One at a time plans for 2p factor sequencing designs

by James Leonard Hansen

A thesis submitted to the Graduate Faculty in partial fulfillment of the requirements for the degree of DOCTOR OF PHILOSOPHY in Mathematics
Montana State University

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This thesis examines 2^p factorial experiments where the order of the application of the factors may be significant. In the experiments considered, the low level of a factor is the absence of a factor, while the high level of the factor is the presence of a factor. The effects of the factors are permanent and each unit may be tested at least p+1 times without the test affecting the unit. The assumptions which relate order effects are examined and a system with algebraic properties is proposed to assist the experimenter in estimating and interpreting order effects. A design and analysis are presented which allow for the estimation of order effects in addition to the usual main effects and interactions. The system for order effects is used to construct one at a time plans which allow for the estimation of order effects and factorial effects in experimental situations where the experimenter can get quick results with random error small in comparison to the effects which are to be estimated.

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ABSTRACT

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CHAPTER I

INTRODUCTION

Factorial experiments are useful when the researcher is investigating the effects of each of a number of factors on the response of some variable. Usually all factors are applied simultaneously to the experimental units and the response is recorded. This is especially true in agricultural experiments where different levels of the treatments may be applied simultaneously and the response is observed and recorded. This type of experimentation was developed by R. A. Fisher [4] in the 1920's and early 1930's. Factorial experimentation is very efficient because every observation supplies information about each factor included in the experiment.

In many industrial experiments where the factors are environments, the factors can not be applied simultaneously, but may be applied in any order. For example, in testing electrical switches or relays, one factor may be vibration and another mechanical shock. In this instance, the factors must be applied sequentially and the order of the application of the factors may be important. R. R. Prarie and W. J. Zimmer treated this problem in two papers published in 1964 and 1968 in the Journal of the American Statistical Society.

The type of sequential experimental design referred to in the Praire and Zimmer papers is related to the order of the application of the factors. This is different from the definition of sequential experimental designs, where observations are obtained in sequence in time and it is to be decided at each point in time whether the experiment is to be continued and possibly what treatment combination is to be used. Therefore, Prairie and Zimmer termed their designs Factor Sequencing Designs (FSD) to distinguish them from Factorial Designs or from Sequential Designs.

In [9], Prairie and Zimmer considered 2^p experiments which apply to the situations where:

a) Each unit may be tested p+1 times without the test itself having an effect on the same unit.

b) There can be no trend effect with successive tests on the same unit.

c) The high level of a factor is the presence of a factor and the low level is the absence of the factor.

d) The effects of the factors are permanent.

The experimental designs discussed in this thesis will always be assumed to satisfy this same set of assumptions.

The usual 2^p factorial designs require 2^p units with one test per unit to estimate all factorial effects. The Factor Sequencing Designs (FSD) developed in [9] require p! units and p+1 tests per unit. In [9], the design and the analysis for full FSD are presented, and in [10], fractions of the full FSD experiment are presented. The purpose of the FSD experiment as presented by Prairie and Zimmer is to determine the importance of the order of application of factors. If order is not important, the factorial effects are estimated in the usual way. But if order is important, they state that the interpretation of the factorial effects is difficult.

If the factors cannot be applied simultaneously, they must be applied in sequence one at a time. Many scientists do their experimental work in single steps, and strive to learn something from each trial or run. These scientists can react quickly to the results of individual runs; however, in order to achieve good results, the experimenter should have effects which are at least three or four times as large as his average random error per trial.

In [3], C. Daniel proposed one at a time plans to produce data of greater value to the experimenter than the sequences of one at a time trials previously used. He indicated that this type of experimentation is economical, but may give biased estimates.

In his paper he described many of these biases as two factor interactions, and then provided sequences of one at a time runs to separate main effects from these two factor interactions and gave methods of estimating each two factor interaction separately.

Factor Sequencing Designs were designed to estimate the effect of the order of application of treatments. But each 2^p FSD requires p! units and (p+1) tests per unit; therefore, one at a time experimentation can be used to determine as quickly as possible if the order of application of the factors makes a difference. The purpose of this thesis is to present a model which will yield the same tests for orders as those presented in [9] and [10] and in addition, will allow for the estimation of the order effects. When one at a time plans are used, the proposed model will also enable the experimenter to interpret his results if order effects are present. If the sequence of one at a time runs is incomplete, the model allows for estimation of the resulting biases in the order parameters. The one at a time plans are constructed to yield maximum information about order effects as early as possible in the experiment.

CHAPTER II

A SYSTEM FOR EXAMINING ORDER EFFECTS

Preliminary Considerations

To facilitate the study of order effects, a model analogous to the usual mixed model will be used with random unit effects and fixed treatment effects. The model used to represent a response for the 2^p FSD is

$$Y_{ij}(f_1,\ldots,f_{j-1}) = m + u_i + \eta_{f_1,\ldots,f_{j-1}} + \theta_{1\ldots j-1} + \epsilon_{ij}$$

where

m = the general mean.

u_i = the effect of the ith unit.

$\eta_{f_1,\ldots,f_{j-1}}$ = the effect of the factors $f_1,\ldots f_{j-1}$, in any order, for j=1 the symbol used is η_1.

$\theta_{1\ldots j-1}$ = the order effect of applying factors $f_1,\ldots,f_{j-1}$ in the specific order $f_1,\ldots,f_{j-1}$.

ϵ_{ij} = the random error associated with the jth test on the ith unit.

For example, in the response

$$Y_{ij}(f_1,f_2) = m + u_i + \eta_{f_1,f_2} + \theta_{12} + \epsilon_{ij}$$

the term θ_{12} indicates the order effect resulting from applying treatments f_1 and f_2 in that specific order; first

f_1 and then f_2. Similarly θ_{21} would indicate the order effect resulting from applying treatments in the order f_2 and then f_1.

The model will be discussed in more detail later. The present section is involved with developing a system to assist is the discussion of order effects. Throughout the discussion, reference will be made to properties of a binary operation. The properties used are the following:

<u>Commutative Property</u>: A binary operation * will be commutative if and only if $a * b = b * a$.

