



Randomization restrictions and the inadvertent split plot in industrial experimentation
by Derek Frank Webb

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in
Statistics

Montana State University

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Abstract:

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Experimental designs run with multiple hard to change factors are correctly analyzed as mixed models. Random effects and variance components are added to the models to account for the restrictions on randomization due to the presence of hard to change factors. Various methods of estimating variance components are examined and a particular method is recommended. The mixed model analysis is compared to the traditional analysis.

Models with particular blocking structures which result in more cost effective experiments and less variable parameter prediction are recommended for factorial experiments with multiple hard to change factors. Response surface designs are also examined and blocking structures recommended.

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IN INDUSTRIAL EXPERIMENTATION

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ABSTRACT

In industrial experimentation there are frequently factors which are costly or time consuming to reset from one run to the next. Given a randomized run order, the experimenter will not reset these hard to change factors when they occur at the same level in consecutive runs. The analysis is then conducted as if full randomization took place when in actuality a split plot structure has been imposed on the model.

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Chapter 1

AN OVERVIEW OF RESTRICTIONS ON RANDOMIZATION IN EXPERIMENTAL DESIGN

The focus of chapter 1 is to provide an overview of randomization and its history in experimental design. This chapter will also examine the effects that are caused when randomization is restricted and their relation to the split-plot design.

In order to facilitate a discussion on randomization, its meaning should be clarified. Consider two definitions of randomization given in Webster's [61] unabridged dictionary. The first definition is:

Controlled distribution (usually) of given tests, factors, samplings, treatments, or units so as to simulate a random or chance distribution and yield unbiased data from which a generalized conclusion can be drawn.

The second definition is:

A random process used in a statistical experiment to reduce or eliminate interference by variables other than those being studied.

A statistician would probably use a combination of these two definitions if asked to explain what randomization is. It is interesting to note that Webster's dictionary uses the word "usually" in the first definition of randomization. This wording alludes to the fact that in an experimental design and its implementation it is quite often the case that certain aspects of an experiment are not randomized.

Randomization, and its implementation in experimental design, has its roots in the classic book The Design of Experiments by R.A. Fisher [17]. Fisher calls randomization "the physical basis of the validity of the test" and proceeds to describe how randomization, especially of treatments to experimental units, is the "essential safeguard" against unknown effects and variables beyond the control of the experimenter. Summarizing Fisher, randomization, when properly carried out, ensures that appropriate estimates of error which perturb the experimenter's data will be used.

Throughout the twentieth century, many classic books on experimental design have been written. They all address randomization to some extent. Several of the more popular texts will be discussed here. Yates' [63] book, Experimental Design, attributes to Fisher the idea of assigning treatments at random to experimental units, and that this random assignment of treatments is "essential to provide a sound basis for the assumption that the deviations used for the estimation of error are independent and contain all those components of error to which the treatment effects are subject, and only those components." One point concerning randomization that Fisher ignores, but Yates discusses is the fact that once a randomization scheme is implemented and an experimental layout is determined, it becomes known information. Yates goes on to say that this information may be incorporated in the subsequent analysis. Thus, Yates is implying that under certain circumstances some experimental layouts determined randomly may be inappropriate. For example, randomly assigning different concentrations of fertilizer to a field may result in a gradient of concentrations across a field. This is an early reference (1965) to the fact that not all randomization schemes are desirable.

The book Experimental Designs by Cochran and Cox [12] has an in-depth discussion of the usefulness of randomization and considers the topic of restricting randomization. Cochran and Cox compare randomization to insurance: Sometimes randomization may not be necessary, but one may not know when that is, so it is safest to always randomize. They do point out that some experiments are very complex and

that randomization of each operation may be too time consuming. In such cases the experimenter may then opt to forgo randomization on certain operations. However, this approach may introduce bias. Bias can be considered as anything which may affect the results of an experiment and is not accounted for. For example, consider a factor such as furnace temperature which is deemed too time consuming to reset to a lower temperature after it has been running at a higher one. Let the factor have five temperature levels; 500°, 520°, 540°, 560°, and 580°. If the experiment is run such that these temperatures occur in increasing order, then the estimates of effects for this factor may be biased if there is some underlying time trend in the running of the experiment. This underlying time trend may be that the experimenter becomes more proficient and accurate using the experimental equipment or measuring devices so that the variability of the response decreases through time. This decrease in variability will be confounded with temperature level. Therefore, the experimenter might examine the results of the experiment and draw some conclusion about temperature which may not be accurate.

In their first chapter, Cochran and Cox devote a section to restricted randomization in which they indicate that certain outcomes resulting from complete randomization may be undesirable. These outcomes could be removed from the total set of potential outcomes from which the experimenter randomly chooses. Thus, restricted randomization may be appropriate in certain experimental situations. Also, the experimenter should be cautious when analyzing data from an experiment which included a restriction on randomization. The appropriate analysis may differ from an analysis which assumes that no restriction on randomization was imposed. Unfortunately, the authors do not provide specific details about how randomization restrictions may alter the analysis.

Design and Analysis of Experiments by Kempthorne [39] is another classic text on the subject of experimental design. Kempthorne discusses the basic principles of randomization formulated by Fisher, as well as randomization tests and dependence

on properly randomized experiments. A very clear discussion of randomization tests is also given by Box, Hunter, and Hunter [8] in their book Statistics for Experimenters. An example from Box, Hunter, and Hunter will serve to illustrate randomization tests as discussed in these two books.

Consider a gardener with eleven tomato plants planted in one long row. He has two fertilizer mixtures, A and B . Mixture B is supposedly an improvement over mixture A . The gardener randomly applies mixture A to 5 plants and mixture B to the remaining 6 plants. At the end of the season, yield in pounds of tomatoes was measured for each plant. The results are as follows.

Fertilizer A	Fertilizer B
29.9	26.6
11.4	23.7
25.3	28.5
16.5	14.2
21.1	17.9
	24.3

$$\bar{y}_A = 20.84 \quad \bar{y}_B = 22.53$$

One of Fisher's most important points about randomization is that if an experiment is run in a randomized fashion, then the researcher can conduct significance tests without any distribution assumptions. For example, if the new fertilizer mixture performed equally as well as the old, then the yield of each tomato plant would be independent of fertilizer treatment. The researcher can test the null hypothesis

H_0 : there is no difference in fertilizer effectiveness,

against the alternative hypothesis

H_a : fertilizer mixture B is more effective than fertilizer mixture A .

Under the null hypothesis, all $\frac{11!}{5!6!} = 462$ ways of allocating the fertilizers A and B to the 11 plants are equally likely. Therefore, the appropriate randomization distribution

under the null hypothesis can be computed by calculating the 462 differences in means ($\bar{y}_B - \bar{y}_A$) associated with the 462 possible fertilizer allocations. The observed difference $\bar{y}_B - \bar{y}_A$ is 1.69, and there are 154 fertilizer arrangements which result in a larger difference. Therefore, a significance level of $\frac{154}{462} = .33$ can be calculated for this experiment. Based on this value, one would fail to reject the null hypothesis.

Randomization distributions can quickly become difficult and time consuming to compute, so Box, Hunter, and Hunter describe the common solution to this problem. If the assumptions are made that the data are simple random samples from two independent normal populations with equal variances then the appropriate test statistic is:

$$t = \frac{\bar{y}_B - \bar{y}_A}{s\sqrt{1/n_A + 1/n_B}} = .44$$

where s^2 is the pooled estimate of the common variance. If the assumptions are correct, then the exact distribution of the test statistic is $t_{n_A+n_B-2} = t_9$, a t -distribution with 9 degrees of freedom. A significance level of .34 can be obtained from one of many computer packages. This is in very close agreement with the significance level calculated using the randomization test.

Fisher is not alone in his advocacy of randomization. For instance, in The Analysis of Variance, Scheffé [53] makes the bold statement: "randomization must be incorporated into the experiment." Currently, this belief is prevalent in the teaching of statistics and the actual implementation of designed experimentation. For instance, in 1995 an article [51] in *The American Statistician* began with the statement: "Deliberate randomization in experimental studies is perhaps the most important contribution our discipline has made to experimental science." In 1999 Jitendra Ganju and James Lucas submitted an article to *The American Statistician* [20] which contained a thorough discussion of "how randomization is discussed in the (statistical) literature." The article discussed experiments where complete randomization is not possible, but there exist some restrictions on randomization. The article then goes on to explain how this can affect significance tests.

Randomization has many benefits, such as protecting against the influence of time-dependent effects, startup effects and one-at-a-time effects. Time-dependent effects are caused by one or more extraneous variables that vary in a systematic fashion over the course of an experiment. Startup effects are caused by the initial startup of equipment in an industrial experiment. All runs associated with a startup may have an additional effect associated with their response. One-at-a-time effects are due to "inherent variability among experimental units" [23]. Some examples are the inability to obtain identical conditions on two identical runs and measurement error. A problem with one-at-a-time effects that may arise if randomization is not used is that the experimenter may "deliberately or inadvertently assign a particular treatment to the 'best' experimental units" [23]. The benefits and the usefulness of randomization are discussed in two articles by Gerald Hahn [23, 24]. Hahn also considers restricting the randomization scheme of an experiment, and even considers the possibility of having no randomization within certain parts of a design. These are not new ideas. Kiefer [33] in 1959 laid out an optimal experimental design approach in which designs are not chosen randomly from a group of designs, but are selected based on some criterion. Kiefer advocated assembling a class of optimal designs wherein all members of the class attain a maximum score based on such criteria as design efficiency, cost of implementation, run order restrictions, or optimality criteria like D or G optimality. A design is then picked from this optimal class of designs.

In 1975, David Harville [25] wrote a compelling article in which he described four of the most popular arguments for randomization in an experimental situation. He then went on to argue that none of those arguments should be taken seriously. The four popular arguments as described in Harville's article are:

1. Randomization allows the experimenter to base inferences for treatment contrasts on randomization models instead of more restrictive normal-theory models.
2. Randomization makes it improbable that factors not included in the assumed

statistical model will be confounded completely with treatment contrasts.

3. Under randomization ordinary estimates of treatment contrasts remain unbiased and confidence regions and hypothesis tests retain (at least approximately) their ascribed properties under a variety of circumstances in which the assumed model is incorrect.
4. Randomization insures that the choice of design is not affected by any biases of preconceived notions on the part of the experimenter.

Harville gives an extensive argument as to why point 1. is valid with or without randomization. He then goes on to describe how a well-chosen and implemented design requires no randomization to guarantee the properties of points 2. through 4. Harville's ideas are extreme in that most experimenters, while restricting randomization in one fashion or another, still try to incorporate it into the experiment whenever possible. In the same article, Harville voices his support for the optimal-design approach (stated previously) as a way of choosing a design, instead of the traditional random approach.

Most experimenters employ a combination of the two approaches laid out by Fisher and Keifer. An experimenter may randomize treatment assignment or run order for certain factor combinations, but may choose not to randomize certain other aspects of an experiment due to, say, cost or difficulty in changing a level of a factor. The remainder of this chapter will be limited to examining randomization restrictions on run order and randomization restrictions due to the resetting of factors.

When restrictions on run order randomization began to appear in the statistical literature, the intention was to suggest ways to guard against the effect of first order time trends on main effects and also to limit the number of factor level changes in an experiment. In many experimental situations, especially in agriculture and industry, there are factors which are very expensive, difficult, or time consuming to change.

Many authors have proposed designs which limit the number of changes of these factors. I will refer to these factors as *hard-to-change factors*.

Daniel and Wilcoxon [13] present certain 2^{p-q} factorial and fractional factorial plans for $p - q = 2, 3, 4, 5$ that are robust against linear and quadratic time trends. For example, if one wanted to run a 2^3 design where it was feared that a linear time trend was present in factor A, a run order such as *aaaaAAAA* drawn at random would be deemed unsatisfactory. Daniel and Wilcoxon eliminate such run orders from consideration, instead focusing on ones which guard against such confounding of time and main effects. To narrow their choice of run orders even further, they use the variance and efficiency of regression coefficients as measures of how well a particular run order "performs." Draper and Stoneman [16] examined all $8! = 40,320$ possible run orders of a 2^3 design. They classified runs according to two criteria:

- 1 Minimize the number of factor level changes,
- 2 Minimize the maximum of the absolute value of the time counts of the three factors,

where time count is defined as the inner product of (1 2 3 4 5 6 7 8) and the column vector of the design matrix corresponding to each factor. Time count gives a direct measure of how much a main effect may be affected by a linear time trend. For instance, if the column of factor A is (-1 1 -1 1 -1 1 -1 1) then the time count would be 4, if the column of factor A is (-1 -1 -1 -1 1 1 1 1) then the time count would be 16. The greater the absolute value of the time count (with maximum of 16), the greater the possible effect of linear time trend. Draper and Stoneman list the "best" designs, but do not give advice as to how to pick one, or how to conduct an analysis on the results of running one of these designs. Dickinson [14] presents a computer program which examines 2^4 and 2^5 designs. The program recommends some run orders which minimize the number of factor level changes and also are robust against linear time trends in the estimates of the main effects.

In a similar article, Joiner and Campbell [31] present a general method of choosing a run order for an experiment. They take into account possible time order dependencies and the cost of changing levels of certain factors. They make the point that the number of possible run orders increases very quickly with respect to the number of factors and the number of levels of each factor in an experiment. So, it becomes infeasible to examine all possible run orders when choosing the "best" one. They describe a technique in which they randomly choose a subset of run orders and then examine this subset to arrive at the "best" one. The criterion used by Joiner and Campbell to select the best run order is $[|\mathbf{X}'\mathbf{X}|^{1/p} \div \text{cost}]$, which is a measure of efficiency of a particular run order, where p is the number of columns of $\mathbf{X}$ and cost is the cost of the experiment based on the number of changes of factor levels necessary to run the experiment. It is interesting to point out that the value of $|\mathbf{X}'\mathbf{X}|^{1/p}$ remains unchanged if the run order changes. The quantity $|\mathbf{X}'\mathbf{X}|^{1/p}$ has the property that if the design is replicated k times then $|\mathbf{X}'\mathbf{X}|^{1/p}$ will be multiplied by k and the $|\mathbf{X}'\mathbf{X}|^{1/p}$ to cost ratio will remain unchanged. In order to select a random subset of run orders from all possible run orders, Joiner and Campbell propose a procedure of selecting probabilities for changing factor levels. As an example, consider a 2^4 design with factor A hard to change. The experimenter might decide to change factor A with probability .3 and the rest of the factors with probability .7. So, for the first run factors A, B, C , and D are randomly chosen ($P(\text{high})=.5$ and $p(\text{low})=.5$) to be at either their high or low level to start out the experiment. For the next run, factor A will be changed to its opposite level with probability .3 and the other factors will be changed to their opposite levels with probability .7. This method of choosing the design continues until all 16 runs have been determined, or a constraint is encountered. For instance, a constraint would occur if all the low levels (8 of them) of factor A were assigned to 8 runs before all 16 runs had been determined. Then, the remaining runs would have to be set at the high level for factor A . This process is repeated until the experimenter has as many run orders as needed, throwing out

replicates. One would then use the measure of efficiency described above to select the best run order from this subset of run orders. This method has the obvious drawback of perhaps not selecting the "best" run order from the set of all run orders.

The above articles as well as many others propose eliminating certain run orders from consideration when choosing a design. This is obviously a restriction on randomization. Another restriction that is not so obvious is the failure to reset a factor when it occurs at the same level in consecutive experimental runs. This idea can be illustrated by considering an experiment with a factor such as oven temperature. Quite often an oven takes a long time to warm up to the desired temperature and it may also be time consuming (or expensive) to change the oven's temperature. When an experiment is run and there are two consecutive runs where oven temperature is at the same value, oven temperature is not brought down to a nominal level (say room temperature) and then brought back up to the desired temperature. Instead oven temperature is left at that desired temperature for both runs. This is a restriction on randomization and may violate the commonly assumed assumption of independent errors in the statistical model. The runs where temperature is not reset may be correlated. This restriction on randomization due to temperature is analogous to a split-plot experiment, where temperature is considered to be the whole-plot treatment. In other words, failing to reset factors at each run imposes a split-plot structure to the design. Although resetting factor levels at each run defeats the purpose of minimizing the number of factor level changes, not resetting factors at the beginning of each run affects the model assumptions. The remainder of this chapter deals with this phenomenon.

An early industrial example of a split-plot design having the problem associated with resetting factors is presented by Wortham and Smith [62]. They provide data for an experiment with two factors: bake time (3 levels) and oven temperature (4 levels). All 12 factor combinations were run and replicated 6 times. The way in which the experiment is carried out is of paramount importance to the analyst. The experiment

was actually conducted (as noted by Hicks [27]) by selecting an oven temperature at random and then placing 3 components into the oven, removing one at random at each of the 3 bake times. This was repeated 4 times, once for each oven temperature. The whole process was replicated 6 times. If the data were analyzed as a completely randomized experiment replicated 6 times one would have overlooked a component of variability associated with the randomization restriction on temperature. The overall variance estimate would have been inflated and tests for the factors would be inaccurate. A correct analysis would have to account for the randomization restriction due to not resetting the temperature. The experiment was actually run as a split-plot design with temperature being the whole-plot treatment and bake time being the split-plot treatment. One way to account for this restriction in the analysis is to introduce a separate error term or variance component to account for the restriction on randomization.

Perhaps the first reference addressing the problem of randomization restrictions by introducing multiple error terms is by Anderson [3]. Anderson provides examples of the use of restriction errors in randomized complete block, nested factorial, and split-plot designs. His examples include a factor which is time consuming to reset, and thus, by definition, is a hard-to-change factor. By not resetting this factor in these experiments, results in creating a split-plot design.

To illustrate Anderson's ideas, consider his following example. Suppose there is interest in running an experiment with two factors, factor *A* with 4 levels and factor *B* with 6 levels. The experiment is to be run with 2 replicates of each treatment combination. Consider factor *A* to be hard-to-change. If a completely randomized design was utilized, factor *A* would technically have to be reset 47 times. This is unacceptable, and so the experimenter runs a randomized complete block design where each of the 4 blocks corresponds to a level of factor *A*. Within each block, 12 runs are made with 2 runs at each level of factor *B*. Notice the restriction on randomization here is due to the fact that factor *A* is not reset until all 12 runs

are carried out across the levels and replicates of factor B . A completely randomized design could have been generated and resulted in having this run order, but to adhere to the principles of randomization, factor A would have had to be reset at each run. Anderson suggests the following linear model with which to analyze the data:

$$y_{ijk} = \mu + A_i + \delta_{(i)} + B_j + AB_{ij} + \epsilon_{(ij)k},$$

where

- y_{ijk} = response for i^{th} level of factor A and j^{th} level of factor B ,
- A_i = effect of i^{th} level of factor A ,
- $\delta_{(i)}$ = restriction error caused by i^{th} level of factor A not being reset,
- B_j = effect of j^{th} level of factor B ,
- AB_{ij} = effect of interaction of i^{th} level of factor A with j^{th} level of factor B ,
- $\epsilon_{(ij)k}$ = error of k^{th} observation, within i^{th} level of factor A and j^{th} level of factor B .

The errors are defined as: $\delta_{(i)} \sim \text{NID}(0, \sigma_w^2)$ and $\epsilon_{(ij)k} \sim \text{NID}(0, \sigma_s^2)$. The w and s subscripts for the variances of the error components indicate whole-plot and split-plot.

It is interesting to note that Dickinson's [14] aforementioned article does mention the problems with not resetting factors at the beginning of each run. He states that the "experimental plans take on some of the aspects of split-plot designs in the presence of setup errors in fixing the levels of the factors." He goes on to say that his methods are valid if the experimenter can assume the errors associated with setting the factor levels are negligible. This may not, in general, be the case and the experimenter should consider a split-plot type analysis.

Anderson and McLean [4] present a paper related to Anderson's [3] in which they discuss linear models which include extra error terms attributable to randomization restrictions. They thoroughly work through three examples, the first one being

the same as the one presented in Anderson [3]. The following statement summarizes the thrust of their paper: "In essence, whenever there is a restriction on a randomization (either from natural causes within the experiment or by the experimenters plan) another error term may be introduced into the model." It is interesting to note that their examples result in "balanced" split-plot structures. This is typically not the case in industrial settings. Many times an experiment is run and only after data is collected does the experimenter (or statistician analyzing the data) realize that a randomization restriction may have occurred. Usually the resultant split-plot structure is not balanced. As an example, consider a 2^3 design with factor A being hard to change and consequently not reset on consecutive run orders at the same level. If a randomized run order is chosen such that the run order for factor A is $AAaaaaAaA$, then an unbalanced split-plot structure results. This run order dictates 4 resets of factor A and creates 5 blocks within which randomization is being restricted.

In 1972, an article originally written by Youden [64] in 1956 appeared in *Technometrics* in which he addressed restriction of randomization in experimentation. Youden raises two points: "randomization is unnecessary if the experimental units are truly independent, and, where the units are not independent and randomization is required a constrained randomization may better serve the needs of the experimenter." In this article additional error terms for the randomization restrictions are not mentioned. Also, even if experimental units are truly independent, failure to reset a factor kept at the same level on consecutive run orders requires the introduction of another error term into the model. These ideas were out-of-date in 1972, but one must realize that this article was written in 1956.

Other references to the topic of randomization restriction appear in more recent literature. In the chapter: 'Factorial Experiments In Completely Randomized Designs,' from the 1989 text Statistical Design and Analysis of Experiments by Mason, Gunst, and Hess [45], the authors say the following: "If 'back-to-back' repeat tests are conducted, the estimate of experimental error can be too small because any

variability associated with setting up and tearing down the equipment would not be present." The authors are referring to not resetting the levels of factors when the same levels of all factors are run twice in a row for the purposes of a replicate point in the experiment. This practice is very undesirable, and it appears that the authors do not expect experimenters to routinely reset factor levels from run to run. Also, additional errors introduced by not resetting the factors are not mentioned. In another chapter 'Nested Designs,' the authors have a section labeled 'Restricted Randomization' in which they discuss restricting run order due to the presence of a hard-to-change factor. They give an example and discuss its similarity to a split-plot experiment. They also warn about the use of restricted randomization without replication. If there is no replication, then there is no estimate of whole-plot error in a split-plot experiment, and consequently there is no test for the main effect that is confounded with the whole plot. They do not provide any details about a proper analysis, nor do they mention resetting factor levels from run to run.

The second part of this chapter focused on research which discussed and occasionally tried to deal with randomization restrictions in experimental designs. In particular, restrictions which were caused by not resetting a factor in the experiment on consecutive runs where it is at the same level were discussed. It is evident from the literature that this type of randomization restriction is important and warrants further investigation.

Chapter 2 summarizes recent results from Ju [32] concerning the implications of not resetting a factor in factorial designs which have a random run order. Chapter 2 also contains new results on runs theory and its application to restrictions on randomization in the factorial experiment. Chapter 3 contains new research which generalizes the results of Chapter 2 to the case of not resetting multiple factors in factorial designs with a random run order. Chapter 4 presents results from Ju [32] and Anbari [1] on blocking structures for factorial designs which contain one factor which is not reset from one run to the next. New research is then presented in

Chapter 4 which generalizes blocking structures to factorial designs with multiple factors which are not reset from one run to the next. These factorial designs with blocking structures are then compared to factorial designs with a random run order and no blocking structure. Chapter 5 presents results from Ju [32] and Anbari [1] on blocking structures for response surface designs which contain one factor which is not reset from one run to the next. New research is then presented in Chapter 5 which generalizes blocking structures to response surface designs with multiple factors which are not reset from one run to the next. Chapter 6 describes the mixed model and presents a thorough discussion of variance component estimation. A particular method is recommended for mixed models which result from industrial experimentation with factors which are not reset from one run to the next when they are at the same level. Chapter 7 presents three examples from industry. These are examples of experiments which contain factors which are difficult to reset and, therefore, are not reset from one run to the next when they remain at the same level.

Chapter 2

THE L^k FACTORIAL EXPERIMENT WITH ONE HARD-TO-CHANGE FACTOR

2.1 The L^k Factorial Experiment

The L^k factorial experiment is one of the most popular experimental designs used in industry. The experiment consists of k factors, each having L levels. All L^k factor-level combinations are included in the experiment. The factors used may be considered as either fixed or random [48]. For this dissertation, a factor will be assumed to be fixed unless otherwise stated.

The L^k factorial experiment is generally conducted using a randomized run order. Most experimenters will then conduct an analysis of the experiment assuming $\mathbf{y} \sim N[\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}]$ where each response, y_i , is independent from all other responses, y_j ($\forall i \neq j$) and all responses have equal variance, σ^2 . In general, this is an oversimplification. The reason why is that most experiments contain factors which are difficult, time consuming, or expensive to change from one level to another. Given that this is the case, the experimenter will not reset (bring down to a nominal level and then back up to the level of interest) a factor on consecutive runs where the factor is at the same level. This practice violates the assumption of independence from one run to the next. Some examples and literature citations related to this were examined at the end of Chapter 1.

2.2 Hard-to-change and Easy-to-change Factors

In order to make a clear distinction between factorial experiments which are not randomized completely and those which are, precise terminology will be defined.

A factor will be said to have been *reset* from one run to the next if it is brought down to a nominal level between runs and then brought back to the level of interest on the following run. A *Hard-To-Change* (HTC) factor will be any factor which is not reset from one run to the next when the level of that factor remains unchanged. A *Easy-To-Change* (ETC) factor will be any factor which is reset from run to run no matter what level is required. An experiment will be called a *completely randomized experiment* if it has a randomized run order and all factors in the experiment are reset at the beginning of each run. An experiment will be called a *randomized experiment* if it has a randomized run order and contains at least one HTC factor. Note that a completely randomized experiment might contain expensive or difficult to reset factors, but the time has been taken to reset these factors at the beginning of each run.

Most industrial experiments contain at least one HTC factor. Every time there are two or more runs in a row where the HTC factor level remains unchanged, a restriction on randomization occurs. This randomization restriction is incorporated into the model and subsequent analysis by the use of variance components, one for each HTC factor. Extensive discussion of this topic can be found in Ju [32], Anbari [1], Ganju [19], and most recently in Lucas [44].

2.3 The 2^3 Factorial Example

An example will be used to illustrate the incorporation of HTC factors into a statistical model. Consider a 2^3 factorial experiment with X_1 being a HTC factor and X_2 and X_3 being ETC factors. The commonly used design matrix for this experiment

is

$$\mathbf{X} = \begin{array}{c|cccc} \text{run} & X_1 & X_2 & X_3 & \\ \hline 1 & 1 & -1 & -1 & -1 \\ 2 & 1 & -1 & -1 & 1 \\ 3 & 1 & -1 & 1 & -1 \\ 4 & 1 & -1 & 1 & 1 \\ 5 & 1 & 1 & -1 & -1 \\ 6 & 1 & 1 & -1 & 1 \\ 7 & 1 & 1 & 1 & -1 \\ 8 & 1 & 1 & 1 & 1 \end{array}$$

Now, consider a randomly chosen run order, 2; 3; 5; 6; 7; 8; 1; 4. The design matrix for this run order would be

$$\mathbf{X} = \begin{array}{c|cccc} \text{run} & X_1 & X_2 & X_3 & \\ \hline 2 & 1 & -1 & -1 & 1 \\ 3 & 1 & -1 & 1 & -1 \\ 5 & 1 & 1 & -1 & -1 \\ 6 & 1 & 1 & -1 & 1 \\ 7 & 1 & 1 & 1 & -1 \\ 8 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 \\ 4 & 1 & -1 & 1 & 1 \end{array},$$

where the lines in the X_1 column separate the blocks that are formed due to resetting the HTC levels of factor X_1 . It is important to notice that within these blocks X_2 and X_3 are completely randomized, but the randomization of X_1 is being restricted within blocks. This restriction on the randomization of X_1 induces a random effect associated with the blocks of X_1 . The correct model is no longer $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ where $\boldsymbol{\beta}$ is a 4×1 vector of fixed effects and $\boldsymbol{\epsilon}$ is a 8×1 vector of overall random errors, but is now the mixed model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \boldsymbol{\epsilon}$ where $\mathbf{u}$ is a 3×1 vector of random effects associated with the 3 blocks created by the HTC factor X_1 , and $\mathbf{Z}$ is a 8×3 design

matrix for random effects (A thorough discussion of the mixed model and variance components is presented in Chapter 6). The fixed and random design matrices for this model are, respectively,

$$\mathbf{X} = \begin{matrix} & \begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 \end{bmatrix} \\ \begin{matrix} 2 \\ 3 \\ 5 \\ 6 \\ 7 \\ 8 \\ 1 \\ 4 \end{matrix} & \end{matrix} \quad \text{and} \quad \mathbf{Z} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix},$$

and the unknown fixed effect and random effect vectors are

$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} \quad \text{and} \quad \mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}.$$

Making common mixed model distributional assumptions that

$$\begin{aligned} \mathbf{E}[\mathbf{u}_i] &= \mathbf{0} \quad \forall i \\ \text{Var}[\mathbf{u}_i] &= \sigma_1^2 \mathbf{I}_{q_i} \\ \text{Cov}[\mathbf{u}_i, \mathbf{u}_j] &= \mathbf{0} \quad \forall i \neq j \\ \mathbf{E}[\boldsymbol{\epsilon}] &= \mathbf{0} \\ \text{Var}[\boldsymbol{\epsilon}] &= \sigma^2 \mathbf{I}_n \\ \text{Cov}[\mathbf{u}_i, \boldsymbol{\epsilon}] &= \mathbf{0} \quad \forall i \end{aligned}$$

allows us to compute the variance of $\mathbf{y}$ as

$$\text{Var}[\mathbf{y}] = \sigma^2 \mathbf{I}_n + \mathbf{Z} \sigma_1^2 \mathbf{Z}' = \sigma^2 \mathbf{I}_n + \sigma_1^2 \mathbf{Z} \mathbf{Z}',$$

where σ^2 is the variance component associated with the overall error ϵ and σ_1^2 is the variance component associated with the random effects due to blocking within factor X_1 . The form of $\mathbf{ZZ}'$ can be shown to be

$$\mathbf{ZZ}' = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

given the previously described form of $\mathbf{Z}$. No matter what run order for the experiment is chosen, $\mathbf{ZZ}'$ will always be an $n \times n$ block diagonal matrix. There will be a 1 on every diagonal entry of $\mathbf{ZZ}'$. There will be a 1 on the i^{th} row and j^{th} column entry of $\mathbf{ZZ}'$ if and only if run i and run j are at the same setting of X_1 and they are in the same block, otherwise there will be a 0 on the i^{th} row and j^{th} column entry of $\mathbf{ZZ}'$ [32]. The 1's in the $\mathbf{ZZ}'$ matrix indicate which runs are correlated with one another, where the covariance between the two runs is σ_1^2 .

