000). Only the F-values corresponding to the orthogonal complements X_1, X_3, X_1X_2, X_1X_3 and $X_1X_2X_3$ are significant at a .05 significance level. The significance of the F-value for the test regarding the orthogonal complement X_1 implies that the hypothesis $\widehat{\mu}\left(\chi_{(1,0,0,0)}\right) = \widehat{\mu}\left(\chi_{(2,0,0,0)}\right) = 0$ is rejected in favor of the alternative hypothesis that both $\widehat{\mu}\left(\chi_{(1,0,0,0)}\right)$ and $\widehat{\mu}\left(\chi_{(2,0,0,0)}\right)$ are different from 0. Since the F-value corresponding to the orthogonal component X_2 is not significant, the hypothesis $\widehat{\mu}\left(\chi_{(0,1,0,0)}\right) = \widehat{\mu}\left(\chi_{(0,2,0,0)}\right) = 0$ is accepted.

Table 3.12: ANOVA Table for the Seat-Belt Experiment.

Orthogonal component	Degrees of freedom	Combined Sum of Squares	Mean Square	F	p-value
X_1	2	3.46217×10^7	1.73109×10^7	85.58	0.000
X_2	2	938539	469270	2.32	0.108
X_3	2	9.54948×10^6	4.77474×10^6	23.61	0.000
X_1X_2	2	2.72745×10^6	1.36373×10^6	6.74	0.002
$X_1X_2^2$	2	570795	285397	1.41	0.253
X_1X_3	2	2.98559×10^6	1.4928×10^6	7.38	0.001
$X_1X_3^2$	2	886587	443294	2.19	0.122
X_2X_3	2	427214	213607	1.06	0.355
$X_2X_3^2$	2	21134	10567	0.05	0.949
$X_1X_2X_3$	2	4.49293×10^6	2.24646×10^6	11.11	0.000
$X_1X_2X_3^2$	2	263016	131508	0.65	0.526
$X_1X_2^2X_3$	2	205537	102768	0.51	0.605
$X_1X_2^2X_3^2$	2	245439	122720	0.61	0.549
residual	54	1.09226×10^7	202270		
total	80	6.88581×10^7			

3.6.2 Statistical inference for normal data on a coset of a finite Abelian group

The data obtained on a regular fraction can be viewed as data structured on a coset of a finite Abelian group. We consider the statistical analysis of such data. Let H be a subgroup of the finite Abelian group G and a an element of G. We assume that the data is obtained on the coset aH in G and let N denote the number of elements of the coset. In order to find a decomposition of the total sum of squares we need a decomposition of the $N \times N$ identity matrix.

First we consider the case where the statistical data is obtained on the principal fraction H of the full factorial design G. In that case we can directly view the data as being structured on the group H and use the theory presented in Section 3.6.1 to analyze the data. By $\mu_{|H} \in \mathbb{R}^H$ we denote the function $\mu \in \mathbb{R}^G$ restricted to H. The theory in Section 3.6.1 gives us a method for testing the hypothesis $\widehat{\mu_{|H}}(\alpha) = \widehat{\mu_{|H}}(\overline{\alpha}) = 0$ (where $\alpha \in \widehat{H}$) against the alternative hypothesis that both of these Fourier coefficients are not equal to 0. The exact relationship between the Fourier coefficients $\widehat{\mu_{|H}} : \widehat{H} \to \mathbb{C}$ and $\widehat{\mu} : \widehat{G} \to \mathbb{C}$ is found using the Poisson summation formula. From Lemma 3.45 we know that all irreducible characters of H can be viewed as an irreducible character of G that is restricted to H. If $\alpha \in \widehat{G}$, then the Fourier coefficients $\widehat{\mu_{|H}}\left(\alpha_{|H}\right)$ and

$\widehat{\mu}(\chi)$, $\chi \in \alpha\widehat{G}_H$, are related according to

$$\widehat{\mu_{|H}}\left(\alpha_{|H}\right) = \frac{1}{|H|}\sum_{h\in H}\mu_{|H}(h)\,\overline{\alpha_{|H}}(h) = \frac{1}{|H|}\sum_{h\in H}\mu(h)\,\overline{\alpha}(h) = \sum_{\chi\in\alpha\widehat{G}_H}\widehat{\mu}(\chi),$$

where the last equality is obtained using (3.7) with $a = 1$. Hence, when we are testing the hypothesis $\widehat{\mu_{|H}}\left(\alpha_{|H}\right) = \widehat{\mu_{|H}}\left(\overline{\alpha_{|H}}\right) = 0$ against the alternative hypothesis that at least one of these Fourier coefficients is different from 0 we are in fact testing the hypothesis

$$\begin{gathered}\textstyle\sum_{\chi\in\alpha\widehat{G}_H}\widehat{\mu}(\chi) = \sum_{\chi\in\overline{\alpha}\widehat{G}_H}\widehat{\mu}(\overline{\chi}) = 0\\ \text{against}\\ \textstyle\sum_{\chi\in\alpha\widehat{G}_H}\widehat{\mu}(\chi) \neq 0 \text{ and } \sum_{\chi\in\overline{\alpha}\widehat{G}_H}\widehat{\mu}(\chi) \neq 0.\end{gathered} \tag{3.30}$$

All hypotheses that can be tested within the framework of harmonic analysis are of the form given in (3.30). If interest is in testing whether $\widehat{\mu}(\alpha) = 0$ for some specific $\alpha \in \widehat{G}$, then it must be reasonable to assume that $\widehat{\mu}(\chi) = 0$ for all $\chi \in \alpha\widehat{G}_H \setminus \alpha$.

When the fractional design on which the data is obtained is not a principal fraction, an additional step is needed. Assume that the statistical data is obtained on the coset aH of G. We denote by $y : G \to \mathbb{R}$ the response function. We only observe the values of this function for $g \in aH$. The expectation function is given by $\mu : G \to \mathbb{R}$ and is defined by $\mu(g) = E[y(g)]$ for all $g \in G$. We define the functions $y_a : G \to \mathbb{R}$ and $\mu_a : G \to \mathbb{R}$ by $y_a(g) = y(ag)$ and $\mu_a(g) = \mu(ag)$, respectively. These functions satisfy $y_a(h) = y(ah)$ and $\mu_a(h) = \mu(ah)$ for all $h \in H$. The observed data in $\{y_a(h) \mid h \in H\}$ is now structured on the group H and we can apply the theory from Section 3.6.1 using the function $y_{a|H} : H \to \mathbb{R}$ as the function that gives the observed values. The Fourier coefficients of the function $\mu_{a|H}$ can be expressed as

$$\begin{aligned}\widehat{\mu_{a|H}}\left(\alpha_{|H}\right) &= \tfrac{1}{H}\textstyle\sum_{h\in H}\overline{\alpha_{|H}}(h)\,\mu_{a|H}(h) = \tfrac{1}{H}\sum_{h\in H}\overline{\alpha}(h)\,\mu_a(h)\\ &= \tfrac{1}{H}\textstyle\sum_{h\in H}\overline{\alpha}(h)\,\mu(ah) = \tfrac{\alpha(a)}{H}\sum_{h\in H}\overline{\alpha}(ah)\,\mu(ah)\\ &= \alpha(a)\textstyle\sum_{\chi\in\alpha\widehat{G}_H}\widehat{\mu}(\chi)\,\overline{\alpha}\chi(a),\end{aligned}$$

where the last equality follows using (3.7). Testing the hypothesis $\widehat{\mu_{a|H}}\left(\alpha_{|H}\right) = \widehat{\mu_{a|H}}\left(\overline{\alpha_{|H}}\right) = 0$ against the alternative hypothesis that at least one of these Fourier coefficients is equal to 0 is equivalent to testing the hypothesis

$$\begin{gathered}\textstyle\sum_{\chi\in\alpha\widehat{G}_H}\widehat{\mu}(\chi)\,\overline{\alpha}\chi(a) = \sum_{\chi\in\overline{\alpha}\widehat{G}_H}\widehat{\mu}(\chi)\,\overline{\alpha}\chi(a) = 0\\ \text{against}\\ \textstyle\sum_{\chi\in\alpha\widehat{G}_H}\widehat{\mu}(\chi)\,\overline{\alpha}\chi(a) \neq 0 \text{ and } \sum_{\chi\in\overline{\alpha}\widehat{G}_H}\widehat{\mu}(\chi)\,\overline{\alpha}\chi(a) \neq 0.\end{gathered} \tag{3.31}$$

When the data is obtained on the coset aH in G then all hypotheses that can be tested within the framework of harmonic analysis are of the form given in (3.31). The theory is illustrated in the next example.

Table 3.13: Design matrix and response data of a 3^{3-1} factorial design.

	Factor			
Run	X_1	X_2	X_3	Response
1	0	0	2	3070
2	0	1	0	5547
3	0	2	1	5735
4	1	0	0	6843
5	1	1	1	6799
6	1	2	2	4968
7	2	0	1	6905
8	2	1	2	6215
9	2	2	0	7145

Example 3.86 Consider the regular fraction of the 3^3 factorial design given in Table 3.13. The fraction is the coset $F = (0,0,2) + H$ in $G = (\mathbb{Z}/3\mathbb{Z})^3$ where the subgroup H is given by

$$\begin{aligned} H &= \{(0,0,0),(0,1,1),(0,2,2),(1,1,2),(1,2,0),(1,0,1),(2,2,1), \\ &\quad (2,0,2),(2,1,0)\}. \end{aligned}$$

The annihilator for H in G is

$$\widehat{G}_H = \{\chi_{(0,0,0)}, \chi_{(1,1,2)}, \chi_{(2,2,1)}\}.$$

We have that $\chi_{(0,0,0)}(g) = 1$, $\chi_{(1,1,2)}(g) = \omega$ and $\chi_{(2,2,1)}(g) = \omega^2$ for all $g \in F$. Hence, using the results in Section 3.4.2 this fraction can be characterized by the defining equation

$$I' = \omega^2 X_1' X_2' \left(X_3'\right)^2 = \omega \left(X_1'\right)^2 \left(X_2'\right)^2 X_3',$$

where $\omega = e^{\frac{2\pi i}{3}}$. The decomposition of the total sum of squares that is obtained using harmonic analysis is presented in Table 3.14. The cosets of $\widehat{G}_H$ in $\widehat{G}$ that correspond to the orthogonal component X_1 are

$$\chi_{(1,0,0)}\widehat{G}_H = \{\chi_{(1,0,0)}, \chi_{(2,1,2)}, \chi_{(0,2,1)}\}$$

and

$$\chi_{(2,0,0)}\widehat{G}_H = \{\chi_{(2,0,0)}, \chi_{(0,1,2)}, \chi_{(1,2,1)}\}.$$

The F-test that corresponds to X_1 tests the hypothesis

$$\begin{aligned} \widehat{\mu}\left(\chi_{(1,0,0)}\right) + \omega\widehat{\mu}\left(\chi_{(2,1,2)}\right) + \omega^2\widehat{\mu}\left(\chi_{(0,2,1)}\right) &= \\ \widehat{\mu}\left(\chi_{(2,0,0)}\right) + \omega\widehat{\mu}\left(\chi_{(0,1,2)}\right) + \omega^2\widehat{\mu}\left(\chi_{(1,2,1)}\right) &= 0 \end{aligned} \tag{3.32}$$

Table 3.14: ANOVA Table for the data in Table 3.13.

Orthogonal component	Degrees of freedom	Combined Sum of Squares	Mean Square	F	p-value
X_1	2	6.20368×10^6	3.10184×10^6	10.71	0.085
X_2	2	511924	255962	0.8835	0.539
X_3	2	6.08926×10^6	3.04463×10^6	10.51	0.087
residual	2	579423	289711		
total	8	1.33843×10^7			

against the alternative hypothesis that both

$$\widehat{\mu}\left(\chi_{(1,0,0)}\right) + \omega\widehat{\mu}\left(\chi_{(2,1,2)}\right) + \omega^2\widehat{\mu}\left(\chi_{(0,2,1)}\right) \neq 0$$

and

$$\widehat{\mu}\left(\chi_{(2,0,0)}\right) + \omega\widehat{\mu}\left(\chi_{(0,1,2)}\right) + \omega^2\widehat{\mu}\left(\chi_{(1,2,1)}\right) \neq 0.$$

The p-value for this test is 0.085 and at a significance level of 0.05 the null-hypothesis (3.32) is accepted. Note that if the Fourier transforms $\widehat{\mu}(\chi)$ that correspond to the orthogonal components $X_1X_2^2X_3$ and X_2X_3 are zero, that is,

$$\widehat{\mu}\left(\chi_{(1,2,1)}\right) = \widehat{\mu}\left(\chi_{(2,1,2)}\right) = \widehat{\mu}\left(\chi_{(0,1,2)}\right) = \widehat{\mu}\left(\chi_{(0,2,1)}\right) = 0,$$

then the hypothesis that is tested

$$\widehat{\mu}\left(\chi_{(1,0,0)}\right) = \widehat{\mu}\left(\chi_{(2,0,0)}\right) = 0.$$

This hypothesis is tested against the alternative hypothesis

$$\widehat{\mu}\left(\chi_{(1,0,0)}\right) \neq 0 \text{ and } \widehat{\mu}\left(\chi_{(2,0,0)}\right) \neq 0.$$

3.7 Possible extensions

The theory of symmetry studies (Viana (2005)) provides another method for statistical analysis of full factorial experiments. Symmetry studies are centered on the notion of data indexed by a finite set of labels upon which certain symmetry transformations can be defined. Briefly, these studies explore the symmetry transformations identified by the set of labels V to facilitate classification, interpretation and statistical analysis of the data $\{y(v) \mid v \in V\}$ indexed by these labels. A finite group G acts on the set V and determines a linear representation of G that operates in a data vector space $\mathcal{V}$. The resulting factorization of $\mathcal{V}$ follows from the construction of the canonical projections of the form given in Theorem 3.12. The theory of symmetry studies has been applied successfully

in different fields: in statistical geometric optics (*e.g.* Lakhsminarayanan and Viana (2005) and Viana and Lakhsminarayanan (2007)) and in the decomposition of the entropy of a finite set of mutually exclusive events (Viana (2006)). A wide variety of applications in biology, chemistry and physics can be found in Viana (2005).

Ledermann (1968) illustrated how symmetry studies can be used to find a decomposition of the total sums of squares for the data observed on a full factorial design. The elements of each set L_j are now merely regarded as labels and no additional structure is assumed for these sets. The labels for the full factorial design are given by $V = L_1 \times L_2 \times \ldots \times L_k$. In this section we, without loss of generality, assume that $L_j = \{1, 2, \ldots, n_j\}$. A symmetry that is consistent with the set of labels is induced by the action of a group G on the set V.

Definition 3.87 (Group action) Given a set V and a group G, a group action of G on V is a function $\varphi : G \times V \to V$ satisfying

1. $\varphi(1, v) = v$ for all $v \in V$,
2. $\varphi(g, \varphi(h, v)) = \varphi(gh, v)$ for all $v \in V$ and $g, h \in G$.

Let S_n denote the symmetric group on the n elements in $\{1, 2, \ldots, n\}$. For instance, for $n = 3$ we have that $S_n = \{1, (12), (13), (23), (123), (132)\}$. In Ledermann (1968) the group $G = S_{n_1} \times S_{n_2} \times \ldots \times S_{n_k}$ is chosen to act on V by the action $\varphi : G \times V \to V$ defined by

$$\varphi(\sigma, v) = (\sigma_1 v_1, \sigma_2 v_2, \ldots, \sigma_k v_k) \tag{3.33}$$

where $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_k) \in G$ and $v = (v_1, v_2, \ldots v_k) \in V$. The action of the group G on V leads to a linear representation $\rho : G \to GL\left(\mathbb{R}^V\right)$ in the data vector space $\mathbb{R}^V$.

Example 3.88 Consider a data vector $y = (y_1, y_2, y_3)^T$ containing statistical data indexed by the labels in a set $V = \{1, 2, 3\}$. We let the group symmetric group S_3 act on D according to $(\sigma, v) = \sigma v$ for all $\sigma \in S_3$ and $v \in V$. A linear representation $\rho : S_3 \to GL\left(\mathbb{R}^3\right)$ of S_3 in $\mathbb{R}^3$ is given by

$$1 \xrightarrow{\rho} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, (12) \xrightarrow{\rho} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, (13) \xrightarrow{\rho} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$(23) \xrightarrow{\rho} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, (123) \xrightarrow{\rho} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \text{ and } (132) \xrightarrow{\rho} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

It is easy to verify that $\rho(\sigma)(y_1, y_2, y_3)^T = (y_{\sigma 1}, y_{\sigma 2}, y_{\sigma 3})$ for all permutations $\sigma \in S_3$. The irreducible characters of the group S_3 are given in Table 3.15. The

Table 3.15: Character table for S_3.

$\sigma \in S_3$	$\chi_1(\sigma)$	$\chi_2(\sigma)$	$\chi_3(\sigma)$
1	1	1	2
(12)	1	−1	0
(13)	1	−1	0
(23)	1	−1	0
(123)	1	1	−1
(132)	1	1	−1

canonical projection matrices as defined in Theorem 3.12 are given by

$$P_1 = \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \; P_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \text{ and } P_3 = \frac{1}{3}\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}.$$

The data vector $y = (y_1, y_2, y_3)^T$ can be written as $A\,y + Q\,y$ where $A = P_1$ and $Q = P_3$, that is,

$$A\,y = \frac{1}{3}\begin{pmatrix} y_1 + y_2 + y_3 \\ y_1 + y_2 + y_3 \\ y_1 + y_2 + y_3 \end{pmatrix} = \overline{y}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

and

$$Q\,y = \frac{1}{3}\begin{pmatrix} 2y_1 - y_2 - y_3 \\ -y_1 + 2y_2 - y_3 \\ -y_1 - y_2 + 2y_3 \end{pmatrix} = \begin{pmatrix} y_1 - \overline{y} \\ y_2 - \overline{y} \\ y_3 - \overline{y} \end{pmatrix}.$$

The vector space $\text{span}\{y_1, y_2, y_3\}$ over $\mathbb{R}$ decomposes into invariant subspaces according to

$$\text{span}\{y_1, y_2, y_3\} = \text{span}\{y_1 + y_2 + y_3\} \oplus \text{span}\{-2y_1 + y_2 + y_3, y_1 - 2y_2 + y_3\}.$$

More precisely, the subspaces $\text{span}\{y_1 + y_2 + y_3\}$ and $\text{span}\{-2y_1 + y_2 + y_3, y_1 - 2y_2 + y_3\}$ are closed under the action of S_3 on the labels in V.

The decomposition $I_n = A_n + Q_n$ with $A_n = \frac{1}{n}ee^T$ and $Q_n = I_n - A_n$ with ee^T the $n \times n$ matrix of ones that in Example 3.88 was obtained for $n = 3$ is called the standard decomposition. The standard decomposition of the $n \times n$ identity matrix is obtained when the symmetric group S_n acts on a set V containing n labels. A derivation of this result for the general n can be found in Section 2.9 of Viana (2005).

The canonical reduction under the action given in (3.33) of the group $S_{n_1} \times S_{n_2} \times \ldots \times S_{n_k}$ on a set $V = L_1 \times L_2 \times \ldots L_k$ of labels is

$$I_N = (A_{n_1} + Q_{n_1}) \otimes (A_{n_2} + Q_{n_2}) \otimes \ldots \otimes (A_{n_k} + \mathcal{Q}_{n_k}).$$

Table 3.16: ANOVA Table for data in Table 3.3 obtained using group actions.

Canonical projection	Degrees of freedom	Sum of Squares	Mean Square	F	p-value
$P_{\{1\}}$	2	3.46217×10^7	1.73109×10^7	85.58	0.000
$P_{\{2\}}$	2	938539	469270	2.32	0.108
$P_{\{3\}}$	2	9.54948×10^6	4.77474×10^6	23.61	0.000
$P_{\{1,2\}}$	4	3.29825×10^6	824563	4.07	0.006
$P_{\{1,3\}}$	4	3.87218×10^6	968045	4.79	0.002
$P_{\{2,3\}}$	4	448348	112087	.554	0.697
$P_{\{1,2,3\}}$	8	5.20692×10^6	650864	3.218	0.005
residual	54	1.09226×10^7	202270		
total	80	6.88581×10^7			

If for $J \subseteq \{1, 2, \ldots, k\}$ we define the function $\delta_J : \{1, 2, \ldots, k\} \to \{0, 1\}$ by

$$\delta_J(j) = \begin{cases} 1 & \text{if } j \in J \\ 0 & \text{otherwise} \end{cases},$$

then the canonical reduction can be expressed as

$$I_N = \sum_{J \subseteq \{1,2,\ldots,k\}} P_J,$$

where

$$P_J = \bigotimes_{j=1}^{k} A_{n_j}^{\delta_J(j)} Q_{n_j}^{1-\delta_J(j)}. \tag{3.34}$$

The resulting decomposition of the total sums of squares is given in Table 3.16. The link with the decomposition given in Table 3.12 is the following. The sums of squares for the canonical projection $P_{\{1,2\}}$ is the total of the sums of squares for the orthogonal components X_1X_2 and $X_1X_2^2$. Moreover, the sums of squares for the canonical projection $P_{\{1,2,3\}}$ is the total of the sums of squares for the orthogonal components $X_1X_2X_3, X_1X_2X_3^2, X_1X_2^2X_3$ and $X_1X_2^2X_3^2$. We like to point out that the canonical projection P_J in (3.34) is simply the projection onto the interaction space H_J as defined in Definition 2.11. The decomposition given in Table 3.16 is commonly referred to as the standard ANOVA decomposition for the full factorial experiment.