<u>Associative Property</u>: A binary operation * will be associative if and only if $(a * b) * c = a * (b * c)$.

To motivate the discussion, consider the following responses

$$Y_{11}(1) = m + u_1 + \eta_1 + \epsilon_{11}$$
$$Y_{12}(f_1) = m + u_1 + \eta_{f_1} + \theta_1 + \epsilon_{12}$$
$$Y_{13}(f_1,f_2) = m + u_1 + \eta_{f_1,f_2} + \theta_{12} + \epsilon_{13}$$
$$Y_{14}(f_1,f_2,f_3) = m + u_1 + \eta_{f_1,f_2,f_3} + \theta_{123} + \epsilon_{14}$$

The response $Y_{11}(1)$ is a preliminary test before any factor has been applied. The response $Y_{12}(f_1)$ is the response after one factor has been applied, and the symbol θ_1 is not subject to an order interpretation. In the response $Y_{13}(f_1, f_2)$, θ_{12} could be denoted by $\theta_1 * \theta_2$ where the star would define an operation on the order effects. Hence,

$$\theta_1 * \theta_2 = \theta_{12}$$

and indicates the order effect of applying treatment f_1 first and then treatment f_2 second. Similarly,

$$\begin{aligned} \theta_1 * \theta_2 * \theta_3 &= \theta_{12} * \theta_3 \\ &= \theta_{123}. \end{aligned}$$

The operation * is well-defined, but is not commutative. If * were commutative,

$$\begin{aligned} \theta_{12} &= \theta_1 * \theta_2 \\ &= \theta_2 * \theta_1 \\ &= \theta_{21}, \end{aligned}$$

which would imply no two factor order effects were present. Thus the assumption of commutivity would eliminate precisely the property of the model which the FSD is used to determine.

Associativity would imply

$$\begin{aligned} \theta_{123} &= \theta_{12} * \theta_3 \\ &= \theta_1 * \theta_2 * \theta_3 \\ &= \theta_1 * \theta_{23}. \end{aligned}$$

Although this concept does not contradict the basic design assumptions as commutivity does, the expression

$\theta_1 * \theta_{23}$ is difficult to interpret. However, the assumption of associativity simplifies the discussion which follows and for this reason will be included in the definition of *.

The following definition is based on the preceding discussion.

Definition 2.1: The associative binary operation * relating order effects is defined by

$$\theta_1 * \theta_2 = \theta_{12}.$$

The operation is extended to three or more effects by repeated operation on the right. For example,

$$\theta_{12} * \theta_3 = \theta_{123}$$

The following lemma is derived from the definition.

Lemma 2.1: Let P and Q represent two permutations of k factors, then if $\theta_P = \theta_Q$, then $\theta_{Pj} = \theta_{Qj}$ for any factor j not a member of the original k factors.

Proof: If $\theta_P = \theta_Q$, then by Definition 2.1

$$\theta_P * \theta_j = \theta_Q * \theta_j$$

or

$$\theta_{Pj} = \theta_{Qj}.$$

For example, if the two order effects θ_{123} and θ_{321} are equal, i.e. $\theta_{123} = \theta_{321}$, then if factor f_5 is applied, Lemma 2.1 with P = 123, Q = 321, and j = 5 implies

$$\theta_{1235} = \theta_{3215}.$$

The above Definition and Lemma will be used to develop a system which aides in the interpretation of results from FSD experiments where order effects are not negligible and assists in developing one at a time plans for these designs. To motivate the discussion, consider the following example of a 2^3 experiment.

Example 2.1: The experiment consists of applying three factors f_1, f_2 and f_3 each at two levels where the low level indicates no treatment is applied and the high level indicates the treatment is applied. Assume there are six units available and the following experiments are performed.

Unit	Application Sequences
1	f_1f_2
2	f_1f_3
3	f_2f_1
4	f_2f_3
5	f_3f_1
6	f_3f_2

In the array given above, the notation f_1f_2 represents an application sequence. The symbol f_1f_2 indicates the unit has been tested three times at this stage of the experiment: first, prior to any treatment; second, after factor f_1 was applied; and third, after the application of factor f_2. A similar interpretation follows for application sequences of more than two factors.

Then suppose the appropriate contrasts have been tested and the following equivalences are determined from the experimental data.

$$\theta_{12} = \theta_{21}$$
$$\theta_{23} = \theta_{32}$$
$$\theta_{31} = \theta_{13}.$$

By applying Lemma 2.1, the following equalities can be derived.

$$\theta_{123} = \theta_{213}$$
$$\theta_{231} = \theta_{321}$$
$$\theta_{132} = \theta_{312}.$$

The above relationships are intuitive because if it is assumed that experimental units are not affected by order after the applications of two factors, the two units should be the same except for experimental error. Therefore, the same response is expected from the two units after applying the same third treatment to each.

However, there is no reason to assume a priori that $\theta_{123} = \theta_{231}$ or $\theta_{123} = \theta_{132}$. It is possible that the three sets could all be non-zero quantities, and in this instance the interpretation would be that three factor order effects occur, but there are no significant two factor order effects. Prairie and Zimmer, in their 1968 paper, presented some fractions of the full FSD design. Some of these fractions involved testing only all possible two factor order combinations by an F test. The above example is intended to illustrate the possibility of a higher order effect, in this case a three factor order effect, even though the test for two factor order effects would not be significant.

Assumptions Regarding Binary Operations In Order Effects

Example 2.1 indicates a need to examine the assumptions underlying order effects. The following discussion will consider two situations and each one will be examined by relating the binary operation to the types of properties it satisfies.

Case 1: The first case considered is the situation where it is known that the set of all order effects of k or fewer factors is insignificant. This prior knowledge gives no information about the set of order effects when more than k factors have been applied. This is equivalent to assuming those properties on the binary operation given in Definition 2.1 and Lemma 2.1 for combining order effects. A situation where this occurs would be as in Example 2.1, and in this instance there could possibly be three distinct three factor order effects for the 2^3, the effects related to (1) θ_{123} and θ_{213}, (2) θ_{231} and θ_{321}, and (3) θ_{132} and θ_{312}, even though two factor effects are absent. Lemma 2.1 gives partial commutativity for effects judged insignificant using experimental data. This means symbols related to two factor order effects which have been determined to be insignificant can be commuted only when they appear in the left-most positions in the sequence.