An alternate way of expressing the model is to always write the fixed effects design matrix $\mathbf{X}$ in standard form and to vary the random effects design matrix $\mathbf{Z}$. Continuing the previous 2^3 example with X_1 being HTC and the run order being 2; 3; 5; 6; 7; 8; 1; 4, the standard form of $\mathbf{X}$ and the form of $\mathbf{Z}$ which reflects the run

order and the fact that X_1 is hard to change are, respectively,

$$X = \begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \quad \text{and} \quad Z = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

The first column of Z contains a 1 in the second and third rows corresponding to the run order, 2; 3; 5; 6; 7; 8; 1; 4, where the second and third runs are at the same level of the HTC factor X_1 . Column two has similar structure in that there is a 1 in the fifth, sixth, seventh, and eighth rows. Column three finishes out the run order with a 1 in the first and forth rows. The ZZ' matrix will now have the form

$$ZZ' = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix}$$

The alternative way of expressing the model with the fixed effects design matrix X given in standard form and the random effects design matrix Z being varied according to the randomized run order and the levels of the HTC factor will be used for the remainder of this dissertation.

2.4 The Expected Variance-Covariance Matrix

In Ju [32] the expected-variance covariance matrix of $\mathbf{y}$ was examined. The following theorem was proven in her dissertation. It is presented here as it was presented in Ju, where the design matrix $\mathbf{X}$ is in standard form and the $\mathbf{Z}$ matrix is varied according to the randomized run order and the levels of the HTC factor.

Theorem 2.1 *The expected variance-covariance matrix $\mathbf{V_E} = E[\text{Var}(\mathbf{y})]$ of a L^k experiment with randomized run order and X_1 being a hard-to-change factor is*

$$\mathbf{V_E} = (\sigma^2 + (1-p)\sigma_1^2)\mathbf{I}_n + (p\sigma_1^2)\mathbf{Z}_1\mathbf{Z}_1'$$

where the expectation is taken with respect to the discrete uniform distribution of possible $\mathbf{Z}\mathbf{Z}'$ matrices and

$$\mathbf{Z}_1 = \begin{bmatrix} \mathbf{J}_1 & & 0 \\ & \mathbf{J}_2 & \\ & & \ddots \\ 0 & & & \mathbf{J}_L \end{bmatrix}_{L^k \times L}, \quad \mathbf{J}_i = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}_{L^{k-1} \times 1},$$

and

$$p = \frac{2}{L^{k-1}(L-1) + 2}.$$

The importance of this result is twofold,

1. Given a randomized run order for a L^k experiment with X_1 being HTC, the probability there will be a 1 in any off-diagonal entry in the $\mathbf{Z}\mathbf{Z}'$ matrix (where a 1 can possibly appear) is p . A 1 in the $\mathbf{Z}\mathbf{Z}'$ matrix indicates that the i^{th} and j^{th} runs have X_1 at the same level and are correlated with covariance σ_1^2 . So, among all randomizations, the i^{th} and j^{th} runs are correlated with probability p .
2. This expected variance-covariance matrix $\mathbf{V_E}$ of the response $\mathbf{y}$ can be used as a standard to compare specific run orders to. Relative to $\mathbf{V_E}$, the experimenter

can judge how “good” a certain run order (that he/she may be interested in running) will be. That is, does a specific run order have better covariance properties (between runs with the HTC factor at the same level) than what is expected from a randomly chosen run order?

2.5 Further Variance-Covariance Matrix Results

Lemma 2.1 *The maximum number of off-diagonal 1's in the $\mathbf{ZZ}'$ matrix for a given run order in an L^k experiment with X_1 as the HTC factor is*

$$(L)(L^{k-1})^2 - L^k = L^k(L^{k-1} - 1).$$

Proof: In the L^k experiment there are L levels of X_1 . There are L^{k-1} runs for each level of X_1 . Because of symmetry, two 1's will appear as off-diagonal entries of $\mathbf{ZZ}'$ every time two runs with X_1 at the same level are run consecutively. The most 1's will occur in the $\mathbf{ZZ}'$ matrix when all runs with X_1 at a certain level are run consecutively. This type of run order will result in $\mathbf{ZZ}'$ being a block diagonal matrix with L blocks, one for each level of factor X_1 . Each block is of size $L^{k-1} \times L^{k-1}$, where L^{k-1} is the number of runs in the experiment at each level of X_1 . So, there are $L(L^{k-1})^2$ possible 1's in $\mathbf{ZZ}'$. There are L^k diagonal 1's which are subtracted from the total resulting in $(L)(L^{k-1})^2 - L^k$ possible off-diagonal 1's.

For certain L^k factorial experiments it is feasible to generate the distribution of all possible $\mathbf{ZZ}'$ matrices. That is, to calculate the probability a $\mathbf{ZZ}'$ matrix will have no 1's as off-diagonal entries, two 1's as off-diagonal entries, up to $L^k(L^{k-1} - 1)$ 1's as off-diagonal entries. The number of off-diagonal 1's is always an even number because $\mathbf{ZZ}'$ is symmetric. The number of 1's as off-diagonal entries is a direct measure of how many runs are correlated due to X_1 being HTC.

Ju [32] examined the $\mathbf{ZZ}'$ matrix for the 2^3 factorial, with X_1 being HTC, in detail. There are $2^3! = 40320$ run orders to consider, but run orders with the same settings of X_1 within blocks do not change the $\mathbf{ZZ}'$ matrix. For this reason, Ju [32] could examine 70 (out of the 40320) different run orders. For example, the run order

1; 2; 3; 5; 6; 7; 8; 4 and the run order 1; 3; 2; 5; 6; 7; 8; 4 result in the same ZZ' matrix. These two run orders also induce the same blocking structure due to the presence of the HTC factor X_1 . For the 2^3 factorial experiment, the assignment of 4 of the runs to the low level of X_1 and the other 4 to the high level of X_1 is arbitrary. The low and high level designations can be switched resulting in half as many runs to consider. For the 2^3 factorial experiment, there are actually only 35 run orders which result in distinct blocking structures as the following theorem shows.

Theorem 2.2 *The number of run orders which result in distinct blocking structures for an L^k factorial experiment with X_1 being HTC are*

$$\frac{L^k!}{(L!)(L^{k-1}!)^L}$$

Proof: Although this theorem was proven in Ju [32], a significantly shorter proof will be given. The proof requires applying the following lemma from Brualdi [11].

Lemma 2.2 *Let S be a multi-set with objects of l different types with finite repetition numbers $n_1, n_2, \dots, n_l$, respectively. Let the size of S be $n = n_1 + n_2 + \dots + n_l$. Then the number of permutations of S equals*

$$\frac{n!}{n_1!n_2!\dots n_l!}$$

To apply Lemma 2.2, note that an L^k factorial experiment contains L levels of factor X_1 and L^k runs, and the runs form a multi-set with L different objects (or levels of factor X_1), each object having repetition numbers L^{k-1} . Thus, there are

$$\frac{L^k!}{L^{k-1}!L^{k-1}!\dots L^{k-1}!} = \frac{L^k!}{(L^{k-1}!)^L}$$

distinct permutations of the runs, where two runs having X_1 at the same level are indistinguishable. There are L levels of X_1 , each assigned to L^{k-1} runs. This assignment is arbitrary. There are $L!$ possible level assignments, or permutations. Hence the number of distinct blocking structures decreases by a factor of $L!$, which matches the result. ◻

The number of distinct blocking structures for a given L^k factorial experiment increases dramatically with the size of the experiment. For instance, a 2^3 experiment has 35 distinct blocking structures, a 2^4 experiment has 6435 distinct blocking structures, and a 3^3 experiment has an incredible 3.797×10^{10} distinct blocking structures. So, it is not practical to completely enumerate the distributions of the ZZ' matrix for any but the smallest L^k designs.

The distribution of ZZ' matrices for the 2^3 factorial experiment with X_1 being HTC will now be derived. The symbols “-” and “+” will be used to represent X_1 at its low level and X_1 at its high level respectively. For a given run, the level at which X_1 is at is all that matters in the construction of the ZZ' matrix. Therefore, a run order such as 1; 2; 4; 5; 6; 7; 8; 3 will be represented as ---++++-. Table 1 contains all 35 run orders which result in distinct blocking structures. There is also a column indicating how many off-diagonal 1's appear in the ZZ' matrix for that particular blocking structure.

Table 1: Run Orders for the 2^3 factorial experiment which result in distinct blocking structures.

Run Order	Ones	Run Order	Ones	Run Order	Ones
-----++++	24	--++--++	8	--++-+-+	4
-----++++-	18	-++++-+--	8	-+-++-+-+	4
-+++++----	18	-++++--+-	8	-+---++-+	4
--+++++---	16	--++++-+-	8	--+-++-+-	4
-++++----+	12	-+-++++--	8	-+-+---++	4
-+----++++	12	-+---++++-	8	-+---+-++	4
---+++-+	12	--+-++++-	8	--+-+---++	4
---+-+---	12	-++-++---	6	-++-+-++-	2
-++----++	10	-++---++-	6	-+-++-+-	2
--+++-+--	10	--++-+++-	6	-++-+-+-	2
--+----+++	10	-++-+-+--	4	-+-+-+-+	0
---++-++	10	-++-.-+-+	4		

Table 2 gives the distribution of the $\mathbf{ZZ}'$ matrix for the 2^3 with X_1 HTC. The first column gives the number of off-diagonal 1's and the second column gives the probability of obtaining that number given a randomly run experiment. The probabilities are arrived at in the following way: from above, there are 3 ways out of 35 of obtaining two off-diagonal 1's, therefore the probability of obtaining two off-diagonal 1's is $\frac{3}{35} = .08571$.

Table 2: The distribution of the ZZ' matrix for the 2^3 factorial experiment with X_1 HTC.

Ones	Probability
0	.02857
2	.08571
4	.25714
6	.08571
8	.20000
10	.11429
12	.11429
16	.02857
18	.05714
24	.02857

Table 2 shows that the probability an experiment with a randomized run order results in all 4 runs with X_1 at the low level being correlated and all 4 runs with X_1 at the high level being correlated is only .02857. Also, the probability that a randomly run experiment results in at most 4 off-diagonal 1's is $.02857 + .08571 + .25714 = .37142$. This demonstrates that a significant proportion of the time, a randomly run 2^3 experiment has very few of the runs correlated.

2.6 Resetting the Hard-To-Change Factor

In a completely randomized L^k factorial experiment the HTC factor X_1 must be reset L^k times, including the initial setup. In a L^k factorial experiment with a randomized run order, the HTC factor X_1 may be reset as few as L times or as many as L^k times. For example, in a 2^3 factorial experiment the run order 1; 3; 4; 2; 5; 6; 7; 8; results in X_1 being reset only 2 times, including the initial setup. The run order 7; 1; 6; 4; 8; 2; 5; 3 results in X_1 being reset 8 times.

The expected number of resets of the HTC factor in a randomized L^k factorial experiment can be easily calculated. Let U equal the number of resets of the HTC factor, where U includes one reset for the initial setup. Counting the number of resets of the HTC factor is equivalent to counting the number of runs formed by the different levels X_1 takes on. For example, consider a 3^2 factorial experiment. The standard design matrix is

$$\mathbf{X} = \begin{array}{c|ccc} \text{run} & X_1 & X_2 & \\ \hline 1 & 1 & -1 & -1 \\ 2 & 1 & -1 & 0 \\ 3 & 1 & -1 & 1 \\ 4 & 1 & 0 & -1 \\ 5 & 1 & 0 & 0 \\ 6 & 1 & 0 & 1 \\ 7 & 1 & 1 & -1 \\ 8 & 1 & 1 & 0 \\ 9 & 1 & 1 & 1 \end{array}$$

Let the 3 levels of X_1 be represented by l (Low), m (Medium), and h (High). Then, the run order 1; 2; 4; 5; 6; 3; 7; 8; 9 would correspond to the levels of X_1 being in the order $l; l; m; m; m; l; h; h; h$. For this example, $U = 4$ and there are also 4 runs of lengths 2, 3, 1, and 3. Every time the HTC factor is reset, a run is begun. There is a one-to-one correspondence between the number of resets of the HTC factor and the associated number of runs created by the levels of the HTC factor. This correspondence allows us to apply the existing theory on runs when studying U .

A comprehensive article on the distribution of runs of k kinds of elements is given in Mood [49]. Mood examines runs of k kinds of elements where there are n_i elements of the i^{th} kind. There are a total of n elements, where $n = \sum_{i=1}^k n_i$. Let r_i denote the number of runs of elements of the i^{th} kind. Mood then shows that

$$E[r_i] = \frac{n_i(n - n_i + 1)}{n},$$

$$\text{Var}[r_i] = \frac{n_i(n_i - 1)(n - n_i + 1)(n - n_i)}{n^2(n - 1)}, \text{ and}$$

$$\text{Cov}[r_i, r_j] = \frac{n_i(n_i - 1)n_j(n_j - 1)}{n^2(n - 1)}.$$

Using these results, it is possible to compute the $E[U]$ and the $\text{Var}[U]$ where $U = r_1 + r_2 + \cdots + r_k$. The expectation of U can be computed as follows

$$\begin{aligned} E[U] &= E[r_1 + r_2 + \cdots + r_k] \\ &= E[r_1] + E[r_2] + \cdots + E[r_k] \\ &= \sum_{i=1}^k \frac{n_i(n - n_i + 1)}{n} \\ &= \frac{n(n + 1) - \sum_{i=1}^k n_i^2}{n}. \end{aligned}$$

The $\text{Var}[U]$ can be computed by use of the fact that

$$\begin{aligned} \text{Var}[U] &= \text{Var}[r_1 + r_2 + \cdots + r_k] \\ &= \sum_{i=1}^k \sum_{j=1}^k \text{Cov}[r_i, r_j] \\ &= \sum_{i=1}^k \text{Var}[r_i] + \sum_{i \neq j}^k \sum_{j=1}^k \text{Cov}[r_i, r_j]. \end{aligned}$$

The $\sum_{i=1}^k \text{Var}[r_i]$ term will be examined first,

$$\begin{aligned} \sum_{i=1}^k \text{Var}[r_i] &= \sum_{i=1}^k \frac{n_i(n_i - 1)(n - n_i + 1)(n - n_i)}{n^2(n - 1)} \\ &= \frac{1}{n^2(n - 1)} \left[\sum_{i=1}^k n_i^2(n^2 + 3n + 1) \right. \\ &\quad \left. - 2 \sum_{i=1}^k n_i^3(n + 1) + \sum_{i=1}^k n_i^4 - n^2 - n^3 \right]. \end{aligned}$$

Next, the covariance term can be expressed as

$$\begin{aligned} \sum_{i \neq j}^k \sum_{j=1}^k \text{Cov}[r_i, r_j] &= \sum_{i \neq j}^k \sum_{j=1}^k \frac{n_i(n_i - 1)n_j(n_j - 1)}{n^2(n - 1)} \\ &= \frac{1}{n^2(n - 1)} \left[\sum_{i=1}^k \sum_{j=1}^k n_i(n_i - 1)n_j(n_j - 1) \right. \end{aligned}$$

$$\begin{aligned}
& - \sum_{i=1}^k n_i^2 (n_i - 1)^2 \Big] \\
& = \frac{1}{n^2(n-1)} \left[\sum_{i=1}^k n_i^2 \left(\sum_{i=1}^k n_i^2 - 2n - 1 \right) \right. \\
& \quad \left. + 2 \sum_{i=1}^k n_i^3 - \sum_{i=1}^k n_i^4 + n^2 \right].
\end{aligned}$$

Simplifying the sum of the expression for the variance and the expression for the covariance yields

$$\text{Var}[U] = \frac{\sum_{i=1}^k n_i^2 [\sum_{i=1}^k n_i^2 + n(n+1)] - 2n \sum_{i=1}^k n_i^3 - n^3}{n^2(n-1)}.$$

The results concerning U , the total number of runs in n objects of k types, can now be applied to the number of resets of the HTC factor X_1 in the L^k factorial experiment. U is equivalent to the number of resets of X_1 where $n = L^k$ is the total number of runs in the L^k factorial experiment, and n_i is the number of runs with the HTC factor at level i . For factorial experiments, n_i is the same for all i , that is $n_i = L^{k-1}$ for $1 \leq i \leq L$. Then,

$$\begin{aligned}
E[U] &= \frac{n(n+1) - \sum_{i=1}^k n_i^2}{n} \\
&= \frac{L^k(L^k+1) - \sum_{i=1}^L (L^{k-1})^2}{L^k} \\
&= \frac{L^k(L^k+1) - L^{2k-1}}{L^k} \\
&= L^k + 1 - L^{k-1},
\end{aligned}$$

and

$$\begin{aligned}
\text{Var}[U] &= \frac{\sum_{i=1}^k n_i^2 [\sum_{i=1}^k n_i^2 + n(n+1)] - 2n \sum_{i=1}^k n_i^3 - n^3}{n^2(n-1)} \\
&= \frac{L^{2k-1} [L^{2k-1} + L^k(L^k+1)] - 2L^k L^{3k-2} - L^{3k}}{L^{2k}(L^k-1)} \\
&= \frac{L^{k-1}(L^k+1) - L^{2k-2} - L^k}{L^k-1} \\
&= \frac{L^{k-1}(L^{k-1}-1)(L-1)}{L^k-1}.
\end{aligned}$$

Table 3 contains the $E[U]$, which is the expected number of resets of the HTC factor for a random run order factorial experiment. The second column of the table gives the ratio of $E[U]$ and L^k where L^k equals the number of resets of the HTC factor for a completely randomized factorial experiment. Note that

$$\lim_{k \rightarrow \infty} \frac{E[U]}{L^k} = 1 - \frac{1}{L}.$$

The last column gives the $\text{Var}[U]$ which equals the variance of the number of resets of the HTC factor.

Table 3: The expected number of resets of one HTC factor for a random run order

L^k	$E[U]$	$E[U]/L^k$	$\text{Var}[U]$
2^2	3	.7500	.6667
2^3	5	.6250	1.7143
2^4	9	.5625	3.7333
2^5	17	.5312	7.7419
2^6	33	.5156	15.7460
2^7	65	.5078	31.7480
2^8	129	.5039	63.7490
3^2	7	.7778	1.5000
3^3	19	.7037	5.5385
3^4	55	.6790	17.5500
3^5	163	.6708	53.5537
3^6	487	.6680	161.5549

The ratio of the expected number of resets of the HTC factor for a random run order factorial experiment to the number of resets of the HTC factor for a completely randomized factorial experiment in Table 3 is useful when considering the cost of running an experiment. Cost may be considered as purely monetary, or may also

involve time, labor, and difficulty in running the experiment. This ratio represents the average cost reduction associated with the HTC factor in running a random run order experiment versus running a completely randomized experiment. For example, the ratio is 56.25% for a 2^4 factorial experiment. On average, the randomized experiment will cost 56.25% of what a completely randomized experiment would cost (in terms of resetting factor levels). There could be significant savings in running a random run order experiment instead of a completely randomized experiment.

Chapter 3

THE L^k FACTORIAL EXPERIMENT WITH C HARD-TO-CHANGE FACTORS

In an industrial setting when an L^k factorial experiment is run there is often more than one HTC factor. In fact, many experimenters will treat all k factors as HTC when running an experiment. This chapter will extend the results in Chapter 2 to the general case where there are c HTC factors, where $1 \leq c \leq k$.

3.1 The Standard X and Z Design Matrices

The standard form of the design matrix X was discussed in Chapter 2, and that form will also be used in this chapter. There will be a different standard form of the design matrix Z for each HTC factor in the L^k factorial experiment. They will be noted Z_1 for the design matrix associated with the HTC factor X_1 , Z_2 for the design matrix associated with the HTC factor X_2 , up to Z_k for the design matrix associated with the HTC factor X_k .

An example will help illustrate the standard forms of the design matrices. Consider a 2^3 factorial experiment with X_1 being HTC. The standard design matrix

$\mathbf{X}$ and standard design matrix $\mathbf{Z}_1$ are, respectively,

$$\mathbf{X} = \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{matrix} \begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{Z}_1 = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}$$

Now, if X_2 is HTC or if X_3 is HTC the standard design matrix $\mathbf{X}$ remains the same, and the standard design matrices $\mathbf{Z}_2$ and $\mathbf{Z}_3$ are, respectively,

$$\mathbf{Z}_2 = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{Z}_3 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

For a L^k factorial experiment with one HTC factor, X_i , the form of the standard design matrix, $\mathbf{Z}_i$, is

$$\mathbf{Z}_i = \mathbf{J}_{L^{i-1}} \otimes \mathbf{I}_L \otimes \mathbf{J}_{L^{k-i}}, \quad (1)$$

where $\mathbf{J}_a$ is a column vector of ones of size $a \times 1$. For example, consider the 2^3 factorial experiment which was discussed above. Let X_2 be HTC. Therefore,

$$\mathbf{J}_{2^{2-1}} = \mathbf{J}_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix},$$

$$I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

and

$$J_{2^{3-2}} = J_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

Inserting these matrices into equation 1 yields

$$\begin{aligned} Z_2 &= \begin{bmatrix} 1 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}, \end{aligned}$$

which matches the expression for Z_2 found above.

3.2 The Permutation Matrix

A permutation matrix is a matrix which reorders either the rows or columns of another matrix [54]. In this chapter, permutation matrices will be used to reorder the rows of the standard design matrices X and Z_i , for $2 \leq i \leq k$. There will be a different permutation matrix for each HTC factor in the L^k factorial experiment. The permutation matrices will be noted $P_1, P_2, \dots, P_k$ for HTC factors $X_1, X_2, \dots, X_k$.

The permutation matrices will be used to reorder the rows of the standard design matrix $\mathbf{X}$ in such a way as to give the column associated with HTC factor X_i the same form as the original column corresponding to HTC factor X_1 . Also, premultiplying $\mathbf{Z}_i$ with permutation matrix $\mathbf{P}_i$ transforms $\mathbf{Z}_i$ in such a way as to result in $\mathbf{P}_i \mathbf{Z}_i = \mathbf{Z}_1$. That is, the standard design matrix $\mathbf{Z}_i$ is transformed into the standard design matrix $\mathbf{Z}_1$. Note that $\mathbf{P}_1 = \mathbf{I}_{L^k}$.

An example will help illustrate the use of permutation matrices. Consider the 2^3 factorial design with X_2 being a HTC factor. The standard design matrices $\mathbf{X}$ and $\mathbf{Z}_2$ were shown to be, respectively

$$\mathbf{X} = \begin{bmatrix} & X_1 & X_2 & X_3 \\ 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{Z}_2 = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}$$

For this example,

$$\mathbf{P}_2 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

This permutation matrix will switch row 3 with row 5 and row 4 with row 6. Premultiplying both $\mathbf{X}$ and $\mathbf{Z}_2$ by $\mathbf{P}_2$ yields, respectively,

$$\mathbf{P}_2 \mathbf{X} = \begin{bmatrix} & X_1 & X_2 & X_3 \\ 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{P}_2 \mathbf{Z}_2 = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}.$$

Now the column in $\mathbf{X}$ corresponding to X_2 has the form the column corresponding to X_1 had originally, and the transformed $\mathbf{Z}_2$ matrix now has the form of $\mathbf{Z}_1$. Aside from the ordering of the columns of $\mathbf{X}$, this transformation gave $\mathbf{X}$ and $\mathbf{Z}_2$ the structure they would have had if X_1 was HTC instead of X_2 .

For all L^k factorial designs with X_i being HTC, where $2 \leq i \leq k$, there will exist a permutation matrix, $\mathbf{P}_i$, with the above properties. This is because of the way the $\mathbf{Z}_i$ matrices were constructed in Section 3.1. Given a specific L^k factorial experiment with X_i being HTC, the form of $\mathbf{P}_i$ can be stated explicitly as

$$\mathbf{P}_i = \left[\sum_{j=1}^L \left(e_j \otimes \mathbf{I}_{L^{i-1}} \otimes e'_j \right) \right] \otimes \mathbf{I}_{L^{k-i}}$$

where e_j is commonly referred to as an elementary column vector and is the j^{th} column of $\mathbf{I}_{L^{i-1}}$. For example, consider the 2^3 factorial experiment which was discussed above. Let X_2 be HTC. Therefore,

$$\mathbf{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \mathbf{e}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

$$\mathbf{I}_{L^{i-1}} = \mathbf{I}_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

and

$$I_{L^{k-i}} = I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Inserting these matrices into the items being summed results in

$$\begin{aligned} e_1 \otimes I_2 \otimes e'_1 &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \end{aligned}$$

and

$$\begin{aligned} e_2 \otimes I_2 \otimes e'_2 &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \end{bmatrix} \\ &= \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \end{bmatrix} \\ &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \end{aligned}$$

So,

$$\begin{aligned} \sum_{j=1}^L (e_j \otimes I_{L-1} \otimes e'_j) &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{aligned}$$

Therefore,

$$\begin{aligned} P_2 &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \end{aligned}$$

which matches the expression for P_2 found above. Searle [54] also points out that the transpose of a permutation matrix is a permutation matrix. In fact, all permutation matrices used in this dissertation are symmetric by nature of their construction [54].

Also, permutation matrices are orthogonal, that is $P^{-1} = P'$.

3.3 The Expected Variance-Covariance Matrix for c HTC Factors

This section contains two theorems which generalize theorem 2.1. Theorem 3.1 will give the form of the expected variance-covariance matrix of an L^k factorial experiment with one HTC factor where the hard to change factor is not necessarily X_1 . Theorem 3.2 will give the form of the expected variance-covariance matrix of an L^k factorial experiment with c HTC factors. The proof of Theorem 3.2 depends on Theorem 3.1.