The decomposition of the total sums of squares given in Table 3.4 is found by letting the group $G = (\mathbb{Z}/3\mathbb{Z})^4$ act on itself by

$$\varphi(g, h) = (g_1 + h_1, g_2 + h_2, g_3 + h_3, g_4 + h_4)$$

for all $g, h \in G$. This action $\varphi : G \times G \to G$ is called the regular action. The regular representation $\rho : G \to GL\left(\mathbb{C}^G\right)$ as defined in Definition 3.13 is used.

In the theory of symmetry studies a design can be defined as a triple consisting of a set of labels V, a group G and a group action φ of G on V. The theory gives an intuitive method for obtaining the standard ANOVA decomposition for full factorial designs using the representation theory of the symmetric group. However, at this moment it is unclear how regular fractions and confounding can be dealt with within this framework.

3.8 Conclusions

We considered coding full factorial designs by finite Abelian groups. Using the character theory of finite Abelian groups we showed that the definitions of regular fractions given by Collombier (1996), Wu and Hamada (2000) and Pistone and Rogantin (2005) are equivalent. An important ingredient in our approach is the special role played by the cosets of the finite Abelian group that codes the full factorial design. We moreover used character theory to prove that any regular fraction when interpreted as a coset is an orthogonal of a certain strength that is related to the resolution of the fraction. This is a generalization of results by Rao and Bose for regular fractions with a prime power as the number of levels.

The standard way to analyze factorial experiments is analysis of variance. Diaconis (1988) and Viana (2005) showed that the well-known decomposition of the total sums of squares in the analysis of variance for full factorial designs naturally arises from harmonic analysis on a finite Abelian group. In this chapter we gave a slight extension by developing the theoretical aspects of harmonic analysis of data structured on cosets of finite Abelian groups.

Ledermann (1968) illustrated how the theory of symmetry studies can be used to find the standard sums of squares decomposition. In this theory a design can be specified by a triple consisting of a set of labels, a group of symmetries and an action of this group on the set of labels. The theory gives an intuitive method for obtaining the standard ANOVA decomposition for full factorial designs. However, at this moment it is unclear how regular fractions can be dealt with within this framework.

Chapter 4

Estimation of Dispersion Parameters

In the previous chapter we assumed that the all observations made in the factorial experiments are statistically independent and that the variance is equal for all observations. In this chapter we abandon these assumptions and assume a mixed linear model for the observed data. The mixed linear model is a generalization of the standard linear model, the generalization being that the data are permitted to exhibit correlation and non-constant variability. In particular, the covariance matrix of the data vector is assumed to follow a linear model. The mixed linear model is used in modern engineering approaches to experimental design like the Taguchi approach. In industrial engineering interest is often in finding the setting for the variables in the production process that minimizes the variability in some quality measure while keeping its mean on target. The impact of the variables on the variability can be taken into account by formulating an appropriate mixed linear model for the data observed in the experiment.

In this chapter we first consider the mixed linear model in its general form. We assume that a random vector Y follows

$$\begin{array}{rcl} \mathrm{E}\,(Y) & = & Z\theta \\ \mathrm{Var}\,(Y) & = & \sum_{i=1}^{v} \alpha_i \, \Gamma_i \end{array} \quad , \tag{4.1}$$

where Z is a known $N \times p$ full rank matrix and $\Gamma_1, \Gamma_2, \ldots, \Gamma_v$ are known $N \times N$ matrices. The parameters $\alpha_1, \alpha_2, \ldots, \alpha_v$ and $\theta = (\theta_1, \theta_2, \ldots, \theta_p)^T$ are unknown. The parameters $\theta_1, \theta_2, \ldots, \theta_p$ and $\alpha_1, \alpha_2, \ldots, \alpha_v$ are called location and dispersion parameters, respectively. Seely (1970b) (see also Seely (1970a)) gives a necessary and sufficient condition for the existence of quadratic unbiased estimators for all the dispersion parameters in the mixed linear model (4.1). In Theorem 4.13 we extend this result by giving a necessary and sufficient condition for the existence of quadratic unbiased estimators that are invariant under translations of the location parameters. Malley (1986) and Liao and Iyer (2000) give estimators for the dispersion parameters in the mixed linear model. The

equivalence of these estimators is shown in Theorem 4.14. In Section 4.4 we consider the estimation of dispersion effects from unreplicated factorial designs. Box and Meyer (1986) initiated the identification of dispersion effects from unreplicated factorial experiments. They did not give an explicit estimation procedure for the dispersion parameters. Estimation methods for the dispersion effects under a linear model for the variance were given in Wiklander (1998) (see also Wiklander and Holm (2003)), Liao and Iyer (2000) and Brenneman and Nair (2001). The equivalence of these estimators is established in Theorems 4.17 and 4.18 for two-level full factorial designs and their regular fractions, respectively. We conclude by giving a definition for a MINQUE estimator for the dispersion effects in two-level full factorial designs and show that the above estimators are MINQUE in this sense.

This chapter is an extended version of Van de Ven (2005) in which the equivalence of the estimators for the dispersion effects was shown. A slightly altered version is accepted for publication in the Journal of Statistical Planning and Inference.

4.1 Examples of the mixed linear model

In the section we briefly consider several applications of the mixed linear model. In two of these examples the mixed linear model is assumed for data observed in a factorial experiment. The first example assumes independent observations and a linear model for the variance. The variance components model (also known as the mixed effects model) is considered in a second example. Another example is the class of weakly stationary time series.

Dispersion effects from factorial experiments

A special instance of the mixed linear model is considered in Wiklander (1998) (see also Wiklander and Holm (2003)), Liao and Iyer (2000) and Brenneman and Nair (2001). In these papers the estimation of dispersion effects using unreplicated (fractional) factorial designs is considered. The model considered in these papers assumes the independence of observations and a linear model for both the expectation as the variance.

Example 4.1 Consider a 2^2 factorial design and assume that the variables may affect both the expectation and the variance of the response variable. Under the assumption that all observations are made independently, a suitable model for the data is given by

$$\mathrm{E}\,(Y) = \begin{pmatrix} 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \tau_\emptyset \\ \tau_1 \\ \tau_2 \end{pmatrix}$$

and Var $(Y) =$

$$\alpha_{\emptyset}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \alpha_1\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \alpha_2\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The parameters τ_1 and τ_2 are called location effects. The parameters α_1 and α_2 are called dispersion effects. Note that since a variance is always positive we have the following restrictions on the dispersion parameters:

$$\alpha_{\emptyset} - \alpha_1 - \alpha_2 \geq 0,\ \alpha_{\emptyset} - \alpha_1 + \alpha_2 \geq 0,\ \alpha_{\emptyset} + \alpha_1 - \alpha_2 \geq 0 \text{ and } \alpha_{\emptyset} + \alpha_1 + \alpha_2 \geq 0.$$

The estimation of dispersion effects from unreplicated (fractional) factorial designs under a linear model for the variance is considered in detail in Section 4.4.

Variance components models

The variance components model is a special case of the mixed linear model. This model has applications in a wide variety of fields including agriculture, industry, biology, genetics and medical research. There is a wide range of textbooks available that deal with the estimation of the parameters in the variance components model. Recent textbooks include Malley (1986), Rao and Kleffe (1988), Searle et al. (1992), Rao (1997) and Cox and Solomon (2003). We will present the model in its general form in Section 4.3. Variance components were briefly introduced in the context of factorial experiments in Section 2.3. The variance components model is the appropriate model for data observed in factorial experiments in which some of the factors are random. For this reason, they are also sometimes referred to as mixed-effects models. We illustrate this class of models by an example of a 2^2 factorial design in which both factors are random.

Example 4.2 Consider a 2^2 factorial design with the levels of the factors X_1 and X_2 coded by $L_1 = L_2 = \{0, 1\}$. If the factors are random and there is assumed to be no interaction between the two factors, then the ANOVA model is given by

$$Y = \begin{pmatrix} \tau_{\emptyset} \\ \tau_{\emptyset} \\ \tau_{\emptyset} \\ \tau_{\emptyset} \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \tau_1(0) \\ \tau_1(1) \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \tau_2(0) \\ \tau_2(1) \end{pmatrix} + \varepsilon.$$

Under the usual assumptions for random factors given in Section 2.3 we find that the expectation and covariance matrix of Y are given by $\mathrm{E}(Y) = (\tau_{\emptyset}, \tau_{\emptyset}, \tau_{\emptyset}, \tau_{\emptyset})^T$

and Var $(Y) =$

$$\sigma^2 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \sigma_1^2 \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix} + \sigma_2^2 \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix},$$

where $\tau_\emptyset, \sigma^2, \sigma_1^2$ and σ_2^2 are unknown parameters. The observations follow a mixed linear model where the dispersion parameters are the error-variance σ^2 and the variance components σ_1^2 and σ_2^2.

In Section 4.3 we will show that if a variance components model is formulated as a mixed linear model, then all dispersion parameters correspond to variances. Note that this implies that each dispersion parameter satisfies $\alpha_j \geq 0$, which is a different restriction than the restriction on the dispersion parameters in the previous example that dealt with the estimation of dispersion effects from unreplicated factorial designs.

Weakly stationary time series

Let $\{y_t \mid t = 1, 2, \ldots, N\}$ denote a process observed in a sequence over time. The observations $Y_t, t = 1, 2, \ldots, N$, form a weakly stationary time series if E $(Y_t) = \mu$ and Cov $(Y_t, Y_{t-i}) = \gamma(i)$, where $\gamma(i)$ is called the autocovariance function. If we let $Y = (Y_1, Y_2, \ldots, Y_N)^T$ then the expectation and covariance matrix of Y are given by E $(Y) = (\mu, \mu, \ldots, \mu)^T$ and

$$\text{Var } (Y) = \begin{pmatrix} \gamma(0) & \gamma(1) & \ldots & \gamma(N-1) \\ \gamma(1) & \gamma(0) & \ldots & \gamma(N-2) \\ \vdots & \vdots & \ddots & \vdots \\ \gamma(N-1) & \gamma(N-2) & \ldots & \gamma(0) \end{pmatrix}.$$

This model is of the form given in (4.1) where the dispersion parameters are the function values of the autocorrelation function, that is, $\alpha_i = \gamma(i-1)$ for $i = 1, 2, \ldots, N$.

4.2 The mixed linear model

In this section we consider the mixed linear model (4.1) in its general form and focus on the estimation of the dispersion parameters $\alpha_i, 1 \leq i \leq v$. In Section 4.2.1 we introduce the class of quadratic estimators for this purpose. A framework for quadratic estimators proposed by Seely (1970b) is presented in Section 4.2.2. In Section 4.2.3 we give necessary and sufficient conditions for the estimability of dispersion parameters and identifiability of the dispersion model. The special class of translation invariant quadratic estimators is considered in Section 4.2.4.

4.2.1 Quadratic estimators

By $\mathcal{M}$ we denote the vector space of symmetric $N \times N$ matrices. The estimators that we consider are the quadratic forms in the vector of observations, that is,

$$Y^T MY, \quad M \in \mathcal{M}. \tag{4.2}$$

The estimators of the form given in (4.2) are called quadratic estimators. The quadratic estimators can be used for estimation of the dispersion parameters in the mixed linear model. We now define the notion of quadratic estimability for dispersion parameters in the mixed linear model.

Definition 4.3 A parameter α_i in the model (4.1) is said to be *quadratically estimable* if there exists a matrix $M \in \mathcal{M}$ for which $\mathrm{E}\left(Y^T MY\right) = \alpha_i$.

The next lemma gives the expectation of a quadratic estimator under the model (4.1).

Lemma 4.4 *For a quadratic form $Y^T MY$ and the model given in (4.1) we have that*

$$E\left(Y^T MY\right) = \sum_{i=1}^{v} \alpha_i tr\left(M\Gamma_i\right) + \theta^T Z^T MZ\theta. \tag{4.3}$$

Proof The proof follows by using the property $\mathrm{tr}\left(M_1 M_2\right) = \mathrm{tr}\left(M_2 M_1\right)$. More precisely,

$$\begin{aligned}
\mathrm{E}\left(Y^T MY\right) &= \mathrm{E}\left(\mathrm{tr}\left(Y^T MY\right)\right) = \mathrm{E}\left(\mathrm{tr}\left(MYY^T\right)\right) = \mathrm{tr}\left(M\mathrm{E}\left(YY^T\right)\right) \\
&= \mathrm{tr}\left(M\left(\mathrm{Var}\left(Y\right) + \mathrm{E}\left(Y\right)\mathrm{E}\left(Y^T\right)\right)\right) \\
&= \mathrm{tr}\left(M\mathrm{Var}\left(Y\right)\right) + \mathrm{tr}\left(M_i\left(Z\theta\right)\left(Z\theta\right)^T\right) \\
&= \mathrm{tr}\left(M\sum_{i=1}^{v}\alpha_i\Gamma_i\right) + \mathrm{tr}\left(\left(Z\theta\right)^T MZ\theta\right) \\
&= \sum_{i=1}^{v}\alpha_i \mathrm{tr}\left(M\Gamma_i j\right) + \theta^T Z^T MZ\theta.
\end{aligned}$$

This completes the proof. □

The variance and covariance of quadratic estimators in the case that the observations in Y are normally distributed are given in the next lemma.

Lemma 4.5 *Under the assumption that the observations in Y are normally distributed random variables satisfying the model (4.1) with $\sum_{j=1}^{v}\alpha_j\Gamma_j$ positive definite we have for all $M_1, M_2 \in \mathcal{M}$ that*

$$\begin{aligned}
&Cov\left(Y^T M_1 Y, Y^T M_2 Y\right) = \\
&2\sum_{i=1}^{v}\sum_{j=1}^{v}\alpha_i\alpha_j tr\left(M_1\Gamma_i M_2\Gamma_j\right) + 4\sum_{i=1}^{v}\alpha_i\theta^T Z^T M_1\Gamma_i M_2 Z\theta.
\end{aligned} \tag{4.4}$$

In particular, we have for all $M \in \mathcal{M}$ that

$$\begin{aligned}
&Var\left(Y^T MY\right) = \\
&2\sum_{i=1}^{v}\sum_{j=1}^{v}\alpha_i\alpha_j tr\left(M\Gamma_i M\Gamma_j\right) + 4\sum_{i=1}^{v}\alpha_i\theta^T Z^T M\Gamma_i MZ\theta.
\end{aligned} \tag{4.5}$$

Proof See Theorem 9.22 (b) and (c) in Schott (1997). □

4.2.2 Framework for quadratic estimators

In this section we describe the framework for quadratic estimators proposed by Seely (1970b) (see also Seely (1970a)) in which quadratic estimators are expressed as inner products of symmetric matrices. We will use this framework when we show the equivalence of different estimators proposed for the dispersion effects in unreplicated factorial designs in Section 4.4. The framework of Seely (1970b) is based on the observation that the vector space $\mathcal{M}$ when endowed with the inner product $\langle \cdot, \cdot \rangle$ defined by $\langle M_1, M_2 \rangle = \text{tr}\,(M_1 M_2)$ is an inner product space. Note that the set of all quadratic estimators is given by $\{\langle M, YY^T \rangle \mid M \in \mathcal{M}\}$.

Given an orthonormal basis $\{Q_i \mid 1 \leq i \leq \dim(\mathcal{M})\}$ for $\mathcal{M}$, every symmetric matrix $M \in \mathcal{M}$ has a unique representation of the form

$$M = \sum_{i=1}^{\dim(\mathcal{M})} \langle M, Q_i \rangle \, Q_i. \tag{4.6}$$

The expansion given in (4.6) is the unique Fourier-Bessel expansion (see Lemma 2.19) of M with respect to the basis $\{Q_i \mid 1 \leq i \leq \dim(\mathcal{M})\}$. A specific orthonormal basis for the vector space of symmetric matrices is now proposed. In proving equality of the estimators for dispersion effects we will use the unique expansion given in (4.6) with respect to this basis. We use a method from Seely (1970b) to construct an orthonormal basis for $\mathcal{M}$ from an orthonormal basis for $\mathbb{R}^N$. Let $\{q_1, q_2, \ldots, q_p\} \subset \mathbb{R}^N$ and define symmetric matrices $Q_{ij}, 1 \leq i \leq j \leq p$, by

$$\begin{array}{ll} Q_{ii} = q_i q_i^T & 1 \leq i \leq p \\ Q_{ij} = \frac{1}{\sqrt{2}} \left(q_i q_j^T + q_j q_i^T \right) & 1 \leq i < j \leq p \end{array} . \tag{4.7}$$

The following theorem tells us that if $\{q_1, q_2, \ldots, q_p\}$ is an orthonormal set in $\mathbb{R}^N$ then the matrices $Q_{ij}, 1 \leq i \leq j \leq p$, form an orthonormal set in $\mathcal{M}$. It also tells us how to construct an orthonormal basis for $\mathcal{M}$ given an orthonormal basis for $\mathbb{R}^N$.

Theorem 4.6 *Let $\{q_1, q_2, \ldots, q_p\}$ be an orthonormal set of vectors in $\mathbb{R}^N$. The set $\{Q_{ij} \mid 1 \leq i \leq j \leq p\}$ with Q_{ij} as defined in (4.7) is an orthonormal set of vectors in the inner product space $(\mathcal{M}, \langle \cdot, \cdot \rangle)$. In particular, if $\{q_1, q_2, \ldots, q_N\}$ is an orthonormal basis for $\mathbb{R}^N$, then the set $\{Q_{ij} \mid 1 \leq i \leq j \leq N\}$ is an orthonormal basis for $(\mathcal{M}, \langle \cdot, \cdot \rangle)$.*

Proof Let the symmetric matrices $A_{ij}, 1 \leq i \leq j \leq p$, be defined by

$$A_{ij} = q_i q_j^T + q_j q_i^T.$$

The inner product $\langle A_{ij}, A_{\ell m} \rangle$ equals

$$\begin{aligned} &\text{tr}\,(A_{ij} A_{\ell m}) = \\ &\text{tr}\left(q_i q_j^T q_\ell q_m^T\right) + \text{tr}\left(q_i q_j^T q_m q_\ell^T\right) + \text{tr}\left(q_j q_i^T q_\ell q_m^T\right) + \text{tr}\left(q_j q_i^T q_m q_\ell^T\right) = \\ &\text{tr}\left(q_j^T q_\ell q_m^T q_i\right) + \text{tr}\left(q_j^T q_m q_\ell^T q_i\right) + \text{tr}\left(q_i^T q_\ell q_m^T q_j\right) + \text{tr}\left(q_i^T q_m q_\ell^T q_j\right) = \\ &q_j^T q_\ell q_m^T q_i + q_j^T q_m q_\ell^T q_i + q_i^T q_\ell q_m^T q_j + q_i^T q_m q_\ell^T q_j. \end{aligned}$$

Let δ_{ij} denote the Kronecker delta. Since $\{q_1, q_2, \ldots, q_p\}$ is a orthonormal set we find that

$$\langle A_{ij}, A_{\ell m} \rangle = \delta_{j\ell}\delta_{im} + \delta_{jm}\delta_{i\ell} + \delta_{i\ell}\delta_{jm} + \delta_{im}\delta_{j\ell} = \begin{cases} 4 & \text{if } i = j = \ell = m \\ 2 & \text{if } i = \ell < j = m \\ 0 & \text{otherwise} \end{cases} .$$

Using this result we find that $\langle Q_{ij}, Q_{\ell m} \rangle = 0$ if $i \neq \ell$ or $j \neq m$ and $\langle Q_{ij}, Q_{ij} \rangle = 1$ for all i and j. The set $\{Q_{ij} \mid 1 \leq i \leq j \leq p\}$ is thus an orthonormal set of vectors in the inner product space $(\mathcal{M}, \langle \cdot, \cdot \rangle)$. If $p = N$ then $\{q_1, q_2, \ldots, q_N\}$ is an orthonormal basis for $\mathbb{R}^N$. The number of elements in the orthonormal set $\{Q_{ij} \mid 1 \leq i \leq j \leq N\}$ is in that case equal to $\frac{1}{2}N(N+1)$ which is $\dim(\mathcal{M})$. We have shown that the set $\{Q_{ij} \mid 1 \leq i \leq j \leq N\}$ is an orthonormal basis for the inner product space $(\mathcal{M}, \langle \cdot, \cdot \rangle)$. □

4.2.3 Quadratic unbiased estimators

In this section we consider the unbiased estimation of the dispersion parameters in the mixed linear model using quadratic estimators. From Lemma 4.4 we find that the expectation of each quadratic form in Y is a linear combination of the dispersion parameters $\alpha_i, 1 \leq i \leq v$, and products of pairs of location parameters $\theta_i\theta_j, 1 \leq i \leq j \leq p$. The following necessary and sufficient condition for a set of quadratic forms to unbiasedly estimate the dispersion parameters is directly obtained from Lemma 4.4.