For example, consider a 2^3 FSD and assume the appropriate two factor order effects have been tested and based on these observations the experimenter assumes $\theta_{12} = \theta_{21}$, $\theta_{13} \neq \theta_{31}$, and $\theta_{23} = \theta_{32}$. Lemma 2.1 indicates the following relationships concerning three factor interactions,

$$\theta_{123} = \theta_{213} \text{ and } \theta_{231} = \theta_{321}.$$

Based on this information the experimenter can plan the remaining experimentation to get the most information with the least expenditure of resources.

Using the assumptions of Case 1, the experimenter can use this system to develop relationships among the order effects. Case 1 could be referred to as the case where two factor order effects judged insignificant commute only on the left of the application sequence.

Case 2: The next situation discussed is one where the symbols related to two factor order effects determined to be insignificant can be commuted anywhere they appear in the complete order sequence. This is equivalent to assuming the binary operation is commutative for the symbols judged insignificant as well as associative for all symbols. The following definition is based on the preceding discussion.

Definition 2.2: The binary operation * is commutative if $\theta_{ij} = \theta_{ji}$, then $\theta_{PijQ} = \theta_{PjiQ}$ for any two sequences of factors P and Q.

Applying the definition with i = 1, j = 2, P = 4 and Q = 35, and if $\theta_{12} = \theta_{12}$, then

$$\theta_{41235} = \theta_{42135}.$$

This Definition can be used to determine the sequence of factors to be run to yield maximum information. For example, consider a 2^3 FSD design where it has been determined that $\theta_{12} = \theta_{21}$, and $\theta_{23} = \theta_{32}$, but that $\theta_{13} \neq \theta_{31}$.

Since $\theta_{12} = \theta_{21}$, Lemma 2.1 implies $\theta_{123} = \theta_{213}$. In addition, $\theta_{23} = \theta_{32}$ and Definition 2.2 implies $\theta_{123} = \theta_{132}$. Hence,

$$\theta_{123} = \theta_{213} = \theta_{132}.$$

Similarly, Lemma 2.1 and Definition 2.2 imply

$$\theta_{312} = \theta_{321} = \theta_{231}.$$

The two sets can be defined as equivalence classes of order effects. The result is intuitive in that if there is only an order effect related to factors A and C, i.e. $\theta_{13} \neq \theta_{31}$, then the position of B in the treatment sequence has no effect, only the relative positions of A and C.

If the experimenter can assume the conditions of Case 2, he can find more relationships among the order effects than he could in Case 1. Case 2, could be referred to as the case where two factor order effects judged insignificant commute anywhere they appear together in the application sequence.

Even if Definition 2.2 can not be assumed a priori, the experiment can be run as in Case 1 where the results of Case 2 are possibilities to be tested for experimentally.

If there is a set of equivalence classes of order effects, the sets can be helpful in interpreting and applying the results of the experiment when order effects are present. For instance, if an FSD is being used to determine factor effects for some industrial process, the order effect could indicate a type of catalytic effect related to the order of application of factors, and the desired results might be achieved only through a specific order of application. When implementing a production process, the knowledge that order effects have been separated into equivalence classes allows for the selection of any particular factor application order sequence from an equivalence class on the basis of optimization in terms of criterion such as production time or cost.

CHAPTER III

ESTIMATION AND INTERPRETATION OF ORDER EFFECTS

Design and Model

The model used is similar to the one discussed by Prairie and Zimmer [9], and is the one stated in equation 2.1. The main difference is the addition of specific representations of order parameters and assumptions concerning these parameters to allow for their estimation and an interpretation of these order effects.

Each factor $f_i (i = 1,\ldots,p)$ has a high level (f_i has been applied) and a low level (f_i has not been applied). Because the effects of the factors are assumed to be permanent, a unit which has received factor f_i at some point must be considered as having the high level of that factor from that time on. In addition, in a complete experiment, every unit will receive each of the p factors in some order and will be tested (p+1) times with the first test occurring before the application of any factor and each succeeding test occurring after the application of each of the p factors.

The design considered in [9] was one where p! groups of r units each were subjected to exactly one of the possible p! orders. A notation for the model was given in Chapter II and is restated here.

(3.1) $$Y_{ij}(f_1,\ldots,f_{j-1}) = m + u_i + \eta_{f_1,\ldots,f_{j-1}} + \theta_{1\ldots j-1} + \epsilon_{ij}$$

$$i = 1,\ldots,r \cdot p!$$

$$j = 1,\ldots,p+1$$

where $Y_{ij}(f_1,\ldots,f_{j-1})$ denotes the response from the jth test on the ith unit resulting from the j-1 factors applied in the application sequence $f_1\ldots f_{j-1}$. The parameters are defined as they were in Chapter II. In addition, it is also assumed that

(1) $e_{ij} \sim NID(0,\sigma_e^2)$

(2) $u_i \sim NID(0,\sigma_u^2)$

(3) There are no interactions among the θ's or between the θ's and the η's.

(4) Let Λ_k be the set of all permutations of k factors, then

(3.2) $$\sum_{L\in\Lambda_k} \theta_L = 0,$$

for $2 \leq k \leq p$.

Example 3.1: If the experiment being run is a 2^3 FSD, then the set of order effects is:

$$\{\theta_{12},\theta_{21},\theta_{13},\theta_{31},\theta_{23},\theta_{123},\theta_{132},\theta_{213},\theta_{231},\theta_{312},\theta_{321}\}$$

and condition (4) would imply

$$\theta_{12} + \theta_{21} = 0,$$

$$\theta_{13} + \theta_{31} = 0,$$

$$\theta_{23} + \theta_{32} = 0,$$

and $$\theta_{123} + \theta_{132} + \theta_{213} + \theta_{231} + \theta_{312} + \theta_{321} = 0$$

Conditions (1) and (2) are usual assumptions for mixed models where the population of inference is infinite. Condition (3) indicates an assumption of independence between the order effects and the factor effects. The order effects are a special type of interaction and to assert they interact with the factor effects would be a redundancy. To assume they interact with each other would imply that orders interact with orders which is also redundant because the test is for order effects and the θ's as defined are order parameters. Condition (4) is imposed to provide a full rank model. However, the assumption does not seem unreasonable because if there is for example an order effect related to f_1 and f_2, the assumption $\theta_{12} + \theta_{21} = 0$ would indicate one order provides an increase to the general mean while the other yields a decrease in the response from the general mean. Similar interpretations hold for order effects for more than two factors, some will decrease the response level and some will increase it, but the deviations from the general mean will add to zero.