Theorem 3.1 *The expected variance-covariance matrix $V_E = E[\text{Var}(\mathbf{y})]$ of an L^k experiment with randomized run order and one hard-to-change factor X_i , where $1 \leq i \leq k$, is*

$$V_E = [\sigma^2 + (1-p)\sigma_i^2] \mathbf{I}_n + (p\sigma_i^2) \mathbf{Z}_i \mathbf{Z}_i'$$

where the expectation is taken with respect to the discrete uniform distribution of possible $\mathbf{Z}\mathbf{Z}'$ matrices, $\mathbf{Z}_i$ is the standard form design matrix for the HTC factor as described in Section 3.1, and

$$p = \frac{2}{L^{k-1}(L-1) + 2}.$$

Proof: If $i = 1$ then apply Theorem 2.1 directly. If $2 \leq i \leq k$ then the experimental model is

$$\mathbf{y} = \mathbf{X}\beta + \mathbf{Z}^* \mathbf{u} + \epsilon,$$

where $\mathbf{Z}^*$ is a random effects design matrix corresponding to the blocks formed by the HTC factor X_i . Premultiply the model with permutation matrix $\mathbf{P}_i$ (Section 3.2) which reorders the rows of the design matrix $\mathbf{X}$ in such a way as to give the column corresponding to X_i the same form as the column corresponding to X_1 in the standard $\mathbf{X}$ design matrix. This also has the effect of reordering the rows of $\mathbf{Z}^*$ such that $\mathbf{P}_i \mathbf{Z}^* = \mathbf{Z}$, where $\mathbf{Z}$ has the form of the $\mathbf{Z}$ matrix in Chapter 2 when X_1 was the HTC factor. The transformed model is

$$\mathbf{P}_i \mathbf{y} = \mathbf{P}_i \mathbf{X} \beta + \mathbf{P}_i \mathbf{Z}^* \mathbf{u} + \mathbf{P}_i \epsilon = \mathbf{X}^* \beta + \mathbf{Z} \mathbf{u} + \epsilon^*.$$

This transformed model matches the form of the model in Chapter 2, except for the fact that the columns of the design matrix $\mathbf{X}$ are in a different order. Apply Theorem 2.1 to the transformed model. The expected variance-covariance matrix is

$$\mathbf{V}_E = [\sigma^2 + (1-p)\sigma_i^2] \mathbf{I}_n + (p\sigma_i^2) \mathbf{Z}_1 \mathbf{Z}_1',$$

where p is as stated in Theorem 3.1 and $\mathbf{Z}_1$ has the standard form stated in Theorem 2.1. The expectation in Theorem 2.1 is with respect to the distribution of $\mathbf{Z}\mathbf{Z}'$ matrices. So, transforming back to the original $\mathbf{Z}^*\mathbf{Z}'$ matrices and using the fact that $\mathbf{P}_i$ is orthogonal [54] and $\mathbf{Z}_1 = \mathbf{P}_i \mathbf{Z}_i$,

$$\begin{aligned} \mathbf{Z}_1 \mathbf{Z}_1' &= \mathbf{E}[\mathbf{Z}\mathbf{Z}'] \\ &= \mathbf{E}[\mathbf{P}_i \mathbf{Z}^* \mathbf{Z}^{*'} \mathbf{P}_i'] \\ &= \mathbf{P}_i \mathbf{E}[\mathbf{Z}^* \mathbf{Z}^{*'}] \mathbf{P}_i'. \end{aligned}$$

Therefore,

$$\begin{aligned} \mathbf{P}_i' \mathbf{Z}_1 \mathbf{Z}_1' \mathbf{P}_i &= \mathbf{P}_i' \mathbf{P}_i \mathbf{E}[\mathbf{Z}^* \mathbf{Z}^{*'}] \mathbf{P}_i' \mathbf{P}_i \\ \mathbf{Z}_i \mathbf{Z}_i' &= \mathbf{E}[\mathbf{Z}^* \mathbf{Z}^{*'}]. \end{aligned}$$

Thus, under the original model,

$$\mathbf{V}_E = [\sigma^2 + (1-p)\sigma_i^2] \mathbf{I}_n + (p\sigma_i^2) \mathbf{Z}_i \mathbf{Z}_i',$$

proving the theorem. ◻

Theorem 3.2 *The expected variance-covariance matrix $\mathbf{V}_E = \mathbf{E}[\text{Var}(\mathbf{y})]$ of an L^k experiment with randomized run order and c hard-to-change factors, $X_1, X_2, \dots, X_c$, where $1 \leq c \leq k$, is*

$$\mathbf{V}_E = \left[\sigma^2 + (1-p) \sum_{i=1}^c \sigma_i^2 \right] \mathbf{I}_n + p \sum_{i=1}^c \sigma_i^2 \mathbf{Z}_i \mathbf{Z}_i'$$

where the expectation is taken with respect to the discrete uniform distribution of possible $\mathbf{Z}\mathbf{Z}'$ matrices, $\mathbf{Z}_i$ is the standard form design matrix for the HTC factor as described in Section 3.1, and

$$p = \frac{2}{L^{k-1}(L-1) + 2}.$$

Proof: If $c = 1$ then apply Theorem 2.1 directly. If $2 \leq c \leq k$ then the experimental model is

$$\mathbf{y} = \mathbf{X}\beta + \mathbf{Z}_1^* \mathbf{u}_1 + \mathbf{Z}_2^* \mathbf{u}_2 + \cdots + \mathbf{Z}_c^* \mathbf{u}_c + \epsilon,$$

where $\mathbf{Z}_i^*$ is a random effects design matrix corresponding to the blocks formed by the HTC factor X_i for $1 \leq i \leq c$. Now, calculate the variance of $\mathbf{y}$ with the typical mixed model distributional assumptions

$$\begin{aligned} \mathbf{E}[\mathbf{u}_i] &= \mathbf{0} \quad \forall i \\ \text{Var}[\mathbf{u}_i] &= \sigma_i^2 \mathbf{I}_{q_i} \\ \text{Cov}[\mathbf{u}_i, \mathbf{u}_j] &= \mathbf{0} \quad \forall i \neq j \\ \mathbf{E}[\epsilon] &= \mathbf{0} \\ \text{Var}[\epsilon] &= \sigma^2 \mathbf{I}_n \\ \text{Cov}[\mathbf{u}_i, \epsilon] &= \mathbf{0} \quad \forall i, \end{aligned}$$

$$\text{Var}[\mathbf{y}] = \sigma_1^2 \mathbf{Z}_1^* \mathbf{Z}_1^{*'} + \sigma_2^2 \mathbf{Z}_2^* \mathbf{Z}_2^{*'} + \cdots + \sigma_c^2 \mathbf{Z}_c^* \mathbf{Z}_c^{*'} + \sigma^2 \mathbf{I}_n.$$

Because it is a linear operator, the expectation of the variance is

$$\mathbf{E}[\text{Var}[\mathbf{y}]] = \sigma_1^2 \mathbf{E}[\mathbf{Z}_1^* \mathbf{Z}_1^{*'}] + \sigma_2^2 \mathbf{E}[\mathbf{Z}_2^* \mathbf{Z}_2^{*'}] + \cdots + \sigma_c^2 \mathbf{E}[\mathbf{Z}_c^* \mathbf{Z}_c^{*'}] + \sigma^2 \mathbf{I}_n.$$

Application of Theorem 3.1 yields,

$$\begin{aligned} \mathbf{V}_E &= \sum_{i=1}^c (1-p) \sigma_i^2 \mathbf{I}_n + p \sigma_1^2 \mathbf{Z}_1 \mathbf{Z}_1' + p \sigma_2^2 \mathbf{Z}_2 \mathbf{Z}_2' + \cdots + p \sigma_c^2 \mathbf{Z}_c \mathbf{Z}_c' + \sigma^2 \mathbf{I}_n \\ &= (1-p) \sum_{i=1}^c \sigma_i^2 \mathbf{I}_n + p \sum_{i=1}^c \sigma_i^2 \mathbf{Z}_i \mathbf{Z}_i' + \sigma^2 \mathbf{I}_n \\ &= \left[\sigma^2 + (1-p) \sum_{i=1}^c \sigma_i^2 \right] \mathbf{I}_n + p \sum_{i=1}^c \sigma_i^2 \mathbf{Z}_i \mathbf{Z}_i'. \quad \square \end{aligned}$$

Chapter 4

PROPOSED 2^k FACTORIAL EXPERIMENTS WITH HARD-TO-CHANGE FACTORS

This chapter will examine various 2^k factorial experiments containing c hard-to-change factors where $1 \leq c \leq k$. Certain experiments having desirable properties will be proposed. These properties will be dependent on the blocking structure which results from the presence of HTC factors. The following properties will be examined in detail.

1. The prediction variance of $\hat{y}$.
2. The cost of running an 2^k experiment containing c HTC factors.
3. Parameter estimation limitations.

4.1 The Prediction Variance of $\hat{y}$

There exists many ways to evaluate an experimental design prior to data collection. Atkinson and Donev [5] provide and discuss various criteria for evaluating an experimental design. In particular, they discuss various optimality criteria such as D-optimality and G-optimality. Many of these optimality criteria either examine the variance of parameter estimators or the variance of prediction estimators. This section will examine the variance of prediction estimators and further generalize the results in the dissertations of Ju [32] and Anbari [1].

A G-optimal design is defined to be a design which minimizes the maximum of the standardized prediction variance over the design region [5]. The G-efficiency of a

design is the ratio of m , the number of parameters in the model, to the maximum of the standardized prediction variance over the design region for that particular design.

That is,

$$G - \text{efficiency} = \frac{m}{\max_{\mathbf{x} \in \mathcal{X}} \text{Var}_{\text{std}}[\hat{y}(\mathbf{x})]}.$$

The standardized variance is defined as

$$\text{Var}_{\text{std}}[\hat{y}(\mathbf{x})] = \frac{n \cdot \text{Var}[\hat{y}(\mathbf{x})]}{\sigma^2}.$$

The maximum is taken over all points in the design space $\mathcal{X}$, n is the number of runs in the experiment, and $\text{Var}[\epsilon_i] = \sigma^2$. The standard design matrix $\mathbf{X}$ has dimension $n \times m$ which corresponds to the n and m used above. In this section, the prediction variance of $\hat{y}$ for experiments containing c HTC factors and having randomized run orders or particular blocking structures based on the HTC factors will be examined.

The 2^k factorial experiment is one of the most common experiments in industry, and therefore, will be the focus of this section. In industry when a 2^k factorial experiment is conducted, it is typically assumed that a completely randomized design was used, that is, $\mathbf{V} = \text{Var}[\mathbf{y}] = \sigma^2 \mathbf{I}$. This is an oversimplification when the experiment contains HTC factors and has a randomized run order, but is not a completely randomized design. Because of this simplification, the experimenter will use $\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$ as the vector of parameter estimators instead of $\tilde{\beta} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$. The effect on the prediction variance of $\hat{y}$ given that $\hat{\beta}$ is used as the parameter estimate and that the experiment contains c HTC factors, $1 \leq c \leq k$, will be examined in this section. For balanced split plot designs Kempthorne [40] states that $\hat{\beta} = \tilde{\beta}$. Therefore, in most cases the experimenter is correct in calculating $\hat{\beta}$ as the parameter estimate, even if $\text{Var}[\mathbf{y}] \neq \sigma^2 \mathbf{I}$.

All balanced blocking structures presented in this chapter are balanced split plot designs, therefore $\hat{\beta} = \tilde{\beta}$ and

$$\text{Var}[\tilde{\beta}] = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} = \text{Var}[\hat{\beta}].$$

Designs with a randomized run order will be compared to designs with specific blocking structures in this chapter. The comparison will be based upon the expected prediction variance for randomized run orders and the prediction variance for run orders with specific blocking structures. The reader should note that for a randomized run order

$$E[\text{Var}[\tilde{\beta}]] = E[(X'V^{-1}X)^{-1}]$$

and

$$\begin{aligned} E[\text{Var}[\hat{\beta}]] &= E[(X'X)^{-1}X'VX(X'X)^{-1}] \\ &= (X'X)^{-1}X'V_EX(X'X)^{-1}, \end{aligned}$$

where V_E is the expected variance-covariance matrix as presented in Ju [32] and generalized in Chapter 3. These two expressions are not equal. For purpose of comparisons, the second expression will be used. This was also the expression used in Ju [32] and Anbari [1].

Calculations of parameter estimators and the variance of parameter estimators are greatly simplified due to orthogonality. A design is an *orthogonal design* if the off-diagonal elements of $X'X$ are all zero (Montgomery [48]). All 2^k factorial designs where the k factors are coded to the standardized levels of ± 1 are orthogonal designs. The addition of center points to a 2^k factorial design also results in an orthogonal design.

4.1.1 The Case With One Hard-To-Change Factor

4.1.1.1 The 2^k Factorial Experiment With a Randomized Run Order

In both Ju [32] and Anbari [1] the prediction variance of $\hat{y}$ was calculated for 2^k factorial experiments containing one HTC factor. The 2^k factorial experiment with a random run order as well as various blocking structures based on the levels of the HTC factor were examined. A synopsis of their results will be presented in order to facilitate a generalization to 2^k factorial experiments with c HTC factors.

Consider a 2^k factorial experiment with a random run order and one HTC factor, X_1 . Let $\hat{\beta} = (X'X)^{-1}X'y$ be the estimate of β assuming $y \sim N[X\beta, \sigma^2 I]$. Also, let there be m parameters in the model including the intercept. Therefore, X is an $2^k \times m$ matrix. Let $E[\text{Var}[y]] = V_E$. The experiment has a random run order and there is one HTC factor present. Therefore, theorem 3.1 states

$$V_E = [\sigma^2 + (1-p)\sigma_1^2]I_n + (p\sigma_1^2)Z_1Z_1'.$$

So, the expected variance of $\hat{\beta}$ can be calculated as follows,

$$\begin{aligned} E[\text{Var}[\hat{\beta}]] &= (X'X)^{-1}X'E[\text{Var}[y]]X(X'X)^{-1} \\ &= (X'X)^{-1}X'V_EX(X'X)^{-1}. \end{aligned}$$

Now, due to orthogonality, $X'X = 2^k I_m$. Therefore,

$$\begin{aligned} E[\text{Var}[\hat{\beta}]] &= \frac{1}{2^{2k}}X'V_EX \\ &= \frac{1}{2^{2k}}X'\left\{[\sigma^2 + (1-p)\sigma_1^2]I_n + (p\sigma_1^2)Z_1Z_1'\right\}X \\ &= \frac{1}{2^{2k}}[\sigma^2 X'X + (1-p)\sigma_1^2 X'X + p\sigma_1^2 X'Z_1Z_1'X] \\ &= \frac{1}{2^k}\sigma^2 I_m + \frac{1}{2^k}(1-p)\sigma_1^2 I_m + \frac{p\sigma_1^2}{2^{2k}}X'Z_1Z_1'X \end{aligned}$$

This implies that for any particular parameter in the model,

$$E[\text{Var}[\hat{\beta}_i]] = a\sigma^2 + b_i\sigma_1^2,$$

where $0 \leq i \leq (m-1)$ (here, m is the number of columns of X), the value of $a = \frac{1}{2^k}$, and the value of b_i depends upon X , Z_1 , i , and m . Note that it is common practice to have $0 \leq i \leq (m-1)$. This results in the intercept of the model being $\hat{\beta}_0$, the parameter $\hat{\beta}_1$ would correspond to X_1 (the first factor in the model), and so on. This result can be easily applied to the equation, $\hat{y} = X\hat{\beta}$, to calculate the expected prediction variance of $\hat{y}$ as follows,

$$E[\text{Var}[\hat{y}]] = XE[\text{Var}[\hat{\beta}]]X'.$$

Therefore, for a given i ,

$$E[\text{Var}[\hat{y}_i]] = \mathbf{x}_i E[\text{Var}[\hat{\beta}]] \mathbf{x}_i',$$

where $\mathbf{x}_i$ is the i^{th} row of the standard design matrix $\mathbf{X}$.

As an example, consider the 2^3 factorial experiment with X_1 being HTC. Let the model contain all main effects and all two factor interactions. This example was also given in Ju [32]. Theorem 3.1 will be used to derive the expected variance of $\hat{\beta}$. Also, Theorem 3.1 states that $p = \frac{1}{3}$ for the 2^3 factorial experiment.

$$\begin{aligned} E[\text{Var}[\hat{\beta}]] &= (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}' E[\text{Var}[\mathbf{y}]] \mathbf{X} (\mathbf{X}'\mathbf{X})^{-1} \\ &= \frac{1}{64} [\sigma^2 \mathbf{X}'\mathbf{X} + (1-p)\sigma_1^2 \mathbf{X}'\mathbf{X} + p\sigma_1^2 \mathbf{X}'\mathbf{Z}_1\mathbf{Z}_1'\mathbf{X}] \\ &= \frac{1}{64} [\sigma^2 \mathbf{X}'\mathbf{X} + (1-\frac{1}{3})\sigma_1^2 \mathbf{X}'\mathbf{X} + \frac{1}{3}\sigma_1^2 \mathbf{X}'\mathbf{Z}_1\mathbf{Z}_1'\mathbf{X}] \\ &= \frac{1}{64} [8\sigma^2 \mathbf{I}_7 + \frac{16}{3}\sigma_1^2 \mathbf{I}_7 + \frac{1}{3}\sigma_1^2 \mathbf{Q}], \end{aligned}$$

where

$$\mathbf{Q} = \mathbf{X}'\mathbf{Z}_1\mathbf{Z}_1'\mathbf{X} = \begin{bmatrix} 32 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 32 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Simplifying the equation to the form

$$E[\text{Var}[\hat{\beta}_i]] = a\sigma^2 + b_i\sigma_1^2,$$

where $0 \leq i \leq 6$ yields

$$\begin{aligned} E[\text{Var}[\hat{\beta}_i]] &= \frac{1}{8}\sigma^2 + \frac{1}{4}\sigma_1^2 & \text{if } 0 \leq i \leq 1 \\ &= \frac{1}{8}\sigma^2 + \frac{1}{12}\sigma_1^2 & \text{if } 2 \leq i \leq 6 \\ E[\text{Cov}[\hat{\beta}_i, \hat{\beta}_j]] &= 0 & \text{if } 0 \leq i < j \leq 6. \end{aligned}$$

It should be pointed out that the parameter estimators for this design's model are not correlated. Now, if one is interested in the $E[\text{Var}[\hat{y}_i]]$ for $i = 2$ then let $\mathbf{x}_2$ be the second row of $\mathbf{X}$. Then,

$$\begin{aligned}
 E[\text{Var}[\hat{y}_2]] &= \mathbf{x}_2 E[\text{Var}[\hat{\beta}]] \mathbf{x}_2' \\
 &= \begin{bmatrix} 1 & 1 & 1 & -1 & 1 & -1 & -1 \end{bmatrix} E[\text{Var}[\hat{\beta}]] \begin{bmatrix} 1 \\ 1 \\ 1 \\ -1 \\ 1 \\ -1 \\ -1 \end{bmatrix} \\
 &= \frac{7}{8}\sigma^2 + \frac{11}{12}\sigma_1^2 \\
 &\approx \frac{7}{8}\sigma^2 + \frac{7.33}{8}\sigma_1^2.
 \end{aligned}$$

It is important to point out that $E[\text{Var}[\hat{y}_i]]$ will be the same $\forall i$ because the $E[\text{Var}[\hat{\beta}]]$ is a diagonal matrix. Therefore, the maximum expected prediction variance of $\hat{y}$, where the maximum is taken over all points in the design space, can be written as

$$\max_{\mathbf{x} \in \mathcal{X}} E[\text{Var}[\hat{y}(\mathbf{x})]] = \mathbf{x}_0 E[\text{Var}[\hat{\beta}]] \mathbf{x}_0',$$

where

$$\mathbf{x}_0 = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \end{bmatrix}.$$

The validity of this equation depends on the following three properties:

1. The maximum expected prediction variance occurs at the corners of the design space, $\mathcal{X}$, for all 2^k designs [5].
2. For all 2^k designs, the corners of the design space correspond to the points of the design.

3. The $E[\text{Var}[\hat{\beta}]]$ is a diagonal matrix.

This simplified calculation of the maximum expected prediction variance of $\hat{y}$ will be used for the remainder of this chapter. It will be shown that this simplification will also hold when the maximum prediction variance of $\hat{y}$ is calculated for a specific design with blocks of equal size. Also, whenever a multiplier of a variance component is reported, it will always be given as a fraction with the denominator being the value 2^k for the design being discussed. This makes comparisons of the maximum prediction variance for different blocking structures straightforward as the numerators only need to be compared.

Table 4 contains the coefficients a and b_i in the formula

$$E[\text{Var}[\hat{\beta}_i]] = a\sigma^2 + b_i\sigma_1^2,$$

where $0 \leq i \leq (m-1)$, for various 2^k factorial experiments with a randomized run order and with X_1 being HTC. This table was given in Anbari [1] and is reproduced here because it will be referenced in the generalization to c HTC factors.

Table 4: The coefficients a and b_i for various 2^k factorial experiments

2^k	a	b_i	
	$\forall i$	$0 \leq i \leq 1$	$i \geq 2$
2^2	$\frac{1}{4}$	$\frac{3}{8}$	$\frac{1}{8}$
2^3	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{1}{12}$
2^4	$\frac{1}{16}$	$\frac{3}{20}$	$\frac{1}{20}$
2^5	$\frac{1}{32}$	$\frac{1}{12}$	$\frac{1}{36}$
2^6	$\frac{1}{64}$	$\frac{3}{68}$	$\frac{1}{68}$
2^7	$\frac{1}{128}$	$\frac{3}{132}$	$\frac{1}{132}$

Table 5 contains the multipliers of σ_1^2 and σ^2 for the maximum expected prediction variance for various 2^k factorial experiments with a randomized run order and with X_1 being HTC.

Table 5: Multipliers of σ_1^2 and σ^2 for the maximum expected prediction variance for various 2^k factorial experiments.

2^k	Parameters In the Model	Variance Multiplier	
		σ^2	σ_1^2
2^2	Main Effects	$\frac{3}{4}$	$\frac{3.50}{4}$
	Main + 2 FI	$\frac{4}{4}$	$\frac{4.00}{4}$
	FullModel	$\frac{4}{4}$	$\frac{4.00}{4}$
2^3	Main Effects	$\frac{4}{8}$	$\frac{5.33}{8}$
	Main + 2 FI	$\frac{7}{8}$	$\frac{7.33}{8}$
	FullModel	$\frac{8}{8}$	$\frac{8.00}{8}$
2^4	Main Effects	$\frac{5}{16}$	$\frac{7.20}{16}$
	Main + 2 FI	$\frac{11}{16}$	$\frac{12.00}{16}$
	FullModel	$\frac{16}{16}$	$\frac{16.00}{16}$
2^5	Main Effects	$\frac{6}{32}$	$\frac{8.89}{32}$
	Main + 2 FI	$\frac{16}{32}$	$\frac{17.78}{32}$
	FullModel	$\frac{32}{32}$	$\frac{32.00}{32}$
2^6	Main Effects	$\frac{7}{64}$	$\frac{10.35}{64}$
	Main + 2 FI	$\frac{22}{64}$	$\frac{24.47}{64}$
	FullModel	$\frac{64}{64}$	$\frac{64.00}{64}$
2^7	Main Effects	$\frac{8}{128}$	$\frac{11.64}{128}$
	Main + 2 FI	$\frac{29}{128}$	$\frac{32}{128}$
	FullModel	$\frac{128}{128}$	$\frac{128.00}{128}$

Table 5 includes values for models containing the main effects only, the main effects and all two-factor interactions, and the full model with all interactions. Note that without center-points or replication there will be no degrees of freedom left to estimate the error in full models and also in models with the main effects and all two-factor interactions for 2^2 and 2^3 designs. This information was given in Anbari

[1] and is reproduced here because it will be referenced in the generalization to c HTC factors.

4.1.1.2 The 2^k Factorial Experiment With Particular Blocking Structures

Various blocking structures for the 2^k factorial experiment will now be examined. As above, assume that X_1 is the HTC factor. The blocking structure is created by having consecutive runs in a randomized experiment at the same level of X_1 (see chapter 2). If the run order of an experiment is randomized without thought to the fact that the experiment contains a HTC factor then the resultant blocking structure will likely be undesirable. The experiment may turn out to be very expensive to run. That is, there may be many resets of the HTC factor. The cost of the experiment will be the topic of Section 4.2. The experiment may also have a larger maximum prediction variance than one obtained with carefully designed blocking. It will be shown that this arises when nondesirable confounding relations exist.

Anbari [1] thoroughly examines blocking structures for 2^k factorial experiments with one HTC factor. Anbari also presented an algorithm which selects confounding relations in the 2^k factorial experiment with one HTC factor which result in the smallest maximum prediction variance for a given block size. Anbari extended the results for 2^k factorial experiments to 2^{k-l} fractional factorial experiments.

Only blocking structures which resulted in blocks containing equal numbers of runs were examined. For example, blocks of size 2 and blocks of size 4 were examined for the 2^3 factorial experiment. A design with blocks of size two results in 4 blocks and a design with blocks of size 4 results in 2 blocks. There are other possibilities, such as one block of size 4 and two blocks of size 2. Blocking structures of that type will be considered in this section.

An example will demonstrate the importance of confounding relations in choosing a blocking structure and how it relates to the maximum prediction variance. Consider the 2^3 factorial experiment with X_1 being HTC. Three models will be discussed;

the main effects model, the main effects and two-factor interactions model, and the full model. Fractional factorial experiments will then be discussed.

For all calculations in this chapter the standard design matrix, $\mathbf{X}$, as given in chapter 2 will be used. This differs from Anbari [1] in that Anbari used design matrices with certain rows interchanged and certain columns interchanged to reflect the blocking structure used. In this chapter the blocking structure will be completely described by the form of the $\mathbf{Z}$ matrix. The standard design matrix, $\mathbf{X}$, for the 2^3 factorial experiment with all main effects and two-factor interactions is:

$$\mathbf{X} = \begin{array}{c|ccccccc} \text{run} & I & X_1 & X_2 & X_3 & X_1X_2 & X_1X_3 & X_2X_3 \\ \hline 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 2 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 3 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 4 & 1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 5 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \\ 6 & 1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 7 & 1 & 1 & 1 & -1 & 1 & -1 & -1 \\ 8 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{array}$$

The standard design matrix, $\mathbf{X}$, for the model containing only main effects would not contain the last three columns of the above design matrix. The full model would contain the following additional column

$$\begin{bmatrix} -1 \\ 1 \\ 1 \\ -1 \\ 1 \\ -1 \\ -1 \\ 1 \end{bmatrix}$$

corresponding to the three-factor interaction term, $X_1X_2X_3$.

When discussing 2^k factorial designs and blocking structures it is common practice to denote the effects of factors by capital Latin letters [48]. The effect of X_1 is denoted by A, the effect of X_2 is denoted by B, and so on. A two-factor interaction effect, say X_2X_3 , is denoted by BC. The letter I represents the "total or average of the entire experiment" [48], that is, the intercept term.

An expression such as $I=A=BC=ABC$ is called a confounding relation. It describes which effects are confounded with each other due to the blocking structure. Confounding results in certain treatment effects being indistinguishable from each other [48]. In the example, $I=A=BC=ABC$, the effects due to factor X_1 , the two-factor interaction X_2X_3 , and the three-factor interaction $X_1X_2X_3$ are confounded with each other. One property of a confounding relation is that all elements of the confounding relation (with the exception of I) can be generated by multiplication of two other elements in the confounding relation.

Anbari [1] showed that the optimal confounding relation for two blocks of size 4 is $I=A$. Any run order such as 5; 7; 6; 8; 1; 3; 4; 2, where the HTC factor X_1 is set up exactly twice, will result in this blocking structure. That is, there will be four runs in a row with X_1 at one level (either -1 or 1) and then four runs in a row with X_1 at the other level. This particular blocking structure does not confound the effect of X_1 with any other factor effect in the model.

The maximum prediction variance of $\hat{y}$ for the model with main effects and two-factor interactions can now be calculated. Earlier, only the expected maximum prediction variance of $\hat{y}$ could be calculated. Although this is a specific example, all run orders which result in two blocks of size 4 based on the $I=A$ confounding relation will have the same ZZ' matrix. Therefore, the expectation over the discrete uniform

distribution of all $\mathbf{ZZ}'$ matrices is not necessary. For this blocking structure,

$$\mathbf{Z} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{ZZ}' = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix},$$

and $\text{Var}[\mathbf{y}] = \mathbf{V} = \sigma^2 \mathbf{I}_8 + \sigma_1^2 \mathbf{ZZ}'$. Therefore,

$$\begin{aligned} \text{Var}[\hat{\beta}] &= (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}' \text{Var}[\mathbf{y}] \mathbf{X} (\mathbf{X}'\mathbf{X})^{-1} \\ &= (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}' \mathbf{V} \mathbf{X} (\mathbf{X}'\mathbf{X})^{-1} \\ &= \frac{1}{64} \mathbf{X}' \mathbf{V} \mathbf{X} \\ &= \frac{1}{64} \mathbf{X}' [\sigma^2 \mathbf{I}_8 + \sigma_1^2 \mathbf{ZZ}'] \mathbf{X} \\ &= \frac{1}{8} \sigma^2 \mathbf{I}_7 + \frac{1}{64} \sigma_1^2 \mathbf{X}' \mathbf{ZZ}' \mathbf{X} \\ &= \frac{1}{8} \sigma^2 \mathbf{I}_7 + \frac{1}{64} \sigma_1^2 \mathbf{Q} \end{aligned}$$

where

$$\mathbf{Q} = \mathbf{X}' \mathbf{ZZ}' \mathbf{X} = \begin{bmatrix} 32 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 32 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

This equation simplifies to the form

$$\text{Var}[\hat{\beta}_i] = a\sigma^2 + b_i\sigma_1^2,$$

where $0 \leq i \leq 6$ yields

$$\begin{aligned}\text{Var}[\hat{\beta}_i] &= \frac{1}{8}\sigma^2 + \frac{1}{2}\sigma_1^2 & \text{if } 0 \leq i \leq 1 \\ &= \frac{1}{8}\sigma^2 & \text{if } 2 \leq i \leq 6 \\ \text{Cov}[\hat{\beta}_i, \hat{\beta}_j] &= 0 & \text{if } 0 \leq i < j \leq 6.\end{aligned}$$

As before, with a randomized run order, the parameter estimators are not correlated. Also, the parameter estimates are the Best Linear Unbiased Estimators (BLUE) for balanced split-plot structures [39]. Having uncorrelated parameter estimators will not necessarily be true for blocking structures having blocks of unequal size as will be pointed out later. Now, the maximum prediction variance of $\hat{y}$ for the model with main effects and two-factor interactions is

$$\begin{aligned}\max_{x \in \mathcal{X}} \text{Var}[\hat{y}(x)] &= x_0 \text{Var}[\hat{\beta}] x_0' \\ &= \frac{7}{8}\sigma^2 + \frac{8}{8}\sigma_1^2.\end{aligned}$$

Anbari [1] showed that the optimal confounding relation for four blocks of size 2 is $I=A=ABC=BC$. A run order such as 1; 4; 5; 8; 3; 2; 7; 6, where the HTC factor X_1 is set up exactly four times, has this optimal confounding property. A run order such as 1; 2; 5; 6; 3; 4; 7; 8 has the confounding relation $I=A=B=AB$ and is therefore not optimal. All run orders with the optimal confounding relation will have the same ZZ' matrix,

$$ZZ' = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}.$$

The non-optimal 1; 2; 5; 6; 3; 4; 7; 8 run order given above has

$$ZZ' = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

The way the confounding relations affect the maximum prediction variance of $\hat{y}$ can be seen by examining the calculation of $\text{Var}[\hat{\beta}]$. For the optimal confounding relation above,

$$\begin{aligned} \text{Var}[\hat{\beta}] &= (X'X)^{-1}X'\text{Var}[y]X(X'X)^{-1} \\ &= \frac{1}{8}\sigma^2 I_7 + \frac{1}{64}\sigma_1^2 Q \end{aligned}$$

where

$$Q = X'ZZ'X = \begin{bmatrix} 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 \end{bmatrix}$$

Note that there is a non-zero diagonal entry in the Q matrix corresponding to the intercept, X_1 , and X_2X_3 . These are two of the terms in the confounding relation. The remaining term in the confounding relation, $X_1X_2X_3$, does not contribute to the $\text{Var}[\hat{\beta}]$ because $X_1X_2X_3$ is not included in the main effects and two-factor interactions model. The i^{th} diagonal entry of the Q matrix will be non-zero only if the i^{th} term

in the model is in the confounding relation [1]. The maximum prediction variance of $\hat{y}$ resulting from this example is

$$\max_{\mathbf{x} \in \mathcal{X}} \text{Var}[\hat{y}(\mathbf{x})] = \frac{7}{8}\sigma^2 + \frac{6}{8}\sigma_1^2.$$

In comparison, the second example with the non-optimal confounding relation has

$$\begin{aligned} \text{Var}[\hat{\beta}] &= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\text{Var}[\mathbf{y}]\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} \\ &= \frac{1}{8}\sigma^2\mathbf{I}_7 + \frac{1}{64}\sigma_1^2\mathbf{Q} \end{aligned}$$

where

$$\mathbf{Q} = \mathbf{X}'\mathbf{Z}\mathbf{Z}'\mathbf{X} = \begin{bmatrix} 16 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 16 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 16 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 16 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

and

$$\max_{\mathbf{x} \in \mathcal{X}} \text{Var}[\hat{y}(\mathbf{x})] = \frac{7}{8}\sigma^2 + \frac{8}{8}\sigma_1^2.$$

For this example, the non-zero diagonal entries correspond to the intercept, X_1 , X_2 , and X_1X_2 . These are the terms in the confounding relation.