Corollary 4.7 *For a set of quadratic forms $Y^T M_i Y, 1 \leq i \leq v$, we have that each $Y^T M_i Y$ is an unbiased estimator for α_i under model (4.1) if and only if $tr(M_i\Gamma_j) = \delta_{ij}$ for all i and j and $Z^T M_i Z = 0$ for all i.*

Let z_i denote the ith column of the matrix Z. Seely (1970b) gives the following necessary and sufficient condition for all dispersion parameters $\alpha_i, 1 \leq i \leq v$, to be quadratically estimable under the model (4.1).

Theorem 4.8 (Seely) *All parameters $\alpha_i, 1 \leq i \leq v$, in model (4.1) are quadratically estimable if and only if the matrixes $\Gamma_1, \Gamma_2, \ldots, \Gamma_v$ are linearly independent and span$\{z_i z_j^T + z_j z_i^T \mid 1 \leq i \leq j \leq p\} \cap$ span$\{\Gamma_i \mid 1 \leq i \leq v\} = \{0\}$.*

Proof See Corollary 1.2 in Seely (1970b). □

An application of this theorem is given in the next example, in which we consider the estimation of dispersion effects from data obtained in an unreplicated 2^2 factorial experiment.

Example 4.9 (Continuation of Example 4.1) The columns of the matrix Z after normalizing are given by

$$q_1 = \frac{1}{2}(1,1,1,1)^T , \; q_2 = \frac{1}{2}(-1,-1,1,1)^T \text{ and } q_3 = \frac{1}{2}(-1,1,-1,1)^T .$$

If we write $z_4 = (1,-1,-1,1)^T$ and $q_4 = \frac{1}{2}\, z_4$ then $\{q_1, q_2, q_3, q_4\}$ is an orthonormal basis for $\mathbb{R}^4$. The matrices $Q_{ij}, 1 \leq i \leq j \leq 4$, defined by

$$\begin{array}{lcll} Q_{ii} & = & q_i q_i^T & = \frac{1}{4} z_i z_i^T \qquad \text{for } 1 \leq i \leq 4, \\ Q_{ij} & = & \frac{1}{\sqrt{2}} \left(q_i q_j^T + q_j q_i^T \right) & = \frac{1}{4\sqrt{2}} \left(z_i z_j^T + z_j z_i^T \right) \qquad \text{for } 1 \leq i < j \leq 4, \end{array}$$

form an orthonormal basis for the linear space of all symmetric matrices of size 4×4. If we expand the matrices in $\Gamma_\emptyset, \Gamma_1$ and Γ_2 with respect to this basis, then we find that

$$\begin{array}{lcl} \Gamma_\emptyset & = & Q_{11} + Q_{22} + Q_{33} + Q_{44}, \\ \Gamma_1 & = & \frac{1}{\sqrt{2}} Q_{12} + \frac{1}{\sqrt{2}} Q_{34}, \\ \Gamma_2 & = & \frac{1}{\sqrt{2}} Q_{13} + \frac{1}{\sqrt{2}} Q_{24}. \end{array}$$

From these Fourier-Bessel expansions it can be seen that

$$\text{span}\left\{ z_i z_j^T + z_j z_i^T \mid 1 \leq i \leq j \leq 3 \right\} \cap \text{span}\left\{ \Gamma_\emptyset, \Gamma_1, \Gamma_2 \right\} = \{0\}.$$

By applying Theorem 4.8 we find that all parameters $\alpha_\emptyset, \alpha_1$ and α_2 are quadratically estimable.

It is easily verified that the only unbiased quadratic estimators for the dispersion parameters $\alpha_\emptyset, \alpha_1$ and α_2 are $\widehat{\alpha}_\emptyset = Y^T M_\emptyset Y$, $\widehat{\alpha}_1 = Y^T M_1 Y$ and $\widehat{\alpha}_2 = Y^T M_2 Y$, respectively, where

$$M_\emptyset = Q_{44},\ M_1 = \sqrt{2}\, Q_{34} \text{ and } M_2 = \sqrt{2}\, Q_{24}.$$

Hence, the unbiased quadratic estimators for the dispersion parameters are

$$\widehat{\alpha}_\emptyset = \frac{1}{4} \left(z_4^T Y \right)^2,\ \widehat{\alpha}_1 = \frac{1}{2} \left(z_3^T Y \right) \left(z_4^T Y \right) \text{ and } \widehat{\alpha}_2 = \frac{1}{2} \left(z_2^T Y \right) \left(z_4^T Y \right).$$

The Ordinary Least Squares estimators for the location effects are

$$\widehat{\theta}_\emptyset = \frac{1}{4} z_1^T Y,\ \widehat{\theta}_1 = \frac{1}{4} z_2^T Y \text{ and } \widehat{\theta}_2 = \frac{1}{4} z_3^T Y.$$

The vector of residuals is given by $R = a\, z_4$ where $a = \frac{1}{4} z_4^T Y$. Observe that the estimators for location effects and dispersion effects are related according to

$$\widehat{\alpha}_\emptyset = 4a^2,\ \widehat{\alpha}_1 = 8a\widehat{\theta}_2 \text{ and } \widehat{\alpha}_2 = 8a\widehat{\theta}_1.$$

Note that if in the previous example we have that $\widehat{\theta}_1$ is large compared to $\widehat{\theta}_2$, then $\widehat{\alpha}_2$ will be large compared to $\widehat{\alpha}_1$, which is clearly undesirable. In order to overcome problems of this kind the estimators for the dispersion parameters are usually restricted to quadratic forms that have the property of translation invariance which we will define in the next section.

4.2.4 Translation invariant quadratic unbiased estimators

From this section onwards we restrict our attention to estimators that are translation invariant quadratic forms. A formal definition of translation invariance for quadratic forms in a random vector Y that follows a linear model $\mathrm{E}(Y) = Z\theta$ is given first.

Definition 4.10 (Translation invariance) A quadratic form $Y^T MY$ is *translation invariant* if it has the property that $(Y + Z\theta)^T M (Y + Z\theta) = Y^T MY$ for all $Y \in \mathbb{R}^N$ and $\theta \in \mathbb{R}^p$.

A condition that is both necessary and sufficient for a quadratic form to be translation invariant is given in the next lemma.

Lemma 4.11 *A quadratic form $Y^T MY$ is translation invariant if and only if $MZ = 0$.*

Proof Clearly, if $MZ = 0$ then $Y^T MY$ is translation invariant. For the converse, assume that $Y^T MY$ is translation invariant. Then for all $\theta \in \mathbb{R}^p$ and $Y \in \mathbb{R}^N$ we have that

$$Y^T MY + \theta^T Z^T MY + Y^T MZ\theta + \theta^T Z^T MZ\theta = Y^T MY,$$

which reduces to

$$-2\theta^T Z^T MY = \theta^T Z^T MZ\theta. \tag{4.8}$$

Note that after substitution of $Y = 0$ in (4.8) we have that $\theta^T Z^T MZ\theta = 0$ for all $\theta \in \mathbb{R}^p$. By taking $\theta = e_i, 1 \le i \le p$, and $\theta = e_i + e_j, 1 \le i < j \le p$, we find that $\theta^T Z^T MZ\theta = 0$ for all $\theta \in \mathbb{R}^p$ implies that $Z^T MZ = 0$. Substituting $Z^T MZ = 0$ in (4.8) we find that $-2\theta^T Z^T MY = 0$ for all $\theta \in \mathbb{R}^P$ and $Y \in \mathbb{R}^N$. By considering all combinations $\theta = e_i$ and $Y = e_j$ with $1 \le i \le p$ and $1 \le j \le N$ and substituting them into $-2\theta^T Z^T MY = 0$ we find that $MZ = 0$. Hence, $MZ = 0$ is also a necessary condition for $Y^T MY$ to be translation invariant. □

By substitution of $MZ = 0$ into the expression for the $\mathrm{Var}\left(Y^T MY\right)$ given in Lemma 4.5 we find that under the normality assumption the variance of a translation invariant quadratic form $Y^T MY$ does not depend on the location parameters. Also the covariance of two translation invariant quadratic forms does not depend on the location parameters.

Imposing the constraint that a symmetric matrix M satisfies $MZ = 0$ is equivalent to requiring that M is of the form

$$M = (I - P_Z)\, B\, (I - P_Z)\,, \tag{4.9}$$

with B a symmetric matrix and $P_Z = Z\left(Z^T Z\right)^- Z^T$, where $\left(Z^T Z\right)^-$ denotes a generalized inverse of $Z^T Z$. The reader is referred to Chapter 1 of Searle (1971) or Chapter 9 of Harville (1997) for a detailed explanation of generalized inverses. Note that $I - P_Z$ is the projection on the orthogonal complement of

the range of Z in $\mathbb{R}^N$ and that for matrices M of the form given in (4.9) we have that

$$Y^T M Y = R^T B R,$$

where $R = (I - P_Z)\, Y$ is the vector containing the residuals after estimating the location parameters using Ordinary Least Squares. That is, restricting to translation invariant quadratic forms is in fact restricting to quadratic forms in the vector of Ordinary Least Squares residuals. In the next lemma we give a necessary and sufficient condition for a set of quadratic estimators to be a set of translation invariant unbiased estimators for the dispersion parameters in the mixed linear model.

Lemma 4.12 *For a set of quadratic forms $Y^T M_i Y, 1 \leq i \leq m$, we have that each $Y^T M_i Y$ is a translation invariant unbiased estimator for α_i under model (4.1) if and only if tr $(M_i \Gamma_j) = \delta_{ij}$ for all i and j and $M_i Z = 0$ for all i.*

Proof First assume that each random variable $Y^T M_i Y$ is a translation invariant unbiased estimator for α_i. Then using the unbiasedness and Corollary 4.7 we find that tr $(M_i \Gamma_j) = \delta_{ij}$ for all i and j and that $Z^T M_i Z = 0$ for all i. From Lemma 4.11 we know that the translation invariance implies that $M_i Z = 0$ for all i. Since, this last condition implies that $Z^T M_i Z = 0$ for all i we find that the conditions tr $(M_i \Gamma_j) = \delta_{ij}$ for all i and j and $M_i Z = 0$ for all i are necessary for the $Y^T M_i Y$ to be a set of translation invariant unbiased estimators for the dispersion parameters in the mixed linear model. To see that the conditions tr $(M_i \Gamma_j) = \delta_{ij}$ for all i and j and $M_i Z = 0$ for all i are sufficient, assume that the matrices $M_i, 1 \leq i \leq v$, satisfy both conditions. Note that $M_i Z = 0$ implies that $Z^T M_i Z = 0$ and, hence, by Corollary 4.7 we have that the $Y^T M_i Y$ are unbiased estimators for the dispersion parameters. The translation invariance follows directly from the condition $M_i Z = 0$ for all i. □

We now set out to derive a necessary and sufficient condition for the quadratic estimability of all dispersion parameters in model (4.1) when estimators are restricted to translation invariant quadratic forms. Note that for a matrix M that satisfies $MZ = 0$ the expectation given in (4.3) reduces to

$$\mathrm{E}\left(Y^T M Y\right) = \sum_{i=1}^{v} \alpha_i \,\mathrm{tr}\,(M \Gamma_i)\,.$$

Let $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_v)^T$ and consider a random vector

$$W = \left(Y^T M_1 Y,\, Y^T M_2 Y,\, \ldots,\, Y^T M_v Y\right)^T, \tag{4.10}$$

where each matrix M_i is symmetric and satisfies $Z^T M_i Z = 0$. The expectation of the random vector W can be written in matrix notation as

$$\mathrm{E}\,(W) = K\,\alpha, \tag{4.11}$$

where

$$K = \begin{pmatrix} \text{tr}\,(M_1\Gamma_1) & \text{tr}\,(M_1\Gamma_2) & \dots & \text{tr}\,(M_1\Gamma_v) \\ \text{tr}\,(M_2\Gamma_1) & \text{tr}\,(M_2\Gamma_2) & \dots & \text{tr}\,(M_2\Gamma_v) \\ \vdots & \vdots & \ddots & \vdots \\ \text{tr}\,(M_v\Gamma_1) & \text{tr}\,(M_v\Gamma_2) & \dots & \text{tr}\,(M_v\Gamma_v) \end{pmatrix}. \tag{4.12}$$

If we fix matrices $M_1, M_2, \dots, M_v$ then (4.11) is a linear model. Using Lemma 2.25 we find that all parameters in this linear model are estimable (by a linear combination of the quadratic forms $Y^T M_i Y, 1 \leq i \leq v$) if and only if the matrix K is full rank. Hence, a necessary and sufficient condition for all dispersion parameters in the model (4.1) to be quadratically estimable by translation invariant quadratic form is the existence of matrices $M_1, M_2, \dots, M_v$, each satisfying $M_i Z = 0$, for which the matrix K in (4.12) is full rank. This is used in the proof of the following theorem.

Theorem 4.13 *Define matrices $A_1, A_2, \dots, A_v$ by $A_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)$. There exists translation invariant unbiased estimators for all dispersion parameters $\alpha_i, 1 \leq i \leq v$, in the model (4.1) if and only if the matrices $A_1, A_2, \dots, A_v$ are linearly independent.*

Proof First we assume that the matrices $A_1, A_2, \dots, A_v$ are linearly dependent and show that this implies the singularity of the matrix K in (4.12) for any choice of the matrices $M_1, M_2, \dots, M_v$. If without loss of generality we let $M_i = (I - P_Z)\,B_i\,(I - P_Z)$ for some $B_i \in \mathcal{M}$, then the elements of the matrix K can be expressed as

$$\begin{aligned} \text{tr}\,(M_i\Gamma_j) &= \text{tr}\,((I - P_Z)\,B_i\,(I - P_Z)\,\Gamma_j) \\ &= \text{tr}\,(B_i\,(I - P_Z)\,\Gamma_j\,(I - P_Z)) \\ &= \text{tr}\,(B_i A_j)\,. \end{aligned}$$

From this last observation it follows that the linear dependence of the matrices $A_1, A_2, \dots, A_v$ implies the linear dependence of the columns of the matrix K and, hence, that the matrix K is not full rank. Note that this observation holds for any choice of the matrices B_i. As a result, the dispersion parameters are not all estimable using translation invariant quadratic forms.

For the converse, we let $M_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)$ and show that for this choice for M_i the matrix K is full rank. The estimability of all dispersion parameter is shown by giving an explicit estimator. First note that the elements of the matrix K with $M_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)$ are given by

$$\text{tr}\,(M_i\Gamma_j) = \text{tr}\,((I - P_Z)\,\Gamma_i\,(I - P_Z)\,\Gamma_j)\,.$$

Using that the matrices $(I - P_Z)$ are idempotent we find that

$$\begin{aligned} \text{tr}\,(M_i\Gamma_j) &= \text{tr}\,((I - P_Z)\,(I - P_Z)\,\Gamma_i\,(I - P_Z)\,(I - P_Z)\,\Gamma_j) \\ &= \text{tr}\,((I - P_Z)\,\Gamma_i\,(I - P_Z)\,(I - P_Z)\,\Gamma_j\,(I - P_Z)) \\ &= \text{tr}\,(A_i A_j)\,. \end{aligned}$$

For the moment assume that the matrix K with $M_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)$ is not full rank. Then because K is a square matrix we have that the rows of K for this choice for M_i are linearly dependent and that there exist $c_1, c_2, \ldots, c_v \in \mathbb{R}$ for which $\sum_{j=1}^{v} c_j \text{tr}\,(A_i A_j) = 0$ for all i. But then also

$$\sum_{i=1}^{v} c_i \sum_{j=1}^{v} c_j \text{tr}\,(A_i A_j) = 0,$$

which implies that

$$\begin{aligned}
\langle \textstyle\sum_{i=1}^{v} c_i A_i, \sum_{i=1}^{v} c_i A_i \rangle &= \text{tr}\left(\textstyle\sum_{i=1}^{v} c_i A_i \sum_{j=1}^{v} c_j A_j\right) \\
&= \text{tr}\left(\textstyle\sum_{i=1}^{v} c_i \sum_{j=1}^{v} c_j A_i A_j\right) \\
&= \text{tr}\left(\textstyle\sum_{i=1}^{v} c_i \sum_{j=1}^{v} c_j A_i A_j\right) \\
&= \textstyle\sum_{j=1}^{v} c_i \sum_{i=1}^{v} c_j \text{tr}\,(A_i A_j) \\
&= 0.
\end{aligned}$$

Because $\langle \cdot, \cdot \rangle$ is an inner product we have that $\langle \sum_{i=1}^{v} c_i A_i, \sum_{i=1}^{v} c_i A_i \rangle = 0$ if and only if $\sum_{i=1}^{v} c_i A_i = 0$. From this we find that if the matrix K with $M_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)$ is not full rank, then the matrices $A_1, A_2, \ldots, A_v$ have to be linearly dependent. This implies that in all cases where the matrices $A_1, A_2, \ldots, A_v$ are linearly independent, we have that the matrix K with $M_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)$ must be full rank. For K full rank unbiased translation invariant estimators for the dispersion parameters can be found using the estimator

$$K^{-1} W, \tag{4.13}$$

for α with $M_i = A_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)$. The unbiasedness of this estimator follows from observing that

$$E\left(K^{-1}W\right) = K^{-1}\text{E}\,(W) = K^{-1}K\alpha = \alpha.$$

Finally, because all the matrices M_i are translation invariant, also linear combinations of these matrices are translation invariant. Hence, the vector W contains translation invariant estimators. □

The estimator $\widehat{\alpha} = K^{-1}W$ for $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_v)^T$ with the matrix K as defined in (4.12) and $M_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)$ that appears in the proof of Theorem 4.2.4 is proposed by Liao and Iyer (2000) for the estimation of dispersion effects from unreplicated fractional factorial designs. This application is considered in more detail in Section 4.4.

Another method for estimating the dispersion parameters was proposed by Malley (1986). Although this method was proposed within the more restricted context of variance components models, it can also be applied for estimation of dispersion parameters in mixed linear models of the general form given in

(4.1). Malley (1986) uses a linearization operation to transform the model for Var (Y) into a simply linear one. The linearization operator that is used is vec (M) which for a matrix M of size $r \times c$ is simply the vector in $\mathbb{R}^{rc}$ formed by stacking the columns of M one upon the other, beginning with column 1 and moving from left to right. An overview of useful properties of the linearization operator vec $(\cdot)$ is given in Section 2.3 of Malley (1986). In this work we only use the property that vec $(M_1)^T$ vec $(M_2) =$ tr $(M_1 M_2)$ for all matrices M_1 and M_2 (provided that the product $M_1 M_2$ is properly defined).

We now give a derivation of the estimator proposed by Malley (1986). To this end we assume that the vector Y follows the mixed linear model given in (4.1) and define the symmetric matrices $A_1, A_2, \ldots, A_v$ by $A_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)$. In addition, we let $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_v)^T$ and $R = (I - P_Z)\,Y$. The linearized covariance matrix of the random vector R can be expressed as

$$\begin{aligned}
\text{vec (Var } (R)) &= \text{vec (Var } ((I - P_Z)\,Y)) \\
&= \text{vec } ((I - P_Z)\,\text{Var } (Y)\,(I - P_Z)) \\
&= \text{vec } ((I - P_Z)\,(\textstyle\sum_{i=1}^{v} \alpha_i \Gamma_i)\,(I - P_Z)) \\
&= \textstyle\sum_{i=1}^{v} \alpha_i\,(\text{vec } (A_j)) \\
&= (\text{vec } (A_1) : \text{vec } (A_2) : \cdots : \text{vec } (A_v))\,\alpha.
\end{aligned}$$

Using that $E\,(R) = 0$ we find that

$$\text{Var } (R) = E\left(RR^T\right) - \text{E } (R)\,\text{E}\left(R^T\right) = E\left(RR^T\right).$$

If we let $V = \text{vec}\left(RR^T\right)$ and $B = (\text{vec } (A_1) : \text{vec } (A_2) : \cdots : \text{vec } (A_v))$, then

$$\text{E } (V) = B\alpha,$$

which is a linear model. The estimator for α proposed by Malley (1986) is the Ordinary Least Squares estimator given by

$$\left(B^T B\right)^{-1} B^T V. \tag{4.14}$$

We now show that the estimator in (4.14) is to be equal to the estimator that was proposed by Liao and Iyer (2000). Recall that the estimator proposed by Liao and Iyer (2000) is the estimator given in (4.13) with K and W as in (4.12) and (4.10), respectively, and with $M_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)$.