Using matrix notation, the model stated in equation 3.1 may be written as

$$\underset{\sim}{Y} = \underset{\sim}{X}^*\begin{pmatrix} m \\ \underset{\sim}{\beta}^* \end{pmatrix} + \underset{\sim}{W}\underset{\sim}{u} + \underset{\sim}{\epsilon} \qquad (3.3)$$

where $\underset{\sim}{Y}$ is the $r(p+1)p! \times 1$ column vector of observations, $\underset{\sim}{X}^*$ is the design matrix with $r(p+1)p!$ rows and $1 + 2^p + \sum_{i=2}^{p} p!/(p-i)!$ columns, β^* is column vector of factor and order parameters with $2^p + \sum_{i=2}^{p} p!/(p-i)!$ rows, $\underset{\sim}{u}$ is the $rp! \times 1$ column vector of unit parameters, $\underset{\sim}{W}$ is the $r(p+1)p! \times rp!$ matrix whose cth column is a column of zeros except for ones in the $[(c-1)(p+1)+1]$th row through the $[c(p+1)]$th row and $\underset{\sim}{\epsilon}$ is the $r(p+1)p! \times 1$ column vector of random errors.

To illustrate the model the responses from a 2^3 are

$$
\begin{aligned}
&Y_{11}(1) = m + u_1 + \eta_1 + \epsilon_{11} \\
&Y_{12}(A) = m + u_1 + \eta_A + \epsilon_{12} \\
&Y_{13}(A,B) = m + u_1 + \eta_{A,B} + \theta_{12} + \epsilon_{13} \\
(3.4)\quad &Y_{14}(A,B,C) = m + u_1 + \eta_{A,B,C} + \theta_{123} + \epsilon_{14} \\
&Y_{21}(1) = m + u_2 + \eta_1 + \epsilon_{21} \\
&\qquad\vdots \qquad\qquad \vdots \\
&Y_{24}(A,C,B) = m + u_2 + \eta_{A,B,C} + \theta_{132} + \epsilon_{24} \\
&\qquad\vdots \qquad\qquad \vdots \\
&Y_{64}(C,B,A) = m + u_6 + \eta_{A,B,C} + \theta_{321} + \epsilon_{64}
\end{aligned}
$$

This model is different from the one proposed in [9] in that Prarie and Zimmer did not include explicit parameters for order effects. However, the model presented in 3.2 has the same number of linearly independent observation vectors, hence their result concerning the rank of the design matrix holds for $\underset{\sim}{X}^*$. The rank of $\underset{\sim}{X}^*$ is

$$(3.5)\qquad \sum_{i=0}^{p} p!/(p-i)!$$

For example, if unit parameters are ignored (the vector $\underset{\sim}{\beta}^*$ does not include unit parameters), then for one replication of a 2^3 FSD, there are 6 units which have η_1, two units each for η_A, η_B, η_C, one unit for each of η_{ij} and its order parameter and one unit for η_{ijk} with the appropriate order parameters, hence there are

$$\sum_{i=0}^{3} 3!/(3-i)! = 1 + 3 + 6 + 6 = 16$$

linearly independent column vectors in $\underset{\sim}{X}^*$ for a 2^3.

The argument can be extended and therefore the rank of $\underset{\sim}{X}^*$ for arbitrary p is as given in Equation 3.5.

The rank of $\underset{\sim}{X}^{*\prime}\underset{\sim}{X}^*$ is the same as the rank of $\underset{\sim}{X}^*$, and the size of the $\underset{\sim}{X}^{*\prime}\underset{\sim}{X}^*$ is equal to the number of columns in $\underset{\sim}{X}^*$. The following discussion will show that a series of constraints on the model parameters will lead to a new model of full rank.

A reparameterization of the factor effects formed by subtracting η_1 from each factor parameter and deleting the column of zeros will reduce the dimension of $\underset{\sim}{X}^*$ by one without changing the rank. Using condition 4, the order effects can be reparameterized to form a full rank model. The following lemmas show that the reparameterization based on condition 4 is sufficient for a full rank model.

<u>Lemma 3.1</u>: In a 2^p FSD experiment, there are

$$\sum_{i=2}^{p} p!/(p-i)!$$ order effects.

Proof: For a fixed i the number of order effects for i factors is the permutation of p factors taken i at a time, i.e. $p!/(p-i)!$. For a 2^p FSD order effects are possible if $i = 2,\ldots,p$. So there are

$$\sum_{i=2}^{p} p!/(p-i)!$$ possible order effects. This completes the proof of the lemma.

Lemma 3.1 implies there are

$$\sum_{i=2}^{3} 3!/(3-i)! = 12$$

order effects for the 2^3 FSD. The twelve effects were enumerated in Example 3.1.

The following lemma will show how many constraints are imposed by condition (4).

<u>Lemma 3.2</u>: For a 2^p FSD experiment condition (4) implies

$$\sum_{i=2}^{p} \binom{p}{i}$$

constraints are imposed on the model defined by Equation 3.1.

Proof: For a fixed set of i factors $2 \leq i \leq p$, there are $\binom{p}{i}$ possible combinations of factors each of which provides one constaint of the form

$$\sum_{L\epsilon\Lambda_i} \theta_L = 0.$$

Consequently, the total number of constraints is given by

$\sum_{i=2}^{p} \binom{p}{i}$. This completes the proof of the lemma.

Lemma 3.2 implies that four constraints are imposed on the 2^3 FSD. The four constraints were given in Example 3.1.