Blocking structures having blocks of unequal size have certain drawbacks. Therefore, the use of blocks of unequal size is discouraged. As an example, consider the 2^3 factorial experiment with X_1 HTC and run order 1; 4; 5; 6; 7; 8; 2; 3. This run order results in two blocks of size 2 and one block of size 4. It makes use of the

confounding relation $I=A=ABC=BC$ for construction of the two blocks of size 2, and the confounding relation $I=A$ for the block of size 4. The ZZ' matrix is as follows,

$$ZZ' = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix}$$

The cost to run this experiment is slightly less than the cost to run an experiment with four blocks of size 2 because the HTC factor is set up three times as opposed to four times. Conversely, it is more expensive to run than an experiment with two blocks of size 4. However, the maximum prediction variance of $\hat{y}$ is larger than those associated with the other blocking structures. For this design,

$$\begin{aligned} \text{Var}[\hat{\beta}] &= (X'X)^{-1}X'\text{Var}[y]X(X'X)^{-1} \\ &= \frac{1}{8}\sigma^2 I_7 + \frac{1}{64}\sigma_1^2 Q \end{aligned}$$

where

$$Q = X'ZZ'X = \begin{bmatrix} 24 & 8 & 0 & 0 & 0 & 0 & 0 & 0 \\ 8 & 24 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 \end{bmatrix},$$

and

$$\max_{x \in \mathcal{X}} \text{Var}[\hat{y}(x)] \geq \frac{7}{8}\sigma^2 + \frac{9}{8}\sigma_1^2.$$

The maximum prediction variance of this design (with the non-optimal blocking structure) occurs at the design point:

$$\mathbf{x}_0 = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \end{bmatrix}.$$

This is because the $\mathbf{X}'\mathbf{Z}\mathbf{Z}'\mathbf{X}$ matrix is a positive semidefinite matrix. That is, it is symmetric and all entries are greater than or equal to zero. Therefore, the maximum occurs at the design point corresponding to all factors at their high level.

Also, note that the $\mathbf{Q}$ matrix has non-zero elements in the (1,2) entry and the (2,1) entry. This results in

$$\text{Cov}[\hat{\beta}_0, \hat{\beta}_1] = \frac{1}{8}\sigma_1^2,$$

that is $\hat{\beta}_0$ and $\hat{\beta}_1$ are correlated.

The previous examples were for the model containing main effects and all two-factor interactions. For the main effects model and the full model, the design matrix, $\mathbf{X}$, will be different. All subsequent calculations will be the same. It should be pointed out that the full model contains $\sum_{i=1}^k \binom{k}{i} = 2^k - 1$ effects [48]. There are only 2^k design points in a 2^k factorial experiment with no center points or replicate points. Therefore, there will be no degrees of freedom left to estimate the error. It is typical, however, to assume the highest order interactions are negligible. In such cases, these terms will be excluded from the model, thereby leaving degrees of freedom for error estimation.

Following are tables 6, 7, 8, 9, 10, and 11 giving the maximum prediction variance for various 2^k factorial experiments with X_1 being HTC and blocking structures based on optimal confounding relations as given in Anbari [1].

Table 6: The maximum prediction variance for the 2^2 factorial experiment with X_1 being HTC.

Block Size	Number of Blocks	Parameters In the Model	#Model Terms In Confounding Relation	Variance Multiplier	
				σ^2	σ_1^2
2	2	Main Effects	2	$\frac{3}{4}$	$\frac{4}{4}$
		Main + 2 FI	2	$\frac{4}{4}$	$\frac{4}{4}$
		Full Model	2	$\frac{4}{4}$	$\frac{4}{4}$

Table 7: The maximum prediction variance for the 2^3 factorial experiment with X_1 being HTC.

Block Size	Number of Blocks	Parameters In the Model	#Model Terms In Confounding Relation	Variance Multiplier	
				σ^2	σ_1^2
4	2	Main Effects	2	$\frac{4}{8}$	$\frac{8}{8}$
		Main + 2 FI	2	$\frac{7}{8}$	$\frac{8}{8}$
		Full Model	2	$\frac{8}{8}$	$\frac{8}{8}$
2	4	Main Effects	2	$\frac{4}{8}$	$\frac{4}{8}$
		Main + 2 FI	3	$\frac{7}{8}$	$\frac{6}{8}$
		Full Model	4	$\frac{8}{8}$	$\frac{8}{8}$

Table 8: The maximum prediction variance for the 2^4 factorial experiment with X_1 being HTC.

Block Size	Number of Blocks	Parameters In the Model	#Model Terms In Confounding Relation	Variance Multiplier	
				σ^2	σ_1^2
8	2	Main Effects	2	$\frac{5}{16}$	$\frac{16}{16}$
		Main + 2 FI	2	$\frac{11}{16}$	$\frac{16}{16}$
		Full Model	2	$\frac{16}{16}$	$\frac{16}{16}$
4	4	Main Effects	2	$\frac{5}{16}$	$\frac{8}{16}$
		Main + 2 FI	2	$\frac{11}{16}$	$\frac{8}{16}$
		Full Model	4	$\frac{16}{16}$	$\frac{16}{16}$
2	8	Main Effects	2	$\frac{5}{16}$	$\frac{4}{16}$
		Main + 2 FI	5	$\frac{11}{16}$	$\frac{10}{16}$
		Full Model	8	$\frac{16}{16}$	$\frac{16}{16}$

Table 9: The maximum prediction variance for the 2^5 factorial experiment with X_1 being HTC.

Block Size	Number of Blocks	Parameters In the Model	#Model Terms In Confounding Relation	Variance Multiplier	
				σ^2	σ_1^2
16	2	Main Effects	2	$\frac{6}{32}$	$\frac{32}{32}$
		Main + 2 FI	2	$\frac{16}{32}$	$\frac{32}{32}$
		Full Model	2	$\frac{32}{32}$	$\frac{32}{32}$
8	4	Main Effects	2	$\frac{6}{32}$	$\frac{16}{32}$
		Main + 2 FI	2	$\frac{16}{32}$	$\frac{16}{32}$
		Full Model	4	$\frac{32}{32}$	$\frac{32}{32}$
4	8	Main Effects	2	$\frac{6}{32}$	$\frac{8}{32}$
		Main + 2 FI	3	$\frac{16}{32}$	$\frac{12}{32}$
		Full Model	8	$\frac{32}{32}$	$\frac{32}{32}$
2	16	Main Effects	2	$\frac{6}{32}$	$\frac{4}{32}$
		Main + 2 FI	8	$\frac{16}{32}$	$\frac{16}{32}$
		Full Model	16	$\frac{32}{32}$	$\frac{32}{32}$

Table 10: The maximum prediction variance for the 2^6 factorial experiment with X_1 being HTC.

Block Size	Number of Blocks	Parameters In the Model	#Model Terms In Confounding Relation	Variance Multiplier	
				σ^2	σ_1^2
32	2	Main Effects	2	$\frac{7}{64}$	$\frac{64}{64}$
		Main + 2 FI	2	$\frac{22}{64}$	$\frac{64}{64}$
		Full Model	2	$\frac{64}{64}$	$\frac{64}{64}$
16	4	Main Effects	2	$\frac{7}{64}$	$\frac{32}{64}$
		Main + 2 FI	2	$\frac{22}{64}$	$\frac{32}{64}$
		Full Model	4	$\frac{64}{64}$	$\frac{64}{64}$
8	8	Main Effects	2	$\frac{7}{64}$	$\frac{16}{64}$
		Main + 2 FI	2	$\frac{22}{64}$	$\frac{16}{64}$
		Full Model	8	$\frac{64}{64}$	$\frac{64}{64}$
4	16	Main Effects	2	$\frac{7}{64}$	$\frac{8}{64}$
		Main + 2 FI	4	$\frac{22}{64}$	$\frac{16}{64}$
		Full Model	16	$\frac{64}{64}$	$\frac{64}{64}$
2	32	Main Effects	2	$\frac{7}{64}$	$\frac{4}{64}$
		Main + 2 FI	12	$\frac{22}{64}$	$\frac{24}{64}$
		Full Model	32	$\frac{64}{64}$	$\frac{64}{64}$

Table 11: The maximum prediction variance for the 2^7 factorial experiment with X_1 being HTC.

Block Size	Number of Blocks	Parameters In the Model	#Model Terms In Confounding Relation	Variance Multiplier	
				σ^2	σ_1^2
64	2	Main Effects	2	$\frac{8}{128}$	$\frac{128}{128}$
		Main + 2 FI	2	$\frac{29}{128}$	$\frac{128}{128}$
		Full Model	2	$\frac{128}{128}$	$\frac{128}{128}$
32	4	Main Effects	2	$\frac{8}{128}$	$\frac{64}{128}$
		Main + 2 FI	2	$\frac{29}{128}$	$\frac{64}{128}$
		Full Model	4	$\frac{128}{128}$	$\frac{128}{128}$
16	8	Main Effects	2	$\frac{8}{128}$	$\frac{32}{128}$
		Main + 2 FI	2	$\frac{29}{128}$	$\frac{32}{128}$
		Full Model	8	$\frac{128}{128}$	$\frac{128}{128}$
8	16	Main Effects	2	$\frac{8}{128}$	$\frac{16}{128}$
		Main + 2 FI	2	$\frac{29}{128}$	$\frac{16}{128}$
		Full Model	16	$\frac{128}{128}$	$\frac{128}{128}$
4	32	Main Effects	2	$\frac{8}{128}$	$\frac{8}{128}$
		Main + 2 FI	6	$\frac{29}{128}$	$\frac{24}{128}$
		Full Model	32	$\frac{128}{128}$	$\frac{128}{128}$
2	64	Main Effects	2	$\frac{8}{128}$	$\frac{4}{128}$
		Main + 2 FI	17	$\frac{29}{128}$	$\frac{34}{128}$
		Full Model	64	$\frac{128}{128}$	$\frac{128}{128}$

This section illustrates the advantages of running a blocked 2^k factorial experiment when there is one HTC factor present. The blocked designs listed in tables 6 through 11 are cheaper to run than a completely randomized experiment and have reduced maximum prediction variance. In fact, many of the blocked designs are super-efficient designs as was pointed out by Anbari [1].

4.1.2 The Case With c Hard-To-Change Factors

4.1.2.1 The 2^k Factorial Experiment With a Randomized Run Order

This section will examine the prediction variance of $\hat{y}$ for the 2^k factorial experiment with c HTC factors. Experiments with random run order as well as particular blocking structures will be considered. For simplicity, assume that $X_1, X_2, \dots, X_c$ are the HTC factors, where $1 \leq c \leq k$.

The general form of the expected prediction variance of $\hat{y}$ for the 2^k factorial experiment with c HTC factors and a random run order will now be developed. The results presented here will generalize the results presented in section 4.1.1.1 to the case of c HTC factors through the use of theorem 3.2.

Consider a 2^k factorial experiment with a random run order and c HTC factors, $X_1, X_2, \dots, X_c$. Let $\hat{\beta} = (X'X)^{-1}X'y$ be the least squares estimate of β and assume $y \sim N[X\beta, \sigma^2 I]$. Also, let m be the number of parameters in the model including the intercept. Therefore, X is a $2^k \times m$ matrix. Let $E[\text{Var}[y]] = V_E$. The experiment has a random run order and there are c HTC factors present. Therefore, theorem 3.2 states

$$V_E = \left[\sigma^2 + (1-p) \sum_{j=1}^c \sigma_j^2 \right] I_n + p \sum_{j=1}^c \sigma_j^2 Z_j Z_j',$$

where $1 \leq j \leq c$, σ_j^2 is the variance component associated with the restriction on randomization due to HTC factor X_j , and Z_j is the standard form design matrix for the HTC factor X_j as described in section 3.1.

So, the expected variance of $\hat{\beta}$ can be calculated as follows,

$$\begin{aligned} E[\text{Var}[\hat{\beta}]] &= (X'X)^{-1}X'E[\text{Var}[y]]X(X'X)^{-1} \\ &= (X'X)^{-1}X'V_EX(X'X)^{-1}. \end{aligned}$$

Now, due to orthogonality, $X'X = 2^k I_m$. Therefore,

$$\begin{aligned} E[\text{Var}[\hat{\beta}]] &= \frac{1}{2^{2k}} X'V_EX \\ &= \frac{1}{2^{2k}} X' \left\{ \left[\sigma^2 + (1-p) \sum_{j=1}^c \sigma_j^2 \right] I_n + p \sum_{j=1}^c \sigma_j^2 Z_j Z_j' \right\} X \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{2^{2k}} \left[\sigma^2 \mathbf{X}'\mathbf{X} + (1-p) \sum_{j=1}^c \sigma_j^2 \mathbf{X}'\mathbf{X} + p \sum_{j=1}^c \sigma_j^2 \mathbf{X}'\mathbf{Z}_j\mathbf{Z}_j'\mathbf{X} \right] \\
&= \frac{1}{2^k} \sigma^2 + \frac{1}{2^k} (1-p) \sum_{j=1}^c \sigma_j^2 + \frac{p}{2^{2k}} \sum_{j=1}^c \sigma_j^2 \mathbf{X}'\mathbf{Z}_j\mathbf{Z}_j'\mathbf{X}.
\end{aligned}$$

This implies that for any particular parameter, β_i , in the model,

$$E[\text{Var}[\hat{\beta}_i]] = a\sigma^2 + \sum_{j=1}^c b_{ij}\sigma_j^2 = a\sigma^2 + b_{i1}\sigma_1^2 + b_{i2}\sigma_2^2 + \cdots + b_{ic}\sigma_c^2,$$

where $1 \leq c \leq k$, the value of $a = \frac{1}{2^k}$, and the value of b_{ij} depends upon $\mathbf{X}$, $\mathbf{Z}_j$, i , and m . As before, $0 \leq i \leq (m-1)$, where m is the number of columns of $\mathbf{X}$. This results in the intercept of the model being $\hat{\beta}_0$, the parameter $\hat{\beta}_1$ would correspond to X_1 (the first factor in the model), and so on.

The expected prediction variance of $\hat{\mathbf{y}}$ can now be calculated as follows:

$$\begin{aligned}
\hat{\mathbf{y}} &= \mathbf{X}\hat{\boldsymbol{\beta}} \\
E[\text{Var}[\hat{\mathbf{y}}]] &= \mathbf{X}E[\text{Var}[\hat{\boldsymbol{\beta}}]]\mathbf{X}'.
\end{aligned}$$

Therefore, for a given i ,

$$E[\text{Var}[\hat{y}_i]] = \mathbf{x}_i E[\text{Var}[\hat{\boldsymbol{\beta}}]] \mathbf{x}_i',$$

where $\mathbf{x}_i$ is the i^{th} row of the standard design matrix $\mathbf{X}$. These calculations are identical to the calculations for the 2^k factorial experiment with one HTC factor except that the form of $E[\text{Var}[\hat{\boldsymbol{\beta}}]]$ is different.

As an example, consider the 2^3 factorial experiment with X_1 , X_2 , and X_3 being HTC. Let the model contain all main effects and all two factor interactions. Theorem 3.2 will be used to derive the expected variance of $\hat{\boldsymbol{\beta}}$. Also, Theorem 3.2 states that $p = \frac{1}{3}$ for the 2^3 factorial experiment with three HTC factors.

$$\begin{aligned}
E[\text{Var}[\hat{\boldsymbol{\beta}}]] &= (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}' E[\text{Var}[\mathbf{y}]] \mathbf{X} (\mathbf{X}'\mathbf{X})^{-1} \\
&= \frac{1}{64} \left[\sigma^2 \mathbf{X}'\mathbf{X} + (1-p)(\sigma_1^2 + \sigma_2^2 + \sigma_3^2) \mathbf{X}'\mathbf{X} + p \sum_{j=1}^3 \sigma_j^2 \mathbf{X}'\mathbf{Z}_j\mathbf{Z}_j'\mathbf{X} \right]
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{64} \left[\sigma^2 \mathbf{X}' \mathbf{X} + \left(1 - \frac{1}{3}\right) (\sigma_1^2 + \sigma_2^2 + \sigma_3^2) \mathbf{X}' \mathbf{X} + \frac{1}{3} \sum_{j=1}^3 \sigma_j^2 \mathbf{X}' \mathbf{Z}_j \mathbf{Z}_j' \mathbf{X} \right] \\
&= \frac{1}{64} \left[8\sigma^2 \mathbf{I}_7 + \frac{16}{3} (\sigma_1^2 + \sigma_2^2 + \sigma_3^2) \mathbf{I}_7 + \frac{1}{3} \sum_{j=1}^3 \sigma_j^2 \mathbf{Q}_j \right],
\end{aligned}$$

where

$$\mathbf{Q}_1 = \mathbf{X}' \mathbf{Z}_1 \mathbf{Z}_1' \mathbf{X} = \begin{bmatrix} 32 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 32 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{Q}_2 = \mathbf{X}' \mathbf{Z}_2 \mathbf{Z}_2' \mathbf{X} = \begin{bmatrix} 32 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 32 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

and

$$\mathbf{Q}_3 = \mathbf{X}' \mathbf{Z}_3 \mathbf{Z}_3' \mathbf{X} = \begin{bmatrix} 32 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 32 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Notice that $\mathbf{Q}_1$, $\mathbf{Q}_2$, and $\mathbf{Q}_3$ all have a nonzero diagonal element in the 1, 1 position.

Also, $\mathbf{Q}_1$ has a nonzero diagonal element in the 2, 2 position, $\mathbf{Q}_2$ has a nonzero

diagonal element in the 3, 3 position, and Q_3 has a nonzero diagonal element in the 4, 4 position. The nonzero element in position 1, 1 represents the effect the presence of the HTC factors have on the expected variance of the intercept, $\hat{\beta}_0$. The nonzero element in position 2, 2 of Q_1 represents the effect the presence of HTC factor X_1 has on the expected variance of $\hat{\beta}_1$. This also holds true for the nonzero element 3, 3 in Q_2 and the nonzero element 4, 4 in Q_3 . In general, Q_j , $1 \leq j \leq c$, will have a nonzero diagonal element in the $j + 1, j + 1$ entry corresponding to the effect of the HTC factor X_j .

The expression, $E[\text{Var}[\hat{\beta}]]$, can now be expressed similarly to the example in section 4.1.1.1 as

$$E[\text{Var}[\hat{\beta}_i]] = a\sigma^2 + b_{i1}(\sigma_1^2) + b_{i2}(\sigma_2^2) + b_{i3}(\sigma_3^2),$$

where $0 \leq i \leq 6$. This yields:

$$\begin{aligned} E[\text{Var}[\hat{\beta}_i]] &= \frac{1}{8}\sigma^2 + \frac{1}{4}(\sigma_1^2 + \sigma_2^2 + \sigma_3^2) & \text{if } i = 0 \\ &= \frac{1}{8}\sigma^2 + \frac{1}{4}\sigma_1^2 + \frac{1}{12}(\sigma_2^2 + \sigma_3^2) & \text{if } i = 1 \\ &= \frac{1}{8}\sigma^2 + \frac{1}{12}\sigma_1^2 + \frac{1}{4}\sigma_2^2 + \frac{1}{12}\sigma_3^2 & \text{if } i = 2 \\ &= \frac{1}{8}\sigma^2 + \frac{1}{12}(\sigma_1^2 + \sigma_2^2) + \frac{1}{4}\sigma_3^2 & \text{if } i = 3 \\ &= \frac{1}{8}\sigma^2 + \frac{1}{12}(\sigma_1^2 + \sigma_2^2 + \sigma_3^2) & \text{if } 4 \leq i \leq 6 \\ E[\text{Cov}[\hat{\beta}_i, \hat{\beta}_j]] &= 0 & \text{if } 0 \leq i < j \leq 6. \end{aligned}$$

Now, if one is interested in the $E[\text{Var}[\hat{y}_i]]$ for $i = 2$ then let x_2 be the second row of X , just like the example in section 4.1.1.1. Then,

$$E[\text{Var}[\hat{y}_2]] = x_2 E[\text{Var}[\hat{\beta}]] x_2'$$

$$\begin{aligned}
&= \begin{bmatrix} 1 & 1 & 1 & -1 & 1 & -1 & -1 \end{bmatrix} E[\text{Var}[\hat{\beta}]] \begin{bmatrix} 1 \\ 1 \\ 1 \\ -1 \\ 1 \\ -1 \\ -1 \end{bmatrix} \\
&= \frac{7}{8}\sigma^2 + \frac{11}{12}\sigma_1^2 + \frac{11}{12}\sigma_2^2 + \frac{11}{12}\sigma_3^2 \\
&= \frac{7}{8}\sigma^2 + \frac{11}{12}(\sigma_1^2 + \sigma_2^2 + \sigma_3^2) \\
&\approx \frac{7}{8}\sigma^2 + \frac{7.33}{8}(\sigma_1^2 + \sigma_2^2 + \sigma_3^2).
\end{aligned}$$

It is important to point out that $E[\text{Var}[\hat{y}_i]]$ will be the same $\forall i$ because the $E[\text{Var}[\hat{\beta}]]$ is a diagonal matrix. Therefore, the maximum expected prediction variance of $\hat{y}$, where the maximum is taken over all points in the design space, can be written as

$$\max_{x \in \mathcal{X}} E[\text{Var}[\hat{y}(x)]] = x_0 E[\text{Var}[\hat{\beta}]] x_0',$$

where

$$x_0 = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \end{bmatrix},$$

analogous to the way it was in section 4.1.1.1.

Table 12 contains the coefficients $a, b_{i1}, b_{i2}, \dots, b_{ic}$ in the formula

$$E[\text{Var}[\hat{\beta}_i]] = a\sigma^2 + b_{i1}\sigma_1^2 + b_{i2}\sigma_2^2 + \dots + b_{ic}\sigma_c^2,$$

where $0 \leq i \leq (m-1)$, for various 2^k factorial experiments with a randomized run order and c HTC factors, $X_1, X_2, \dots, X_c$. The table is indexed by the coefficients a and b_{ij} , where $1 \leq j \leq c$. For example, if one is interested in $E[\text{Var}[\hat{\beta}_3]]$ for a 2^5 factorial experiment with $c = 4$ HTC factors, the value of $b_{0,3}$ and the value of $b_{3,3}$ would be $\frac{1}{12}$. The value of b_{ij} remains the same for a given 2^k factorial experiment as long as there are at least j HTC factors. The values in this table are identical to the values in Table 4.

Table 12: The coefficients $a, b_{i1}, b_{i2}, \dots, b_{ic}$ for factorial experiments with a randomized run order and c HTC factors.

2^k	a	b_{ij}	b_{ij}
	$\forall i$	$i \in \{0, j\}$	$i \notin \{0, j\}$
2^2	$\frac{1}{4}$	$\frac{3}{8}$	$\frac{1}{8}$
2^3	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{1}{12}$
2^4	$\frac{1}{16}$	$\frac{3}{20}$	$\frac{1}{20}$
2^5	$\frac{1}{32}$	$\frac{1}{12}$	$\frac{1}{36}$
2^6	$\frac{1}{64}$	$\frac{3}{68}$	$\frac{1}{68}$
2^7	$\frac{1}{128}$	$\frac{3}{132}$	$\frac{1}{132}$

Table 13 contains the multipliers of σ^2 and σ_j^2 , where $1 \leq j \leq c$, for the maximum expected prediction variance for various 2^k factorial experiments with a randomized run order and c HTC factors, $X_1, X_2, \dots, X_c$. Table 13 will include values for models containing the main effects only, the main effects and all two-factor interactions, and the full model with all interactions. The values in this table are identical to the values in table 5.

Table 13: The multipliers of σ^2 and σ_j^2 for the maximum expected prediction variance factorial experiments with a randomized run order and c HTC factors.

2^k	Parameters In the Model	Variance Multiplier	
		σ^2	σ_j^2
2^2	Main Effects	$\frac{3}{4}$	$\frac{3.50}{4}$
	Main + 2 FI	$\frac{4}{4}$	$\frac{4.00}{4}$
	Full Model	$\frac{4}{4}$	$\frac{4.00}{4}$
2^3	Main Effects	$\frac{4}{8}$	$\frac{5.33}{8}$
	Main + 2 FI	$\frac{7}{8}$	$\frac{7.33}{8}$
	Full Model	$\frac{8}{8}$	$\frac{8.00}{8}$
2^4	Main Effects	$\frac{5}{16}$	$\frac{7.20}{16}$
	Main + 2 FI	$\frac{11}{16}$	$\frac{12.00}{16}$
	Full Model	$\frac{16}{16}$	$\frac{16.00}{16}$
2^5	Main Effects	$\frac{6}{32}$	$\frac{8.89}{32}$
	Main + 2 FI	$\frac{16}{32}$	$\frac{17.78}{32}$
	Full Model	$\frac{32}{32}$	$\frac{32.00}{32}$
2^6	Main Effects	$\frac{7}{64}$	$\frac{10.35}{64}$
	Main + 2 FI	$\frac{22}{64}$	$\frac{24.47}{64}$
	Full Model	$\frac{64}{64}$	$\frac{64.00}{64}$
2^7	Main Effects	$\frac{8}{128}$	$\frac{11.64}{128}$
	Main + 2 FI	$\frac{29}{128}$	$\frac{32.00}{128}$
	Full Model	$\frac{128}{128}$	$\frac{128.00}{128}$

A randomized run order is a reasonable way to conduct an experiment. A random run order is cheaper, in terms of resetting the HTC factors, than a completely randomized run order, and only has slightly higher maximum expected prediction variance. For example, consider the following table where the number of resets of

the HTC factors for both completely randomized and randomized 2^k designs with c HTC factors are given. The multipliers of σ^2 and σ_j^2 , where $1 \leq j \leq c$, for the maximum prediction variance and the maximum expected prediction variance are also given for completely randomized and randomized designs respectively. Note that the maximum prediction variance for a completely randomized 2^k factorial experiment is $P\sigma^2 + P\sigma_1^2 + \dots + P\sigma_c^2$, where P is the number of parameters in the model. This result follows from the Kiefer-Wolfowitz equivalence theorem. For a thorough discussion, see Anbari [1], Kiefer and Wolfowitz [34] [35], and Kiefer [36] [37] [38].

Table 14: The comparison of cost and prediction variance for randomized and completely randomized 2^k factorial experiments with c HTC factors.