Theorem 4.14 *The estimation methods proposed by Malley (1986) and Liao and Iyer (2000) give the same estimates for the parameters $\alpha_1, \alpha_2, \ldots, \alpha_v$ in the mixed linear model (4.1).*

Proof The result follows from observing that

$$\begin{aligned}
\left(B^T B\right)_{i,j} &= \text{vec } (A_i)^T\,\text{vec } (A_j) = \text{tr } (A_i A_j) \\
&= \text{tr } ((I - P_Z)\,\Gamma_i\,(I - P_Z)\,(I - P_Z)\,\Gamma_j\,(I - P_Z)) \\
&= \text{tr } ((I - P_Z)\,(I - P_Z)\,\Gamma_i\,(I - P_Z)\,(I - P_Z)\,\Gamma_j) \\
&= \text{tr } ((I - P_Z)\,\Gamma_i\,(I - P_Z)\,\Gamma_j) = \text{tr } (A_i \Gamma_j) = K_{i,j}
\end{aligned}$$

and

$$\begin{aligned}
\left(B^T V\right)_j &= \text{vec } (A_j)^T \text{ vec } \left(RR^T\right) = \text{tr } \left(A_j RR^T\right) \\
&= \text{tr } \left(A_j \left(I - P_Z\right) Y \left(\left(I - P_Z\right) Y\right)^T\right) \\
&= \text{tr } \left(\left(I - P_Z\right) \Gamma_j \left(I - P_Z\right) \left(I - P_Z\right) YY^T \left(I - P_Z\right)\right) \\
&= \text{tr } \left(\left(I - P_Z\right) \Gamma_j \left(I - P_Z\right) YY^T\right) = \\
&= \text{tr } \left(A_j YY^T\right) = \text{tr } \left(Y^T A_j Y\right) = Y^T A_j Y = W_j.
\end{aligned}$$

□

4.3 Variance components model

The variance component model is the appropriate model when some of the factors in an experiment have random effects. Recent textbooks dealing exclusively with the variance components model include Malley (1986), Rao and Kleffe (1988), Searle et al. (1992), Rao (1997) and Cox and Solomon (2003). The model is given in matrix notation by

$$Y = Z\theta + \sum_{j=1}^{v} U_j b_j, \tag{4.15}$$

where Z is a known $N \times p$ matrix and θ is a vector of unknown fixed parameters. The matrices U_j in (4.15) are known $N \times c_j$ matrices. Usually it is assumed that $U_1 = I_N$. The b_j are unknown random vectors that satisfy

$$\begin{aligned}
\text{E } (b_j) &= 0 && \text{for } j = 1, 2, \ldots, v; \\
\text{Var } (b_j) &= \sigma_j^2 \, I_{c_j} && \text{for } j = 1, 2, \ldots, v; \\
\text{Cov } (b_i, b_j) &= 0 && \text{for } i \neq j.
\end{aligned}$$

The parts $Z\theta$ and $\sum_{i=1}^{v} U_j b_j$ in (4.15) are usually referred to as the fixed and random part, respectively. Interest is in estimating the parameters $\theta_i, 1 \leq i \leq p$, and the variances $\sigma_j^2, 1 \leq j \leq v$.

4.3.1 Relation with mixed linear model

The variance components model given in (4.15) is a special instance of the mixed linear model in (4.1). The expectation of the random vector Y of observations under the variance components model is E $(Y) = Z\theta$ and the covariance matrix of Y is

$$\begin{aligned}
\text{Var } (Y) &= \text{Var } \left(\textstyle\sum_{j=1}^{v} U_j b_j\right) = \textstyle\sum_{j=1}^{v} \text{Var } (U_j b_j) \\
&= \textstyle\sum_{j=1}^{v} U_j \text{Var } (b_j) \, U_j^T = \textstyle\sum_{j=1}^{v} \sigma_j^2 U_j U_j^T.
\end{aligned}$$

Hence, the variance components model can be formulated as in (4.1) with matrices $\Gamma_j = U_j U_j^T$ and coefficients $\alpha_j = \sigma_j^2$. However, note that we have a restriction on the parameters α_j in the model. All parameters α_j need to be positive because they refer to the variances σ_j^2.

4.3.2 MINQUE estimation of variance components

MINQUE (MInimum Norm Quadratic Unbiased Estimation) estimation was introduced for uncorrelated heteroscedastic data in Rao (1970) and for variance components models in Rao (1972). This method of estimation considers unobservable "natural" estimates for the dispersion parameters and finds translation invariant quadratic unbiased estimates for the dispersion parameters $\alpha_1, \alpha_2, \ldots, \alpha_v$ that are closest to these natural estimates. The distance between an estimate and the natural estimate for each parameter is defined by a matrix norm which is usually taken to be the Euclidean norm. Consider the variance components model given in (4.15) with $U_1 = I_N$ and σ_1^2 the error variance. The vectors b_j in the model are unknown. However, if the vectors b_j were known then a natural estimator for the parameter $\alpha_j = \sigma_j^2$ would be $\frac{1}{c_j} b_j^T b_j$. We can express the variance components model (4.15) in the more compact form

$$Y = Z\theta + Ub,$$

where $U = (U_1 : U_2 : \cdots : U_v)$ and $b = \left(b_1^T : b_2^T : \cdots : b_v^T\right)^T$. In this notation the natural estimator for α_j can be expressed as $b^T \Delta_j b$ where Δ_j is a suitably defined diagonal matrix. In contrast the proposed estimator is of the form $Y^T M_j Y$ where the symmetric matrix M_j satisfies $M_j Z = 0$. That is, the proposed estimator is of the form

$$Y^T M_j Y = b^T U^T M_j U b.$$

The quadratic form $Y^T M_j Y$ is said to be a MINQUE estimator of α_j if the matrix M_j is determined such that a specified matrix norm $\left|\left|U^T M_j U - \Delta_j\right|\right|$ is minimized subject to the conditions $M_j Z = 0$ and $\text{tr}\left(M_j U_i U_i^T\right) = \delta_{ij}$ that force unbiasedness and translation invariance of the quadratic estimator. If the Euclidean norm $||M||_2 = \sqrt{\text{tr}\,(M^2)}$ is used then

$$\begin{aligned} \left|\left|U^T M_j U - \Delta_j\right|\right|_2^2 &= \text{tr}\left(U^T M_j U - \Delta_j\right)\left(U^T M_j U - \Delta_j\right) \\ &= \text{tr}\left(U^T M_j U U^T M_j U\right) + \text{tr}\left(\Delta_j^2\right) - 2\text{tr}\left(\Delta_j U^T M_j U\right) \end{aligned}$$

Note that $\Delta_j^2 = \Delta_j$ since Δ_j is a diagonal matrix with diagonal elements that are either zero or one. Since exactly c_i of these diagonal elements equal 1 we have that $\text{tr}\left(\Delta_j^2\right) = \text{tr}\,(\Delta_j) = c_j$. The part $\text{tr}\left(\Delta_j U^T M_j\right)$ can be simplified as

$$\text{tr}\left(\Delta_j U^T M_j U\right) = \text{tr}\left(U \Delta_j U^T M_j\right) = \text{tr}\left(U_j U_j^T M_j\right) = \text{tr}\left(M_j U_j U_j^T\right) = 1.$$

Hence, $\left|\left|U^T M_j U - \Delta_j\right|\right|_2^2 = \text{tr}\left(U^T M_j U U^T M_j U\right) + c_i - 2$. To find the MINQUE estimator we need to find the solution M_j of the problem

$$\begin{array}{l} \min \text{tr}\,(M_j V M_j V) \\ \text{subject to} \\ \left\{ \begin{array}{lcl} M_j Z & = & 0 \\ \text{tr}\left(M_j U_i U_i^T\right) & = & \delta_{ij} \text{ for } i = 1, 2, \ldots, v \end{array} \right. \end{array} \tag{4.16}$$

where $V = UU^T = \sum_{i=1}^{v} U_i U_i^T$.

In most cases the variance components $\sigma_i^2, 1 \leq i \leq v$, are not all equal. For this reason Rao (1973) proposes to express the difference $U^T M_j U - \Delta_j$ in terms of the standardized random vectors $s_i = {\sigma_i}^{-1} b_i$. In this way the quadratic form

$$s^T \Lambda^{\frac{1}{2}} \left(U^T M_j U - \Delta_j\right) \Lambda^{\frac{1}{2}} s$$

is obtained, where

$$\Lambda = \begin{pmatrix} \sigma_1^2 I_{c_1} & 0 & \cdots & 0 \\ 0 & \sigma_2^2 I_{c_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_v^2 I_{c_v} \end{pmatrix}.$$

If the standardized vectors and the Euclidean norm are used, then the minimization problem that needs to be solved in order to find the MINQUE estimators is

$$\begin{array}{l} \min \text{tr}\,(M_j V_\star M_j V_\star) \\ \text{subject to} \\ \left\{ \begin{array}{lcl} M_j Z & = & 0 \\ \text{tr}\left(M_j U_i U_i^T\right) & = & \delta_{ij} \text{ for } i = 1, 2, \ldots, v \end{array} \right. \end{array} \tag{4.17}$$

where

$$V_\star = \sum_{i=1}^{v} \sigma_i^2 U_i U_i^T. \tag{4.18}$$

The variance components σ_i^2 are unknown. However, if there is some a priori knowledge of the approximate ratios of σ_i^2, then we can substitute these into (4.18) and solve the minimization for the $V_\star$ computed.

The solution to the minimization problems (4.16) and (4.17) is given in the next theorem. Let V a positive definite matrix of size $N \times N$ and define the inner product $(\cdot, \cdot)_V : \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$ by $(a, b)_V = a^T V^{-1} b$. The projection operator onto the space spanned by the columns of Z using this inner product is

$$P = Z\left(Z^T V^{-1} Z\right)^- Z^T V^{-1},$$

where M^- denotes a generalized inverse of M.

Theorem 4.15 (Rao) *The minimum of tr* $(MVMV)$ *subject to the conditions*

$$\begin{cases} MZ & = & 0 \\ tr\left(M\Gamma_i\right) & = & a_i \text{ for } i = 1, 2, \ldots, v \end{cases}$$

is attained at

$$M = \sum_{i=1}^{v} \lambda_i V^{-1} \left(I - P\right) \Gamma_i V^{-1} \left(I - P\right)$$

where the vector $\lambda = \left(\lambda_1, \lambda_2, \ldots, \lambda_v\right)^T$ *is determined from the system* $S\lambda = a$ *of equations with* $a = \left(a_1, a_2, \ldots, a_v\right)^T$ *and the elements of the matrix* S *are given by* $S_{i,j} = tr\left(V^{-1}\left(I - P\right)\Gamma_i V^{-1}\left(I - P\right)\Gamma_j\right)$.

Proof See Rao (1972) p. 114. □

The solution to the minimization problem of (4.17) when the a priori values for the variance components are taken to be $\sigma_1^2 = 1$ and $\sigma_i^2 = 0$ for $i \neq 1$ was called the MINQUEO by Searle et al. (1992).

4.4 Dispersion effects from factorial designs

In this section we discuss the the estimation of dispersion effects from unreplicated two-level factorial designs and focus on the estimation methods that assume a mixed linear model for the data. Box and Meyer (1986) were the first to consider identifying both location and dispersion effects from unreplicated two-level fractional factorial designs. Since the publication of their paper a number of different procedures (both iterative and non-iterative) have been proposed for estimating the location and dispersion effects (Wang (1989); Nelder and Lee (1991); Engel and Huele (1996); Bergman and Hynén (1997); Wiklander (1998); Liao and Iyer (2000); McGrath and Lin (2001); Brenneman and Nair (2001); Wiklander and Holm (2003)). An overview and a critical analysis of most of these procedures is given by Brenneman and Nair (2001). In their paper they note that the analysis of location and dispersion effects is an intrinsically difficult problem and show that all methods proposed so far suffer from bias to some extent.

Most of the papers consider a log-linear model for the dispersion effects. However, several estimation methods have been proposed for cases in which a linear structure for the dispersion effects is more applicable. Under a linear structure for dispersion effects, non-iterative estimation methods were proposed by Wiklander (1998) (see also Wiklander and Holm (2003)), Liao and Iyer (2000) and Brenneman and Nair (2001). Brenneman and Nair (2001) suggest a linear regression of the squared residuals. This method can be applied for any design and the model in (4.1) provided that the matrices $\Gamma_i, 1 \leq i \leq v$, are diagonal. Liao and Iyer (2000) describe a general method for finding quadratic forms in the vector of observations that estimate the dispersion parameters $\alpha_1, \alpha_2, \ldots, \alpha_v$

in model (4.1). This estimator was already presented in its general form in Section 4.2.4. Although the estimation method proposed by Liao and Iyer (2000) applies to any design, the content of the paper is mainly restricted to estimation in two-level factorial designs. Liao and Iyer (2000) also present a method to construct two-level fractional factorial designs that are A-optimal for this method of estimation when there is only one factor responsible for the dispersion effects. The estimators proposed by Wiklander (1998) and Wiklander and Holm (2003) are sums of products of specific pairs of linear estimators of negligible (higher order) location effects. The use of this method is restricted to two-level factorial designs and regular fractions of such designs. Surprisingly, the three proposed methods for estimation are equivalent when the design is a two-level factorial design or a regular fraction of such a design. In this section a proof for the equivalence of these estimation methods is given.

The following additional notation will be used in this section. The design matrix $Z = (z_1 : z_2 : \ldots : z_p)$ is an $N \times p$ matrix with columns denoted by $z_1, z_2, \ldots, z_p$. We let the column z_1 correspond to the constant term in the model, *i.e.*, all entries in this column be equal to 1. The other columns of Z each correspond to a main-effect or interaction-effect. The jth entry in these columns equals 1 when the corresponding factor is at its high level and -1 when it is at its lower level in run j. The matrices $\Gamma_i, 1 \leq i \leq v$, are diagonal matrices. We let $\Gamma_1 = I$ and let the other matrices correspond to main-effects or interaction-effects. The jth diagonal element of Γ_i is 1 if the corresponding factor or interaction is at its higher level and -1 otherwise. Note that we do not assume that the location model and the dispersion model involve the same factors and interactions. As a consequence, the column z_i in Z and the diagonal of Γ_i do not necessarily coincide for $i \neq 1$.

In this section both full two-level factorial designs and regular fractions of these designs are considered. We assume that there is no confounding of the effects to which the matrices $\Gamma_i, 1 \leq i \leq v$, correspond. By Z_{ext} we denote the extended design matrix. In case of a full factorial design this is the $N \times N$ matrix that comes from extending the design matrix Z with all columns that correspond to location effects that are not in the model. In the case of a regular fraction the matrix Z_{ext} is defined as any non-unique matrix that results from extending the matrix Z to an $N \times N$ matrix for which the columns correspond to a maximum set of unconfounded effects. This will be illustrated in Section 4.4.2.

We let the operator $\circ$ denote the Hadamard product for vectors, *i.e.*, for $a = (a_1, a_2, \ldots, a_N)^T$ and $b = (b_1, b_2, \ldots, b_N)^T$ we let $a \circ b = (a_1 b_1, a_2 b_2, \ldots, a_N b_N)^T$. The columns of the extended design matrix Z_{ext} for a full factorial design form a group under this operation. Finally, by diag (M) we denote the diagonal of the matrix M as a column vector.

4.4.1 Estimation methods

Wiklander (1998) (see also Wiklander and Holm (2003)), Liao and Iyer (2000) and Brenneman and Nair (2001) proposed non-iterative methods for the esti-

mation of the dispersion effects in the model given in (4.1). The three methods for estimating the dispersion effects are described in this section.

Wiklander and Holm

Wiklander (1998) describes a method for finding estimators for the parameters $\alpha_1, \alpha_2, \ldots, \alpha_v$ when the design is a two-level full factorial design. In Wiklander and Holm (2003) the method is illustrated for regular fractions of such designs. Wiklander (1998) and Wiklander and Holm (2003) use the Ordinary Least Squares estimators of the negligible location effects to construct their estimators. A similar approach was used by Bergman and Hynén (1997) to construct a test statistic for testing for dispersion effects. The method for a 2^n full factorial design can be described as follows. Let Z_{ext} denote the $N \times N$ matrix resulting from extending the design matrix $Z = (z_1 : z_2 : \ldots : z_p)$ with columns corresponding to all effects that are not in the location model. The ith column of Z_{ext} is denoted by z_i. Wiklander (1998) and Wiklander and Holm (2003) propose a one-to-one transformation of the elements of Y into new random variables

$$T_i = \frac{1}{N} z_i^T Y \text{ for } 1 \leq i \leq N. \tag{4.19}$$

Note that the random variables $T_1, T_2, \ldots, T_p$ are unbiased estimators for the location effects. These estimators need not be independent. The estimators for the dispersion parameters are constructed using products of specific pairs of random variables in the set $\{T_i \mid p+1 \leq i \leq N\}$. More precisely, for any pair (i, j) such that diag $(\Gamma_\ell) = z_i \circ z_j$ and $p+1 \leq i \leq j \leq N$ we have that NT_iT_j is an unbiased estimator for α_ℓ. The estimator for α_ℓ proposed by Wiklander (1998) and Wiklander and Holm (2003) is the average of all such estimators with different i and j. This is the estimator that we consider in this chapter. Wiklander (1998) and Wiklander and Holm (2003) also propose a reduced estimator consisting of the maximum number of independent estimators NT_iT_j. We do not consider this reduced estimator here.

For a regular fraction a slight modification is needed. Let $s = k - m$, then the extended design matrix of a regular 2^{k-m} fraction is equal to that of a 2^s full factorial design up to the signs of the columns. If for a certain pair (i, j) with $p+1 \leq i \leq j \leq N$ and $\ell \in \{1, 2, \ldots, v\}$ we have diag $(\Gamma_\ell) = z_i \circ z_j$, then $E(NT_iT_j) = \alpha_\ell$. If, on the other hand, diag $(\Gamma_\ell) = -z_i \circ z_j$, then $E(-NT_iT_j) = \alpha_\ell$. The proposed unbiased estimator for α_ℓ is the average of all estimators $\pm NT_iT_j$ of these two types.

Liao and Iyer

The estimation method proposed by Liao and Iyer (2000) was considered in Section 4.2.4. For this reason we only briefly summarize their method here. In order to estimate the dispersion parameters in the model (4.1), Liao and Iyer (2000) define matrices $A_1, A_2, \ldots, A_v$ of the form

$$A_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)\,, \tag{4.20}$$

where P_Z is the projection matrix onto the column space of Z, *i.e.*

$$P_Z = Z\left(Z^T Z\right)^- Z^T,$$

where $\left(Z^T Z\right)^-$ denotes a generalized inverse of $Z^T Z$ (see Chapter 1 of Searle (1971) and Chapter 9 of Harville (1997) for a definition). Note that $I - P_Z$ is the projection on the orthogonal complement of the range of Z, *i.e*, onto the space spanned by the columns in Z_{ext} that are not in Z. Define the vector $W = \left(Y^T A_1 Y, Y^T A_2 Y, \ldots, Y^T A_v Y\right)^T$ and the matrix K by

$$K = \begin{pmatrix} \text{tr}\,(A_1\Gamma_1) & \text{tr}\,(A_1\Gamma_2) & \ldots & \text{tr}\,(A_1\Gamma_v) \\ \text{tr}\,(A_2\Gamma_1) & \text{tr}\,(A_2\Gamma_2) & \ldots & \text{tr}\,(A_2\Gamma_v) \\ \vdots & \vdots & \ddots & \vdots \\ \text{tr}\,(A_v\Gamma_1) & \text{tr}\,(A_v\Gamma_2) & \ldots & \text{tr}\,(A_v\Gamma_v) \end{pmatrix}. \tag{4.21}$$

If K is invertible then

$$K^{-1}W \tag{4.22}$$

is an unbiased estimator for $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_v)^T$.

For the case $v = 2$ Liao and Iyer (2000) propose a method to determine regular two-level fractional factorial designs of resolution at least III that are A-optimal for estimating the parameters α_1 and α_2 using this method.

Brenneman and Nair

Under model (4.1) with the Γ_i diagonal, Brenneman and Nair (2001) propose using a linear regression of the squared residuals after estimating the location effects using Ordinary Least Squares estimation. The covariance matrix of the vector R of residuals is given by

$$\text{Var}\,(R) = \text{Var}\,((I - P_Z)\,Y) = (I - P_Z)\,\text{Var}\,(Y)\,(I - P_Z)\,.$$

Given model (4.1) this matrix can be expressed in terms of the parameters $\alpha_1, \alpha_2, \ldots, \alpha_v$ by

$$\text{Var}\,(R) = \sum_{1 \le j \le v} \alpha_j\,(I - P_Z)\,\Gamma_j\,(I - P_Z) = \sum_{1 \le j \le v} \alpha_j A_j,$$

with A_j defined as in (4.20). Let $R^\star$ denote the vector of squared residuals. Since $E\,(R) = 0$ the model for the squared residuals is given by

$$E\,(R^\star) = \text{diag}\,(\text{Var}\,(R)) = B\alpha,$$

where

$$B = \begin{pmatrix} \text{diag}\,(A_1) & : & \text{diag}\,(A_2) & : & \ldots & : & \text{diag}\,(A_v) \end{pmatrix}.$$

If B is full rank then an unbiased estimator for α is

$$\left(B^T B\right)^{-1} B^T R^\star. \tag{4.23}$$

For the case of a two-level full factorial design, let $p_\ell, 2 \leq \ell \leq v$, denote the number of pairs of columns z_i and z_j in Z for which diag $(\Gamma_\ell) = z_i \circ z_j$. By R_i we denote the ith element of the vector R of residuals. Brenneman and Nair (2001) showed if $2 \leq \ell \leq v$ and $N > 2\,(p - p_\ell)$ then

$$\frac{1}{N - 2\,(p - p_\ell)} \left(\sum_{i:(\Gamma_\ell)_{i,i}=1} R_i^2 - \sum_{i:(\Gamma_\ell)_{i,i}=-1} R_i^2 \right) \tag{4.24}$$

is an unbiased estimator for α_ℓ. Brenneman and Nair (2001) do not give an explicit expression for the estimator of α_1 that is obtained using their method. For $N > p$ the estimator for α_1 obtained using a linear regression of the squared residuals is equal to

$$\frac{1}{N - p} \sum_{1 \leq i \leq N} R_i^2. \tag{4.25}$$

This can be shown by explicitly calculating (4.23). When the design is a regular fraction then the expression for α_1 given in (4.25) remains valid. However, a slight adjustment must be made to (4.24). That is, for regular fractions p_ℓ should be defined as the number of pairs of columns z_i and z_j in Z for which diag $(\Gamma_\ell) = \pm\, z_i \circ z_j$. A detailed proof of the results can be found in Brenneman and Nair (2001) (for the full factorial case) and Appendix A of this thesis.