If the number of constraints is subtracted from the number of order effects, the number of parameters present after imposing the constraints is given by Lemma 3.1 and Lemma 3.2.

$$\sum_{i=2}^{p} p!/(p-i)! - \sum_{i=2}^{p} \binom{p}{i} = \sum_{i=2}^{p} \binom{p}{i} i! - \sum_{i=2}^{p} \binom{p}{i}$$

$$= \sum_{i=2}^{p} \binom{p}{i}\left(i!-1\right).$$

The next lemma indicates the number of order parameters to be estimated after imposing the constraints equals the number of degrees of freedom for order effects in the 2^p FSD design.

Lemma 3.3: In a 2^p FSD experiment there are

$$\sum_{i=2}^{p} \binom{p}{i}(i!-1)$$ degrees of freedom for order effects.

Proof: The number of degrees of freedom is equal to the number of linearly independent comparisons which can be formed between order effects of the same set L of i factors. Hence, each of the $\binom{p}{i}$ combinations can be permuted in i! ways which implies there are $(i!-1)$ independent comparisons which can be formed and for fixed i there are $\binom{p}{i}(i!-1)$ degrees of freedom. Since $2 \leq i \leq p$, the total degrees of freedom for order effects in a 2^p FSD design is

$$\sum_{i=2}^{p} \binom{p}{i}(i!-1).$$ This completes the proof of the lemma.

Lemma 3.3 is illustrated using the 2^3 FSD experiment described in Example 3.1. There are $\binom{3}{2} = 3$ combinations of two factors. They are {12, 13, 23} . Each combination can be permuted in 2! = 2 ways, and only one linearly independent comparison of these two order effects can be obtained. Thus there is (2!-1) = 1 independent effect for each combination. Similarly, there is $\binom{3}{3} = 1$ combinations of the three factors, and there are 3! = 6 order effects. Among these six order effects only five linearly independent comparisons can be made. Therefore there are

$$\sum_{i=2}^{3} \binom{3}{i}(i!-1) = 3\cdot 1 + 1\cdot 5$$
$$= 8$$

independent order effects for the 2^3 FSD.

The rank of $\underset{\sim}{X}^*$ can be decomposed as follows:

$$\sum_{i=0}^{p} p!/(p-i)! = \sum_{i=0}^{p} \binom{p}{i} i!$$

$$= \sum_{i=0}^{p} \binom{p}{i} + \sum_{i=0}^{p} \binom{p}{i}(i!-1).$$

Because the first expression on the right equals 2^p and the first two terms of the second expression are zero,

$$\sum_{i=0}^{p} p!/(p-i)! = 2^p + \sum_{i=2}^{p} \binom{p}{i}(i!-1)$$

$$= 1 + (2^p-1) + \sum_{i=2}^{p} \binom{p}{i}(i!-1)$$

where the expressions on the right correspond to the degrees of freedom for the mean, factors and orders respectively.

The above discussion implies that $\underset{\sim}{X}^*$ can be reparameterized to form a full rank model. The reparameterization can be accomplished by multiplication on the right by a matrix $\underset{\sim}{M}$. The design matrix $\underset{\sim}{X}$ used will be one which contains the appropriate contrasts for factor effects.

The factorial representation and nomenclature for 2^p experiments is given in many tests, eg., [8]. For a 2^p factorial experiment, the treatment combination can be represented as an n-tuple, $(X_1, X_2, \ldots, X_n)$ where each $X_i = \pm 1$. Thus the factorial representation for the result of a single run of in a 2^3 may be written as

$$\left\{m + 1/2[AX_1 + BX_2 + CX_3 + (AB)X_1X_2 + (AC)X_1X_3 + (BC)X_2X_3 + (ABC)X_1X_2X_3]\right\}$$

where m = the general mean

X_i = -1 at the low level of A, B or C for $i = 1, 2, 3$, respectively.

= +1 at the high level of the corresponding factor.

The symbols (AB), et cetera are not products, they represent interactions. The parenthesis will usually be omitted. This representation simplifies the discussion of one at a time plans in Chapters IV and V.

A matrix $\underset{\sim}{M}$ such that $\underset{\sim}{X}^*\underset{\sim}{M} = \underset{\sim}{X}$ exists by the results concerning generalized inverses of Chapter I of Searle [11].

After the reparameterization the model becomes

(3.6) $$\underset{\sim}{Y} = \underset{\sim}{X} \binom{m}{\underset{\sim}{\beta}} + \underset{\sim\sim}{Wu} + \underset{\sim}{\epsilon}.$$

For an example of $\underset{\sim}{X}$ from a 2^3 FSD with $r = 1$, see the Appendix. Also,

$$\binom{m}{\underset{\sim}{\beta}}' = (m, A, B, C, AB, AC, BC, ABC, \theta_{12}, \theta_{13}, \theta_{23}, \theta_{123}, \theta_{132}, \theta_{213}, \theta_{231}, \theta_{312}).$$

Examples of responses are:

$$Y_{11}(1) = m + 1/2\{-A - B - C + AB + AC + BC - ABC\} + u_1 + \epsilon_{11}$$

$$Y_{12}(A) = m + 1/2\{A - B - C - AB - AC + BC + ABC\} + u_1 + \epsilon_{12}$$

$$Y_{13}(A,B) = m + 1/2\{A + B - C + AB - AC - BC - ABC\} + \theta_{12} + u_1 + \epsilon_{13}$$

$$\vdots \qquad\qquad \vdots$$

$$Y_{32}(B,A) = m + 1/2\{A + B - C + AB - AC - BC - ABC\} - \theta_{12} + u_3 + \epsilon_{32}$$

$$\vdots \qquad\qquad \vdots$$

The model used is analogous to the mixed model of random unit effects and fixed treatment effects. The analysis of the design will be explained in the next section.

Analysis

The analysis of the design given in the previous section is based on the analysis presented in [9]. The procedure used was to transform the model by a linear transformation and then to analyze the transformed model using the method of least squares. The same technique is used in the section which follows.

In the discussion which follows, it will be desirable to use a method of multiplication of two matrices which is different from the usual matrix multiplication. This method called the direct product is very useful when working with blocks of submatrices. The following definition is given by Graybill [5].