2^k	Parameters in The Model	Completely Randomized		Randomized		
		Variance Multiplier	Cost	Variance Multiplier		Cost
		$\sigma^2 = \sigma_j^2$		σ^2	σ_j^2	
2^2	Main Effects	$\frac{3}{4}$	$4c$	$\frac{3}{4}$	$\frac{3.50}{4}$	$3c$
	Main + 2 FI	$\frac{4}{4}$	$4c$	$\frac{4}{4}$	$\frac{4.00}{4}$	$3c$
	Full Model	$\frac{4}{4}$	$4c$	$\frac{4}{4}$	$\frac{4.00}{4}$	$3c$
2^3	Main Effects	$\frac{4}{8}$	$8c$	$\frac{4}{8}$	$\frac{5.33}{8}$	$5c$
	Main + 2 FI	$\frac{7}{8}$	$8c$	$\frac{7}{8}$	$\frac{7.33}{8}$	$5c$
	Full Model	$\frac{8}{8}$	$8c$	$\frac{8}{8}$	$\frac{8.00}{8}$	$5c$
2^4	Main Effects	$\frac{5}{16}$	$16c$	$\frac{5}{16}$	$\frac{7.20}{16}$	$9c$
	Main + 2 FI	$\frac{11}{16}$	$16c$	$\frac{11}{16}$	$\frac{12.00}{16}$	$9c$
	Full Model	$\frac{16}{16}$	$16c$	$\frac{16}{16}$	$\frac{16.00}{16}$	$9c$
2^5	Main Effects	$\frac{6}{32}$	$32c$	$\frac{6}{32}$	$\frac{8.89}{32}$	$17c$
	Main + 2 FI	$\frac{16}{32}$	$32c$	$\frac{16}{32}$	$\frac{17.78}{32}$	$17c$
	Full Model	$\frac{32}{32}$	$32c$	$\frac{32}{32}$	$\frac{32.00}{32}$	$17c$
2^6	Main Effects	$\frac{7}{64}$	$64c$	$\frac{7}{64}$	$\frac{10.35}{64}$	$33c$
	Main + 2 FI	$\frac{22}{64}$	$64c$	$\frac{22}{64}$	$\frac{24.47}{64}$	$33c$
	Full Model	$\frac{64}{64}$	$64c$	$\frac{64}{64}$	$\frac{64.00}{64}$	$33c$
2^6	Main Effects	$\frac{7}{128}$	$128c$	$\frac{7}{128}$	$\frac{11.64}{128}$	$65c$
	Main + 2 FI	$\frac{22}{128}$	$128c$	$\frac{22}{128}$	$\frac{32.00}{128}$	$65c$
	Full Model	$\frac{64}{128}$	$128c$	$\frac{64}{128}$	$\frac{128.00}{128}$	$65c$

The experimenter's prior knowledge of the variability associated with setting up the HTC factors in the 2^k factorial experiment may lead to a simplification of the calculation of the the maximum expected prediction variance of $\hat{y}$. For example, assume that the experimenter conducts a 2^k factorial experiment with c HTC factors

and is willing to assume $\sigma_1^2 = \sigma_2^2 = \dots = \sigma_c^2$. For simplicity, let all the variance components be equal to a common value, σ_c^2 . Then, the the expected variance of $\hat{\beta}$ can be expressed as follows:

$$\begin{aligned} E[\text{Var}[\hat{\beta}]] &= \frac{1}{2^k} \sigma^2 + \frac{1}{2^k} (1-p) \sum_{j=1}^c \sigma_j^2 + \frac{1}{2^{2k}} p \sum_{j=1}^c \sigma_j^2 \mathbf{X}' \mathbf{Z}_j \mathbf{Z}_j' \mathbf{X} \\ &= \frac{1}{2^k} \sigma^2 + \frac{c}{2^k} (1-p) \sigma_c^2 + \frac{1}{2^{2k}} p \sigma_c^2 \sum_{j=1}^c \mathbf{X}' \mathbf{Z}_j \mathbf{Z}_j' \mathbf{X} \end{aligned}$$

This implies that for any particular parameter in the model,

$$E[\text{Var}[\hat{\beta}_i]] = a\sigma^2 + \sum_{j=1}^c b_{ij}\sigma_j^2 = a\sigma^2 + \sigma_c^2 \sum_{j=1}^c b_{ij},$$

where $0 \leq i \leq (m-1)$ (here, m is the number of columns of $\mathbf{X}$), $1 \leq c \leq k$, the value of $a = \frac{1}{2^k}$, and the value of b_{ij} depends upon $\mathbf{X}$, $\mathbf{Z}_j$, i , and m . As before, $0 \leq i \leq (m-1)$. This results in the intercept of the model being $\hat{\beta}_0$, the parameter $\hat{\beta}_1$ would correspond to X_1 (the first factor in the model), and so on.

The expected prediction variance of $\hat{y}$ is calculated just as before,

$$\hat{y} = \mathbf{X}\hat{\beta}$$

$$E[\text{Var}[\hat{y}]] = \mathbf{X}E[\text{Var}[\hat{\beta}]]\mathbf{X}'.$$

Therefore, for a given i ,

$$E[\text{Var}[\hat{y}_i]] = \mathbf{x}_i E[\text{Var}[\hat{\beta}]] \mathbf{x}_i',$$

where $\mathbf{x}_i$ is the i^{th} row of the standard design matrix $\mathbf{X}$.

To illustrate this simplification, just as before, consider the 2^3 factorial experiment with X_1 , X_2 , and X_3 being HTC. The expression, $E[\text{Var}[\hat{\beta}]]$, was found to be:

$$\begin{aligned} E[\text{Var}[\hat{\beta}_i]] &= \frac{1}{8} \sigma^2 + \frac{1}{4} (\sigma_1^2 + \sigma_2^2 + \sigma_3^2) & \text{if } i = 0 \\ &= \frac{1}{8} \sigma^2 + \frac{1}{4} \sigma_1^2 + \frac{1}{12} (\sigma_2^2 + \sigma_3^2) & \text{if } i = 1 \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{8}\sigma^2 + \frac{1}{12}\sigma_1^2 + \frac{1}{4}\sigma_2^2 + \frac{1}{12}\sigma_3^2 \quad \text{if } i = 2 \\
&= \frac{1}{8}\sigma^2 + \frac{1}{12}(\sigma_1^2 + \sigma_2^2) + \frac{1}{4}\sigma_3^2 \quad \text{if } i = 3 \\
&= \frac{1}{8}\sigma^2 + \frac{1}{12}(\sigma_1^2 + \sigma_2^2 + \sigma_3^2) \quad \text{if } 4 \leq i \leq 6 \\
E[\text{Cov}[\hat{\beta}_i, \hat{\beta}_j]] &= 0 \quad \text{if } 0 \leq i < j \leq 6.
\end{aligned}$$

Now, with the assumption of equal variance components, $E[\text{Var}[\hat{\beta}]]$ is now:

$$\begin{aligned}
E[\text{Var}[\hat{\beta}_i]] &= \frac{1}{8}\sigma^2 + \frac{3}{4}\sigma_c^2 \quad \text{if } i = 0 \\
&= \frac{1}{8}\sigma^2 + \frac{5}{12}\sigma_c^2 \quad \text{if } 1 \leq i \leq 3 \\
&= \frac{1}{8}\sigma^2 + \frac{3}{12}\sigma_c^2 \quad \text{if } 4 \leq i \leq 6 \\
E[\text{Cov}[\hat{\beta}_i, \hat{\beta}_j]] &= 0 \quad \text{if } 0 \leq i < j \leq 6.
\end{aligned}$$

In general, if the experimenter is willing to assume that all the variance components are equal, then

$$E[\text{Var}[\hat{\beta}_i]] = a\sigma^2 + b_i\sigma_c^2.$$

For this example, it was previously shown that the maximum prediction variance of $\hat{y}$ was

$$\max_{\mathbf{x} \in \mathcal{X}} E[\text{Var}[\hat{y}(\mathbf{x})]] = \frac{7}{8}\sigma^2 + \frac{11}{12}(\sigma_1^2 + \sigma_2^2 + \sigma_3^2).$$

The simplification of assuming that the variance components are all equal implies

$$\begin{aligned}
\max_{\mathbf{x} \in \mathcal{X}} E[\text{Var}[\hat{y}(\mathbf{x})]] &= \frac{7}{8}\sigma^2 + \frac{33}{12}\sigma_c^2 \\
&= \frac{7}{8}\sigma^2 + \frac{22}{8}\sigma_c^2.
\end{aligned}$$

Table 15 contains the coefficients a and b_i in the formula

$$E[\text{Var}[\hat{\beta}_i]] = a\sigma^2 + b_i\sigma_c^2,$$

where $0 \leq i \leq (m-1)$, for various 2^k factorial experiments with a randomized run order and c HTC factors, $X_1, X_2, \dots, X_c$. Also, it is assumed that $\sigma_1^2 = \sigma_2^2 = \dots = \sigma_c^2$.

Table 15: The coefficients a and b_i for various 2^k factorial experiments with a randomized run order and c HTC factors.

2^k	a	b_i	b_i	b_i
	$\forall i$	$i = 0$	$1 \leq i \leq c$	$c < i$
2^2	$\frac{1}{4}$	$\frac{3c}{8}$	$\frac{3}{8} + \frac{c-1}{8}$	$\frac{c}{8}$
2^3	$\frac{1}{8}$	$\frac{c}{4}$	$\frac{1}{4} + \frac{c-1}{12}$	$\frac{c}{12}$
2^4	$\frac{1}{16}$	$\frac{3c}{20}$	$\frac{3}{20} + \frac{c-1}{20}$	$\frac{c}{20}$
2^5	$\frac{1}{32}$	$\frac{c}{12}$	$\frac{1}{12} + \frac{c-1}{36}$	$\frac{c}{36}$
2^6	$\frac{1}{64}$	$\frac{3c}{68}$	$\frac{3}{68} + \frac{c-1}{68}$	$\frac{c}{68}$
2^7	$\frac{1}{128}$	$\frac{3c}{132}$	$\frac{3}{132} + \frac{c-1}{132}$	$\frac{c}{132}$

Table 16 contains the multipliers of σ^2 and σ_c^2 for the maximum expected prediction variance for various 2^k factorial experiments with a randomized run order and c HTC factors, $X_1, X_2, \dots, X_c$. Also, it is assumed that $\sigma_1^2 = \sigma_2^2 = \dots = \sigma_c^2$. Table 16 will include values for models containing the main effects only, the main effects and all two-factor interactions, and the full model with all interactions.

Table 16: The multipliers of σ^2 and σ_c^2 for the maximum expected prediction variance for factorial experiments with a randomized run order and c HTC factors.

2^k	Parameters In the Model	Variance Multiplier	
		σ^2	σ_c^2
2^2	Main Effects	$\frac{3}{4}$	$\frac{3.50c}{4}$
	Main + 2 FI	$\frac{4}{4}$	$\frac{4.00c}{4}$
	Full Model	$\frac{4}{4}$	$\frac{4.00c}{4}$
2^3	Main Effects	$\frac{4}{8}$	$\frac{5.33c}{8}$
	Main + 2 FI	$\frac{7}{8}$	$\frac{7.33c}{8}$
	Full Model	$\frac{8}{8}$	$\frac{8.00c}{8}$
2^4	Main Effects	$\frac{5}{16}$	$\frac{7.20c}{16}$
	Main + 2 FI	$\frac{11}{16}$	$\frac{12.00c}{16}$
	Full Model	$\frac{16}{16}$	$\frac{16.00c}{16}$
2^5	Main Effects	$\frac{6}{32}$	$\frac{8.89c}{32}$
	Main + 2 FI	$\frac{16}{32}$	$\frac{17.78c}{32}$
	Full Model	$\frac{32}{32}$	$\frac{32.00c}{32}$
2^6	Main Effects	$\frac{7}{64}$	$\frac{10.35c}{64}$
	Main + 2 FI	$\frac{22}{64}$	$\frac{24.47c}{64}$
	Full Model	$\frac{64}{64}$	$\frac{64.00c}{64}$
2^7	Main Effects	$\frac{8}{128}$	$\frac{11.64c}{128}$
	Main + 2 FI	$\frac{29}{128}$	$\frac{32c}{128}$
	Full Model	$\frac{128}{128}$	$\frac{128.00c}{128}$

4.1.2.2 The 2^k Factorial Experiment With Particular Blocking Structures

Various blocking structures for the 2^k factorial experiment will now be discussed. The major difference between the case with c HTC factors and the case with one HTC factor in section 4.1.1.2. is that there will be multiple Z matrices. For each

HTC factor, there will be a Z matrix which completely describes the restrictions on randomization due to that HTC factor.

Anbari [1] developed an algorithm for generating optimal confounding relations for 2^k factorial experiments with 1 HTC factor. The optimal confounding relations in section 4.1.1.2 were generated by this algorithm. Anbari also discusses the fact that the algorithm produces optimal confounding relations for 2^k factorial experiments containing c HTC factors. All optimal confounding relations used in this section will be generated by this algorithm.

The 2^3 factorial experiment will be used as an example of the use of confounding relations to develop blocking structures when there are c HTC factors. First, consider the case where $c = 2$. That is, there are 2 HTC factors, X_1 and X_2 . The model containing all main effects and two-factor interactions will be considered.

Blocking structures are best visualized by the use of the standard design matrix, X for the 2^3 factorial experiment with all main effects and two-factor interactions:

$$X = \begin{array}{c|ccccccc} \text{run} & I & X_1 & X_2 & X_3 & X_1X_2 & X_1X_3 & X_2X_3 \\ \hline 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 2 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 3 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 4 & 1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 5 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \\ 6 & 1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 7 & 1 & 1 & 1 & -1 & 1 & -1 & -1 \\ 8 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{array}$$

With 1 HTC factor, the number of blocks is easily specified. For example, if X_1 were the only HTC factor, then the run order 1; 3; 2; 4; 5; 7; 6; 8 has two blocks of size 4. With two HTC factors, there will be blocks created by each of the HTC factors. For example, the run order 2; 1; 3; 4; 6; 5; 8; 7 has two blocks of size 4 created

by X_1 and four blocks of size 2 created by X_2 . Rearranging the $\mathbf{X}$ matrix clearly demonstrates this:

$$\mathbf{X} = \begin{array}{c} \text{run} \\ 2 \\ 1 \\ 3 \\ 4 \\ 6 \\ 5 \\ 8 \\ 7 \end{array} \begin{bmatrix} I & X_1 & X_2 & X_3 & X_1X_2 & X_1X_3 & X_2X_3 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & -1 \end{bmatrix}$$

The lines in the X_1 and X_2 columns separate the blocks that are formed due to resetting the HTC factors. Notice that the block size for all blocks created by HTC factor X_1 is four. Similarly, the blocks created by HTC factor X_2 are all of size 2. There are run orders that result in fewer blocks, but have the undesirable property of unequal block size. For example, the run order 1; 2; 3; 4; 7; 8; 5; 6 has the following blocking structure:

$$\mathbf{X} = \begin{array}{c} \text{run} \\ 1 \\ 2 \\ 3 \\ 4 \\ 7 \\ 8 \\ 5 \\ 6 \end{array} \begin{bmatrix} I & X_1 & X_2 & X_3 & X_1X_2 & X_1X_3 & X_2X_3 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 \end{bmatrix}$$

Now, there are only three blocks formed by X_2 . This experiment is slightly cheaper to run than the 2^3 factorial design which has 4 blocks of size 2 for HTC factor X_2 . It

does, however, have the same undesirable properties indicated in Section 4.1.1.2 for blocking structures of unequal block size. The maximum prediction variance will be larger in comparison to experiments with blocking structures having equal block size, and some parameter estimators will be correlated.

The optimal confounding relation for a 2^3 factorial experiment with X_1 and X_2 HTC, with X_1 creating two blocks of size 4, and X_2 creating four blocks of size 2 is $I=A=B=AB$.

The maximum prediction variance of $\hat{y}$ for the model with main effects and two-factor interactions can now be determined. Because there are two HTC factors, there will be a matrix, Z_1 , which describes the blocking structure of X_1 and a matrix, Z_2 , which describes the blocking structure of X_2 . For this example,

$$Z_1 = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}, \quad Z_1 Z_1' = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix},$$

and

$$Z_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad Z_2 Z_2' = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

This blocking structure yields $\text{Var}[\mathbf{y}] = \mathbf{V} = \sigma^2 \mathbf{I}_8 + \sigma_1^2 \mathbf{Z}_1 \mathbf{Z}_1' + \sigma_2^2 \mathbf{Z}_2 \mathbf{Z}_2'$.
Therefore,

$$\begin{aligned}
 \text{Var}[\hat{\beta}] &= (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}' \text{Var}[\mathbf{y}] \mathbf{X} (\mathbf{X}'\mathbf{X})^{-1} \\
 &= (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}' \mathbf{V} \mathbf{X} (\mathbf{X}'\mathbf{X})^{-1} \\
 &= \frac{1}{64} \mathbf{X}' \mathbf{V} \mathbf{X} \\
 &= \frac{1}{64} \mathbf{X}' [\sigma^2 \mathbf{I}_8 + \sigma_1^2 \mathbf{Z}_1 \mathbf{Z}_1' + \sigma_2^2 \mathbf{Z}_2 \mathbf{Z}_2'] \mathbf{X} \\
 &= \frac{1}{8} \sigma^2 \mathbf{I}_7 + \frac{1}{64} \sigma_1^2 \mathbf{X}' \mathbf{Z}_1 \mathbf{Z}_1' \mathbf{X} + \frac{1}{64} \sigma_2^2 \mathbf{X}' \mathbf{Z}_2 \mathbf{Z}_2' \mathbf{X} \\
 &= \frac{1}{8} \sigma^2 \mathbf{I}_7 + \frac{1}{64} \sigma_1^2 \mathbf{Q}_1 + \frac{1}{64} \sigma_2^2 \mathbf{Q}_2
 \end{aligned}$$

where

$$\mathbf{Q}_1 = \mathbf{X}' \mathbf{Z}_1 \mathbf{Z}_1' \mathbf{X} = \begin{bmatrix} 32 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 32 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

and

$$\mathbf{Q}_2 = \mathbf{X}' \mathbf{Z}_2 \mathbf{Z}_2' \mathbf{X} = \begin{bmatrix} 16 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 16 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 16 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 16 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

This equation simplifies to the form

$$\text{Var}[\hat{\beta}_i] = a\sigma^2 + b_{i1}\sigma_1^2 + b_{i2}\sigma_2^2,$$

where $0 \leq i \leq 6$ yields

$$\begin{aligned}
 \text{Var}[\hat{\beta}_i] &= \frac{1}{8}\sigma^2 + \frac{1}{2}\sigma_1^2 + \frac{1}{4}\sigma_2^2 & \text{if } 0 \leq i \leq 1 \\
 &= \frac{1}{8}\sigma^2 + \frac{1}{4}\sigma_2^2 & \text{if } i = 2 \\
 &= \frac{1}{8}\sigma^2 & \text{if } i = 3 \\
 &= \frac{1}{8}\sigma^2 + \frac{1}{4}\sigma_2^2 & \text{if } i = 4 \\
 &= \frac{1}{8}\sigma^2 & \text{if } i \geq 5 \\
 \text{Cov}[\hat{\beta}_i, \hat{\beta}_j] &= 0 & \text{if } 0 \leq i < j \leq 6.
 \end{aligned}$$

As before, with a randomized run order, the parameter estimators are not correlated. For this design, the maximum prediction variance of $\hat{y}$ for the model with main effects and two-factor interactions is

$$\begin{aligned}
 \max_{x \in \mathcal{X}} \text{Var}[\hat{y}(x)] &= x_0 \text{Var}[\hat{\beta}] x_0' \\
 &= \frac{7}{8}\sigma^2 + \frac{8}{8}\sigma_1^2 + \frac{8}{8}\sigma_2^2.
 \end{aligned}$$

The only other balanced blocking structure possible for the 2^3 factorial experiment with 2 HTC factors is one where there are four blocks of size 2 for HTC factor X_1 and eight blocks of size 1 for HTC factor X_2 . This particular structure results in the resetting of X_2 at the beginning of each run. In effect, this makes X_2 ETC.

The same difficulty results if all three factors are HTC. The optimal confounding relation for all three factors HTC is $I=A=B=C=AB=AC=BC=ABC$. This results in two blocks of size 4 for X_1 , four blocks of size 2 for X_2 , and 8 blocks of size 1 for X_3 . Therefore, the third factor will be reset at the beginning of each run. This results in X_3 being ETC. There are other run orders which result in blocking structures where all three of the HTC factors are set up less than 8 times. For instance, the run order

1; 2; 4; 3; 7; 8; 6; 5 results in the following blocking structure:

run	I	X_1	X_2	X_3	X_1X_2	X_1X_3	X_2X_3
1	1	-1	-1	-1	1	1	1
2	1	-1	-1	1	1	-1	-1
4	1	-1	1	1	-1	-1	1
$X =$ 3	1	-1	1	-1	-1	1	-1
7	1	1	1	-1	1	-1	-1
8	1	1	1	1	1	1	1
6	1	1	-1	1	-1	1	-1
5	1	1	-1	-1	-1	-1	1

Factor X_1 creates two blocks of size 4, factor X_2 creates two blocks of size 2 and one block of size 4, and factor X_3 creates three blocks of size 2 and two blocks of size 1. This run order results in blocks of unequal size and therefore the analysis will result in parameter estimators being correlated and the maximum prediction variance of $\hat{y}$ being larger than that associated with the blocking structure with confounding relation $I=A=B=C=AB=AC=BC=ABC$. Therefore, in general, for 2^k factorial experiments with $c = k$ HTC factors, the experimenter is better served by choosing one HTC factor to be ETC.

The following tables (Tables 17 to 21) contain the optimal confounding relations for 2^k factorial experiments with c HTC factors, where $2 \leq c \leq (k - 1)$. For a particular HTC factor, the confounding relations generate blocks of equal size. The column labeled "Block Size" in the tables refers to the size of blocks generated by the c HTC factors. This information is expressed in the form of a c -tuple. For example, for the 2^3 factorial experiment with 2 HTC factors, the column "Block Size" would contain (4, 2) because HTC factor X_1 creates two blocks of size 4 and HTC factor X_2 creates four blocks of size 2.

The reader should be aware that for most confounding relations given, there may be more than one way to assign blocks to the c HTC factors. The algorithm by

Anbari [1] gives the optimal confounding relation, but does not state how to assign the blocks generated by it. At this time, no algorithm for doing this is known to exist. Two examples are given in the tables where the terms in the confounding relations are labeled to inform the reader of which HTC factor they are creating blocks for. The two examples given are for the 2^4 and 2^5 experiments with 2 HTC factors. The notation is as follows: A(1) corresponds to associating blocks formed by the term A in the confounding relation with HTC factor X_1 , AB(2) corresponds to associating blocks formed by the term AB in the confounding relation with HTC factor X_2 , and so on.

Table 17: The optimal confounding relations for 2^3 factorial experiments with c HTC factors.

# of HTC Factors	Block Size	Confounding Relation
2	(4, 2)	$I = A = B = AB$

Table 18: The optimal confounding relations for 2^4 factorial experiments with c HTC factors.

# of HTC Factors	Block Size	Confounding Relation
2	(8, 4)	$I = A = B = AB$
2	(4, 2)	$I = A(1) = BCD(1) = ABCD(1) = B(2) = AB(2) = CD(2) = ACD(2)$
3	(8, 4, 2)	$I = A = B = C = AB = AC = BC = ABC$

Table 19: The optimal confounding relations for 2^5 factorial experiments with c HTC factors.

# of HTC Factors	Block Size	Confounding Relation
2	(16, 8)	$I = A = B = AB$
2	(8, 4)	$I = A = B = CDE = AB = ACDE = BCDE = ABCDE$
2	(4, 2)	$I = A(1) = CD(1) = BCE(1) = BDE(1) = ACD(1) = ABCE(1) = ABDE(1) = B(2) = CE(2) = DE(2) = AB(2) = ACE(2) = ADE(2) = BCD(2) = ABCD(2)$
3	(16, 8, 4)	$I = A = B = C = AB = AC = BC = ABC$
3	(8, 4, 2)	$I = A = B = C = DE = AB = AC = ADE = BC = BDE = CDE = ABC = ABDE = ACDE = BCDE = ABCDE$
4	(16, 8, 4, 2)	$I = A = B = C = D = AB = AC = AD = BC = BD = CD = ABC = ABD = ACD = BCD = ABCD$

Table 20: The optimal confounding relations for 2^6 factorial experiments with c HTC factors.

# of HTC Factors	Block Size	Confounding Relation
2	(32, 16)	$I = A = B = AB$
2	(16, 8)	$I = A = B = CDEF = AB = ACDEF = BCDEF = ABCDEF$
2	(8, 4)	$I = A = B = CEF = DE = AB = ACEF = ADE = BCEF = BDE = CDF = ABCEF = ABDE = ACDF = BCDF = ABCDF$
2	(4, 2)	$I = A = B = CF = DF = EF = AB = ACF = ADF = AEF = BCF = BDF = BEF = CD = CE = DE = ABCF = ABDF = ABEF = ACD = ACE = ADE = BCD = BCE = BDE = CDEF = ABCD = ABCE = ABDE = ACDEF = BCDEF = ABCDEF$
3	(32, 16, 8)	$I = A = B = C = AB = AC = BC = ABC$
3	(16, 8, 4)	$I = A = B = C = DEF = AB = AC = ADEF = BC = BDEF = CDEF = ABC = ABDEF = ACDEF = BCDEF = ABCDEF$
3	(8, 4, 2)	$I = A = B = C = DF = EF = AB = AC = ADF = AEF = BC = BDF = BEF = CDF = CEF = DE = ABC = ABDF = ABEF = ACDF = ACEF = ADE = BCDF = BCEF = BDE = CDE = ABCDF = ABCEF = ACDE = ABDE = BCDE = ABCDE$

Table 20: The optimal confounding relations for 2^6 factorial experiments with c HTC factors.

# of HTC Factors	Block Size	Confounding Relation
4	(32, 16, 8, 4)	$I = A = B = C = D = AB = AC = AD = BC = BD = CD = ABC = ACD = BCD = ABD = ABCD$
4	(16, 8, 4, 2)	$I = A = B = C = D = EF = AB = AC = AD = AEF = BC = BD = BEF = CD = CEF = DEF = ABC = ABD = ABEF = ACD = ACEF = ADEF = BCD = BCEF = BDEF = CDEF = ABCD = ABDEF = ABCEF = ACDEF = BCDEF = ABCDEF$
5	(32, 16, 8, 4, 2)	$I = A = B = C = D = E = AB = AC = AD = AE = BC = BD = BE = CD = CE = DE = ABC = ABD = ABE = ACD = ACE = ADE = BCD = BCE = BDE = CDE = ABCD = ABCE = ABDE = ACDE = BCDE = ABCDE$

Table 21: The optimal confounding relations for 2^7 factorial experiments with c HTC factors.

# of HTC Factors	Block Size	Confounding Relation
2	(64, 32)	$I = A = B = AB$
2	(32, 16)	$I = A = B = CDEFG = AB = ACDEFG = BCDEFG = ABCDEFG$
2	(16, 8)	$I = A = B = CEFG = DE = AB = ACEFG = ADE = BCEFG = BDE = CDFG = ABCEFG = ABDE = ACDFG = BCDFG = ABCDFG$
2	(8, 4)	Optimal confounding relation Generator : $I = A = B = CFG = DF = EG$
2	(4, 2)	Optimal confounding relation Generator : $I = A = B = CG = DG = EG = FG$
3	(64, 32, 16)	$I = A = B = C = AB = AC = BC = ABC$
3	(32, 16, 8)	$I = A = B = C = DEFG = AB = AC = ADEFG = BC = BDEFG = CDEFG = ABC = ABDEFG = ACDEFG = BCDEFG = ABCDEFG$
3	(16, 8, 4)	Optimal confounding relation Generator : $I = A = B = C = DFG = EF$
3	(8, 4, 2)	Optimal confounding relation Generator : $I = A = B = C = DG = EG = FG$
4	(64, 32, 16, 8)	$I = A = B = C = D = AB = AC = AD = BC = BD = CD = ABC = ABD = ACD = BCD = ABCD$

Table 21: The optimal confounding relations for 2^7 factorial experiments with c HTC factors.

# of HTC Factors	Block Size	Confounding Relation
4	(32, 16, 8, 4)	Optimal confounding relation Generator : $I = A = B = C = D = EFG$
4	(16, 8, 4, 2)	Optimal confounding relation Generator : $I = A = B = C = D = EG = FG$
5	(64, 32, 16, 8, 4)	Optimal confounding relation Generator : $I = A = B = C = D = E$
5	(32, 16, 8, 4, 2)	Optimal confounding relation Generator : $I = A = B = C = D = E = FG$
6	(64, 32, 16, 8, 4, 2)	Optimal confounding relation Generator : $I = A = B = C = D = E = F$

Following are Tables 22 to 26, which give the maximum prediction variance for various 2^k factorial experiments with c HTC factors, $X_1, X_2, \dots, X_c$. Optimal blocking structures are generated by using the optimal confounding relations in Tables 17 to 21 and the algorithm presented in Anbari [1]. For many of the designs listed, it is possible for the maximum prediction variance to vary depending on the way the blocks are assigned to the c HTC factors. As was stated prior to tables 17 through 21, no algorithm exists for assigning blocks in a manner which results in the lowest expected maximum prediction variance. The two examples of assigning blocks for the 2^4 and 2^5 designs with 2 HTC factors given in Tables 18 and 19 result in super efficient designs for models with main effects and two factor interactions. The maximum prediction variance given in the following tables for these two designs is based on those block assignments.

Table 22: The maximum prediction variance for the 2^3 factorial experiment with c HTC factors.