4.4.2 Equivalence of estimation methods

In this section we show that the three methods of estimation described in Section 4.4.1 give the same estimates for the dispersion parameters in model (4.1) for two-level full factorial designs and regular fractions of these designs.

Full factorial designs

Consider a 2^k full factorial design. Before we show equality of the estimators, we first give a lemma that we need in the proof. Recall that the extended design matrix Z_{ext} for a two-level full factorial design is the $N \times N$ matrix that comes from extending the design matrix Z with all columns corresponding to the location effects that are not in the model. The columns in the extended design matrix Z_{ext} of a full factorial design form a group with the Hadamard product $\circ$. The identity element in this group is the vector of length N with each element equal to 1. We will denote this identity element by z_1. The proof of the next lemma uses the group property and orthogonality of the columns in Z_{ext}.

Lemma 4.16 *Let z_i and z_j be columns in the extended design matrix Z_{ext} of a two-level full factorial design and let Γ denote a diagonal matrix with a column of Z_{ext} as its diagonal, then we have*

$$z_i^T \Gamma z_j = \begin{cases} N & \text{if } diag\,(\Gamma) = z_i \circ z_j \\ 0 & \text{otherwise} \end{cases}.$$

Proof If the diagonal of Γ equals the column z_ℓ of Z_{ext}, then

$$z_i^T \Gamma z_j = (z_i \circ z_\ell)^T z_j = \begin{cases} N & \text{if } z_j = (z_i \circ z_\ell) \\ 0 & \text{otherwise} \end{cases}.$$

Since all elements of z_i are non-zero we have

$$z_j = z_i \circ z_\ell \Leftrightarrow z_i \circ z_j = z_i \circ z_i \circ z_\ell = z_1 \circ z_\ell = z_\ell = \text{diag}\,(\Gamma),$$

which completes the proof. □

Our main theorem shows the equivalence of the three estimation methods discussed in Section 4.4.1 when the design is a 2^k full factorial design.

Theorem 4.17 *Assume that data is obtained on an unreplicated two-level full factorial design. The estimation methods proposed by (i) Wiklander (1998) and Wiklander and Holm (2003), (ii) Liao and Iyer (2000) and (iii) Brenneman and Nair (2001) all give the same estimates for the parameters $\alpha_1, \alpha_2, \ldots, \alpha_v$ in (4.1).*

Proof We will first show equality of the estimators proposed by Wiklander (1998) and Liao and Iyer (2000). First consider the estimation method proposed by Liao and Iyer (2000) and described in Section 4.4.1. We show that the matrix K given in (4.21) is a diagonal matrix. Let $q_1, q_2, \ldots, q_N$ denote the columns in the extended design matrix Z_{ext} after normalization, *i.e.*, $q_i = \frac{z_i}{\sqrt{N}}$ for all i, and let the matrices Q_{ij} be defined as in (4.7). Since $\{q_1, q_2, \ldots, q_N\}$ is an orthonormal basis for $\mathbb{R}^N$ it follows from Theorem 4.6 that $\{Q_{ij} \mid 1 \le i \le j \le N\}$ is an orthonormal basis for the inner product space $(\mathcal{M}, \langle \cdot, \cdot \rangle)$. By (4.6) we have that each matrix Γ_ℓ has a unique representation of the form

$$\Gamma_\ell = \sum_{1 \le i \le j \le N} \langle \Gamma_\ell, Q_{ij} \rangle \, Q_{ij}.$$

The coefficient of the matrix $Q_{ii}, i = 1, \ldots, N$, in this representation equals

$$\langle \Gamma_\ell, Q_{ii} \rangle = \text{tr}\,\left(\Gamma_\ell q_i q_i^T\right) = q_i^T \Gamma_\ell q_i = \frac{1}{N} z_i^T \Gamma_\ell z_i = \delta_{\ell 1}.$$

The coefficients of matrix Q_{ij} where $i \neq j$ are given by

$$\langle \Gamma_\ell, Q_{ij} \rangle = \frac{1}{\sqrt{2}} \text{tr}\,\left(\Gamma_\ell q_i q_j^T + \Gamma_\ell q_j q_i^T\right) = \sqrt{2} q_i^T \Gamma_\ell q_j.$$

Using $q_i = \frac{z_i}{\sqrt{N}}$ and Lemma 4.16 we find

$$\langle \Gamma_\ell, Q_{ij} \rangle = \frac{\sqrt{2}}{N} z_i^T \Gamma_\ell z_j = \begin{cases} \sqrt{2} & \text{if diag}\,(\Gamma_\ell) = z_i \circ z_j \\ 0 & \text{otherwise} \end{cases}.$$

The matrix Γ_1 can be expressed in terms of the matrices Q_{ij} in the following way

$$\Gamma_1 = \sum_{1 \le i \le N} Q_{ii}. \tag{4.26}$$

The matrices $\Gamma_\ell, 2 \le \ell \le v$, are given in terms of the matrices Q_{ij} by

$$\Gamma_\ell = \sqrt{2} \sum Q_{ij}, \tag{4.27}$$

where the summation is over all different pairs (i, j) for which $1 \le i \le j \le N$ and $z_i \circ z_j = \text{diag}\,(\Gamma_\ell)$. Note that since $z_1, z_2, \ldots, z_p$ are columns in Z and the columns $z_{p+1}, z_{p+2}, \ldots, z_N$ of Z_{ext} are orthogonal to span $\{z_1, z_2, \ldots, z_p\}$ we have

$$(I - P_Z)\, Q_{ij}\, (I - P_Z) = \begin{cases} Q_{ij} & \text{if } p+1 \le i \le j \le N \\ 0 & \text{otherwise} \end{cases}.$$

The matrix A_1 defined in (4.20) is uniquely represented in terms of the matrices Q_{ij} by

$$A_1 = \sum_{p+1 \le i \le N} Q_{ii}. \tag{4.28}$$

Let Ω_ℓ denote the set of all pairs (i, j) with $p + 1 \le i \le j \le N$ for which $z_i \circ z_j = \text{diag}\,(\Gamma_\ell)$. The matrices $A_\ell, 2 \le \ell \le v$, defined in (4.20) are uniquely represented by

$$A_\ell = \sqrt{2} \sum_{(i,j) \in \Omega_\ell} Q_{ij}. \tag{4.29}$$

The elements of the matrix K are given by

$$\text{tr}\,(A_\ell \Gamma_j) = \langle A_\ell, \Gamma_j \rangle. \tag{4.30}$$

Substituting (4.26), (4.27), (4.28) and (4.29) into (4.30) and using that the matrices Q_{ij} form an orthonormal set we find

$$\text{tr}\,(A_\ell \Gamma_j) = \begin{cases} N - p & \text{if } j = \ell = 1 \\ 2\,|\Omega_\ell| & \text{if } 2 \le j = \ell \le v \\ 0 & \text{otherwise} \end{cases}.$$

Hence, the matrix K is a diagonal matrix with

$$(N - p,\, 2\,|\Omega_2|\,,\, 2\,|\Omega_3|\,,\, \ldots,\, 2\,|\Omega_v|)^T$$

as its diagonal. The estimator for α_1 proposed by Liao and Iyer (2000) is

$$\frac{1}{N-p} Y^T A_1 Y. \tag{4.31}$$

The estimator proposed for $\alpha_\ell, 2 \leq \ell \leq v$, is

$$\frac{1}{2\left|\Omega_\ell\right|} Y^T A_\ell Y. \tag{4.32}$$

For $2 \leq \ell \leq v$, we find that after substitution of A_ℓ in (4.32) by its expansion given in (4.29) and replacing Q_{ij} and T_i using (4.7) and (4.19), respectively, the estimator for α_ℓ in (4.32) can be written as

$$\begin{aligned} \tfrac{1}{2\left|\Omega_\ell\right|} Y^T A_\ell Y &= \tfrac{1}{\sqrt{2}\left|\Omega_\ell\right|} \textstyle\sum_{(i,j)\in\Omega_\ell} Y^T Q_{ij} Y \\ &= \tfrac{1}{N\left|\Omega_\ell\right|} \textstyle\sum_{(i,j)\in\Omega_\ell} z_i^T Y z_j^T Y \\ &= \tfrac{1}{N\left|\Omega_\ell\right|} \textstyle\sum_{(i,j)\in\Omega_\ell} N T_i N T_j \\ &= \tfrac{1}{\left|\Omega_\ell\right|} \textstyle\sum_{(i,j)\in\Omega_\ell} N T_i T_j. \end{aligned} \tag{4.33}$$

Recall from Section 4.4.1 that the estimator for α_ℓ proposed by Wiklander (1998) and Wiklander and Holm (2003) was the average of all NT_iT_j over pairs (i, j) with $p + 1 \leq i \leq j \leq N$ for which $\operatorname{diag}(\Gamma_\ell) = z_i \circ z_j$. This is exactly the right-hand side of (4.33). Now, for α_1 we find that after substitution of A_1 in (4.31) by its expansion given in (4.28) and replacing Q_{ij} and T_j using (4.7) and (4.19), respectively, we find that the estimator in (4.31) can be expressed as

$$\begin{aligned} \tfrac{1}{N-p} Y^T A_1 Y &= \tfrac{1}{N-p} \textstyle\sum_{p+1\leq i\leq N} Y^T Q_{ii} Y \\ &= \tfrac{1}{N-p} \textstyle\sum_{p+1\leq i\leq N} \tfrac{1}{N} z_i^T Y z_i^T Y \\ &= \tfrac{1}{N(N-p)} \textstyle\sum_{p+1\leq i\leq N} N T_i N T_i \\ &= \tfrac{1}{N-p} \textstyle\sum_{p+1\leq i\leq N} N T_i^2. \end{aligned} \tag{4.34}$$

To see that the right-hand side of (4.34) is equal to the estimator proposed by Wiklander (1998) and Wiklander and Holm (2003) observe that $z_i \circ z_j = z_1$ if and only if $i = j$.

We will now show equality of the estimators proposed by Liao and Iyer (2000) and Brenneman and Nair (2001). The estimator for $\alpha_\ell, 2 \leq \ell \leq v$, proposed by Brenneman and Nair (2001) is given in (4.24). Observe that this estimator can be written as a quadratic form in the residuals,

$$\frac{1}{N - 2\left(p - p_\ell\right)} \left(\sum_{i:(\Gamma_\ell)_{i,i}=1} R_i^2 - \sum_{i:(\Gamma_\ell)_{i,i}=-1} R_i^2 \right) = \frac{1}{N - 2\left(p - p_k\right)} R^T \Gamma_\ell R. \tag{4.35}$$

Since the location effects are estimated using Ordinary Least Squares we have that

$$R = \left(I - P_Z\right) Y. \tag{4.36}$$

Substituting (4.36) into the right-hand side of (4.35) we find that the proposed estimator equals

$$\frac{1}{N - 2\left(p - p_\ell\right)} Y^T \left(I - P_Z\right) \Gamma_\ell \left(I - P_Z\right) Y = \frac{1}{N - 2\left(p - p_\ell\right)} Y^T A_\ell Y, \tag{4.37}$$

with A_ℓ given in (4.20). Note that there are $\frac{N}{2}$ pairs of columns z_i and z_j in Z_{ext} such that $z_i \circ z_j = \text{diag}\,(\Gamma_\ell)$. For p_ℓ of these pairs both z_i and z_j are in Z (by the definition of p_ℓ). For all other $p - 2p_\ell$ columns z_i in Z there exists a column $z_j, p+1 \leq j \leq N$, of Z_{ext} such that $z_i \circ z_j = \text{diag}\,(\Gamma_\ell)$. The number $|\Omega_\ell|$ of columns z_i and z_j with $p+1 \leq i \leq j \leq N$ for which $z_i \circ z_j = \text{diag}\,(\Gamma_\ell)$ is, hence, $\frac{N}{2} - p_\ell - (p - 2p_\ell) = \frac{N}{2} - (p - p_\ell)$. Substitution of $\frac{N}{2} - (p - p_\ell) = |\Omega_\ell|$ into (4.37) gives

$$\frac{1}{2\,|\Omega_\ell|} Y^T A_\ell Y,$$

which equals (4.32). The estimator for α_1 obtained using a linear regression of the squared residuals is

$$\frac{1}{N-p} \sum_{1 \leq i \leq N} R_i^2 = \frac{1}{N-p} R^T \Gamma_1 R = \frac{1}{N-p} Y^T A_1 Y,$$

which equals (4.31). Hence, also the estimators for α_ℓ proposed by Brenneman and Nair (2001) and Liao and Iyer (2000) are equal for all $1 \leq \ell \leq v$. □

Regular fractions

We now show the equivalence of the estimation methods proposed by Wiklander and Holm (2003), Liao and Iyer (2000) and Brenneman and Nair (2001) for regular 2^{k-m} fractions of two-level factorial designs. Let $N = 2^{k-m}$ denote the number of runs in the fraction. Recall that the extended design matrix for a regular fraction is defined as any non-unique matrix that results from extending the matrix Z to a $N \times N$ matrix for which the columns correspond to a maximal set of unconfounded effects. In the full factorial case the columns in the extended design matrix form a group with respect to the Hadamard product. For regular fractions the columns of an extended design matrix do not always have this property. This is illustrated by the next example.

Example Consider the regular 2^{3-1} fractional factorial design given in Table 4.1. The matrix Z consisting of the columns in the table is a $N \times N$ matrix with columns corresponding to a maximal set of unconfounded effects. Hence, $Z_{\text{ext}} = Z$ is an extended design matrix for the design. Let z_i denote the ith column in Table 4.1, then $Z_{\text{ext}} = \begin{pmatrix} z_1 & : & z_2 & : & z_3 & : & z_4 \end{pmatrix}$. For this extended design matrix we have that $z_2 \circ z_3 = -z_4$. Since $-z_4$ is not a column in the extended design matrix Z_{ext}, the columns z_1, z_2, z_3 and z_4 do not form a group with the Hadamard product $\circ$.

We have shown that the columns of the extended design matrix for regular fractions in general do not form a group with operation $\circ$. However, if Z_{ext} is an extended design matrix for a regular two-level fractional factorial design and z_i and z_j are columns in Z_{ext} then either $z_i \circ z_j$ or $-z_i \circ z_j$ is a column in Z_{ext}. We will use this property to proof that the three methods also give the same estimators in regular fractions of two-level factorial designs. The next theorem states the equivalence for regular two-level fractional factorial designs.

Table 4.1: Fraction of the 2^3 factorial design with $I = -X_1X_2X_3$.

Run	I	X_1	X_2	X_3
1	1	-1	-1	-1
2	1	1	-1	1
3	1	-1	1	1
4	1	1	1	-1

Theorem 4.18 *Assume that data is obtained on a regular fraction of a two-level full factorial design. The estimation methods proposed by (i) Wiklander and Holm (2003), (ii) Liao and Iyer (2000) and (iii) Brenneman and Nair (2001) all give the same estimates for the parameters $\alpha_1, \alpha_2, \ldots, \alpha_v$ in (4.1).*

Proof We will first show that the methods proposed by Wiklander and Holm (2003) and Liao and Iyer (2000) yield the same estimates. First consider the estimation method proposed by Liao and Iyer (2000) and described in Section 4.4.1. We show that the matrix K given in (4.21) is a diagonal matrix. Let $q_1, q_2, \ldots, q_N$ denote the columns in the extended design matrix Z_{ext} after normalization, *i.e.*, $q_i = \frac{z_i}{\sqrt{N}}$ for all i. Let matrices Q_{ij} be defined as in (4.7). Then we have

$$\langle \Gamma_\ell, Q_{ij} \rangle = \begin{cases} -\sqrt{2} & \text{if diag } (\Gamma_\ell) = -z_i \circ z_j \\ \sqrt{2} & \text{if diag } (\Gamma_\ell) = z_i \circ z_j \\ 0 & \text{otherwise} \end{cases} .$$

Using the expansion in (4.6) the matrices Γ_ℓ can be written in terms of matrices Q_{ij} as follows

$$\Gamma_\ell = \begin{cases} \sum_{1 \le i \le N} Q_{ii} & \text{for } \ell = 1 \\ \sqrt{2} \sum_{+} Q_{ij} - \sqrt{2} \sum_{-} Q_{ij} & \text{for } 2 \le \ell \le v \end{cases} . \tag{4.38}$$

where $\sum_+$ and $\sum_-$ denote the sums over all pairs $(i,j), 1 \le i \le j \le N$, for which $z_i \circ z_j = \text{diag } (\Gamma_\ell)$ and $z_i \circ z_j = -\text{diag } (\Gamma_\ell)$, respectively. Let $\Omega_{\ell+}$ and $\Omega_{\ell-}$ denote the sets of all pairs $(i,j), p+1 \le i \le j \le N$, for which $z_i \circ z_j = \text{diag } (\Gamma_\ell)$ and $z_i \circ z_j = -\text{diag } (\Gamma_\ell)$, respectively. Then the matrices A_ℓ can be written in terms of the matrices Q_{ij} as follows

$$A_\ell = \begin{cases} \sum_{p+1 \le i \le N} Q_{ii} & \text{for } \ell = 1 \\ \sqrt{2} \sum_{(i,j) \in \Omega_{\ell+}} Q_{ij} - \sqrt{2} \sum_{(i,j) \in \Omega_{\ell-}} Q_{ij} & \text{for } 2 \le \ell \le v \end{cases} . \tag{4.39}$$

Using the expansions (4.38) and (4.39) and the orthonormality of the matrices

Q_{ij} we find that the elements in the matrix K given in (4.21) are

$$\text{tr } (A_\ell \Gamma_j) = \langle A_\ell, \Gamma_j \rangle = \begin{cases} N-p & \text{if } j = \ell = 1 \\ 2\left(|\Omega_{\ell+}| + |\Omega_{\ell-}|\right) & \text{if } 2 \leq j = \ell \leq v \\ 0 & \text{otherwise} \end{cases} .$$

Hence, also for regular fractions we have that the matrix K is diagonal. We find that the estimator for α_1 proposed by Liao and Iyer (2000) is

$$\frac{1}{N-p} Y^T A_1 Y, \tag{4.40}$$

which in (4.34) is shown to be equal to

$$\frac{1}{N-p} \sum_{p+1 \leq i \leq N} N T_i^2.$$

Note that also in the case of a regular fraction the columns in Z_{ext} satisfy $z_i \circ z_j = z_1$ if and only if $i = j$, from which the equality of the estimators for α_1 proposed by Liao and Iyer (2000) and Wiklander and Holm (2003) follows. The estimator for $\alpha_\ell, 2 \leq \ell \leq v$, proposed by Liao and Iyer (2000) is

$$\frac{1}{2\left(|\Omega_{\ell+}| + |\Omega_{\ell-}|\right)} Y^T A_\ell Y. \tag{4.41}$$

This estimator can be expressed as

$$\begin{aligned} &\frac{1}{2\sqrt{2}\left(|\Omega_{\ell+}| + |\Omega_{\ell-}|\right)} \left(\sum\nolimits_{(i,j) \in \Omega_{\ell+}} Y^T Q_{ij} Y - \sum\nolimits_{(i,j) \in \Omega_{\ell-}} Y^T Q_{ij} Y \right) \\ &= \frac{1}{2\left(|\Omega_{\ell+}| + |\Omega_{\ell-}|\right)} \left(\sum\nolimits_{(i,j) \in \Omega_{\ell+}} N T_i T_j + \sum\nolimits_{(i,j) \in \Omega_{\ell-}} (-N T_i T_j) \right), \end{aligned} \tag{4.42}$$

which is the estimator proposed by Wiklander and Holm (2003) for a regular fraction.