<u>Definition 3.1</u>: Direct Product: Let $\underset{\sim}{P}$ be a $m_2 \times n_2$ matrix and let $\underset{\sim}{Q}$ be an $m_1 \times n_1$ matrix; then the direct product of $\underset{\sim}{P}$ and $\underset{\sim}{Q}$ written $\underset{\sim}{P} \otimes \underset{\sim}{Q}$ is a matrix $\underset{\sim}{T}$ of size $m_1 m_2 \times n_1 n_2$ defined by

$$\underset{\sim}{T} = [t_{ij}] = [\underset{\sim}{P} q_{ij}].$$

The symbol $\underset{\sim}{I}$ will always denote an identity matrix and $\underset{\sim}{J}$ will always denote a matrix with every element equal to one.

The model defined by equation 3.6 is of full rank, but the Gauss-Markov Theorem does not apply because the Y's are not independent. The non-independence is a result of the following theorem.

<u>Theorem 3.1</u>: For the model given by Equation 3.6,

(1) $E(\underset{\sim}{Y}) = \underset{\sim}{X}\begin{pmatrix} m \\ \underset{\sim}{\beta} \end{pmatrix}$

(2) $\mathrm{Var}(\underset{\sim}{Y}) = \sigma_\epsilon^2 \underset{\sim}{I} + \sigma_u^2 [\underset{\sim}{J} \otimes \underset{\sim}{I}]$

Proof: Applying conditions 1 and 2 of expression 3.2,

(1) $$E(\underset{\sim}{Y}) = E\left(\underset{\sim}{X}\begin{pmatrix} m \\ \underset{\sim}{\beta} \end{pmatrix} + \underset{\sim}{W}\underset{\sim}{u} + \underset{\sim}{\epsilon}\right)$$
$$= E\, \underset{\sim}{X}\begin{pmatrix} m \\ \underset{\sim}{\beta} \end{pmatrix} + E(\underset{\sim}{W}\underset{\sim}{u}) + E(\underset{\sim}{\epsilon})$$
$$= \underset{\sim}{X}\begin{pmatrix} m \\ \underset{\sim}{\beta} \end{pmatrix} + \underset{\sim}{W}E(\underset{\sim}{u})$$
$$= \underset{\sim}{X}\begin{pmatrix} m \\ \underset{\sim}{\beta} \end{pmatrix}$$

(2) $$\mathrm{Var}(\underset{\sim}{Y}) = E\left(\underset{\sim}{Y} - \underset{\sim}{X}\begin{pmatrix} m \\ \underset{\sim}{\beta} \end{pmatrix}\right)^2$$
$$= E(\underset{\sim}{W}\underset{\sim}{u} + \underset{\sim}{\epsilon})^2 = E(\underset{\sim}{\epsilon}^2) + E(\underset{\sim}{W}\underset{\sim}{u}\underset{\sim}{\epsilon}) + E(\underset{\sim}{\epsilon}\underset{\sim}{W}\underset{\sim}{u}) + \underset{\sim}{W}\, E(\underset{\sim}{u}\underset{\sim}{u}')\underset{\sim}{W}'$$
$$= \sigma_\epsilon^2 \underset{\sim}{I} + \sigma_u^2 \underset{\sim}{W}\underset{\sim}{W}'$$
$$= \sigma_\epsilon^2 \underset{\sim}{I} + \sigma_u^2 [\underset{\sim}{J} \otimes \underset{\sim}{I}]$$

where the $\underset{\sim}{I}$ associated with σ_ϵ^2 is the identity of order $r(p+1)p!$, and $[J \otimes I]$ is the direct product of a $\underset{\sim}{J}$ matrix of size $(p+1) \times (p+1)$ and $\underset{\sim}{I}$ is the identity of order $rp!$. Hence, $[\underset{\sim}{J} \otimes \underset{\sim}{I}]$ is a square matrix of order $r(p+1)p!$ which is the same dimension as the identity associated with σ_ϵ^2.

The Gauss-Markov Theorem for least squares estimation can be applied to a transformed vector $\underset{\sim}{Z} = \underset{\sim}{T}\underset{\sim}{Y}$ if

$$\text{Var}(\underset{\sim}{Z}) = \sigma_\epsilon^2 \underset{\sim}{I}.$$

Therefore, the transformation must satisfy

$$\begin{aligned}
\text{Var}(\underset{\sim}{Z}) &= \text{Var}(\underset{\sim}{T}\underset{\sim}{Y}) \\
&= \underset{\sim}{T}\ \text{Var}(\underset{\sim}{Y})\underset{\sim}{T} \\
&= \underset{\sim}{T}[\sigma_\epsilon^2 \underset{\sim}{I} + \sigma_u^2 \underset{\sim}{W}\underset{\sim}{W}']\underset{\sim}{T}' \\
&= \sigma_\epsilon^2 \underset{\sim}{T}\underset{\sim}{T} + \sigma_u^2 \underset{\sim}{T}\underset{\sim}{W}(\underset{\sim}{T}\underset{\sim}{W})' \\
&= \sigma_\epsilon^2 \underset{\sim}{I}
\end{aligned}$$

Hence the matrix $\underset{\sim}{T}$ must satisfy the following two conditions:

$$(1) \qquad \underset{\sim}{T}\underset{\sim}{T}' = \underset{\sim}{I}$$

$$(2) \qquad (\underset{\sim}{T}\underset{\sim}{W})(\underset{\sim}{T}\underset{\sim}{W})' = 0$$

or equivalently

$$\underset{\sim}{T}\underset{\sim}{W} = 0.$$

If $r = 1$, a matrix which satisfies the above conditions is

$$(3.7) \qquad \underset{\sim}{T} = [\underset{\sim}{H} \otimes \underset{\sim}{I}]$$

where $\underset{\sim}{T}$ is a rectangular matrix of dimension $pp! \times (p+1)p!$ and $\underset{\sim}{H}$ is a $p \times p+1$ matrix which is a Helmert matrix with the first row deleted (see Searle [11], page 33).

$$\underset{\sim}{H} = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} & 0 & \cdots & 0 \\ 1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6} & \cdots & 0 \\ \vdots & & \vdots & & \\ \frac{1}{\sqrt{p(p+1)}} & \frac{1}{\sqrt{p(p+1)}} & \frac{1}{\sqrt{p(p+1)}} & \cdots & \frac{-p}{\sqrt{p(p+1)}} \end{bmatrix}$$

For r replications of the FSD experiment, the desired matrix is

$$\underset{\sim}{T} = [\underset{\sim}{T} \otimes \underset{\sim}{j}']$$

where $\underset{\sim}{T}$ is defined as above and $\underset{\sim}{j}'$ is a $r \times 1$ column vector of ones. An example of a matrix $\underset{\sim}{T}$ for one replication of a 2^3 is the Appendix.