# of HTC Factors	Block Size	Parameters In the Model	Variance Multiplier		
			σ^2	σ_1^2	σ_2^2
2	(4, 2)	Main Effects	$\frac{4}{8}$	$\frac{8}{8}$	$\frac{6}{8}$
		Main + 2 FI	$\frac{7}{8}$	$\frac{8}{8}$	$\frac{8}{8}$
		Full Model	$\frac{8}{8}$	$\frac{8}{8}$	$\frac{8}{8}$

Table 23: The maximum prediction variance for the 2^4 factorial experiment with c HTC factors.

# of HTC Factors	Block Size	Parameters In the Model	Variance Multiplier			
			σ^2	σ_1^2	σ_2^2	σ_3^2
2	(8, 4)	Main Effects	$\frac{5}{16}$	$\frac{16}{16}$	$\frac{12}{16}$	
		Main + 2 FI	$\frac{11}{16}$	$\frac{16}{16}$	$\frac{16}{16}$	
		Full Model	$\frac{16}{16}$	$\frac{16}{16}$	$\frac{16}{16}$	
2	(4, 2)	Main Effects	$\frac{5}{16}$	$\frac{8}{16}$	$\frac{6}{16}$	
		Main + 2 FI	$\frac{11}{16}$	$\frac{8}{16}$	$\frac{10}{16}$	
		Full Model	$\frac{16}{16}$	$\frac{16}{16}$	$\frac{16}{16}$	
3	(8, 4, 2)	Main Effects	$\frac{5}{16}$	$\frac{16}{16}$	$\frac{12}{16}$	$\frac{8}{16}$
		Main + 2 FI	$\frac{11}{16}$	$\frac{16}{16}$	$\frac{16}{16}$	$\frac{14}{16}$
		Full Model	$\frac{16}{16}$	$\frac{16}{16}$	$\frac{16}{16}$	$\frac{16}{16}$

Table 24: The maximum prediction variance for the 2^5 factorial experiment with c HTC factors.

# of HTC Factors	Block Size	Parameters In the Model	Variance Multiplier				
			σ^2	σ_1^2	σ_2^2	σ_3^2	σ_4^2
2	(16, 8)	Main Effects	$\frac{6}{32}$	$\frac{32}{32}$	$\frac{24}{32}$		
		Main + 2 FI	$\frac{16}{32}$	$\frac{32}{32}$	$\frac{32}{32}$		
		Full Model	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{32}{32}$		
2	(8, 4)	Main Effects	$\frac{6}{32}$	$\frac{16}{32}$	$\frac{12}{32}$		
		Main + 2 FI	$\frac{16}{32}$	$\frac{16}{32}$	$\frac{16}{32}$		
		Full Model	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{32}{32}$		
2	(4, 2)	Main Effects	$\frac{6}{32}$	$\frac{8}{32}$	$\frac{6}{32}$		
		Main + 2 FI	$\frac{16}{32}$	$\frac{12}{32}$	$\frac{14}{32}$		
		Full Model	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{32}{32}$		
3	(16, 8, 4)	Main Effects	$\frac{6}{32}$	$\frac{32}{32}$	$\frac{24}{32}$	$\frac{16}{32}$	
		Main + 2 FI	$\frac{16}{32}$	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{28}{32}$	
		Full Model	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{32}{32}$	
3	(8, 4, 2)	Main Effects	$\frac{6}{32}$	$\frac{16}{32}$	$\frac{12}{32}$	$\frac{8}{32}$	
		Main + 2 FI	$\frac{16}{32}$	$\frac{24}{32}$	$\frac{20}{32}$	$\frac{16}{32}$	
		Full Model	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{32}{32}$	
4	(16, 8, 4, 2)	Main Effects	$\frac{6}{32}$	$\frac{32}{32}$	$\frac{24}{32}$	$\frac{16}{32}$	$\frac{10}{32}$
		Main + 2 FI	$\frac{16}{32}$	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{28}{32}$	$\frac{22}{32}$
		Full Model	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{32}{32}$	$\frac{32}{32}$

Table 25: The maximum prediction variance for the 2^6 factorial experiment with c HTC factors.

# of HTC Factors	Block Size	Parameters In the Model	Variance Multiplier					
			σ^2	σ_1^2	σ_2^2	σ_3^2	σ_4^2	σ_5^2
2	(32, 16)	Main Effects	$\frac{7}{64}$	$\frac{64}{64}$	$\frac{48}{64}$			
		Main + 2 FI	$\frac{22}{64}$	$\frac{64}{64}$	$\frac{64}{64}$			
		Full Model	$\frac{64}{64}$	$\frac{64}{64}$	$\frac{64}{64}$			
2	(16, 8)	Main Effects	$\frac{7}{64}$	$\frac{32}{64}$	$\frac{24}{64}$			
		Main + 2 FI	$\frac{22}{64}$	$\frac{32}{64}$	$\frac{32}{64}$			
		Full Model	$\frac{64}{64}$	$\frac{64}{64}$	$\frac{64}{64}$			
2	(8, 4)	Main Effects	$\frac{7}{64}$	$\frac{16}{64}$	$\frac{12}{64}$			
		Main + 2 FI	$\frac{22}{64}$	$\frac{24}{64}$	$\frac{20}{64}$			
		Full Model	$\frac{64}{64}$	$\frac{64}{64}$	$\frac{64}{64}$			
2	(4, 2)	Main Effects	$\frac{7}{64}$	$\frac{8}{64}$	$\frac{6}{64}$			
		Main + 2 FI	$\frac{22}{64}$	$\frac{32}{64}$	$\frac{20}{64}$			
		Full Model	$\frac{64}{64}$	$\frac{64}{64}$	$\frac{64}{64}$			
3	(32, 16, 8)	Main Effects	$\frac{7}{64}$	$\frac{64}{64}$	$\frac{48}{64}$	$\frac{32}{64}$		
		Main + 2 FI	$\frac{22}{64}$	$\frac{64}{64}$	$\frac{64}{64}$	$\frac{56}{64}$		
		Full Model	$\frac{64}{64}$	$\frac{64}{64}$	$\frac{64}{64}$	$\frac{64}{64}$		
3	(16, 8, 4)	Main Effects	$\frac{7}{64}$	$\frac{32}{64}$	$\frac{24}{64}$	$\frac{16}{64}$		
		Main + 2 FI	$\frac{22}{64}$	$\frac{32}{64}$	$\frac{32}{64}$	$\frac{28}{64}$		
		Full Model	$\frac{64}{64}$	$\frac{64}{64}$	$\frac{64}{64}$	$\frac{64}{64}$		

Table 25: The maximum prediction variance for the 2^6 factorial experiment with c HTC factors.

[illegible]

Table 26: The maximum prediction variance for the 2^7 factorial experiment with c HTC factors.

# of HTC Factors	Block Size	Parameters In the Model	Variance Multiplier						
			σ^2	σ_1^2	σ_2^2	σ_3^2	σ_4^2	σ_5^2	σ_6^2
2	(64, 32)	Main Effects	$\frac{8}{128}$	$\frac{128}{128}$	$\frac{96}{128}$				
		Main + 2 FI	$\frac{29}{128}$	$\frac{128}{128}$	$\frac{128}{128}$				
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$				
2	(32, 16)	Main Effects	$\frac{8}{128}$	$\frac{64}{128}$	$\frac{48}{128}$				
		Main + 2 FI	$\frac{29}{128}$	$\frac{128}{128}$	$\frac{64}{128}$				
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$				
2	(16, 8)	Main Effects	$\frac{8}{128}$	$\frac{32}{128}$	$\frac{24}{128}$				
		Main + 2 FI	$\frac{29}{128}$	$\frac{48}{128}$	$\frac{40}{128}$				
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$				
2	(8, 4)	Main Effects	$\frac{8}{128}$	$\frac{16}{128}$	$\frac{12}{128}$				
		Main + 2 FI	$\frac{29}{128}$	$\frac{32}{128}$	$\frac{24}{128}$				
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$				
2	(4, 2)	Main Effects	$\frac{8}{128}$	$\frac{8}{128}$	$\frac{6}{128}$				
		Main + 2 FI	$\frac{29}{128}$	$\frac{48}{128}$	$\frac{26}{128}$				
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$				

Table 26: The maximum prediction variance for the 2^7 factorial experiment with c HTC factors.

# of HTC Factors	Block Size	Parameters In the Model	Variance Multiplier						
			σ^2	σ_1^2	σ_2^2	σ_3^2	σ_4^2	σ_5^2	σ_6^2
3	(64, 32, 16)	Main Effects	$\frac{8}{128}$	$\frac{128}{128}$	$\frac{96}{128}$	$\frac{64}{128}$			
		Main + 2 FI	$\frac{29}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{112}{128}$			
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$			
3	(32, 16, 8)	Main Effects	$\frac{8}{128}$	$\frac{64}{128}$	$\frac{48}{128}$	$\frac{32}{128}$			
		Main + 2 FI	$\frac{29}{128}$	$\frac{128}{128}$	$\frac{64}{128}$	$\frac{56}{128}$			
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$			
3	(16, 8, 4)	Main Effects	$\frac{8}{128}$	$\frac{32}{128}$	$\frac{24}{128}$	$\frac{16}{128}$			
		Main + 2 FI	$\frac{29}{128}$	$\frac{48}{128}$	$\frac{40}{128}$	$\frac{32}{128}$			
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$			
3	(8, 4, 2)	Main Effects	$\frac{8}{128}$	$\frac{16}{128}$	$\frac{12}{128}$	$\frac{8}{128}$			
		Main + 2 FI	$\frac{29}{128}$	$\frac{64}{128}$	$\frac{40}{128}$	$\frac{26}{128}$			
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$			
4	(64, 32, 16, 8)	Main Effects	$\frac{8}{128}$	$\frac{128}{128}$	$\frac{96}{128}$	$\frac{64}{128}$	$\frac{40}{128}$		
		Main + 2 FI	$\frac{29}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{112}{128}$	$\frac{88}{128}$		
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$		

Table 26: The maximum prediction variance for the 2^7 factorial experiment with c HTC factors.

# HTC Factors	Block Size	Parameters In the Model	Variance Multiplier						
			σ^2	σ_1^2	σ_2^2	σ_3^2	σ_4^2	σ_5^2	σ_6^2
4	(32, 16, 8, 4)	Main Effects	$\frac{8}{128}$	$\frac{64}{128}$	$\frac{48}{128}$	$\frac{32}{128}$	$\frac{20}{128}$		
		Main + 2 FI	$\frac{29}{128}$	$\frac{64}{128}$	$\frac{64}{128}$	$\frac{56}{128}$	$\frac{44}{128}$		
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$		
4	(16, 8, 4, 2)	Main Effects	$\frac{8}{128}$	$\frac{32}{128}$	$\frac{24}{128}$	$\frac{16}{128}$	$\frac{10}{128}$		
		Main + 2 FI	$\frac{29}{128}$	$\frac{80}{128}$	$\frac{56}{128}$	$\frac{40}{128}$	$\frac{28}{128}$		
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$		
5	(64, 32, 16, 8, 4)	Main Effects	$\frac{8}{128}$	$\frac{128}{128}$	$\frac{96}{128}$	$\frac{64}{128}$	$\frac{40}{128}$	$\frac{24}{128}$	
		Main + 2 FI	$\frac{29}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{112}{128}$	$\frac{88}{128}$	$\frac{64}{128}$	
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	
5	(32, 16, 8, 4, 2)	Main Effects	$\frac{8}{128}$	$\frac{64}{128}$	$\frac{48}{128}$	$\frac{32}{128}$	$\frac{20}{128}$	$\frac{12}{128}$	
		Main + 2 FI	$\frac{29}{128}$	$\frac{96}{128}$	$\frac{80}{128}$	$\frac{64}{128}$	$\frac{48}{128}$	$\frac{34}{128}$	
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	
6	(64, 32, 16, 8, 4, 2)	Main Effects	$\frac{8}{128}$	$\frac{128}{128}$	$\frac{96}{128}$	$\frac{64}{128}$	$\frac{40}{128}$	$\frac{24}{128}$	$\frac{14}{128}$
		Main + 2 FI	$\frac{29}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{112}{128}$	$\frac{88}{128}$	$\frac{64}{128}$	$\frac{44}{128}$
		Full Model	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$	$\frac{128}{128}$

4.1.3 Choosing a Run Order for the 2^k Factorial Experiment

This section, will examine methods of choosing a run order when running a 2^k factorial experiment. Traditionally, a 2^k factorial experiment is recommended to be run with a completely random run order. This is optimal in theory, but is rarely practical or even possible in practice. In general, the driving force in industry behind choosing an experiment to run is cost. Cost can be associated with the expense of experimental units, runs, and the time involved with resetting HTC factors. In manufacturing situations time can easily be the most cost prohibitive part of an

experiment, therefore resetting HTC factors is usually not done. This section will narrowly define cost as the number of resets of the HTC factors. The cost of running 2^k factorial experiments will be examined in detail. The maximum prediction variance of 2^k factorial experiments will also be examined.

The number of resets of one HTC factor for various 2^k factorial experiments was examined in detail in Section 2.6. Those results will now be extended. Three types of run orders will be examined: completely randomized, randomized run order, and blocked. Let U_{CR} be the number of resets of the HTC factors for a given 2^k factorial experiment with a completely randomized run order, let U_R be the number of resets of the HTC factors for a given 2^k factorial experiment with a randomized run order, and let U_B be the number of resets of the HTC factors for a given 2^k factorial experiment with a blocked run order. The setup of a HTC factor at the beginning of an experiment is considered to be a reset.

For a completely randomized run order, each HTC factor must be reset 2^k times. Therefore, for a 2^k factorial experiment with c HTC factors, there will be $c \cdot 2^k$ resets of the HTC factors. That is, $U_{CR} = c \cdot 2^k$.

For a randomized run order, each HTC factor may be reset as few as 2 times, or as many as 2^k times. The $E[U_R]$, where the expectation is taken over all possible run orders, for a 2^k factorial experiment with one HTC factor is

$$E[U_R] = \frac{n}{2} + 1,$$

where $n = 2^k$ is the total number of runs. Therefore, for a 2^k factorial experiment with c HTC factors,

$$E[U_R] = \frac{cn}{2} + c = c \cdot 2^{k-1} + c.$$

For a run order with a blocking structure generated by the HTC factors, the number of resets of the HTC factors, U_B , will be equal to the number of blocks. For example, consider a 2^4 factorial experiment with 2 HTC factors and block size of (4, 2). There will be 4 blocks of size 4 created by HTC factor X_1 and 8 blocks of size 2 created by HTC factor X_2 . Therefore, $U_B = 12$.

Following are Tables 27 to 32, which give U_{CR} , U_R , and U_B for various 2^k factorial experiments with c HTC factors, $X_1, X_2, \dots, X_c$.

Table 27: The U_{CR} , U_R , and U_B values for the 2^2 factorial experiments with c HTC factors.

# of HTC Factors	U_{CR}	$E[U_R]$	Block Size	U_B
1	4	3	(2)	2
2	8	6	(2, 1)	6

Table 28: The U_{CR} , U_R , and U_B values for the 2^3 factorial experiments with c HTC factors.

# of HTC Factors	U_{CR}	$E[U_R]$	Block Size	U_B
1	8	5	(4)	2
			(2)	4
2	16	10	(4, 2)	6
3	24	15	(4, 2, 1)	14

Table 29: The U_{CR} , U_R , and U_B values for the 2^4 factorial experiments with c HTC factors.

# of HTC Factors	U_{CR}	$E[U_R]$	Block Size	U_B
1	16	9	(8)	2
			(4)	4
			(2)	8
2	32	18	(8, 4)	6
			(4, 2)	12
3	48	27	(8, 4, 2)	14
4	64	36	(8, 4, 2, 1)	30

Table 30: The U_{CR} , U_R , and U_B values for the 2^5 factorial experiments with c HTC factors.

# of HTC Factors	U_{CR}	$E[U_R]$	Block Size	U_B
1	32	17	(16)	2
			(8)	4
			(4)	8
			(2)	16
2	64	34	(16, 8)	6
			(8, 4)	12
			(4, 2)	24
3	96	51	(16, 8, 4)	14
			(8, 4, 2)	28
4	128	68	(16, 8, 4, 2)	30
5	160	85	(16, 8, 4, 2, 1)	62

Table 31: The U_{CR} , U_R , and U_B values for the 2^6 factorial experiments with c HTC factors.

# of HTC Factors	U_{CR}	$E[U_R]$	Block Size	U_B
1	64	33	(32)	2
			(16)	4
			(8)	8
			(4)	16
			(2)	32
2	128	66	(32, 16)	6
			(16, 8)	12
			(8, 4)	24
			(4, 2)	48
3	192	99	(32, 16, 8)	14
			(16, 8, 4)	28
			(8, 4, 2)	56
4	256	132	(32, 16, 8, 4)	30
			(16, 8, 4, 2)	60
5	320	165	(32, 16, 8, 4, 2)	62
6	384	198	(32, 16, 8, 4, 2, 1)	126

Table 32: The U_{CR} , U_R , and U_B values for the 2^7 factorial experiments with c HTC factors.

# of HTC Factors	U_{CR}	$E[U_R]$	Block Size	U_B
1	128	65	(64)	2
			(32)	4
			(16)	8
			(8)	16
			(4)	32
			(2)	64
2	256	130	(64, 32)	6
			(32, 16)	12
			(16, 8)	24
			(8, 4)	48
			(4, 2)	96
3	384	195	(64, 32, 16)	14
			(32, 16, 8)	28
			(16, 8, 4)	56
			(8, 4, 2)	112
4	512	260	(64, 32, 16, 8)	30
			(32, 16, 8, 4)	60
			(16, 8, 4, 2)	120
5	640	325	(64, 32, 16, 8, 4)	62
			(32, 16, 8, 4, 2)	124
6	768	390	(64, 32, 16, 8, 4, 2)	126
7	896	455	(64, 32, 16, 8, 4, 2, 1)	254

It is easy to see from the tables that a 2^k factorial experiment with blocks based on the HTC factors results in a run order that minimizes the number of resets. The least expensive experiment to run, in terms of the number of resets of the HTC factors, is the one with the largest blocks. However, if the maximum prediction variance is considered, the experiment with the largest blocks may not be the most desirable to run. For example, consider a 2^5 factorial experiment with 2 HTC factors, X_1 and X_2 . The following table displays the maximum prediction variance and cost of running a 2^5 factorial experiment where the experimenter is interested in fitting a model with all main effects and two-factor interactions. Completely randomized, randomized, and blocked run orders are considered.

Table 33: The maximum prediction variance and cost of running a 2^5 factorial experiment

Run Order	Variance Multiplier			Cost
	σ^2	σ_1^2	σ_2^2	
Completely Randomized	$\frac{16}{32}$	$\frac{16}{32}$	$\frac{16}{32}$	$U_{CR} = 64$
Randomized	$\frac{16}{32}$	$\frac{17.78}{32}$	$\frac{17.78}{32}$	$U_R = 34$
Block Size (16,8)	$\frac{16}{32}$	$\frac{32}{32}$	$\frac{32}{32}$	$U_B = 6$
Block Size (8,4)	$\frac{16}{32}$	$\frac{16}{32}$	$\frac{16}{32}$	$U_B = 12$
Block Size (4,2)	$\frac{16}{32}$	$\frac{12}{32}$	$\frac{14}{32}$	$U_B = 24$

According to this table, the experimenter could choose a blocked run order of block size (8,4) when running a 2^5 factorial experiment with 2 HTC factors. The blocked run order of block size (8,4) results in a low cost and a small maximum prediction variance in comparison to other run orders. The experimenter might also be inclined to choose a blocked run order of block size (4,2) because this blocked run order has lower cost than a randomized run order and has the smallest maximum prediction variance of all the designs listed.

4.1.4 The Most Cost Efficient Run Order for the 2^k Factorial Experiment - Extensions and Future Research

The properties of experiments with randomized run orders and experiments with run orders based on blocks created by the levels of the HTC factors have been examined. Another type of run order which can be useful when running experiments with all the factors being HTC is the one-at-a-time experiment. A one-at-a-time experiment is conducted by only changing the level of one factor from one run to the next. This results in run orders for experiments which are the most cost effective to run (in terms of resetting HTC factors).

For example, consider a 2^3 factorial experiment with 3 HTC factors. The expected number of resets of the 3 HTC factors for a randomized run order is 15 (see table 4.24). The number of resets of the 3 HTC factors for the blocking structure (4,2,1) is 14. The one-at-a-time experiment results in 8 resets of the 3 HTC factors. The one-at-a-time experiment is significantly cheaper to run than either the randomized run order experiment or the blocked experiment.

Extensive research has been done in the field of one-at-a-time experiments. For example, Tiahrt and Weeks [59] and Dickinson [14] examine various one-at-a-time 2^k factorial experiments. A second article by Tiahrt [58] examines various one-at-a-time 2^{k-p} factorial experiments.

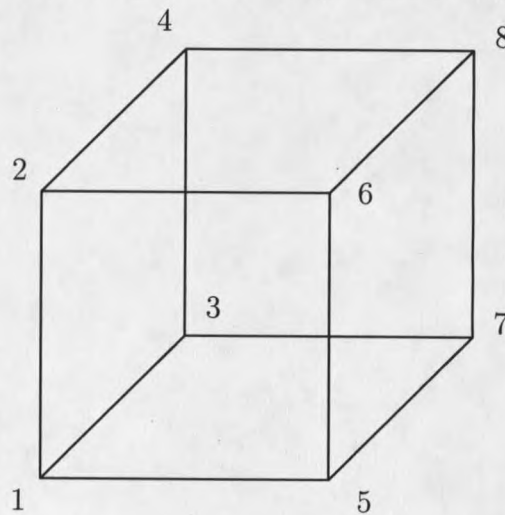
The 2^3 factorial experiment with all three factors being HTC will be used as an example to illustrate properties of one-at-a-time experiments. Notation will be developed to describe one-at-a-time run orders. The commonly used run order for

this experiment is:

run	X_1	X_2	X_3
1	-1	-1	-1
2	-1	-1	1
3	-1	1	-1
4	-1	1	1
5	1	-1	-1
6	1	-1	1
7	1	1	-1
8	1	1	1

The design space can be illustrated by Picture 4.1. Graph theory notation will be used to discuss the design space. For a good introduction to graph theory see Brualdi [11] or Liu [43].

4.1 The 2^3 Factorial Experiment Space



Picture 4.1 is called a *graph* and every point in Picture 4.1 is called a *vertex* and is numbered. The numbers correspond to the runs in the commonly used run order presented earlier. Therefore, vertex 1 corresponds to all 3 HTC factors being at their low level, vertex 2 corresponds to $X_1 = -1$, $X_2 = -1$, and $X_3 = 1$, and so on. All the lines connecting the vertices are called *edges*. Each edge connects two

runs which when occurring consecutively in an experiment result in only one change of one of the 3 HTC factors. For example, vertices 6 and 8 are connected by an edge. This implies that if runs 6 and 8 occur consecutively in an experiment, then the level of only one factor is changed. For this example, if the experimenter goes from run 6 to 8 then the level of factor X_2 is changed from low to high and the other 2 factors remain at the same level.

If the experimenter chooses a run order such as 1;2;4;3;7;5;6;8, then tracing this run order (with your pencil) through the graph results in visiting all the vertices exactly once via an edge. This tracing is called a *walk* and if the *walk* never covers an edge more than once it is called a *trail*. A trail that starts at one vertex and returns there after visiting every other vertex exactly once is called a *Hamilton cycle* and a trail that starts at one vertex and visits every other vertex (ending up somewhere) is called a *Hamilton chain*. Every Hamilton cycle is a special case of a Hamilton chain. Every one-at-a-time experiment can be expressed as a Hamilton chain given the respective graph. The run order 1;2;4;3;7;5;6;8 is an example of a one-at-a-time experiment and can be written as:

run	X_1	X_2	X_3
1	-1	-1	-1
2	-1	-1	1
4	-1	1	1
3	-1	1	-1
7	1	1	-1
5	1	-1	-1
6	1	-1	1
8	1	1	1

For sake of argument, consider an 2^3 factorial experiment that always starts at run 1. Then, there are 18 possible Hamilton chains (one-at-a-time experiments). Given that there are 8 different runs at which the experiment may begin, there are

$18 \times 8 = 144$ Hamilton chains for the 2^3 factorial experiment. The Hamilton chains beginning at vertex 1 are presented in Table 34. Along with the run order of each Hamilton chain are columns which list the number of changes made to each HTC factor. Note that the initial setup could be considered as a change to each HTC factor from a cost perspective, but the initial setup is not included in this table.

Table 34: The Hamilton chains beginning at vertex 1 for the 2^3 factorial experiment.

Run Order	X_1	X_2	X_3
1; 2; 6; 5; 7; 3; 4; 8	3	1	3
1; 2; 6; 5; 7; 8; 4; 3	2	1	4
1; 2; 6; 8; 4; 3; 7; 5	3	2	2
1; 2; 4; 8; 6; 5; 7; 3	2	3	2
1; 2; 4; 3; 7; 5; 6; 8	1	3	3
1; 2; 4; 3; 7; 8; 6; 5	1	2	4
1; 5; 6; 2; 4; 3; 7; 8	3	1	3
1; 5; 6; 2; 4; 8; 7; 3	4	1	2
1; 5; 6; 8; 7; 3; 4; 2	2	2	3
1; 5; 7; 3; 4; 2; 6; 8	3	3	2
1; 5; 7; 3; 4; 8; 6; 2	4	2	1
1; 5; 7; 8; 6; 2; 4; 3	2	3	2
1; 3; 4; 2; 6; 5; 7; 8	1	3	3
1; 3; 4; 2; 6; 8; 7; 5	1	4	2
1; 3; 4; 8; 7; 5; 6; 2	2	2	3
1; 3; 7; 5; 6; 2; 4; 8	3	3	1
1; 3; 7; 5; 6; 8; 4; 2	2	4	1
1; 3; 7; 8; 4; 2; 6; 5	3	2	2

Tiahrt [59] [58] also lists Hamilton chains for various 2^{k-p} factorial designs and recommends these one-at-a-time experiments for situations when experimental situations dictate the use of very restricted randomized run orders.

Table 4.30 illustrates that an experimenter may want to choose one Hamilton chain over another. For example, the run order 1;2;6;5;7;3;4;8 results in 4 changes of factor X_1 , 1 change of factor X_2 , and 3 changes of factor X_3 . Therefore, if the experimenter knows that factor X_2 is more costly, or harder, to change than the other two factors, the experimenter may choose this design over the others. Tiahrt makes no distinction between the different Hamilton chains and offers no analysis based on choosing one particular design.

The one-at-a-time factorial experiment offers the experimenter an extremely cheap design to implement, but not without a price in the precision of estimation of coefficients in the model. The exact penalty for running an experiment of this type is currently not known. Future areas of research include the following:

1. Combinatorial results which give the total number of Hamilton cycles and chains for various 2^k and 2^{k-p} factorial experiments.
2. The correct analysis of such one-at-a-time factorial experiments when a particular Hamilton chain is chosen.
3. Comparisons between completely randomized run orders, randomized run orders, blocked run orders based on the levels of HTC factors, and one-at-a-time run orders. These comparisons can be made using appropriate metrics such as cost to run the experiment defined by the number of resets of HTC factors, and the maximum prediction variance $\hat{y}$.

Chapter 5

RESPONSE SURFACE DESIGNS

Response surface designs are extensively used in industry to characterize and optimize processes. Both Ju [32] and Anbari [1] examine response surface designs with one HTC factor. Response surface designs with randomized run orders and run orders with blocking structures based upon the HTC factor were considered. A general approach to handling response surface designs with c HTC factors, randomized run orders, and run orders with blocking structure based on the HTC factors will be presented in this chapter.

The relationship between the response, y , and the levels of the factors, X_i (where the factors are quantitative), can be expressed as follows:

$$y_u = \Phi(X_{1u}, X_{2u}, \dots, X_{ku})$$

where

y_u = the response at the u^{th} observation,

$u = 1, 2, \dots, n$ where n is the size of the design, or the number of runs in the experiment,

Φ = is the response surface function,

X_{iu} = the level of the i^{th} factor, $1 \leq i \leq k$, at the u^{th} observation.

This notation is very similar to that given by Cochran and Cox [12]. It has been altered slightly to be consistent with notation previously used in this dissertation.

Typically, Φ is an unknown function and the response surface is approximated by the response surface model

$$y_u = f(X_{1u}, X_{2u}, \dots, X_{ku}) + \epsilon_u$$

where the assumptions of $E[\epsilon_u] = 0$ and $\text{Var}[\epsilon_u] = \sigma^2 \forall u$ are made (Myers and Montgomery [50]). The function, f , can be most any function, but is typically a first or second order polynomial in $X_1, X_2, \dots, X_k$. This chapter will focus on second order models and will consider two of the most commonly used second order designs in industry, the central composite design (Box and Wilson [9]) and the Box-Behnken design (Box and Behnken [10]).

The model for a second order response surface design with no HTC factors can be written in matrix form as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}.$$

For response surface designs with one HTC factor, the model can be written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \boldsymbol{\epsilon}.$$

These models have the same form as those presented in Chapter 2 for L^k factorial experiments with one HTC factor. The $\mathbf{X}$ matrix is the standard design matrix which is described in Chapters 2 and 3. The $\mathbf{Z}$ matrix is a design matrix for the random effects in the model due HTC factor X_1 . This $\mathbf{Z}$ matrix will have the same structure as those in Chapter 2, which are dependent upon the structure of the standard design matrix $\mathbf{X}$.