We will now show that the estimation methods proposed by Liao and Iyer (2000) and Brenneman and Nair (2001) are equal. The estimator for $\alpha_\ell, 2 \leq \ell \leq v$, proposed by Brenneman and Nair (2001) is given by

$$\frac{1}{N - 2(p - p_\ell)} \left(\sum_{i:(\Gamma_\ell)_{i,i}=1} R_i^2 - \sum_{i:(\Gamma_\ell)_{i,i}=-1} R_i^2 \right) = \frac{1}{N - 2(p - p_\ell)} Y^T A_\ell Y, \tag{4.43}$$

where $p_\ell, 2 \leq \ell \leq v$, denotes the number of pairs of columns z_i and z_j in Z for which $\text{diag } (\Gamma_\ell) = \pm z_i \circ z_j$. There are $\frac{N}{2}$ pairs of columns in Z_{ext} for which $z_i \circ z_j = \pm \text{diag } (\Gamma_\ell)$. For all other $p - 2p_\ell$ columns z_i in Z there exists a column $z_j, p+1 \leq j \leq N$, of Z_{ext} such that $z_i \circ z_j = \pm \text{diag } (\Gamma_\ell)$. The

Table 4.2: A non-regular fraction of the 2^4 factorial design.

Run	X_1	X_2	X_3	X_4
1	-1	-1	-1	-1
2	1	-1	-1	-1
3	-1	-1	1	-1
4	1	1	1	-1
5	-1	1	-1	1
6	1	1	-1	1
7	1	-1	1	1
8	-1	1	1	1

number $|\Omega_{\ell+}| + |\Omega_{\ell-}|$ of columns z_i and z_j with $p+1 \leq i \leq j \leq N$ for which $z_i \circ z_j = \pm\text{diag}\,(\Gamma_\ell)$ is, hence, $\frac{N}{2} - p_\ell - (p - 2p_\ell) = \frac{N}{2} - (p - p_\ell)$. Substitution of $\frac{N}{2} - (p - p_\ell) = |\Omega_{\ell+}| + |\Omega_{\ell-}|$ into (4.43) gives (4.41) which is the estimator proposed by Liao and Iyer (2000). The estimator for α_1 obtained using a linear regression of the squared residuals is given in (4.25) and equals

$$\frac{1}{N-p} \sum_{1 \leq i \leq N} R_i^2 = \frac{1}{N-p} R^T \Gamma_1 R = \frac{1}{N-p} Y^T A_1 Y.$$

The expression on the right-hand side is the estimator in (4.40) proposed by Liao and Iyer (2000). Hence, also the estimators for α_ℓ proposed by Brenneman and Nair (2001) and Liao and Iyer (2000) are equal for all $1 \leq \ell \leq v$. □

Non-regular fractions of 2^p designs

The use of methods proposed by Liao and Iyer (2000) and Brenneman and Nair (2001) is not limited to factorial designs and regular fractions of these designs. The equivalence, however, does not generalize to non-regular fractions of two-level factorial designs. This is shown by the next example.

Example 4.19 To illustrate that the estimators for the dispersion effects obtained with methods proposed by Liao and Iyer (2000) and Brenneman and Nair (2001) may differ in the case of a non-regular two-level factorial design, we consider the non-regular fraction of the 2^4 factorial design given in Table 4.2. We consider a main-effects model for the mean and assume that only the factor X_1 has a possible dispersion effect. The estimator for the vector $\alpha = (\alpha_1, \alpha_2)^T$ proposed by Liao and Iyer (2000) is given in (4.22). We find the dispersion effect

α_2 associated with factor X_1 is estimated by $Y^T M_{\mathrm{LI}} Y$ with M_{LI} given by

$$\begin{pmatrix} -0.125 & -0.125 & 0.221 & 0.029 & 0.183 & 0.067 & 0.029 & -0.279 \\ -0.125 & 0.221 & -0.067 & -0.029 & 0.067 & -0.163 & -0.029 & 0.125 \\ 0.221 & -0.067 & -0.125 & -0.029 & -0.279 & 0.125 & -0.029 & 0.183 \\ 0.029 & -0.029 & -0.029 & 0.029 & 0.029 & -0.029 & 0.029 & -0.029 \\ 0.183 & 0.067 & -0.279 & 0.029 & -0.125 & -0.125 & 0.029 & 0.221 \\ 0.067 & -0.163 & 0.125 & -0.029 & -0.125 & 0.221 & -0.029 & -0.067 \\ 0.029 & -0.029 & -0.029 & 0.029 & 0.029 & -0.029 & 0.029 & -0.029 \\ -0.279 & 0.125 & 0.183 & -0.029 & 0.221 & -0.067 & -0.029 & -0.125 \end{pmatrix}.$$

The estimator for the vector α proposed by Brenneman and Nair (2001) is given in (4.23). For the dispersion effect α_2 of factor X_1 we find the estimator $Y^T M_{\mathrm{BN}} Y$ with M_{BN} given by

$$\begin{pmatrix} -0.125 & -0.125 & 0.246 & 0.004 & 0.134 & 0.116 & 0.004 & -0.254 \\ -0.125 & 0.246 & -0.116 & -0.004 & 0.116 & -0.237 & -0.004 & 0.125 \\ 0.246 & -0.116 & -0.125 & -0.004 & -0.254 & 0.125 & -0.004 & 0.134 \\ 0.004 & -0.004 & -0.004 & 0.004 & 0.004 & -0.004 & 0.004 & -0.004 \\ 0.134 & 0.116 & -0.254 & 0.004 & -0.125 & -0.125 & 0.004 & 0.246 \\ 0.116 & -0.237 & 0.125 & -0.004 & -0.125 & 0.246 & -0.004 & -0.116 \\ 0.004 & -0.004 & -0.004 & 0.004 & 0.004 & -0.004 & 0.004 & -0.004 \\ -0.254 & 0.125 & 0.134 & -0.004 & 0.246 & -0.116 & -0.004 & -0.125 \end{pmatrix}.$$

The entries of the matrices M_{LI} and M_{BN} were first computed exactly and only replaced by numerical values in the end. Given symmetric matrices A and B we have that the statement $Y^T AY = Y^T BY$ is true for all $Y \in \mathbb{R}^N$ if and only if $A = B$. Since some of the entries in the matrices M_{LI} and M_{BN} differ, the equality of the estimators obtained using the two methods does not hold for general $Y \in \mathbb{R}^N$.

4.4.3 MINQUE estimation of dispersion effects

MINQUE estimation is usually discussed in relation to variance components models. However, the estimators for the dispersion effects in two-level factorial designs and their regular fractions that we considered Section 4.4.1 can also be shown to be MINQUE estimators. Brenneman and Nair (2001) mention that the estimator they propose is a special case of the MINQUE estimator that has been studied in the variance components literature. Liao and Iyer (2000) also remark that the parameter estimates given in (4.13) are MINQUE estimators for the dispersion parameters. A precise argument for this, however, is lacking in both papers. We add a precise argument for this remark which is similar to the argument that Rao (1972) uses to justify the MINQUE property. To this end, we let

$$Y = Z\theta + \varepsilon$$

where ε is used to denote the random part. If ε were exactly known, then a natural estimator for the dispersion parameter α_j would have been $\frac{1}{N}\varepsilon^T\Gamma_j\varepsilon$. However, the proposed estimator is Y^TM_jY where the matrix M_j satisfies $M_jZ = 0$ and tr $(M_j\Gamma_i) = \delta_{ij}$ for all i. Note that for all matrices M_j satisfying $M_jZ = 0$ we have that $Y^TM_jY = \varepsilon^TM_j\varepsilon$. The MINQUE estimator for α_j is the translation invariant unbiased quadratic form Y^TM_jY where M_j minimizes

$$\left|\left|\frac{\Gamma_j}{N} - M_j\right|\right|$$

for some matrix norm $||\cdot||$. If the Euclidean norm is chosen, then

$$\begin{aligned}\left|\left|\tfrac{\Gamma_j}{N} - M_j\right|\right|_2^2 &= \text{tr}\left(\tfrac{\Gamma_j}{N} - M_j\right)\left(\tfrac{\Gamma_j}{N} - M_j\right)\\ &= \tfrac{1}{N^2}\text{tr}\,(\Gamma_j\Gamma_j) - \tfrac{2}{N}\text{tr}\,(M_j\Gamma_j) + \text{tr}\left(M_j^2\right)\\ &= \text{tr}\left(\tfrac{1}{N^2}I_N\right) - \text{tr}\left(\tfrac{2}{N}M_j\Gamma_j\right) + \text{tr}\left(M_j^2\right).\end{aligned}$$

Using Lemma 4.4 we find that if Y^TM_jY is an unbiased translation invariant estimator for α_j, then we must have that tr $(M_j\Gamma_j) = 1$ which implies that

$$\left|\left|\frac{\Gamma_j}{N} - M_j\right|\right|_2^2 = \frac{1}{N} - \frac{2}{N} + \text{tr}\left(M_j^2\right) = -\frac{1}{N} + \text{tr}\left(M_j^2\right).$$

Hence, finding the MINQUE estimator for the dispersion parameter α_j requires that we find the unbiased translation invariant quadratic form Y^TM_jY that minimizes tr $\left(M_j^2\right)$. That is, we need to solve the minimization problem

$$\begin{aligned}&\min \text{tr}\left(M_j^2\right)\\ &\text{subject to}\\ &\begin{cases} M_jZ &= 0\\ \text{tr}\,(M_j\Gamma_i) &= \delta_{ij} \text{ for } i = 1, 2, \ldots, v\end{cases}.\end{aligned}$$

The solution to this problem is found using Theorem 4.15 and by taking $V = I_N$. Note that for this choice of V we have that

$$P = Z\left(Z^TZ\right)^-Z^T = P_Z$$

and

$$S_{i,j} = \text{tr}\,((I - P_Z)\,\Gamma_i\,(I - P_Z)\,\Gamma_j) = K_{i,j}$$

with K is the matrix given in (4.21). Using that $S = K$ we find that the solution for λ of the equation $S\lambda = e_j$ is the jth column of the matrix K^{-1}. Note that K is symmetric implies that K^{-1} is symmetric. This implies that the solution of $K\lambda = e_j$ is also the jth row of the matrix K^{-1}. It is now easily verified that the vector $K^{-1}W$ in (4.22) contains a set of translation invariant unbiased estimators Y^TM_jY for the dispersion parameters α_j for which $||M_j||_2^2$ is minimized.

4.5 Conclusions

In this chapter we considered the estimation of the dispersion parameters in a mixed linear model. In particular, translation invariant unbiased quadratic estimators were considered. For the general model a necessary and sufficient condition for the existence of translation invariant unbiased quadratic estimators for all dispersion parameters was given. The estimation methods for the dispersion parameters in the mixed linear model proposed by Malley (1986) and Liao and Iyer (2000) were shown to be equivalent. Special attention was given to the estimation of dispersion effects from unreplicated two-level factorial designs. The estimators proposed by Wiklander (1998), Liao and Iyer (2000) and Brenneman and Nair (2001) for dispersion effects under a linear dispersion model were shown to be equivalent for full factorial designs and their regular fractions. Moreover, we gave a definition for the MINQUE estimator of the dispersion effects in these designs and showed that the above estimators for dispersion effects are MINQUE in this sense.

Chapter 5

Two-Step Designs

The material of this chapter is a slightly modified version of Van Berkum et al. (2005). The primary inspiration came from consulting on experimental design of a sticker manufacturer early in the year 2000. The sticker manufacturer wanted to investigate the influence of several variables in the production of stickers on a quality measure related to adhesion. The production process of stickers consists of two separate steps. In the first step mixing and coating of adhesive ingredients results in the intermediate product of a master roll. This master roll is slit to narrow rolls which in the second step are stored and converted to stickers after some period of time. In both steps eight variables with a possible influence on the quality measure were identified. The role of certain variables in the process was not fully understood from previous experiments in which the two steps were analyzed separately. It was argued that this could be the result of failing to consider interactions between variables in different steps of manufacturing and that a design of resolution IV examining the influence of variables from both steps was needed. For economic reasons the number of master rolls that could be produced for the experiment was restricted to sixteen. Running a completely randomized 2^{16-11}_{IV} fractional factorial design was not an option because it required the production of thirty-two master rolls. However, due to the specific experimental environment it was possible to expose different parts of a master roll to different settings with respect to the variables in the second step. The experiments in which the same master roll is used in several runs are an example of fractional factorial split-plot experiments (Kempthorne (1952), p. 318). More recent papers dealing with fractional factorial split-plot experiments include Bingham and Sitter (1999), Bisgaard (2000), Bingham and Sitter (2003), Bingham et al. (2004) and Castillo et al. (2005). In the sticker example a fractional factorial split-plot design for the two-step production process was constructed by first choosing a 2^{8-4}_{IV} design for the first step. This resulted in the production of sixteen master rolls. The design was extended to a 2^{16-11}_{IV} design in which two slit rolls from each of these master rolls were used. Throughout this chapter we use the name two-step designs to refer to designs that are constructed in this way.

The proposed design is not fully randomized since each master roll is used in two runs of the two-step design. The restricted randomization makes that the assumption of independent observations that is commonly made is not valid in this case. Therefore, the standard way of hypothesis testing using F-tests cannot be applied. However, Bisgaard (2000) and Bingham and Sitter (2001) have shown that methods for testing the significance of effects in fractional factorial split-plot designs are only slightly more complicated than the standard ways of testing in fully randomized fractional factorial experiments.

In the sticker example it was not clear a priori which two-factor interactions were likely to be present. In other cases, interest may be in finding an efficient two-step design that identifies a given set of effects. In this chapter we present a search algorithm that can be used for this purpose. The algorithm is a modified version of the algorithm in Franklin and Bailey (1977). Our modifications are needed in order to maintain the split-plot structure of the designs and to be able to find a design that requires the production of a minimal number of intermediate products. The design is extended in such a way that the number of runs in the extended design is also minimized.

The outline of this chapter is as follows. In Section 5.1 we give some further details about of the proposed experimental design. The appropriate model and methods for analysis are given in Section 5.2. The modified Franklin and Bailey algorithm for constructing efficient two-step designs is described in Section 5.3.

5.1 Example of a two-step design

The special form of the designs that we consider is illustrated in the next example in which we consider a simplified version of the production process of stickers described in the introduction of this chapter.

Example 5.1 For simplicity we assume that only four different variables are considered in each of the steps. A fractional 2^{4-1}_{IV} design in X_1, X_2, X_3 and X_4 with the defining relation[1] $I = X_1X_2X_3X_4$ is used for the first step. For the second step the design is extended to a 2^{8-4}_{IV} design in $X_1, X_2, \ldots, X_8$ using the generators $X_6 = X_1X_2X_5$, $X_7 = X_1X_3X_5$ and $X_8 = X_2X_3X_5$ (in addition to the generator $X_4 = X_1X_2X_3$). The design is given in Table 5.1. Note that narrow rolls slit from the same master roll are in the second step of the production process further processed to stickers under different conditions.

The two-step designs that we propose for investigating the important effects in two-step production processes are a special application case of split-plot designs. Split-plot designs are factorial designs with a restricted randomization. Like many other types of experimental designs, split-plots designs were originally used in agriculture (see Yates (1937), Kempthorne (1952) and Cochran

[1] In this chapter we use the classical notation for the 2^{k-m} fractional factorial designs. The levels are coded using $L_1 = L_2 = \ldots = L_k = \{-1, 1\}$. In this chapter the product $\prod_{j\in J} X_J, J \subseteq \{1, 2, \ldots, k\}$, is used to denote the effect $\sum_{d\in D} v_J(d)\, y(d)$ where $v_J(d) = \prod_{j\in J} d_j$.

Table 5.1: The 2^{4-1}_{IV} design that is extended to a 2^{8-4}_{IV} design in Example 5.1.

Master roll	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	Sticker
1	−1	−1	−1	−1	−1	−1	−1	−1	1
					1	1	1	1	2
2	−1	−1	1	1	−1	−1	1	1	3
					1	1	−1	−1	4
3	−1	1	−1	1	−1	1	−1	1	5
					1	−1	1	−1	6
4	−1	1	1	−1	−1	1	1	−1	7
					1	−1	−1	1	8
5	1	−1	−1	1	−1	1	1	−1	9
					1	−1	−1	1	10
6	1	−1	1	−1	−1	1	−1	1	11
					1	−1	1	−1	12
7	1	1	−1	−1	−1	−1	1	1	13
					1	1	−1	−1	14
8	1	1	1	1	−1	−1	−1	−1	15
					1	1	1	1	16

and Cox (1957)). Recently, split-plot designs have regained interest because of their applicability in robust design (see Bisgaard (2000) and Bingham and Sitter (2003)) and, even more recently, in combinatorial and high-throughput experimentation for drug and material development (Castillo et al. (2005)).

Some recent papers deal with the problem of finding good fractional factorial split-plot designs (see Bingham and Sitter (1999), Bingham and Sitter (2003) and Bingham et al. (2004)). In these papers the quality of the designs is judged using the minimum aberration criterion introduced in Fries and Hunter (1980). The minimum aberration criterion is a generalization of the resolution criterion and uses the word-length pattern to judge the quality of the design. For a 2^{k-m} fractional factorial design F the word-length pattern is defined as the vector $W = (A_1(F), A_2(F), \ldots, A_k(F))$ where $A_j(F)$ denotes the number of words of length j in the defining relation for F. A fraction F_1 is said to have less aberration than F_2 if $A_r(F_1) < A_r(F_2)$ and $A_j(F_1) = A_j(F_2)$ for $j = 1, \ldots, r-1$. The minimum aberration criterion treats all effects of the same order equally and is therefore especially useful when sound knowledge about which effects might be present is lacking. In those cases the minimum aberration criterion can be used to compare designs of equal resolution.

5.2 Model and analysis

We consider a two-step production process where in the first step k_1 variables and in the second step k_2 variables may affect the quality of the final product. Two levels are chosen for each variable and we assume the corresponding factors to be fixed. For the first step a $2^{k_1-m_1}$ design is used. This design is extended to a 2^{k-m} factorial design of desired resolution and with $k = k_1 + k_2$ and $m = m_1 + m_2$. The extended design will also be denoted by $2^{(k_1+k_2)-(m_1+m_2)}$. We will use the name two-step design to refer to a design constructed in this way. We assume that the full factorial design is coded by the elements in the set $D = \{-1, 1\}^k$ and let $F \subset D$ denote the regular 2^{k-m} fraction that corresponds to the extended design.

An ANOVA model (see Section 2.3) is used to describe the relation between the quality (response) and the variables in the production process. The standard ANOVA decomposition of the total sums of squares will be used to analyze the results. The model needs to take into account that observations made on the products constructed using the same intermediate product are may be correlated. This is done by including an extra error term that is nested within the factors of the first step. We let the indices in the set $W := \{1, ..., k_1\}$ correspond to variables from the first step and the indices $\{k_1 + 1, ..., k\}$ to variables in the second step. The full model (not fully identifiable on the fraction F due to confounding) for the $2^{(k_1+k_2)-(m_1+m_2)}$ two step design is

$$y(d) = \sum_{I \subseteq \{1,\ldots,k\}} \tau_I(d_I) + \eta(d_W) + \varepsilon(d), \tag{5.1}$$

where $\eta(d_W) \sim N(0, \sigma_\eta)$ is the additional error induced by the restricted ran-

Table 5.2: The 2^2 design extended to the 2^{4-1} design with $X_4 = X_1X_2X_3$.

Intermediate product	X_1	X_2	X_3	X_4	Final product
1	-1	-1	-1	-1	1
			1	1	2
2	-1	1	-1	1	3
			1	-1	4
3	1	-1	-1	1	5
			1	-1	6
4	1	1	-1	-1	7
			1	1	8

domization. We now impose the constraints given in (2.20) on the parameters $\tau_I(d_I)$ in model (5.1). The model is illustrated in the next example.

Example 5.2 In this example we consider a two-step production process and assume that in each step two variables may affect the quality of the final product. To investigate the influence of these four variables a 2^2 full factorial design is chosen for the first step. This design is extended to a 2^{4-1} design using the generator $X_4 = X_1X_2X_3$. The resulting design is presented in Table 5.2. It is assumed that there are no interactions influencing the quality. The following model is formulated

$$y(d) = \tau_\emptyset + \tau_1(d_1) + \tau_2(d_2) + \eta(d_1, d_2) + \tau_3(d_3) + \tau_4(d_4) + \varepsilon(d), \qquad (5.2)$$

where $\eta(d_1, d_2) \sim N\left(0, \sigma_\eta^2\right)$, $\varepsilon(d) \sim N\left(0, \sigma^2\right)$ and all random terms are assumed independent. If the usual constraints

$$\sum_{d_j \in \{-1,1\}} \tau_j(d_j) = 0 \text{ for } j = 1, 2, 3, 4,$$

are used for obtaining identifiability, then the model (5.2) can be reformulated as

$$Y = Z\tau + U_\eta\tau_\eta + U_\varepsilon\tau_\varepsilon,$$

where $U_\varepsilon = I_8$ and the matrices U_η and X are given by

$$U_\eta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \text{ and } Z = \begin{pmatrix} 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

The vector $\tau = (\tau_\emptyset, \tau_1, \tau_2, \tau_3, \tau_4)$ contains the unknown location parameters. The vectors τ_η and τ_ε contain independent random variables with mean 0 and variance σ_η^2 and σ^2, respectively. The sums of squares are given by

$$MS_1 = \left(x_1^T y\right)^2, MS_2 = \left(x_2^T y\right)^2, MS_3 = \left(x_3^T y\right)^2, MS_4 = \left(x_4^T y\right)^2,$$

and

$$MS_\eta = \left(x_\eta^T y\right)^2 \text{ and } MS_\varepsilon = \frac{1}{2}\left(\left(x_{\varepsilon_1}^T y\right)^2 + \left(x_{\varepsilon_2}^T y\right)^2\right),$$

where

$$\begin{aligned} x_1 &= \tfrac{1}{\sqrt{8}}(-1,-1,-1,-1,1,1,1,1)^T, & x_2 &= \tfrac{1}{\sqrt{8}}(-1,-1,1,1,-1,-1,1,1)^T \\ x_3 &= \tfrac{1}{\sqrt{8}}(-1,1,-1,1,-1,1,-1,1)^T, & x_4 &= \tfrac{1}{\sqrt{8}}(-1,1,1,-1,1,-1,-1,1)^T \\ x_\eta &= \tfrac{1}{\sqrt{8}}(1,1,-1,-1,-1,-1,1,1)^T, & x_{\varepsilon_1} &= \tfrac{1}{\sqrt{8}}(1,-1,1,-1,-1,1,-1,1)^T \\ x_{\varepsilon_2} &= \tfrac{1}{\sqrt{8}}(1,-1,-1,1,1,-1,-1,1)^T. \end{aligned}$$

The expected mean squares can be found by writing the model in the form

$$\begin{aligned} \mathrm{E}(Y) &= Z\tau \\ \mathrm{Var}(Y) &= \sigma^2 I + \sigma_\eta^2 U_\eta U_\eta^T \end{aligned},$$

and using Lemma 4.4. The expected mean squares are given in Table 5.3.