The following theorem follows from the definition of $\underset{\sim}{T}$.

Theorem 3.2: For $\underset{\sim}{Y}$ defined by Equation 3.6, and $\underset{\sim}{T}$ defined Equation 3.7. If $\underset{\sim}{Z} = \underset{\sim}{T}\underset{\sim}{Y}$, then

(1) $\underset{\sim}{Z}$ is normal

(2) $E(\underset{\sim}{Z}) = \underset{\sim}{T}\underset{\sim}{X}\binom{m}{\underset{\sim}{\beta}}$

(3) $Var(\underset{\sim}{Z}) = \sigma_\epsilon^2 \underset{\sim}{I}$.

Proof: The proof follows from Theorem 3.1 and a well known result from multivariate analysis (see Anderson Theorem

2.4.5) which states if X is $N(\mu, V)$ and if $Z = DX$ then X is $N(D\mu, DVD')$. Hence, Y normal implies $Z = TY$ is normal and

$$E(Z) = E(TY) = TE(Y) = TX\binom{m}{\beta}$$

and

$$\begin{aligned} Var(Z) &= T\, Var(Y) T' \\ &= T[\sigma_{\epsilon}^{2} I + \sigma_{u}^{2} WW']T' \\ &= \sigma_{\epsilon}^{2} TT' + \sigma_{u}^{2} TW(TW)' \\ &= \sigma_{\epsilon}^{2} I \end{aligned}$$

where I is of order $rp \cdot p! \times rp \cdot p!$. This completes the proof.

The first row of TX is all zeros because the transformation removes the mean effect as well as the unit effects. A full rank model for Z will result if the first column of TX is deleted, and the parameter m deleted from the parameter vector. Set R equal to the matrix TX with the first column deleted, then

$$Z = R\beta + \epsilon \tag{3.8}$$

where R is a

$$rpp! \times \sum_{i=1}^{p} \frac{p!}{(p-i)!}$$

matrix of full column rank, $\underset{\sim}{\beta}$ is a

$$\sum_{i=1}^{p} \frac{p!}{(p-i)!} \times 1$$

column vector of parameters, and $\underset{\sim}{\epsilon}$ is a rpp! $\times$ 1 vector of random errors.

Because the mean and unit effects have been removed, all that remains for degrees of freedom are those for treatments, orders and error. By Theorem 3.2, $\underset{\sim}{Z}$ is normally distributed with $\text{Var}(\underset{\sim}{Z}) = \sigma_{\epsilon}^{2}\underset{\sim}{I}$; therefore, by the Gauss-Markov Theorem the best linear unbiased estimate of $\underset{\sim}{\beta}$ is

(3.9) $$\hat{\underset{\sim}{\beta}} = (\underset{\sim}{R}'\underset{\sim}{R})^{-1}\underset{\sim}{R}'\underset{\sim}{Z}$$

If order is neglected, a new parameter vector is formed, composed only of factor effects,

$$\underset{\sim}{\beta}_1' = (A, B, C, AB, \ldots).$$

Corresponding to this parameter vector, a design matrix $\underset{\sim}{R}_1$ of order rpp! $\times$ (2^p-1) can be found by

(3.10) $$\underset{\sim}{R}_1 = \underset{\sim}{R}\begin{bmatrix}\underset{\sim}{I} \\ \underset{\sim}{0}\end{bmatrix}$$

where $\begin{bmatrix}\underset{\sim}{I} \\ \underset{\sim}{0}\end{bmatrix}$ is an augmented matrix with $\underset{\sim}{I}$ the $(2^p-1) \times (2^p-1)$ identity and $\underset{\sim}{0}$ is a null matrix of order

$$\left(\sum_{i=1}^{p} \frac{p!}{(p-i)!} - (2^p-1)\right) \times (2^p-1).$$

The vector of factor effects $\underset{\sim}{\beta}_1$ is estimated by

(3.11) $$\hat{\underset{\sim}{\beta}}_1 = (\underset{\sim}{R}_1'\underset{\sim}{R}_1)^{-1}\underset{\sim}{R}_1'\underset{\sim}{Z}$$

For a 2^3 FSD with $r = 1$, the matrices $\underset{\sim}{R}$, $(\underset{\sim}{R}'\underset{\sim}{R})^{-1}$, $\underset{\sim}{R}_1$ and $(\underset{\sim}{R}'_1\underset{\sim}{R}_1)^{-1}$ are given in the Appendix.

A partition of the total sum of squares $\underset{\sim}{Z}'\underset{\sim}{Z}$ is

$$\underset{\sim}{Z}'\underset{\sim}{Z} = \underset{\sim}{Z}'[\underset{\sim}{I} - \underset{\sim}{R}(\underset{\sim}{R}'\underset{\sim}{R})^{-1}\underset{\sim}{R}']\underset{\sim}{Z} + \underset{\sim}{Z}'[\underset{\sim}{R}(\underset{\sim}{R}'\underset{\sim}{R})^{-1}\underset{\sim}{R}' - \underset{\sim}{R}_1(\underset{\sim}{R}_1'\underset{\sim}{R}_1)^{-1}\underset{\sim}{R}_1']\underset{\sim}{Z}$$
$$+ \underset{\sim}{Z}'[\underset{\sim}{R}_1(\underset{\sim}{R}_1'\underset{\sim}{R}_1)^{-1}\underset{\sim}{R}_1']\underset{\sim}{Z}$$

where all of the matrices in the brackets are idempotent. Using Equation 3.10, it can be shown that all cross products are zero. The first term of the partition is the error sum of squares associated with fitting the full model. The second term is the sum of squares associated with fitting order effects only and the third term is the sum of squares for factor effects.