5.1 The Expected Variance-Covariance Matrix for One HTC Factor

In Ju [32] a theorem was presented which gave the expected-variance covariance matrix of $\mathbf{y}$ for a second order response surface design with one HTC factor having L levels. That theorem will be presented here as it was in Ju and also in the notational form of Chapters 2 and 3 so that the results can easily be generalized to second order response surface designs with c HTC factors.

Theorem 5.1 *The expected variance-covariance matrix $V_E = E[\text{Var}(\mathbf{y})]$ of a second order response surface model with k factors, a randomized run order, and X_1 being a hard-to-change factor is*

$$V_E = \sigma^2 I_n + \sigma_1^2 V_2$$

where:

$$V_2 = \begin{bmatrix} V_{21} & & 0 \\ & V_{22} & \\ 0 & & V_{2L} \end{bmatrix}_{n \times n}$$

and $n = \sum_{i=1}^L n_i$ where n_i is the number of runs when the HTC factor, X_1 , is at level i , $1 \leq i \leq L$, and:

$$V_{2i} = \begin{bmatrix} 1 & p_i & \cdots & p_i \\ p_i & 1 & \cdots & p_i \\ \vdots & \vdots & \ddots & \vdots \\ p_i & \cdots & p_i & 1 \end{bmatrix}_{n_i \times n_i}$$

where:

$$p_i = \frac{2(n_i - 2)!}{n!} \sum_{r=0}^{n_i-2} \frac{(n - r - 1)!}{(n_i - r - 2)!}$$

The above theorem will now be presented using notation from Chapters 2 and 3.

Theorem 5.2 *The expected variance-covariance matrix $V_E = E[\text{Var}(\mathbf{y})]$ of a second order response surface model with k factors, a randomized run order, and X_1 being a hard-to-change factor is*

$$V_E = \sigma^2 I_n + \sigma_1^2 W_1 + \sigma_1^2 Z_1 Z_1'$$

where the expectation is taken with respect to the distribution of possible $Z Z'$ matrices and $n = \sum_{i=1}^U n_i$ where n_i is the number of runs when the HTC factor, X_1 , is at level i given the run order in the standard design matrix X , U is the number of runs (or blocks) the HTC factor creates, and:

$$W_1 = \bigoplus_{i=1}^L [(1 - p_i) I_{n_i}]$$

and:

$$\mathbf{Z}_1 = \begin{bmatrix} \sqrt{p_1} \mathbf{J}_1 & & 0 \\ & \sqrt{p_2} \mathbf{J}_2 & \\ & & \ddots \\ 0 & & & \sqrt{p_L} \mathbf{J}_L \end{bmatrix}_{n \times L}, \quad \mathbf{J}_i = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}_{n_i \times 1},$$

and

$$p_i = \frac{2(n_i - 2)!}{n!} \sum_{r=0}^{n_i-2} \frac{(n - r - 1)!}{(n_i - r - 2)!}.$$

Notice that the difference between Theorem 5.2 and Theorem 2.1 is that there is a different p_i for each block of the block diagonal matrix $\mathbf{Z}_1 \mathbf{Z}'_1$. In Theorem 2.1 there was only one p for all the blocks in $\mathbf{Z}_1 \mathbf{Z}'_1$. To incorporate this difference into the equation for $\mathbf{V}_E$, the coefficients, p_i , are brought into the structure of $\mathbf{Z}_1 \mathbf{Z}'_1$. This difference is also the reason for the matrix $\mathbf{W}_1$. Both of the matrices, $\mathbf{Z}_1 \mathbf{Z}'_1$ and $\mathbf{W}_1$, are standard design matrices. Standard design matrices were introduced in Chapter 3 and their structures are completely dependent on the structure of the design matrix $\mathbf{X}$. The general form of $\mathbf{X}$ will be described through the following example.

The following example will help illustrate Theorem 5.2 using the notation of Chapters 2 and 3. Consider a central composite design (CCD) with three factors: X_1 , X_2 , and X_3 , where X_1 is HTC. For simplicity, consider a non-rotatable face-centered

cube design with 2 center points. The standard form of the design matrix, $\mathbf{X}$, is

$$\mathbf{X} = \begin{array}{c|cccc} \begin{array}{l} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \end{array} & \begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & 0 & -1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

There are many possible ways to describe the design matrix for a face-centered cube design. For this Thesis, the standard form of the design matrix, $\mathbf{X}$, for a face-centered cube design will first have the 2^{k-1} factorial points listed with X_1 at its low level, followed by two star points corresponding to X_1 at its low and high levels, respectively, then the 2^{k-1} factorial points listed with X_1 at its high level, followed by the remaining $2k - 2$ star points with X_1 at its intermediate level, and concluding with the center points.

For this example, there are three levels of the HTC factor: -1 , 0 , and 1 . Due to the structure of the standard design matrix, $\mathbf{X}$, there are three blocks formed by the HTC factor X_1 . Therefore, $U = 3$ and $n_1 = 5$, $n_2 = 5$, and $n_3 = 6$. There are 16 runs, so $n = 16$. Notice that if X_2 were the HTC factor instead of X_1 , then $U = 8$

and $n_1 = 2$, $n_2 = 2$, $n_3 = 2$, $n_4 = 2$, $n_5 = 2$, $n_6 = 1$, $n_7 = 1$, and $n_8 = 4$. The values of the p_i are: $p_1 = \frac{2}{13} \approx .1538$, $p_2 = \frac{2}{13} \approx .1538$, and $p_3 = \frac{2}{12} \approx .1667$. The standard design matrix, W_1 , has the form:

[illegible]

and the standard form of the design matrix $Z_1 Z_1'$ is

$$Z_1 Z_1' = \begin{bmatrix} \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & \frac{2}{13} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} & \frac{2}{12} \end{bmatrix}$$

5.2 The Expected Variance-Covariance Matrix for c HTC Factors

The theorems and justifications presented here are very similar to Theorems 3.1 and 3.2. The main differences are that there is a different p_i for each block of the block diagonal matrix $Z_i Z_i'$ and that there is no closed form expression for the permutation matrices, P_i , because of the myriad of possible response surface designs.

Theorem 5.3 *The expected variance-covariance matrix $V_E = E[\text{Var}(\mathbf{y})]$ of a second order response surface model with k factors, a randomized run order, and one hard-to-change factor X_i , where $1 \leq i \leq k$, is*

$$V_E = \sigma^2 I_n + \sigma_i^2 W_i + \sigma_i^2 Z_i Z_i'$$

where the expectation is taken with respect to the discrete uniform distribution of possible $\mathbf{Z}\mathbf{Z}'$ matrices, $\mathbf{Z}_i$ and $\mathbf{W}_i$ are the standard form design matrices for the HTC factor as described in Sections 3.1 and 5.1, and

$$p_i = \frac{2(n_i - 2)!}{n!} \sum_{r=0}^{n_i-2} \frac{(n - r - 1)!}{(n_i - r - 2)!}.$$

Proof: If $i = 1$ then apply Theorem 5.2 directly. If $2 \leq i \leq k$ then the experimental model is

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}^*\mathbf{u} + \boldsymbol{\epsilon},$$

where $\mathbf{Z}^*$ is a random effects design matrix corresponding to the blocks formed by the HTC factor X_i . Premultiply the model with permutation matrix $\mathbf{P}_i$ (Section 3.2) which reorders the rows of the design matrix $\mathbf{X}$ in such a way as to give the column corresponding to X_i the same form as the column corresponding to X_1 in the standard $\mathbf{X}$ design matrix. This also has the effect of reordering the rows of $\mathbf{Z}^*$ such that $\mathbf{P}_i\mathbf{Z}^* = \mathbf{Z}$, where $\mathbf{Z}$ has the form of the $\mathbf{Z}$ matrix in Chapter 2 when X_1 was the HTC factor. The transformed model is

$$\mathbf{P}_i\mathbf{y} = \mathbf{P}_i\mathbf{X}\boldsymbol{\beta} + \mathbf{P}_i\mathbf{Z}^*\mathbf{u} + \mathbf{P}_i\boldsymbol{\epsilon} = \mathbf{X}^*\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \boldsymbol{\epsilon}^*.$$

This transformed model matches the form of the model in Chapter 5, except for the fact that the columns of the design matrix $\mathbf{X}$ are in a different order. Apply Theorem 5.2 to the transformed model. The expected variance-covariance matrix is

$$\mathbf{V}_E = \sigma^2\mathbf{I}_n + \sigma_i^2\mathbf{W}_1 + \sigma_i^2\mathbf{Z}_1\mathbf{Z}_1'$$

where p_i is as stated in Theorem 5.2 and $\mathbf{Z}_1$ and $\mathbf{W}_1$ have the standard form stated in Theorem 5.2. The expectation in Theorem 5.2 is with respect to the discrete uniform distribution of $\mathbf{Z}\mathbf{Z}'$ matrices. So, transforming back to the original $\mathbf{Z}^*\mathbf{Z}^{*'}$ matrices and using the fact that $\mathbf{P}_i$ is orthogonal [54] and $\mathbf{Z}_1 = \mathbf{P}_i\mathbf{Z}_i$,

$$\begin{aligned} \mathbf{Z}_1\mathbf{Z}_1' &= \mathbf{E}[\mathbf{Z}\mathbf{Z}'] \\ &= \mathbf{E}[\mathbf{P}_i\mathbf{Z}^*\mathbf{Z}^{*'}\mathbf{P}_i'] \\ &= \mathbf{P}_i\mathbf{E}[\mathbf{Z}^*\mathbf{Z}^{*'}]\mathbf{P}_i'. \end{aligned}$$

Thus,

$$P_i' Z_1 Z_1' P_i = P_i' P_i E[Z^* Z^{*'}] P_i' P_i,$$

implying

$$Z_i Z_i' = E[Z^* Z^{*'}].$$

Also, under the original model, $W_1 = P_i W_i$, therefore, $P_i' W_1 = W_i$. Thus, under the original model,

$$V_E = \sigma^2 I_n + \sigma_i^2 W_i + \sigma_i^2 Z_i Z_i'$$

proving the theorem. ◻

To illustrate the notation of Theorem 5.3, consider the central composite design (CCD) which was used to illustrate Theorem 5.2. There are three factors: X_1 , X_2 , and X_3 , and for this example, let X_2 be HTC. Therefore, $U = 8$ and $n_1 = 2$, $n_2 = 2$, $n_3 = 2$, $n_4 = 2$, $n_5 = 2$, $n_6 = 1$, $n_7 = 1$, and $n_8 = 4$. There are 16 runs, so $n = 16$. The values of the p_i remain the same as the previous example and are: $p_1 = \frac{2}{13} \approx .1538$, $p_2 = \frac{2}{13} \approx .1538$, and $p_3 = \frac{2}{12} \approx .1667$. The standard design matrix, W_2 , has the

[illegible]

and the standard form of the design matrix $Z_2 Z_2'$ is

[illegible]

For this example, the permutation matrix P_2 has the form:

$$P_2 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

This permutation matrix switches rows 3,4 with 7,8 and switches rows 5,6 with 11,12. Premultiplying the Standard design matrix $\mathbf{X}$ for this design with this permutation matrix results in reordering the rows such that the column corresponding to X_2 will have the structure the column corresponding to X_1 had prior to premultiplying by P_2 .

Theorem 5.4 *The expected variance-covariance matrix $V_E = E[\text{Var}(\mathbf{y})]$ of second order response surface model with k factors, randomized run order, and c hard-to-change factors, $X_1, X_2, \dots, X_c$, where $1 \leq c \leq k$, is*

$$V_E = \sigma^2 \mathbf{I}_n + \sum_{i=1}^c \sigma_i^2 \mathbf{W}_i + \sum_{i=1}^c \sigma_i^2 \mathbf{Z}_i \mathbf{Z}_i'$$

where the expectation is taken with respect to the discrete uniform distribution of possible $\mathbf{Z}\mathbf{Z}'$ matrices, $\mathbf{Z}_i$ and $\mathbf{W}_i$ are the standard form design matrices for the HTC factor as described in Sections 3.1 and 5.1, and

$$p_i = \frac{2(n_i - 2)!}{n!} \sum_{r=0}^{n_i-2} \frac{(n - r - 1)!}{(n_i - r - 2)!}.$$

Proof: If $c = 1$ then apply Theorem 5.2 directly. If $2 \leq c \leq k$ then the experimental model is

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}_1^* \mathbf{u}_1 + \mathbf{Z}_2^* \mathbf{u}_2 + \cdots + \mathbf{Z}_c^* \mathbf{u}_c + \boldsymbol{\epsilon},$$

where $\mathbf{Z}_i^*$ is a random effects design matrix corresponding to the blocks formed by the HTC factor X_i for $1 \leq i \leq c$. Now, calculate the variance of $\mathbf{y}$ with the typical mixed model distributional assumptions

$$\begin{aligned} \mathbf{E}[\mathbf{u}_i] &= \mathbf{0} \quad \forall i \\ \text{Var}[\mathbf{u}_i] &= \sigma_i^2 \mathbf{I}_{q_i} \\ \text{Cov}[\mathbf{u}_i, \mathbf{u}_j] &= \mathbf{0} \quad \forall i \neq j \\ \mathbf{E}[\boldsymbol{\epsilon}] &= \mathbf{0} \\ \text{Var}[\boldsymbol{\epsilon}] &= \sigma^2 \mathbf{I}_n \\ \text{Cov}[\mathbf{u}_i, \boldsymbol{\epsilon}] &= \mathbf{0} \quad \forall i, \end{aligned}$$

$$\text{Var}[\mathbf{y}] = \sigma_1^2 \mathbf{Z}_1^* \mathbf{Z}_1^{*'} + \sigma_2^2 \mathbf{Z}_2^* \mathbf{Z}_2^{*'} + \cdots + \sigma_c^2 \mathbf{Z}_c^* \mathbf{Z}_c^{*'} + \sigma^2 \mathbf{I}_n.$$

Because it is a linear operator, the expectation of the variance is

$$\mathbf{E}[\text{Var}[\mathbf{y}]] = \sigma_1^2 \mathbf{E}[\mathbf{Z}_1^* \mathbf{Z}_1^{*'}] + \sigma_2^2 \mathbf{E}[\mathbf{Z}_2^* \mathbf{Z}_2^{*'}] + \cdots + \sigma_c^2 \mathbf{E}[\mathbf{Z}_c^* \mathbf{Z}_c^{*'}] + \sigma^2 \mathbf{I}_n.$$

Application of Theorem 5.3 yields,

$$\mathbf{V}_E = \sigma^2 \mathbf{I}_n + \sum_{i=1}^c \sigma_i^2 \mathbf{W}_i + \sum_{i=1}^c \sigma_i^2 \mathbf{Z}_i \mathbf{Z}_i'.$$

5.3 Blocking With the Central Composite Design

This section will examine blocking structures for central composite designs (CCDs) based on orthogonal blocking, where the CCD contains HTC factors. A CCD is a 2^k factorial or a 2^{k-p} fractional factorial combined with $2k$ axial points or star points and some number of center points [50]:

X_1	X_2	$\dots$	X_k
$-\alpha$	0	$\dots$	0
α	0	$\dots$	0
0	$-\alpha$	$\dots$	0
0	α	$\dots$	0
0	0	$\dots$	$-\alpha$
0	0	$\dots$	α
0	0	$\dots$	0

The value of α is frequently chosen such that $\alpha = 1$ which yields a face-centered cube design or α is chosen such that the design is rotatable. A rotatable design has constant

$$\frac{n \cdot \text{VAR}[\hat{y}(\mathbf{x})]}{\sigma^2}$$

for all points $\mathbf{x}$ equidistant from the center of the design space.

A CCD can have many runs and, therefore, take a long time to complete. Carrying out the experiment under constant conditions (same day, same batch of material, same operator, etc...) may be difficult. Therefore, blocking of the CCD into homogeneous batches of runs is often employed.

A desirable method of blocking is that of orthogonal blocking. Simply stated, orthogonal blocking implies that the block effects are orthogonal to model coefficients [50]. Therefore, estimation of the model coefficients is not affected by the presence of blocks.

Myers and Montgomery [50] present the following requirements for orthogonal blocking in second order designs. They state that blocking effects are orthogonal to regression coefficients if:

1. Each block itself is a first-order orthogonal design.
2. For each design variable, the sum of squares contribution from each block is proportional to the block size.

Many CCDs can have orthogonal blocking structures. Condition 1 above holds if factorial points are blocked such that the blocks, linear coefficients, and two-factor interactions are all orthogonal and star points are placed in their own block. Condition 2 above holds if the number of center points, their position in existing blocks and the α value are chosen with care. Quite often the value of α which results in orthogonal blocking is the same (or very close to) the value of α which results in rotatability of the design.

Blocking structures for CCDs with HTC factors will now be recommended. The recommended designs presented here differ from the ones presented in Ju [32] in that Ju presents designs which limit the number of changes of a HTC factor. Those designs do not create orthogonal blocking structures. The designs presented here will limit the number of changes of the HTC factors and preserve the orthogonal blocking structure.

As an example, consider a four factor CCD. Initially, consider all factors to be ETC. The four factor CCD can be blocked orthogonally and be rotatable. The design matrix with main effects only is as follows:

Run	X_1	X_2	X_3	X_4	Block
1	-1	-1	-1	-1	1
2	-1	-1	1	1	1
3	-1	1	-1	1	1
4	-1	1	1	-1	1
5	1	-1	-1	1	1
6	1	-1	1	-1	1
7	1	1	-1	-1	1
8	1	1	1	1	1
9 - 10	0	0	0	0	1
11	-1	-1	-1	1	2
12	-1	-1	1	-1	2
13	-1	1	-1	-1	2
14	-1	1	1	1	2
15	1	-1	-1	-1	2
16	1	-1	1	1	2
17	1	1	-1	1	2
18	1	1	1	-1	2
19 - 20	0	0	0	0	2
21	2	0	0	0	3
22	-2	0	0	0	3
23	0	2	0	0	3
24	0	-2	0	0	3
25	0	0	2	0	3
26	0	0	-2	0	3
27	0	0	0	2	3
28	0	0	0	-2	3
29 - 30	0	0	0	0	3

where the vector, 0 0 0 0, corresponds to two runs at the center of the design space.

The defining relationship for blocks 1 and 2 is $I = ABCD$. The value of α in block 3 for which the blocks are orthogonal and the design is rotatable is $\alpha = 2$. There are three blocks as indicated by the column labeled *Block* and also by the horizontal lines. Each block is of size 10 and contains 2 center points. The run order of this experiment would then be randomized within each block.

Now, consider the above CCD with X_1 being HTC. Within the two orthogonal blocks containing the 2^4 design, blocking structures from Chapter 4 can be used. Due to the orthogonal blocking structure, 2 blocks of size 8 for the HTC factor is not possible. Examining Table 4.5 also reveals that this is not the optimal size for blocks for a 2^4 factorial experiment with a HTC factor. The optimal size for blocks is 4. That implies that there need to be 4 blocks. This is easily accomplished within the confines of orthogonal blocking by using the confounding relation $I = A = ABCD = BCD$. Therefore, a recommended blocking structure for a CCD with 4 factors and 1 HTC factor is:

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
9 - 10	0	0	0	0
11	0	0	0	0
12	0	0	2	0
13	0	0	-2	0
14	0	2	0	0
15	2	0	0	0
16	-2	0	0	0
17	0	-2	0	0
18	0	0	0	2
19	0	0	0	-2
20	0	0	0	0
21 - 22	0	0	0	0
23	-1	-1	-1	1
24	-1	-1	1	-1
25	-1	1	-1	-1
26	-1	1	1	1
27	1	-1	-1	-1
28	1	-1	1	1
29	1	1	-1	1
30	1	1	1	-1

where the vector, $0\ 0\ 0\ 0$, corresponds to two runs at the center of the design space. The short horizontal lines indicate the blocks formed by HTC factor X_1 and the long horizontal lines indicate the orthogonal blocks. This design results in 8 resets of the HTC factor X_1 assuming X_1 is not reset between blocks. If X_1 is reset between blocks then this design results in 10 resets of the HTC factor. Factor X_1 may be reset between blocks even if it is kept at the same level from run to run between blocks. This is because blocks are typically run on different days or other time periods. Therefore there will be an initial setup (reset) of X_1 at the beginning of each block. A randomized run order, on average, results in 21.87 resets of the HTC factor X_1 assuming X_1 is not reset between blocks. If X_1 is reset between blocks, then a randomized run order, on average, results in at least 21.87 resets of the HTC factor. Finding the exact average number of resets for a randomized run order is a combinatorial problem for future research. The result of 21.87 resets is a direct application of the formula

$$E[U] = \frac{n(n+1) - \sum_{i=1}^k n_i^2}{n}$$

from chapter 2 where U is the number of resets of the HTC factor, n is the number of runs, and n_i is the number of runs with the HTC factor at level i .

Now, consider the previous example with X_1 and X_2 being HTC factors. The optimal confounding relation from Chapter 4 for a 2^4 factorial experiment with X_1 having 4 blocks of size 4 and X_2 having 8 blocks of size 2 is $I = A = B = CD = AB = ACD = BCD = ABCD$. Therefore, a recommended blocking structure for a CCD with 4 factors and 2 HTC factors, X_1 and X_2 , is:

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
9 - 10	0	0	0	0
11	0	0	0	0
12	0	0	2	0
13	0	0	-2	0
14	0	2	0	0
15	2	0	0	0
16	-2	0	0	0
17	0	-2	0	0
18	0	0	0	2
19	0	0	0	-2
20	0	0	0	0
21 - 22	0	0	0	0
23	-1	-1	-1	1
24	-1	-1	1	-1
25	-1	1	-1	-1
26	-1	1	1	1
27	1	-1	-1	-1
28	1	-1	1	1
29	1	1	-1	1
30	1	1	1	-1

where the vector, $0\ 0\ 0\ 0$, corresponds to two runs at the center of the design space. The short horizontal lines indicate the blocks formed by HTC factors X_1 and X_2 , the long horizontal lines indicate the orthogonal blocks. This design results in 8 resets of HTC factor X_1 and 13 resets of HTC factor X_2 assuming that X_1 and X_2 are not reset between blocks. If X_1 and X_2 are reset between blocks then this design results in 10 resets of X_1 and 15 resets of X_2 . A randomized run order would, on average, results in 43.74 resets of the HTC factors X_1 and X_2 assuming X_1 and X_2 are not reset between blocks. Just as the previous example, if X_1 and X_2 are reset between blocks, then a randomized run order, on average, results in at least 43.74 resets of the HTC factors.

5.4 Blocking With the Box-Behnken Design

This section will examine blocking structures for Box Behnken designs (BBDs) based on orthogonal blocking, where the BBD contains HTC factors. Box Behnken designs were proposed by Box and Behnken [10] in 1960. They are three level designs for fitting second-order response surfaces. The structure of a BBD is quite simple and relies on the construction of balanced incomplete block designs. For example, consider the BBD in Myers and Montgomery [50] created from a balanced incomplete block design. There are three factors, X_1 , X_2 , and X_3 , and three blocks. The structure of the balanced incomplete block design is:

	X_1	X_2	X_3
Block1	×	×	
Block2	×		×
Block3		×	×

The BBD is then created by having 4 runs for the first block where X_1 and X_2 take on the levels of a 2^2 design and $X_3 = 0$. There are 4 runs for the second block, but this time X_1 and X_3 take on the levels of a 2^2 factorial design and $X_2 = 0$. This same

method is used for the third block, and then the design is augmented with n_c center points. The design matrix for this example is:

X_1	X_2	X_3
-1	-1	0
-1	1	0
1	-1	0
1	1	0
-1	0	-1
-1	0	1
1	0	-1
1	0	1
0	-1	-1
0	-1	1
0	1	-1
0	1	1
0	0	0

The BBD is similar in size to the CCD. For example, a CCD with $k = 3$ factors contains $14 + n_c$ design points and a BBD with 3 factors contains $12 + n_c$ design points. The BBD can also be blocked orthogonally, for certain values of k , just like the CCDs.

Blocking structures for BBDs with HTC factors will now be recommended. The designs will limit the number of changes of the HTC factors and preserve the orthogonal blocking structure. The recommended designs presented here differ slightly from the ones presented in Ju [32]. An example will help illustrate the recommended blocking structures and also point out the differences between the blocking structures presented here and the blocking structures presented in Ju.

Consider a four factor BBD. Initially, consider all factors to be ETC. The four factor BBD can be blocked orthogonally. The design matrix with main effects only

is:

Run	X_1	X_2	X_3	X_4	Block
1	-1	-1	0	0	1
2	-1	1	0	0	1
3	1	-1	0	0	1
4	1	1	0	0	1
5	0	0	-1	-1	1
6	0	0	-1	1	1
7	0	0	1	-1	1
8	0	0	1	1	1
9 - 10	0	0	0	0	1
11	-1	0	0	-1	2
12	-1	0	0	1	2
13	1	0	0	-1	2
14	1	0	0	1	2
15	0	-1	-1	0	2
16	0	-1	1	0	2
17	0	1	-1	0	2
18	0	1	1	0	2
19 - 20	0	0	0	0	2
21	-1	0	-1	0	3
22	-1	0	1	0	3
23	1	0	-1	0	3
24	1	0	1	0	3
25	0	-1	0	-1	3
26	0	-1	0	1	3
27	0	1	0	-1	3
28	0	1	0	1	3
29 - 30	0	0	0	0	3

where the vector, $0\ 0\ 0\ 0$, corresponds to two runs at the center of the design space. There are three orthogonal blocks as indicated by the column labeled *Block* and are separated by the horizontal lines. Each block is size 10 and contains 2 center points. The run order of this experiment would then be randomized within each block.

Now, consider the above BBD with X_1 being HTC. Within the three orthogonal blocks, various blocking structures based on the levels of X_1 can be used. The blocking structure recommended by Ju [32] is:

Run	X_1	X_2	X_3	X_4	Block
1	-1	-1	0	0	1
2	-1	1	0	0	1
3	0	0	0	0	2
4	0	0	1	1	2
5	0	0	1	-1	2
6	0	0	-1	-1	2
7	0	0	0	0	2
8	0	0	-1	1	2
9	1	-1	0	0	3
10	1	1	0	0	3
11	-1	0	0	-1	4
12	-1	0	0	1	4
13 - 14	0	0	0	0	5
15	0	-1	1	0	5
16	0	1	1	0	5
17	0	1	-1	0	5
18	0	-1	-1	0	5
19	1	0	0	1	6
20	1	0	0	-1	6
21	-1	0	-1	0	7
22	-1	0	1	0	7
23	0	0	0	0	8
24	0	1	0	1	8
25	0	0	0	0	8
26	0	-1	0	-1	8
27	0	1	0	-1	8
28	0	-1	0	1	8
29	1	0	0	0	9
30	1	0	-1	0	9

where the vector, $0\ 0\ 0\ 0$, corresponds to two runs at the center of the design space. The short horizontal lines indicate the blocks formed by HTC factor X_1 and the long horizontal lines indicate the orthogonal blocks. This design results in 9 resets of the HTC factor X_1 , which includes the original setup. A randomized run order would, on average, results in 17.8 resets of the HTC factor X_1 .

Now, consider the same BBD with X_1 being HTC. A somewhat different blocking structure will now be recommended. This blocking structure also results in 9 resets of the HTC factor X_1 . The difference is that this blocking structure can also be used for a BBD with $k = 4$ and c HTC factors, where $1 \leq c \leq 4$. The blocking structure is:

Run	X_1	X_2	X_3	X_4	Block
1	-1	-1	0	0	1
2	-1	1	0	0	1
3	1	-1	0	0	2
4	1	1	0	0	2
5	0	0	-1	-1	3
6	0	0	-1	1	3
7	0	0	1	-1	3
8	0	0	1	1	3
9 - 10	0	0	0	0	3
11	-1	0	0	-1	4
12	-1	0	0	1	4
13	1	0	0	-1	5
14	1	0	0	1	5
15	0	-1	-1	0	6
16	0	-1	1	0	6
17	0	1	-1	0	6
18	0	1	1	0	6
19 - 20	0	0	0	0	6
21	-1	0	-1	0	7
22	-1	0	1	0	7
23	1	0	-1	0	8
24	1	0	1	0	8
25	0	-1	0	-1	9
26	0	-1	0	1	9
27	0	1	0	-1	9
28	0	1	0	1	9
29 - 30	0	0	0	0	9

where the vector, $0\ 0\ 0\ 0$, corresponds to two runs at the center of the design space.

The short horizontal lines in the X_1 column indicate the blocks formed by HTC factor X_1 and the long horizontal lines indicate the orthogonal blocks. The design with one HTC factor results in 9 resets of the HTC factor X_1 , counting the original setup. A randomized run order would, on average, results in 17.8 resets of the HTC factor X_1 .

The horizontal lines in the X_2 and X_3 columns indicate blocks formed if the design had three HTC factors: X_1 , X_2 , and X_3 . The number of resets of all HTC factors is 37. A randomized run order with 3 HTC factors would, on average, result in 53.4 resets of the HTC factors. The blocking structures presented here are based on results presented in Chapter for 2^2 factorial experiments with 2 HTC factors.