We are now going to derive the expected mean squares for the full model given in (5.1) with the constraints in (2.20) imposed on the parameters. By Z_{full} we denote the design matrix for the full model after imposing the constraints on the parameters. The matrix Z_{full} has size $N \times 2^k$ where $N = 2^{k-m}$ and typically contains the same column several times. The linear dependence of the columns of the matrix Z_{full} implies that the full model is never identifiable. The design matrix Z_{full} for the full model is used in deriving the expected mean squares for the model (5.1) given in the next theorem. In this theorem we use $X_J, J \subseteq \{1,2,\ldots,k\}$, to denote the effect $X_{j_1} X_{j_2} \ldots X_{j_m}$.

Theorem 5.3 *Let F be a $2^{(k_1+k_2)-(m_1+m_2)}$ two-step design. Let C_J for some $J \subseteq \{1,2,\ldots k\}$ be the set containing all subsets $I \subseteq \{1,2,\ldots,k\}$ for which X_I*

is completely confounded with X_J on the design F. For the expectation of MS_J, the mean sum of squares for X_J, one has

$$E\left(MS_J\right) = \sigma^2 + \delta\left(J\right) 2^{k_2-m_2}\sigma_\eta^2 + 2^{k-m}\left(\sum_{I\in C_J} s_J\left(I\right)\tau_I\right)^2, \qquad (5.3)$$

where

$$\delta\left(J\right) = \begin{cases} 1 & \text{if there exists an } I \in C_J \text{ that satisfies } I \subseteq \{1,2,\ldots,k_1\}, \\ 0 & \text{otherwise,} \end{cases}$$

and

$$s_J\left(I\right) = \begin{cases} 1 & \text{if } X_I = \ X_J \text{ on } F \\ -1 & \text{if } X_I = -X_J \text{ on } F \end{cases}.$$

Proof The full model can be written in the following form

$$\begin{aligned} \mathrm{E}\left(Y\right) &= Z_{\text{full}}\,\tau, \\ \mathrm{Var}\left(Y\right) &= \sigma^2 I + \sigma_\eta^2 U_\eta U_\eta^T. \end{aligned}$$

Note that this is a special case of the mixed linear model given in (4.1). In particular, $\Gamma_1 = I, \Gamma_2 = U_\eta U_\eta^T, \alpha_1 = \sigma^2$ and $\alpha_2 = \sigma_\eta^2$. We will use this later to compute the expectation of the mean sum of squares. Let the set $\mathcal{T}$ contain subsets $J \subseteq \{1,2,\ldots,k\}$ in such a way that the set $\{X_J \mid J \in \mathcal{T}\}$ is a maximal set of effects that are orthogonal on F. Without loss of generality we assume that $\emptyset \in \mathcal{T}$. If by $z_J, J \in \mathcal{T}$, we denote the column in Z_{full} that corresponds to the factor Z_J, then an orthonormal basis for $\mathbb{R}^N$ is given by $\{q_J \mid J \in \mathcal{T}\}$ where $q_J = \frac{1}{\sqrt{N}} z_J$. The standard decomposition of the total sums of squares SS_T is now given by

$$SS_T = \sum_{J\in\mathcal{T}\setminus\{\emptyset\}} SS_J,$$

Table 5.3: Expected mean squares for the design in Table 5.2 under model (5.2).

MS	E (MS)
MS_1	$\sigma^2 + 2\,\sigma_\eta^2 + 8\,\tau_1^2$
MS_2	$\sigma^2 + 2\,\sigma_\eta^2 + 8\,\tau_2^2$
MS_η	$\sigma^2 + 2\,\sigma_\eta^2$
MS_3	$\sigma^2 + 8\,\tau_3^2$
MS_4	$\sigma^2 + 8\,\tau_4^2$
MS_ε	σ^2

where

$$SS_J = \left(q_J^T Y\right)^2 = Y^T q_J q_J^T Y \quad \text{for } J \in \mathcal{T} \setminus \{\emptyset\}.$$

All sums of squares correspond to one degree of freedom since rank $\left(q_J q_J^T\right) = 1$. Hence, $MS_J = SS_J$ for all J. We compute the expectation of MS_J using Lemma 4.4. Substitution of $M = q_J q_J^T, \Gamma_1 = I$ and $\Gamma_2 = U_\eta U_\eta^T$ into (4.3) gives

$$\mathrm{E}\left(MS_J\right) = \sigma^2 + \sigma_\eta^2 \, q_J^T \, U_\eta U_\eta^T \, q_J + \left(q_J^T Z_{\text{full}} \, \tau\right)^2.$$

For each z_I, for $I \subseteq \{1, 2, \ldots, k\}$, we have that

$$q_J^T z_I = \begin{cases} s_J\left(I\right) \frac{N}{\sqrt{N}} = s_J\left(I\right) \sqrt{N} & \text{if } J \in C_I, \\ 0 & \text{otherwise,} \end{cases}$$

from which we find that

$$\left(q_J^T Z_{\text{full}} \, \tau\right)^2 = N \left(\sum_{I \in C_J} s_J\left(I\right) \tau_I \right)^2 = 2^{k-m} \left(\sum_{I \in C_J} s_J\left(I\right) \tau_I \right)^2.$$

In addition, we have that

$$q_J^T U_\eta = \begin{cases} 0 & \text{if there exists an } I \in C_J \text{ for which } I \subseteq \{1, 2, \ldots, k_1\}, \\ \frac{2^{k_2 - m_2}}{\sqrt{N}} 1^T & \text{otherwise,} \end{cases}$$

where 1 is used to denote the all-one-vector of length $(k_1 - m_1)$. Hence,

$$\begin{aligned} q_J^T U_\eta U_\eta^T q_J &= \delta\left(J\right) \left(\frac{2^{(k_2 - m_2)}}{\sqrt{N}} \right)^2 2^{(k_1 - m_1)} \\ &= \delta\left(J\right) \frac{2^{2(k_2 - m_2)}}{2^{(k_1 - m_1) - (k_2 - m_2)}} 2^{(k_1 - m_1)} \\ &= \delta\left(J\right) 2^{(k_2 - m_2)}, \end{aligned}$$

which completes the proof. □

From Theorem 5.3 we find that sets of confounded effects can be divided into two groups based on the variance of the corresponding contrast. The group with the larger variance $\sigma^2 + 2^{k_2 - m_2} \sigma_\eta^2$ is formed by the sets containing a main effect from the first step or interaction consisting of only factors from the first step. The other group has error variance σ^2. A similar result is stated in Bisgaard (2000) in the context of fractional factorial split-plot experiments. In our application the factors from the first and second step are the whole-plot and sub-plot factors, respectively. Two methods might be used to test whether there are significant effects in fractional factorial split-plot designs (Bisgaard (2000), Bingham and Sitter (2001)). The first one uses normal probability plots (see Daniel (1959)), the second is the usual way of testing hypothesis when analysis of variance is applied. It is clear that the expectations of the mean squares can be divided into two groups, depending on the value of $\delta\left(J\right)$. For each of these

groups a normal probability plot can be drawn to see if there are significant effects. If there is at least one set of confounded effects C_J for which it can be assumed that all the effects are zero, then the mean sum of squares of these relations yield an estimate for the error term of the group involved, *i.e.* for σ^2 in the second group and for $\sigma^2 + 2^{k_2-m_2}\sigma_\eta^2$ in the first group. In that case the formal way of testing using F-tests can be applied.

Note that effects that are confounded with an interaction containing only factors from the first step are in two-step designs estimated with a larger variance and fewer error degrees of freedom than in completely randomized designs. Hence, if possible two-step designs should be performed in such a way that the factors varied in the first step are either of less interest or likely to have large effects.

5.3 Construction of two-step designs

In this section we present an algorithm that finds two-step designs that identify a given set of effects while minimizing the number of required intermediate products. The algorithm is a modified version of the algorithm of Franklin and Bailey (1977). The Franklin and Bailey algorithm finds two-level regular fractional factorial designs with minimal number of runs that identify a given set of effects. In Franklin (1985) the algorithm is extended to construct fractions of symmetric n^k factorial designs where $n \geq 2$ is prime. The algorithm finds a suitable fractional factorial 2^{k-m} design by searching through a table in order to find a set of m effects to be confounded with the mean. These effects are selected in such a way that none of the effects from the set that needs to be identified appears in the group generated by these m effects. We propose a modified version of the algorithm in Franklin and Bailey (1977) to construct efficient two-step designs. The modifications are needed because our first objective is now to minimize the number of different intermediate products (instead of the total number of final products) that need to be produced for the experiment. To find an efficient $2^{(k_1+k_2)-(m_1+m_2)}$ design for the two production proces we first fix values for m_1 and m_2 (depending on m_1) and use a modified search table in order to keep the special structure of the $2^{(k_1+k_2)-(m_1+m_2)}$ split-plot design. In Section 5.3.1 we describe the original Franklin and Bailey algorithm. The necessary modifications are discussed in detail in Section 5.3.2. A full description of the modified algorithm is given in Section 5.3.3.

5.3.1 The Franklin and Bailey algorithm

We first need some extra definitions. The algorithm constructs a 2^{k-m} starting from a full factorial design in $k-m$ factors. These $k-m$ factors are called *basic factors*. Franklin and Bailey (1977) define the *basic effects group* as the Abelian group generated by the basic factors. The factors that are not basic factors are called the *added factors*. Now note that equating each added factor to one of the elements in the basic effects group completely determines the

confounding structure for the design. The corresponding equations are called *defining contrasts*. For a set of defining contrasts the *defining contrast group* is defined as the group generated by the defining contrasts. Finally, Franklin and Bailey (1977) distinguish between eligible and ineligible effects. The *eligible effects* are those effects that can be chosen as a defining contrast, whereas the *ineligible effects* cannot be chosen.

The first step of the algorithm is establishing the set consisting of all ineligible effects. In factorial designs ineligible effects correspond to effects that are not assumed zero (including all effects that are to be estimated), products of two effects to be estimated and products of an effect to be estimated and an effect not to be estimated but assumed unequal to zero. Having determined this set of ineligible effects, the next step is determining a starting value for m. Franklin and Bailey (1977) suggest to choose m such that the largest subgroup generated by main effects that is completely contained in the eligible effects set contains not more than 2^{k-m} members. Then $k-m$ factors are chosen at random to be the basic factors. A two-way table with 2^{k-m} rows headed by the basic effects group and m columns headed by the added factors is constructed.

Let the set B consist of all the subsets J of $\{1, 2, \ldots, k\}$ for which the factor X_J is in the basic effects group. The interaction $X_{J\cup\{i\}}$ between X_J and an added factor X_i is placed in the row indexed by X_J and the column indexed by X_i only when it corresponds to an eligible effect. The table is searched for a set of m defining contrasts, one selected from each of the columns. A simple search routine is used to find such a set. An effect is added to the group of defining contrasts only if the resulting defining contrast group does not contain any ineligible effects. If the set of defining contrasts (with less than m elements) cannot be extended then the last added element is removed and (if available) another element from the same column is chosen. The algorithm stops when a suitable design is found. If no suitable design is found, a new set of $k-m$ basic factors (if available) is selected and the steps of constructing the table and searching of defining contrasts are repeated for this new set of basic factors. In case no such new set exists m is decreased by one and all steps starting with the selection of the basic factors are repeated. A short illustration of the algorithm is given in Example 5.4, which is adapted from Franklin and Bailey (1977).

Example 5.4 Suppose we want to find the smallest possible balanced 2^{5-m} fractional design that can be used to estimate each of the main effects X_1, X_2, X_3, X_4 and X_5 and the interaction effects X_1X_2 and X_2X_5. The largest groups in the ineligible effects set (*e.g.* the group generated by X_1, X_2 and X_3) contain eight members. Hence, 2 is chosen to be a starting value for m. When X_1, X_2 and X_3 are chosen as basic factors the Table 5.4 is constructed. A minimal design found by the algorithm is the one defined by $X_4 = X_2X_3$ and $X_5 = X_1X_3$.

Table 5.4: Eligible-Effects Table constructed in Example 5.4 (− denotes an ineligible effect).

	X_4	X_5
I	−	−
X_1	−	−
X_2	−	−
X_1X_2	−	−
X_3	−	−
X_1X_3	$X_1X_3X_4$	$X_1X_3X_5$
X_2X_3	$X_2X_3X_4$	−
$X_1X_2X_3$	$X_1X_2X_3X_4$	$X_1X_2X_3X_5$

5.3.2 Modifications needed for constructing two-step designs

Some minor modifications to the just sketched Franklin and Bailey algorithm are needed to make it suitable for constructing two-step designs. Before discussing the modifications some notation is given. Recall that for the first step a $2^{k_1-m_1}$ design is chosen. This design is extended to a 2^{k-m} design, where $k = k_1 + k_2$. Let m_2 equal $m - m_1$. The set of all effects to be estimated is denoted by TE. All effects outside TE are assumed to be zero. The subset of TE of main factors in the first step and interactions containing only factors from the first step is called TE_1 and we denote its number of elements by $e(1)$. Let TE_2 equal $TE \backslash TE_1$ and e(2) be the number of elements in this set. The next modifications are needed. First, instead of just one start value for m, now values for both m_1 and m_2 are needed. The value

$$m_1 = k_1 - \lceil {}^2\log(e(1) + 2) \rceil \tag{5.4}$$

is an upper bound, since for smaller values of m_1 there are not enough degrees of freedom to estimate all effects in $TE(1)$. Given a value for m_1 an upper bound on m_2, based on the degrees of freedom needed to estimate all effects in $TE(2)$, is

$$m_2 = k_2 + k_1 - m_1 - \lceil {}^2\log(2^{k_1-m_1} + e(2) + 1) \rceil \ . \tag{5.5}$$

To obtain the special structure of the two-step design $k_1 - m_1$ basic factors have to be chosen from the first step and $k_2 - m_2$ from the second step. Another modification concerns the set of ineligible effects. When constructing two-step designs effects that are a product of an added factor from the first step and at least one basic factor from the second step must be considered ineligible. Effects that are a product of an added factor from the second step and an effect from the basic effects group that contains only main factors from the first step must

also be considered ineligible. A two-way table can now be constructed in the same way as described by Franklin and Bailey (1977). The first m_1 columns correspond to added factors from the first step, the remaining m_2 columns each to an added factor from the second step. The way of searching the defining contrasts can be left unchanged.

If for a given combination of m_1 and m_2 a suitable design cannot be found for any set of $k - m$ basic factors then the value of m_1 and/or m_2 should be adjusted. If not more than $m_1 - 1$ defining contrasts are found then a $2^{k_1-m_1}$ design that can be used to estimate all effects in TE_1 does not exist. In this case the value of m_1 should be decreased by one and a new value for m_2 needs to be computed using (5.5). In all other cases in which a suitable design is not found p_2 should be decreased by one if $m_2 > 0$ and m_1 should be decreased by one in case $m_2 = 0$ and $m_1 > 1$. Each time the value of m_1 is decreased the value of m_2 needs to be updated using (5.5). The search procedure stops if a suitable design is found or if

$$(m_1 = 0 \ \wedge \ m_2 = 1) \ \vee \ (m_1 = 1 \ \wedge \ m_2 = 0) \ .$$

5.3.3 An algorithm for constructing two-step designs

The modified version of the algorithm of Franklin and Bailey (1977) is given below. The expression DC appearing first in step 5 denotes the set of all up to then selected defining contrasts. NC is used to refer to the set of all effects that cannot be chosen as a design generator.

1. Choose the following start values for m_1 and m_2

$$\begin{aligned} m_1 &= k_1 - \lceil {}^2\log(e(1) + 2) \rceil \\ m_2 &= k_2 + k_1 - m_1 - \lceil {}^2\log(2^{k_1-m_1} + e(2) + 1) \rceil \ . \end{aligned}$$

2. Choose a set of basic factors, such that $k_1 - m_1$ factors are from the first step and $k_2 - m_2$ factors are from the second step of the process.

3. Determine the set NC. The effects that cannot be chosen as design generator are

   (a) All effects of the set TE and all products of two effects of this set.

   (b) Products of an added factor from the first step with an effect from the basic effects group that contains at least one factor from the second step.

   (c) Products of an added factor from the second step and an effect from the basic effects group that contains only effects from the first step of the process.

4. Construct a table with 2^{k-m} rows and m columns. The rows correspond to the basic effects. Columns 1 to m_1 each correspond to one of the added factors from the first step and the other columns correspond to added

Table 5.5: Table constructed with the modified algorithm in Example 5.6.

	X_4	X_6	X_7	X_8
I	–	–	–	–
X_1	–	–	–	–
X_2	–	–	–	–
X_1X_2	–	–	–	–
X_3	–	–	–	–
X_1X_3	$X_1X_3X_4$	–	–	–
X_2X_3	$X_2X_3X_4$	–	–	–
$X_1X_2X_3$	$X_1X_2X_3X_4$	–	–	–
X_5	–	–	–	–
X_1X_5	–	$X_1X_5X_6$	–	–
X_2X_5	–	$X_2X_5X_6$	–	–
$X_1X_2X_5$	–	$X_1X_2X_5X_6$	–	–
X_3X_5	–	$X_3X_5X_6$	–	–
$X_1X_3X_5$	–	$X_1X_3X_5X_6$	$X_1X_3X_5X_7$	$X_1X_3X_5X_8$
$X_2X_3X_5$	–	$X_2X_3X_5X_6$	$X_2X_3X_5X_7$	$X_2X_3X_5X_8$
$X_1X_2X_3X_5$	–	$X_1X_2X_3X_5X_6$	$X_1X_2X_3X_5X_7$	$X_1X_2X_3X_5X_8$

factors from the second step. The entry of a cell in row i and column j is equal to $X_{J\cup\{i\}}$, where X_J is the basic effect that corresponds to row J and X_i is the added factor that corresponds to column i, but only if the effect $X_{J\cup\{i\}}$ is not an element of the set NC. Otherwise the entry is empty.

Remark 5.5 The modified algorithm may also be used when interactions between factors from the first and second step appear in the set of effects to be estimated.

Example 5.6 Let X_1, X_2, X_3 and X_4 be all possible relevant factors from the first step and X_5, X_6, X_7 and X_8 those from the second step. Suppose we are looking for a design to estimate all main effects and the interactions X_1X_2, X_5X_7 and X_5X_8. Starting values for m_1 and m_2 are respectively 1 and 3. In step 4 Table 5.5 is constructed.

The set DC is initialized and is equal to $\{I\}$. In each column an effect has to be found. This effect defines a design generator, because the added factor of the column involved can be expressed in basic factors by use of this effect. The search for effects is started in column zero. During the search there is always an actual column and for each column with number less or equal to the actual column a row pointer is defined. This pointer

points to the actual row of that column. The actual column at this point is zero with row pointer zero.

Go to the next column and make the row pointer of that column zero.

Go to the next row in the actual column, *i.e.* increase the row pointer by one. If there is no row available go to step 5.5.

Consider the effect in the actual row and column. Check whether all generalized interactions between this effect and the already selected defining contrasts of the set DC can be chosen, *i.e.* they should not be element of the set NC. If this is not the case, then go back to step 5.5

Add the effect that has been found in step 5.5 to the set DC, as well as all generalized interactions between this effect and the already selected defining contrasts of the set DC. If the actual column is the last column, then a possible design with defining contrasts has been found. To find all possible designs one should go to step 5.5. If the actual column is not the last column, one should go to step 5.5.

If the actual column is the first column, then go to step 5.5. If not then the previous column becomes the actual column without changing the row pointer of that column and go to 5.5.