The degrees of freedom for factor effects are 2^p-1, and by Lemma 3.3, the degree of freedom for order effects are

$$\sum_{i=2}^{p} \binom{p}{i}\left(i!-1\right).$$

The total degrees of freedom are rpp!, and by subtraction, those for error are

$$rpp! - (2^p-1) - \sum_{i=2}^{p} \binom{p}{i}(i!-1)$$

The preceding discussion can be summarized in the following Analysis of Variance table.

Table 3.1

Source (SV)	Degrees of Freedom (DF)	Sum of Squares (SS)
Total	$rpp!$	$\underset{\sim}{Z}'\underset{\sim}{Z}$
Factors	2^p-1	$\underset{\sim}{Z}'[\underset{\sim}{R}_1(\underset{\sim}{R}_1'\underset{\sim}{R}_1)^{-1}\underset{\sim}{R}_1']\underset{\sim}{Z}$
Orders	$\sum_{i=2}^{p} \binom{p}{i}(i!-1)$	$\underset{\sim}{Z}'[\underset{\sim}{R}(\underset{\sim}{R}'\underset{\sim}{R})^{-1}\underset{\sim}{R} - \underset{\sim}{R}_1(\underset{\sim}{R}_1'\underset{\sim}{R}_1)^{-1}\underset{\sim}{R}_1']\underset{\sim}{Z}$
Error	$rpp! - (2^p-1) - \sum_{i=2}^{p} \binom{p}{i}(i!-1)$	$\underset{\sim}{Z}'[\underset{\sim}{I} - \underset{\sim}{R}(\underset{\sim}{R}'\underset{\sim}{R})^{-1}\underset{\sim}{R}]\underset{\sim}{Z}$

The expected mean squares corresponding to the sums of squares of Table 3.1 are

$$\sigma_e^2 + [\underset{\sim}{\beta}_1'(\underset{\sim}{R}_1'\underset{\sim}{R}_1)\underset{\sim}{\beta}_1]/DF$$

$$\sigma_e^2 + [\underset{\sim}{\beta}'(\underset{\sim}{R}'\underset{\sim}{R})\underset{\sim}{\beta} - \underset{\sim}{\beta}_1'(\underset{\sim}{R}_1'\underset{\sim}{R}_1)\underset{\sim}{\beta}_1]/DF$$

$$\sigma_e^2$$

for factors, orders and error, respectively.

Because the matrices in the quadratic forms for the sums of squares are idempotent with cross product zero, under the null hypothesis of no factor and no order effects the sums of squares are independently distributed as σ^2 times a χ^2 variable. Thus the F-test can be used to test the hypothesis that order effects are all neglible, also the factorial effects can be tested by the appropriate F-test.

In the situation where the order effects are negligible, the factorial effects would be estimated by $\hat{\underset{\sim}{\beta}}_1$. If the order effects are significant, $\hat{\underset{\sim}{\beta}}$ provides an estimate of the factorial and order effects. In this situation, the discussion of Chapter Two applies and aides in the interpretation of the order effects. Two examples are presented to illustrate the analysis and to illustrate the use of this design in interpreting factor and order effects when order effects are significant.

Examples

In [9], examples are provided to illustrate the model presented in that paper. The same data is used in the following two examples to show that the model and design presented in this thesis leads to the same F tests for order effects and for factorial effects.

Example 3.2: The following set of observations is obtained from the data of Table II of [9].

$$\underset{\sim}{Y}' = (56.258,\ 56.579,\ 52.661,\ 51.315,\ 55.500,\ 57.461,\ 57.475,\ 50.396,\ 58.515,\ 56.323,\ 62.023,\ 61.673,\ 56.583,\ 56.924,\ 56.111,\ 62.085,\ 54.217,\ 55.914,\ 53.974,\ 49.754,\ 56.034,\ 57.895,\ 55.440,\ 62.863)$$

The model used is the one given by (3.3). Now using the transformation $\underset{\sim}{Z} = \underset{\sim}{T}\underset{\sim}{Y}$, the vector of transformed observations $\underset{\sim}{Z}$ is

$$\underset{\sim}{Z}' = (-0.227,\ 3.068,\ 3.335,\ -1.387,\ -0.812,\ 5.556,\ 1.550,\ -3.759,\ -2.355,\ -0.241,\ 0.524,\ -4.803,\ -1.200,\ 0.891,\ 4.285,\ -1.316,\ 1.245,\ -5.548).$$

The best estimate of $\underset{\sim}{\beta}$ given by (3.9) is

$$\hat{\underset{\sim}{\beta}}' = (.62,\ -1.19,\ .27,\ .60,\ -.65,\ -.39,\ .47,\ -3.66,\ .88,\ -.23,\ -4.7,\ -5.67,\ 3.62,\ 4.71,\ -4.59).$$

By neglecting order the best estimate of β_1 given by (3.10) is

$$\hat{\underset{\sim}{\beta}}_1' = (3.06, -3.39, .019, .58, -.76, -.26, .47).$$

In Table 3.2, the analysis of variance corresponding to Table 3.1 is given.

Table 3.2

SV	DF	SS	MS	F	P-value
Total	18	154.18			
Factors	7	56.99	8.14	10.71	.0387
Orders	8	94.91	11.86	15.61	.0229
Error	3	2.28	.76		

The test of significance indicates that the order effects are significant. Therefore the model given in (3.9) is used. Table 3.3 lists the parameters, estimates, standard errors and tests of significance for this model. The t entry in the table is the usual t-test of significance where

$$t_n = \frac{\text{estimated effect}}{\text{standard error of estimate}} .$$

The estimates of the variances are given by

$$\hat{\text{Var}}(\underset{\sim}{k}'\hat{\underset{\sim}{\beta}}) = \underset{\sim}{k}(\underset{\sim}{R}'\underset{\sim}{R})^{-1}\underset{\sim}{k}'\hat{\sigma}_e^2 .$$

For this example, $(\underset{\sim}{R}'\underset{\sim}{R})^{-1}$ is given in the Appendix.