The search procedure with the current set of basic factors has been finished. If there is another set of basic factors available for the same values of m_1 and m_2, and if one wants to find all possible designs, then go to step 2. Otherwise go to step 5.5.

Stop the search procedure if a suitable design has been found or if the following holds

$$(m_1 = 0 \ \wedge \ m_2 = 1) \ \vee \ (m_1 = 1 \ \wedge \ m_2 = 0) \ .$$

In other cases the value of m_1 and/or m_2 should be adjusted. In the case that for all possible sets of basic factors (with the current values of m_1 and m_2) not more than $m_1 - 1$ defining contrasts have been found or if $m_2 = 0$ and $m_1 > 1$, then first the value of m_1 must be decreased by one and a new value for m_2 needs to be computed using (5.5). Otherwise, only the value of m_2 must be decreased by one. Go to step 2 after these adjustments.

Example 5.7 (Continuation of Example 5.6) For the problem given in Example 5.6 the set

$$DC = \{I, \, X_1X_3X_4, \, X_1X_5X_6, \, X_2X_3X_5X_7, \, X_1X_2X_3X_5X_8\}$$

of defining contrasts is found. Note that in this case a resolution IV design can be found by extending the set of ineligible effects (constructed

in step 3) to include all interactions containing less than four factors. The resolution IV design found by the algorithm is given by

$$DC = \{I,\ X_1X_2X_3X_4,\ X_1X_2X_5X_6,\ X_2X_3X_5X_7,\ X_1X_3X_5X_8\}.$$

This is the design given in Table 5.1.

Note that the updating procedure for m_1 and m_2 in step 12 guarantees that we find a fractional factorial split-plot design that requires a minimal number of intermediate products. The algorithm always terminates because in the worst case m_1 and m_2 will decrease until $m_1 = m_2 = 0$, in which case the $2^{k_1+k_2}$ full factorial design is found.

5.4 Conclusions

In this chapter we discussed a real-life industrial problem from a two-step production process. In this problem an intermediate product from the first step is split into several parts in order to allow further processing in the second step. The situation can be handled by using a fractional factorial split-plot design. The use of a fractional factorial split-plot design can reduce the costs of an experiment as well as the time that is necessary to perform the experiment. The analysis is similar to the analysis in completely randomized experiments apart from adding an extra error term for the randomization restriction. The usual F-test and normal probability plots can be used to test for significant effects. However, care must be taken in order to use the appropriate error variance in assessing the significance, because the effects that are confounded with an interaction containing only factors from the first step are in these designs estimated with a larger variance and fewer error degrees of freedom. Fractional factorial split-plot designs for analyzing two-step production processes that require the production of a minimal number of intermediate products can be constructed using the modified version of the Franklin and Bailey algorithm that we proposed in this chapter. Generalization of this concept to multi-step production processes seems straightforward.

Appendix A

The Brenneman and Nair Estimators

Brenneman and Nair (2001) propose a linear regression of the squared residuals for estimating the dispersion effects in two-level factorial designs. In their paper they give an expression for the estimators for $\alpha_2, \alpha_3, \ldots, \alpha_v$ when the design is a two-level full factorial design. They do not give expressions for the estimator for α_1 in case of a full factorial design and the estimators for $\alpha_1, \alpha_2, \ldots, \alpha_v$ when the design is a regular two-level fractional factorial design. In this section we deduce expressions for the estimators of $\alpha_1, \alpha_2, \ldots, \alpha_v$ obtained using the method proposed by Brenneman and Nair (2001) for cases in which the design is a two-level full factorial design or a regular fraction of such a design.

Let for $1 \leq i \leq v$ the matrices A_i be defined by $A_i = (I - P_Z)\,\Gamma_i\,(I - P_Z)$. The unbiased estimator for $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_v)^T$ proposed by Brenneman and Nair (2001) is $\left(B^T B\right)^{-1} B^T R^\star$ where $R^\star$ denotes the vector of squared residuals and the matrix B is given by

$$B = \left(\text{ diag } (A_1) \;\; : \;\; \text{diag } (A_2) \;\; : \;\; \ldots \;\; : \;\; \text{diag } (A_v) \right).$$

The expressions for the estimators in terms of the squared residuals are given in the next theorem.

Theorem A.1 *Assume that data is obtained on a a two-level full factorial design or regular fraction of such a design. If $p < N$ and $2\,(p - p_\ell) < N$ for all $\ell, 2 \leq \ell \leq N$, then the estimator for the dispersion parameter α_ℓ proposed by Brenneman and Nair (2001) is given by*

$$\begin{array}{ll} \frac{1}{N-p} \sum_{1 \leq j \leq N} R_j^2 & \text{if } \ell = 1 \\ \frac{1}{N-2(p-p_\ell)} \left(\sum_{j:(\Gamma_\ell)_{j,j}=1} R_j^2 - \sum_{j:(\Gamma_\ell)_{j,j}=-1} R_j^2 \right) & \text{if } 2 \leq \ell \leq v \end{array},$$

where p denotes the number of columns of the design matrix Z and p_ℓ denotes the number of pairs of columns in the design matrix Z for which diag $(\Gamma_\ell) = \pm\, z_i \circ z_j$

Proof In the case of a regular fraction or full factorial design we have that $Z^T Z = I$, which implies that $P_Z = ZZ^T$. Using that P_Z and $\Gamma_\ell, 1 \leq \ell \leq k$, are symmetric matrices we find that

$$\text{diag}\,(A_\ell) = \text{diag}\,(\Gamma_\ell) - 2\text{diag}\,(\Gamma_\ell P_Z) + \text{diag}\,(P_Z \Gamma_\ell P_Z)\,.$$

To simplify this expression for diag (A_ℓ) note that diag $(\Gamma_\ell P_Z)$ equals

$$\text{diag}\,(\Gamma_\ell) \circ \text{diag}\,(P_Z) = \frac{1}{N}\text{diag}\,(\Gamma_\ell) \circ \text{diag}\left(ZZ^T\right) = \frac{p}{N}\text{diag}\,(\Gamma_\ell)$$

To find a different expression for diag $(P_Z \Gamma_\ell P_Z) = \text{diag}\left(ZZ^T \Gamma_\ell ZZ^T\right)$ observe that the elements of the matrix $Z^T \Gamma_\ell Z$ are given by

$$\left(Z^T \Gamma_\ell Z\right)_{ij} = \left(\text{diag}\,(\Gamma_\ell) \circ z_i\right)^T z_j = \begin{cases} -N & \text{if } z_i \circ z_j = -\text{diag}\,(\Gamma_\ell) \\ N & \text{if } z_i \circ z_j = \text{diag}\,(\Gamma_\ell) \\ 0 & \text{otherwise} \end{cases}.$$

Note that all rows and columns of $Z^T \Gamma_\ell Z$ have at most one non-zero element. We find that $ZZ^T \Gamma_\ell Z = (c_1 : c_2 : \ldots : c_p)$ where the column c_j is given by

$$c_j = \begin{cases} -Nz_i & \text{if } z_i = -z_j \circ \text{diag}\,(\Gamma_\ell) \text{ is a column in } Z \\ Nz_i & \text{if } z_i = z_j \circ \text{diag}\,(\Gamma_\ell) \text{ is a column in } Z \\ 0 & \text{otherwise} \end{cases}.$$

As a consequence,

$$\left(ZZ^T \Gamma_\ell ZZ^T\right)_{r,r} = \sum (c_j)_r \, (z_j)_r \,, \tag{A.1}$$

where the summation is over all j for which there exists an $i, 1 \leq i \leq p$, such that $z_i \circ z_j = \pm\,\text{diag}\,(\Gamma_\ell)$. For j satisfying this condition and the corresponding i we have that $(c_j)_r \, (z_j)_r$ equals

$$N\,(z_j \circ \text{diag}\,(\Gamma_\ell))_r \, (z_j)_r = N\,(z_j)_r \,\text{diag}\,(\Gamma_\ell)_r \, (z_j)_r = N\text{diag}\,(\Gamma_\ell)_r \,.$$

Since all p columns z_i in Z satisfy $z_i \circ z_i = \text{diag}\,(\Gamma_1)$,

$$\left(Z\left(Z^T \Gamma_1 Z\right) Z^T\right)_{r,r} = Np\,(\text{diag}\,(\Gamma_1))_r \,.$$

The number of pairs z_i and z_j of columns in Z that satisfy diag $(\Gamma_\ell) = z_i \circ z_j$ equals p_ℓ and since each of these pairs appears twice in the sum in (A.1) we find for ℓ such that $2 \leq \ell \leq v$,

$$\left(Z\left(Z^T \Gamma_\ell Z\right) Z^T\right)_{r,r} = 2Np_\ell\,(\text{diag}\,(\Gamma_\ell))_r \,.$$

Hence, we have found that diag $(P_Z \Gamma_\ell P_Z)$ equals

$$\frac{1}{N^2}\text{diag}\left(ZZ^T \Gamma_\ell ZZ^T\right) = \begin{cases} \frac{p}{N}\text{diag}\,(\Gamma_1) & \text{if } \ell = 1 \\ \frac{2p_\ell}{N}\text{diag}\,(\Gamma_\ell) & \text{if } 2 \leq \ell \leq v \end{cases}.$$

The diagonal of matrix A_ℓ is a multiple of the diagonal of the matrix Γ_ℓ, in particular,

$$\text{diag}\,(A_\ell) = \begin{cases} \frac{N-p}{N}\text{diag}\,(\Gamma_1) & \text{if } \ell = 1 \\ \frac{N-2(p-p_\ell)}{N}\text{diag}\,(\Gamma_m) & \text{if } 2 \leq \ell \leq v \end{cases}.$$

The conditions $p < N$ and $2\,(p - p_\ell) < N$ imply that none of the columns $\text{diag}\,(A_\ell)\,, 1 \leq \ell \leq v$, in B equals zero. Since the columns of B are all multiples of different diagonals of the matrices $\Gamma_i, 1 \leq i \leq v$, the matrix B is orthogonal. The matrix $\left(B^T B\right)^{-1} B^T$ is

$$\left(B^T B\right)^{-1} B^T = \begin{pmatrix} \frac{1}{N-p}\left(\text{diag}\,(\Gamma_1)^T\right) \\ \frac{1}{N-2(p-p_2)}\left(\text{diag}\,(\Gamma_2)^T\right) \\ \vdots \\ \frac{1}{N-2(p-p_v)}\left(\text{diag}\,(\Gamma_v)^T\right) \end{pmatrix}.$$

The estimator for α_1 proposed by Brenneman and Nair (2001) is the first element of $\left(B^T B\right)^{-1} B^T R^\star$ and is given by

$$\frac{1}{N-p}\sum_{1 \leq i \leq N} R_i^2.$$

The estimator for the dispersion effect $\alpha_\ell, 2 \leq \ell \leq v$, is given by

$$\frac{1}{N-2\,(p-p_\ell)}\left(\sum_{i:(\Gamma_\ell)_{i,i}=1} R_i^2 - \sum_{i:(\Gamma_\ell)_{i,i}=-1} R_i^2\right).$$

This completes the proof. □

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Summary

Equivalences in Design of Experiments

The statistical theory of experimental designs was initiated by Fisher in the 1920s in the context of agricultural experiments performed at the Rothamsted Experimental Station. Applications of experimental designs in industry started in the 1930s, but really took off after World War II. The second half of the 20th century witnessed both a widespread application of experimental designs in industrial settings and tremendous advances in the mathematical and statistical theory. Recent technological developments in biology (DNA microarrays) and chemical engineering (high-throughput reactors) generated new challenges in experimental design. So experimental designs is a lively subject with a rich history from both an applied and theoretical point of view.

This thesis is mainly an exploration of the mathematical framework underlying factorial designs, an important subclass of experimental designs. Factorial designs are probably the most widely used type of experimental designs in industry. The literature on experimental designs is either example-based with lack of general statements and clear definitions or so abstract that the link to real applications is lost. With this thesis we hope to contribute to closing this gap. By restricting ourselves to factorial designs it is possible to provide a framework which is mathematically rigorous yet applicable in practice.

A mathematical framework for factorial designs is given in Chapter 2. Each of the subsequent chapters is devoted to a specific topic related to factorial designs.

In Chapter 3 we study coding full factorial designs by finite Abelian groups. This idea was introduced by Fisher in the 1940s to study confounding. Confounding arises when one performs only a fraction of a full factorial design. Using the character theory of finite Abelian groups we show that definitions of so-called regular fractions given by Collombier (1996), Wu and Hamada (2000) and Pistone and Rogantin (2005) are equivalent. An important ingredient in our approach is the special role played by the cosets of the finite Abelian group. We moreover use character theory to prove that any regular fraction when interpreted as a coset is an orthogonal array of a certain strength related to the resolution of that fraction. This is a generalization of results by Rao and Bose for regular fractions of symmetric factorial designs with a prime power as the

number of levels.

The standard way to analyze factorial designs is analysis of variance. Diaconis and Viana have shown that the well-known sums of squares decomposition in analysis of variance for full factorial designs naturally arises from harmonic analysis on a finite Abelian group. We give a slight extension of their setup by developing the theoretical aspects of harmonic analysis of data structured on cosets of finite Abelian groups.

In Chapter 4 we study the estimation of dispersion parameters in a mixed linear model. This is the common model behind modern engineering approaches to experimental design like the Taguchi approach. We give necessary and sufficient conditions for the existence of translation invariant unbiased estimators for the dispersion parameters in the mixed linear model. We show that the estimators for the dispersion parameters in Malley (1986) and Liao and Iyer (2000) are equivalent.

In the 1980s Box and Meyer initiated the identification of dispersion effects from unreplicated factorial experiments. They did not give an explicit estimation procedure for the dispersion parameters. We show that the well-known estimators for dispersion effects proposed by Wiklander (1998), Liao and Iyer (2000) and Brenneman and Nair (2001) coincide for two-level full factorial designs and their regular fractions. Moreover, we give a definition for MINQUE estimator for the dispersion effects in two-level full factorial designs and show that the above estimators are MINQUE in this sense.

Finally, in Chapter 5 we study a real-life industrial problem from a two-step production process. In this problem an intermediate product from step 1 is split into several parts in order to allow further processing in step 2. This type of situation is typically handled by using a split-plot design. However, in this specific example running a full factorial split-plot design was not feasible for economic reasons. We show how to apply recently developed analysis methods for fractional factorial split-plot designs developed by Bisgaard, Bingham and Sitter. Finally, we modified the algorithm in Franklin and Bailey (1977) to generate fractional factorial split-plot designs that identify a given set of effects while minimizing the number of required intermediate products.

Samenvatting

Equivalenties in de Theorie van Proefopzetten

De statistische theorie van proefopzetten werd in de jaren twintig van de vorige eeuw geïntroduceerd door Fisher, toen werkzaam bij het landbouwkundig proefstation Rothamsted. De eerste toepassingen van deze theorie in de industrie vonden plaats in de jaren dertig, maar de echte acceptatie van deze theorie door de industrie kwam er pas na de Tweede Wereldoorlog. In de jaren volgend op de oorlog nam het gebruik van proefopzetten in de industrie sterk toe en werden er grote vooruitgangen geboekt in de ontwikkeling van de gerelateerde wiskundige en statistische theorie. Recente technologische ontwikkelingen in biologie (DNA microarrays) en scheikundige technologie (high-troughput reactoren) leverden nieuwe uitdagingen voor het opzetten van experimenten. Kortom de theorie van proefopzetten is een dynamisch onderwerp met een rijke historie vanuit zowel theoretisch als toegepast oogpunt.

Dit proefschrift is vooral een uiteenzetting van het wiskundige raamwerk dat ten grondslag ligt aan de factoriële proefopzetten, een belangrijke categorie proefopzetten. Factoriële proefopzetten zijn waarschijnlijk de meest gebruikte proefopzetten in de industrie. Literatuur over proefopzetten is vaak ofwel gebaseerd op voorbeelden met een gebrek aan algemene stellingen en duidelijke definities ofwel zo abstract dat het verband met toepassingen in de praktijk ver te zoeken is. Met dit proefschrift hopen we een bijdrage te leveren aan het overbruggen van deze kloof tussen theorie en praktijk. Door ons te beperken tot factoriële proefopzetten is het mogelijk een raamwerk te geven dat zowel wiskundig correct als hanteerbaar in de praktijk is.

Het wiskundig raamwerk voor factoriële proefopzetten wordt beschreven in hoofdstuk 2. Elk van de daaropvolgende hoofdstukken is gewijd aan specifiek onderwerp gerelateerd aan factoriële proefopzetten.

In hoofdstuk 3 bestuderen we het coderen van volledige factoriële proefopzetten door middel van een eindige abelse groep. Dit idee werd in de jaren veertig door Fisher geïntroduceerd om de verstrengeling van effecten te bestuderen. Verstrengeling vindt plaats wanneer slechts een fractie van een volledige factoriële proefopzet wordt uitgevoerd. Met behulp van de karaktertheorie van eindige abelse groepen laten we zien dat definities van zogenaamde reguliere fracties zoals gegeven in Collombier (1996), Wu en Hamada (2000) en Pistone

en Rogantin (2005) equivalent zijn. Een belangrijk element in onze benadering is de special rol van de cosets van de eindige abelse groep. We gebruiken de karaktertheorie tevens om te laten zien dat elke regulier fractie, wanneer deze geïnterpreteerd wordt als een coset, een orthogonale array is waarvan de sterkte gerelateerd is aan de resolutie van de fractie. Dit is een generalisatie van de resultaten van Rao en Bose voor regular fracties van symmetrische factoriële proefopzetten waar het aantal niveaus een priemmacht is.

De gebruikelijke methode om factoriële proefopzetten te analyseren is door middel van variantie-analyse. Diaconis en Viana hebben laten zien dat de bekende decompositie van de totale kwadratensom in de variantie-analyse voor een volledige factoriële proefopzet op een natuurlijke manier volgt uit de harmonische analyse op de eindige abelse groep. Wij geven een kleine uitbreiding van hun aanpak door de theoretische aspecten van harmonische analyse voor data gestructureerd op de cosets van eindige abelse groepen te ontwikkelen.

In hoofdstuk 4 bestuderen we het schatten van de dispersie parameters in een mixed linear model. Dit is het gebruikelijke model achter moderne toepassingen van proefopzetten voor productontwikkeling, zoals de Taguchi methode. We geven noodzakelijke en voldoende voorwaarden voor het bestaan van translatie invariante zuivere kwadratische schatters voor de dispersie parameters in het model. Tevens laten we zien dat de schatters voor de dispersie parameters gegeven in Malley (1996) en Liao en Iyer (2000) equivalent zijn.

In de jaren tachtig stelden Box en Meyer voor om dispersie effecten te identificeren door gebruik te maken van factoriële proefopzetten zonder herhalingen. Zij gaven echter geen expliciete schattingsprocedure voor de dispersie parameters. We laten zien dat de bekende schatters voor de dispersie effecten voorgesteld door Wiklander (1998), Liao en Iyer (2000) en Brenneman en Nair (2001) samenvallen voor volledige factoriële proefopzetten met alle factoren op twee niveaus en hun regulier fracties. Daarnaast geven we een definitie voor de MINQUE schatter voor de dispersie effecten in volledige factoriële proefopzet met alle factoren op twee niveaus en laten we zien dat de eerder genoemde schatters MINQUE zijn.

Tenslotte bestuderen we in hoofdstuk 5 een vraagstuk vanuit de industrie dat betrekking heeft op een twee-stappen productie proces. In dit proces wordt een halfproduct na de eerste stap gesplitst in enkele delen om verdere productie in de tweede stap te ondergaan. In een dergelijke situatie wordt gewoonlijk gebruik gemaakt van een split-plot proefopzet. Echter, in dit specifieke voorbeeld was het uitvoeren van een volledige factoriële split-plot proefopzet vanwege financiële redenen niet haalbaar. We laten zien hoe de recent door Bisgaard, Bingham en Sitter ontwikkelde analysemethoden voor fractionele factoriële split-plot proefopzetten gebruikt kunnen worden. Het algoritme van Franklin en Bailey (1977) werd aangepast om zo fractionele factoriële split-plot proefopzetten te construeren die een gegeven set van effecten identificeren en tegelijkertijd het aantal vereiste halfproducten minimaliseren.

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Curriculum Vitae

Peter van de Ven was born in 's-Hertogenbosch, the Netherlands, on March 21, 1978. He attended grammar school at the Beekvliet Gymnasium, Sint-Michielsgestel, where he obtained his degree in June 1995. Peter went on to study Engineering Mathematics at the Eindhoven University of Technology, where he received his Master of Science (M.Sc.) degree from the Department of Mathematics and Computer Science in August 2001. In parallel he studied Health Psychology at the University of Tilburg, where he obtained a Master of Arts (M.A.) degree from the Department of Social Sciences in January 2003. Peter started his Ph.D. research in February 2003 in the Statistical Information and Modelling group of the research institute EURANDOM. His research focussed on several topics in design of experiments. Peter defends his thesis on May 21, 2007, at the Eindhoven University of Technology. On June 1, 2007, he joins the Design of Experiments group of the Southampton Statistical Science Research Institute (S3RI) as a Research Fellow.