5.5 Related Research and Future Work

Blocking structures for factorial and response surface designs which contain HTC and ETC factors is an active area of current research and a rich area for future research. Recent research includes the work of Huang, Chen, and Voelkel [30] where 2^k factorial experiments with c HTC factors are examined. They recommend blocking structures which result in minimum-aberration designs [18]. The prediction variance and the problem of correlated estimators of the model coefficients is not considered. Bingham and Sitter [6] continue the research of Huang, Chen, and Voelkel by examining 2^k fractional factorial experiments with c HTC factors. They present an algorithm for generating nonisomorphic two-level fractional factorial designs and rank designs based on the minimum aberration criterion.

Future research topics include:

1. The calculation of the maximum prediction variance of response surface designs with HTC factors.
2. The creation of an algorithm for generating blocking structures for CCDs with c HTC factors within the framework of orthogonal blocking. Possible criterion for choosing superior blocking structures might be cost of resetting the HTC factors and maximum prediction variance.

3. How blocking structures and the presence of HTC factors affect the correlation of estimators of model coefficients for response surface designs.
4. The relationship between the number of changes of HTC factors and the magnitude of the maximum prediction variance.

Chapter 6

THE MIXED MODEL

In this chapter, the mixed model will be developed followed by a description of various methods of variance component estimation. The methods will be compared based on their usefulness in estimating variance components in experimental design situations with hard-to-change and easy-to-change factors. Variance Components by Searle, Casella, and McCulloch [55] is this chapter's primary reference and will not be referenced further. Secondary references will be cited when appropriate.

This chapter will recommend the best variance component estimation technique for the mixed models encountered in industrial situations where there are HTC and ETC factors. Mixed model applications including variance component estimation will be presented in Chapter 7 in the form of examples from real industrial experiments.

6.1 Mixed Model Related-Definitions

In an experimental design situation, the researcher is interested in the effects on the variable of interest, or the response that are associated with different factor levels. The effects of a factor may be classified as either *fixed effects* or *random effects*. A factor will be defined as a fixed effects factor if a finite set of levels of that factor are included in the experiment, and this set of levels represent all possible levels of interest to the experimenter. A factor will be defined as a random effects factor if a finite but randomly chosen subset of levels are included in the experiment. This subset of levels is randomly chosen from either a very large or infinite collection of levels of the factor.

If an experiment contains only fixed effects then the experiment would be analyzed using a *fixed effects model*. If an experiment contains only random effects then the experiment would be analyzed using a *random effects model*. If an experiment contains both fixed and random effects then the experiment would be analyzed using a *mixed model*. This is the case with the randomized run order designs discussed earlier. This chapter is concerned with mixed model analysis.

The following three definitions are needed to categorize the type of data being analyzed. First, a *cell* will be defined as the "intersection" of one level of every factor (fixed and random) being considered. As an example, consider an experiment with two factors, A and B , each having a low and high level. One Particular cell occurs at the low level of factor A and at the low level of factor B . This experiment has 4 possible cells. An experiment will be said to have *balanced data*, or just be referred to as *balanced* if each cell contains the same number of observations. An experiment will be said to have *unbalanced data*, or just be referred to as *unbalanced* if it is not balanced.

6.2 The Mixed Model

The general mixed model will be expressed as

$$y = X\beta + \sum_{i=1}^c Z_i u_i + \epsilon,$$

or equivalently

$$y = X\beta + Zu + \epsilon,$$

where

$$Z = (Z_1 Z_2 \cdots Z_c) \quad \text{and} \quad u = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_c \end{pmatrix}.$$

The matrices and vectors used in the above model have the following sizes and ranks,

- $\mathbf{y}$ = $n \times 1$ response vector,
 $\mathbf{X}$ = $n \times p$ known fixed effects design matrix of rank r ,
 $\mathbf{Z}_i$ = $n \times q_i$ known random effects design matrix of rank r_i ,
 $\boldsymbol{\beta}$ = $p \times 1$ vector of unknown fixed effects,
 $\mathbf{u}_i$ = $q_i \times 1$ vector of unknown random effects,
 $\boldsymbol{\epsilon}$ = $n \times 1$ vector of random errors.

The design matrices $\mathbf{X}$ and $\mathbf{Z}$ are known matrices of zeros and ones. The matrix $\mathbf{X}$ is the typical design matrix used in linear models. The matrix $\mathbf{Z}$ is the matrix which describes the restrictions on randomization due to the presence of hard-to-change factors. The structure of this matrix was described in Chapter 2.

The following distributional assumptions will be used unless otherwise stated:

$$\begin{aligned}
 E[\mathbf{u}_i] &= \mathbf{0} \quad \forall i \\
 \text{Var}[\mathbf{u}_i] &= \sigma_i^2 \mathbf{I}_{q_i} \\
 \text{Cov}[\mathbf{u}_i, \mathbf{u}_j] &= \mathbf{0} \quad \forall i \neq j \\
 E[\boldsymbol{\epsilon}] &= \mathbf{0} \\
 \text{Var}[\boldsymbol{\epsilon}] &= \mathbf{R} \\
 \text{Cov}[\mathbf{u}_i, \boldsymbol{\epsilon}] &= \mathbf{0} \quad \forall i.
 \end{aligned}$$

In general, $\text{Var}[\boldsymbol{\epsilon}] = \mathbf{R} = \sigma^2 \mathbf{I}_n$. The collection of scalars $(\sigma_1^2 \sigma_2^2 \dots \sigma_c^2 \sigma^2)$ are referred to as the variance components of the mixed model. It is easily shown that $E[\mathbf{y}] = \mathbf{X}\boldsymbol{\beta}$. Also,

$$\text{Var}[\mathbf{y}] = \sum_{i=1}^c \mathbf{Z}_i \text{Var}[\mathbf{u}_i] \mathbf{Z}_i' + \text{Var}[\boldsymbol{\epsilon}] = \sum_{i=1}^c \sigma_i^2 \mathbf{Z}_i \mathbf{Z}_i' + \mathbf{R} = \mathbf{R} + \mathbf{Z} \mathbf{D} \mathbf{Z}',$$

where

$$\mathbf{D} = \text{Var}[\mathbf{u}] = \bigoplus_{i=1}^c \sigma_i^2 \mathbf{I}_{q_i}.$$

6.3 Variance Component Estimation

When dealing with mixed models, the experimenter is frequently interested in estimating the fixed effects vector $\boldsymbol{\beta}$. In this dissertation the emphasis will also be

on estimating β . If the experimenter is interested in u , then prediction, instead of estimation, is necessary because u is a random vector. The simplest case is when $\text{Var}[y] = R + ZDZ'$ is known. If the variance of y is known then the solution to Henderson's [26] mixed model equations,

$$\begin{bmatrix} X'R^{-1}X & X'R^{-1}Z \\ Z'R^{-1}X & Z'R^{-1}Z + D^{-1} \end{bmatrix} \begin{bmatrix} \tilde{\beta} \\ \tilde{u} \end{bmatrix} = \begin{bmatrix} X'R^{-1}y \\ Z'R^{-1}y \end{bmatrix},$$

yields $\tilde{\beta}$ and $\tilde{u}$, where

$$\tilde{\beta} = [X'(ZDZ' + R)^{-1}X]^{-1}X'(ZDZ' + R)^{-1}y$$

and

$$\tilde{u} = DZ'(ZDZ' + R)^{-1}(y - X\tilde{\beta}).$$

The fixed effects solution, $\tilde{\beta}$, is the best linear unbiased estimator (BLUE) of β and the random effects prediction, $\tilde{u}$, is the best linear unbiased predictor (BLUP) of u . A BLUE is defined as an estimator of β which is a linear function of the response y , say $Ay + k$, that is unbiased and has minimum variance over all other linear unbiased estimators. A BLUP is defined as a predictor of u (not an estimator because u is random), say $A^*y + k^*$, that is unbiased and has minimum variance over all other linear unbiased predictors. If the variance of y is unknown, then D and R must be estimated before any estimation of β or prediction of u can be calculated. Estimating D and R implies estimating the vector of variance components $(\sigma_1^2 \sigma_2^2 \cdots \sigma_c^2 \sigma^2)$.

The remainder of this section will be devoted to examining several methods of variance component estimation. The methods will be divided into two classes, one which involves balanced data and one which involves unbalanced data.

6.3.1 Balanced Data Variance Component Estimation

6.3.1.1 The ANOVA Method

The most basic and commonly used variance component estimation procedure for balanced data is called the ANOVA method. This method consists of equating

the sums of squares of the ANOVA table to their expectations. The expectations will consist of linear combinations of the variance components. This system of $c + 1$ equations with $c + 1$ unknown variance components is then solved for and the resultant solutions are the estimators of the variance components. Note that the sums of squares of the fixed effects need not be computed because their expected sums of squares will not contain any variance components.

A simple example will help to illustrate this method. Consider a 2^3 design with factor A being hard-to-change and factors B and C being easy-to-change. All factors are considered fixed effects factors. By restricting randomization, the design was planned to restrict the number of times the factor A level has to be reset at four. Blocks were set up based on the generators $L_1 = A$ and $L_2 = ABC$. Suppose that the following restricted randomization scheme was chosen to be run:

A	B	C
1	1	1
1	-1	-1
-1	1	1
-1	-1	-1
1	1	-1
1	-1	1
-1	1	-1
-1	-1	1

where the lines in the factor A column represent how the blocks were formed based on the restriction on randomization.

The experimenter is interested in fitting a first-order model with no interaction terms. Because of the presence of the hard-to-change factor and the way the experiment was set up there are 4 blocks of size 2. These blocks are considered random and an extra term must be introduced into the model to account for this. The correct

model is the following mixed model:

$$y = X\beta + Zu + \epsilon,$$

where

- y = 8×1 response vector,
- X = 8×4 known fixed effects design matrix of rank r ,
- Z = 8×4 known random effects design matrix of rank r_i ,
- β = 4×1 vector of unknown fixed effects $(\beta_0 \beta_1 \beta_2 \beta_3)'$,
- u = 4×1 vector of unknown random effects $(u_1 u_2 u_3 u_4)'$,
- ϵ = 8×1 vector of random errors.

The design matrices have the following structure:

$$X = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \quad \text{and} \quad Z = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

There is only one factor of random effects in this model, and it corresponds to the block structure of factor A . I will refer to this factor of random effects as "Block". Thus, there are two variance components that need to be estimated: the component associated with Block (σ_1^2) and the component associated with the overall random error (σ^2). The matrix formulation for the sum of squares associated with Block is

$$SS_{Block} = y'(I - H_x)Z[Z'(I - H_x)Z]^{-1}Z'(I - H_x)y,$$

and the sum of squares associated with the overall error is

$$SSE = y'(I - H)y$$

where $H_x = X(X'X)^{-1}X'$ and $H = (XZ)[(XZ)'(XZ)]^{-1}(XZ)'$. The calculations of the expected sum of squares for both **SSBlock** and **SSE** are as follows:

$$\begin{aligned}
 E[SSE] &= \text{tr}[(I - H)\text{Var}[y]] + E[y]'(I - H)E[y] \\
 &= \text{tr}[(I - H)(\sigma^2 I_8 + ZDZ')] + \beta'X'(I - H)X\beta \\
 &= \sigma^2 \text{tr}[I_8 - H] + 0 \\
 &= \sigma^2 \text{rank}[I_8 - H] \\
 &= 2\sigma^2
 \end{aligned}$$

and

$$\begin{aligned}
 E[SSBlock] &= \text{tr}[(I - H_x)Z[Z'(I - H_x)Z]^{-1}Z'(I - H_x)(\sigma^2 I_8 + ZDZ')] \\
 &\quad + \beta'X'(I - H_x)Z[Z'(I - H_x)Z]^{-1}Z'(I - H_x)X\beta \\
 &= \frac{1}{4}(8)(2\sigma_1^2 + \sigma^2) \\
 &= 4\sigma_1^2 + 2\sigma^2.
 \end{aligned}$$

Equating the sums of squares to their expected mean squares yields the following ANOVA estimators of the variance components:

$$\hat{\sigma}^2 = \frac{SSE}{2} \text{ and } \hat{\sigma}_1^2 = \frac{SSBlock - SSE}{4}.$$

The benefits and drawbacks of the ANOVA method will now be discussed. The ANOVA estimators are unbiased and can also be shown to have minimum variance among all quadratic unbiased estimators (MVQU)[22]. These results do not require any normality assumptions. If one makes the assumption that $y \sim N[X\beta, R + ZDZ']$, then the ANOVA estimators have minimum variance among all unbiased estimators (MVUE)[21], not just among quadratic estimators. The drawback to ANOVA estimators is that they may be negative. All subsequent methods of variance components to be examined also have this drawback. This problem will be discussed in more detail at the end of this chapter.

Two other methods of variance component estimation which may be applied to balanced data are the maximum likelihood (ML) and the restricted maximum likelihood (REML) estimation methods. The details of these two methods and their properties will be discussed in this chapter's subsection on unbalanced data.

In general, under a balanced data situation, the ANOVA method is easiest to employ and has better properties than the ML method. The ANOVA estimators are also equal to the REML estimators under balanced data [2]. This result does not hold for unbalanced data. With the advent of fast computing packages, the simplicity of calculations becomes less of an issue and the experimenter may just use REML estimators for all balanced data situations. This recommendation of the REML method for balanced data is consistent with the recommendation of the REML method for unbalanced data discussed in the next section.

6.3.2 Unbalanced Data Variance Component Estimation

The methods of variance component estimation which will be considered here are Henderson's Methods I, II, and III; maximum likelihood (ML) estimation; and restricted maximum likelihood (REML) estimation. The minimum-norm quadratic unbiased equation (MINQUE) method will be discussed very briefly.

6.3.2.1 Henderson's Methods

Henderson's Method I is very closely related to the ANOVA method and a matrix generalization of the ANOVA method will aid in discussing Henderson's Method I. The ANOVA method consists of calculating $c + 1$ sums of squares, 1 for each of the c random effects factors and one for the overall error. Label these $c + 1$ sums of squares as the vector $\mathbf{s}$. Then, the expectation of each row of $\mathbf{s}$ is a linear combination of the $c + 1$ variance components $\boldsymbol{\sigma} = (\sigma_1^2 \ \sigma_2^2 \ \cdots \ \sigma_c^2 \ \sigma^2)$. Using this notation, the expectation of $\mathbf{s}$ can be expressed as $\mathbf{C}\boldsymbol{\sigma}$, where $\mathbf{C}$ is a matrix whose rows are the linear combinations of $\boldsymbol{\sigma}$ corresponding to each of the $c + 1$ sums of squares. Then, the ANOVA estimators of $\boldsymbol{\sigma}$ are $\tilde{\boldsymbol{\sigma}} = \mathbf{C}^{-1}\mathbf{s}$ (providing that $\mathbf{C}$ is nonsingular). Henderson's

Method I consists of formulating quadratic forms $y'Ay$ for each factor in the model. Once quadratic forms have been specified, their expectations are calculated. Just like the ANOVA method, these expectations are then set equal to their respective sums of squares and the variance components are then solved for.

Henderson's Method I only works for random effects models. The reason why uses the fact that if a model has both fixed and random effects then $X'AX \neq 0$. For balanced data it was the case that $X'AX=0$. This is important because $E[y'Ay] = \text{tr}[A\Sigma] + \beta'X'AX\beta$ and if $X'AX \neq 0$ then the expected sums of squares have fixed effect terms in them. Therefore, if the variance components are solved for, the solutions will be functions of the fixed effects, which are unknown quantities.

Like the ANOVA estimators, Henderson's Method I estimators are unbiased, and are equal to ANOVA estimators for balanced data. A drawback is that they are limited to random effects models only. They may also produce negative variance component estimators.

Henderson's Method II is an attempt to use the simplicity of method I on mixed models, not just random effects models. The problem with mixed models and unbalanced data is that $X'AX \neq 0$. Method II involves adjusting the data such that it can be considered as coming from a random effects model instead of a mixed model. This ensures that $X'AX=0$ for all quadratic forms. Henderson proposed adjusting the data in the following way. Consider the model

$$y = 1_n\mu + X\beta + Zu + \epsilon.$$

Let L be a matrix chosen such that

$$y_o = y - XLy = 1_n\mu_o + Zu + \epsilon_o,$$

where μ_o is an adjusted overall mean dependent on L and $\epsilon_o = (I - XL)\epsilon$ is an adjusted overall error dependent on L and y_o is the adjusted data which now comes from a random effects model. Notice that L must be chosen such that

$$y - XLy = 1_n\mu + X\beta + Zu + \epsilon - XL1_n\mu - XLX\beta - XLZu - XL\epsilon$$

$$= \mu(1_n - XL1_n) + (I - XL)X\beta + (I - XL)Zu + (I - XL)\epsilon$$

reduces to

$$y - XLy = 1_n\mu_0 + Zu + \epsilon_0.$$

Searle, Casella, and McCulloch [55] give a description of how to compute L . They also note that L must satisfy 3 conditions:

- (i) $XLZ = 0$
- (ii) $XL \propto 1_n$
- (iii) $(I - XL)X = 1_nt'$ for some row vector t' .

Once this transformation to a random effects model is made Henderson's Method I is employed. One drawback to Method II is that for the three conditions on L to hold there must be no interaction terms between random effects and fixed effects in the model. This is a serious drawback and Henderson went on to present Method III to overcome this deficiency. Aside from this drawback, Method II has similar properties to Method I: the variance component estimators are unbiased and for balanced data Method II estimators are the same as ANOVA estimators.

Henderson's Method III is very similar in spirit to method II. The basic idea is that the data is transformed in such a way as to create a purely random model. Then, the ANOVA method is used on that new model. Unlike Method II, Method III can handle mixed models with interaction terms between the fixed effects and the random effects. To apply Method III, start out with the basic mixed model:

$$y = X\beta + Zu + \epsilon$$

and then transform the data to the purely random model:

$$(I - H_x)y = (I - H_x)Zu + (I - H_x)\epsilon,$$

where $H_x = X(X'X)^{-1}X'$. Then use the ANOVA method on the transformed random model. The drawback to this method is that there may be more than one way

to express the quadratic forms necessary to use the ANOVA method. Searle, Casella, and McCulloch [55] point out that this occurs when there are two or more crossed random factors. The mixed models discussed in this dissertation generally result in models with random factors, due to randomization restrictions, that are not crossed. Thus, Method III will work fine on these mixed models. Mixed models with two or more crossed random factors can be dealt with using the ML or REML methods described in the following subsection. Aside from this drawback, Method III has similar properties to Method I and Method II: the variance component estimators are unbiased and for balanced data Method III estimators are the same as ANOVA estimators.

6.3.2.2 Maximum Likelihood and Restricted Maximum Likelihood

The Maximum Likelihood (ML) and Restricted Maximum Likelihood (REML) methods are very different than Henderson's methods and the ANOVA method. ML and REML methods are based on maximizing a likelihood function and, therefore, require a distribution assumption. Most commonly, the researcher will assume that $y \sim N[X\beta, \Sigma]$ where $\Sigma = R + ZDZ'$ in the mixed model setting. As noted earlier, $R = \text{Var}[\epsilon] = \sigma^2 I_n$ and $D = \text{Var}[u] = \bigoplus_{i=1}^c \sigma_i^2 I_i$.

The assumption of normality allows us to write out the likelihood function as

$$L(\beta, \Sigma|y) = \frac{1}{(2\pi)^{\frac{1}{2}} |\Sigma|^{\frac{1}{2}}} e^{-\frac{1}{2}(y-x\beta)' \Sigma^{-1} (y-x\beta)}.$$

Once a likelihood function is defined, it is maximized over the vectors of fixed effects and variance components $\beta = (\beta_1 \ \beta_2 \ \dots \ \beta_p)'$ and $\sigma = (\sigma_1^2 \ \sigma_2^2 \ \dots \ \sigma_c^2 \ \sigma^2)'$. These maximizers, which will be referred to as $\tilde{\beta}$ and $\tilde{\sigma}$, are then the estimators of β and σ .

Most commonly the likelihood function, $L(\beta, \Sigma|y)$, is not directly maximized. It is more convenient mathematically to maximize the log likelihood function

$$\log[L(\beta, \Sigma|y)] = -\frac{n}{2} \ln(2\pi) - \frac{1}{2} \ln(\Sigma) - \frac{1}{2} (y - x\beta)' \Sigma^{-1} (y - x\beta).$$

The log likelihood function is called the score function, $S(\beta, \Sigma)$, and maximization is achieved through calculus techniques. The derivatives of $S(\beta, \Sigma)$ with respect to β and σ are

$$\frac{\partial L}{\partial \sigma} = -\frac{1}{2} \text{tr}(\Sigma^{-1} Z_i Z_i') + \frac{1}{2} (y - X\beta)' \Sigma^{-1} Z_i Z_i' \Sigma^{-1} (y - X\beta)$$

for $i = 0, \dots, c$ and

$$\frac{\partial L}{\partial \beta} = X' \Sigma^{-1} y - X' \Sigma^{-1} X \beta.$$

Equating these derivatives to zero yields the following equations

$$\tilde{\beta} = (X' \tilde{\Sigma}^{-1} X)^{-1} X' \tilde{\Sigma}^{-1} y$$

and

$$\text{tr}(Z_i' \tilde{\Sigma}^{-1} Z_i) = y'(I - \tilde{H})' \tilde{\Sigma}^{-1} Z_i Z_i' \tilde{\Sigma}^{-1} (I - \tilde{H}) y$$

for $i = 0, \dots, c$ and $\tilde{H} = X(X' \tilde{\Sigma}^{-1} X)^{-1} X' \tilde{\Sigma}^{-1}$. There are $c + 1$ equations which must be solved for the $c + 1$ variance components. Because these equations are nonlinear in $\sigma = (\sigma_1^2 \ \sigma_2^2 \ \dots \ \sigma_c^2 \ \sigma^2)'$, the solution is obtained via numerical iteration. Also, since $\tilde{\sigma}$ are maximum likelihood estimations they must reside in the parameter space of σ . This requires that $\sigma_i \geq 0$ for all i . Thus, if a variance component has a negative estimate, that estimate is set equal to zero. Searle, Casella, and McCulloch [55] point out that solving this system of equations by numerical iteration is difficult. There are many software packages available to handle this problem. The package used for work in this dissertation is the SAS PROC MIXED procedure [52]. This procedure uses the Newton-Raphson algorithm to solve the system of equations.

A drawback to ML estimation is that it does not take into account the degrees of freedom associated with the fixed effects. For a simplistic example, consider x_i identically and independently distributed $N(\mu, \sigma^2)$ for $i = 1, \dots, n$. The unbiased ANOVA estimate of σ^2 is $\hat{\sigma}^2 = \sum_i (x_i - \bar{x})^2 / (n - 1)$, whereas the biased ML estimate is $\tilde{\sigma}^2 = \sum_i (x_i - \bar{x})^2 / (n)$. The REML method does take into account the degrees of freedom associated with the fixed effects. The REML method uses a transformation

of the data vector $\mathbf{y}$ and its associated model. This transformation is chosen in such a way as to completely eliminate the fixed effects from the model no matter what the value of $\mathbf{y}$.

In order to transform the data vector $\mathbf{y}$ and eliminate the fixed effects from the model a matrix $\mathbf{K}$ must be chosen such that

$$\mathbf{K}'\mathbf{y} = \mathbf{K}'\mathbf{X}\boldsymbol{\beta} + \mathbf{K}'\mathbf{Z}\mathbf{u} + \mathbf{K}'\boldsymbol{\epsilon} = \mathbf{K}'\mathbf{Z}\mathbf{u} + \mathbf{K}'\boldsymbol{\epsilon} \quad \forall \boldsymbol{\beta}.$$

In other words, $\mathbf{K}$ must be chosen such that $\mathbf{K}'\mathbf{X}\boldsymbol{\beta} = \mathbf{0} \quad \forall \boldsymbol{\beta}$. This is accomplished by letting $\mathbf{K}'\mathbf{K}$ be the full rank factorization of $(\mathbf{I} - \mathbf{H}_x)$, where $\mathbf{H}_x = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$. The resultant model is $\mathbf{K}'\mathbf{y} = \mathbf{K}'\mathbf{Z}\mathbf{u} + \mathbf{K}'\boldsymbol{\epsilon}$. One then assumes that $\mathbf{K}'\mathbf{y} \sim N[\mathbf{0}, \mathbf{K}'\mathbf{Z}\mathbf{D}\mathbf{Z}'\mathbf{K} + \mathbf{R}]$ and then follows the ML procedure on this reduced model.

ML and REML have some very desirable asymptotic properties. Although the variance component estimators are not unbiased; they are consistent. That is, $\tilde{\boldsymbol{\sigma}}$ converges in probability to $\boldsymbol{\sigma}$. In fact, $\tilde{\boldsymbol{\sigma}}$ has an asymptotic distribution of $N[\boldsymbol{\sigma}, \mathbf{I}(\boldsymbol{\sigma})^{-1}]$ where $\mathbf{I}(\boldsymbol{\sigma})^{-1}$ is the inverse of Fisher's information matrix and its form is described in detail in Searle, Casella, and McCulloch [55], and also in Miller [47]. REML estimators are also exactly equal to ANOVA estimators in the balanced data case. ML and REML estimation is computationally intense, but with modern computer packages this is not a drawback unless a very large number of variance components are being estimated.

6.3.3 Conclusions and Recommendations

All variance component estimation procedures examined here, with the exception of ML and REML, have the undesirable feature of producing negative estimators. A negative estimate may be taken to be an indication that the model being used is incorrect or that the variance component is zero. Quite often, when the researcher is using the ANOVA method or Henderson's methods, a negative variance component estimate is set equal to zero. A general discussion of negative estimators can be found

in LaMotte [42] and Styan and Pukelsheim [57]. A discussion of negative estimators and their relation to an incorrect model can be found in Hocking [28] [29] and Smith and Murray [56]. The ML and REML procedures always give nonnegative variance component estimators because the estimators are required to be in the parameter space.

The recommended variance component estimation procedure for the types of mixed models encountered in experimental design situations with randomization restrictions due to not resetting hard-to-change factors is REML. In the balanced data setting the REML estimators equal the ANOVA estimators, and in the unbalanced data setting there is no ambiguity as to what quadratic forms to use in contrast to what occurs in Henderson's method III. REML also can be used on any mixed model with random effects and fixed effects, crossed or not. REML estimators are less biased than ML estimators and have desirable asymptotic properties. There is also minimal concern regarding the computational difficulty due to the computational speed of today's computer.

Chapter 7

EXAMPLES

This chapter will examine experiments from industry which contained HTC and ETC factors. These experiments were run and analyzed in a traditional fashion assuming a completely randomized run order, even though HTC factors were present.

7.1 A Box-Behnken design

A Box-Behnken design was conducted in the fall of 1998 at a major computer component manufacturing company. The purpose of the experiment was to improve the performance of a wrapper machine. The wrapper machine is used to package product in an air-tight bag. Three factors were deemed important by engineering for creating a strong seal on the bag the product was placed in. These factors were spacing of the seal crimper (X_1), speed at which the machine was run (X_2), and temperature of the seal crimper (X_3).

Due to the manufacturing process and the mechanics of the machine, speed and spacing were HTC factors and temperature was an ETC factor. The experimenters were aware that spacing was a HTC factor and organized the runs in such a way as to create 4 blocks based on the levels of spacing. Speed and temperature were then randomized within these blocks. When the experiment began, the experimenters realized that speed was also a HTC factor and therefore did not reset if from run to run where speed was at the same level.

The following matrix displays the run order in which the experiment was carried out. The HTC factors are spacing (X_1) and speed (X_2). The ETC factor is

temperature (X_3). The lines in the matrix represent restrictions on randomization due to the presence of the HTC factors, spacing and speed.

X_1	X_2	X_3
0	1	-1
0	1	1
0	0	0
1	0	1
1	0	-1
1	-1	0
1	1	0
-1	1	0
-1	-1	0
-1	0	-1
-1	0	1
0	0	0
0	-1	-1
0	-1	1
0	0	0

The experiment was carried out and analyzed using the following model:

$$y = X\beta + \epsilon,$$

where the typical assumption of independent and identical error structure, $E[\epsilon] = 0$ and $\text{Var}[\epsilon] = \sigma^2 I_n$, was made.

Analysis revealed that the main effects of speed and temperature were significant at the $\alpha = .05$ level. The spacing main effect, all two factor interactions, and all squared terms were non-significant. Therefore, the experimenters focused their energy on improving the process by only examining the two significant factors, speed and temperature. They also excluded the speed-by-temperature interaction because the analysis indicated it was very non-significant.

A more appropriate analysis should include the restrictions on randomization which occurred during the experiment. Using results from the previous chapters, the correct model is;

$$y = X\beta + Zu + \epsilon,$$

where

run	X_1	X_2	X_3	X_{12}	X_{13}	X_{23}	X_1^2	X_2^2	X_3^2
1	1	0	1	-1	0	0	-1	0	1
2	1	0	1	1	0	0	1	0	1
3	1	0	0	0	0	0	0	0	0
4	1	1	0	1	0	1	0	1	0
5	1	1	0	-1	0	-1	0	1	0
6	1	1	-1	0	-1	0	0	1	1
7	1	1	1	0	1	0	0	1	1
8	1	-1	1	0	-1	0	0	1	1
9	1	-1	-1	0	1	0	0	1	1
10	1	-1	0	-1	0	1	0	1	0
11	1	-1	0	1	0	-1	0	1	0
12	1	0	0	0	0	0	0	0	0
13	1	0	-1	-1	0	0	1	0	1
14	1	0	-1	1	0	0	-1	0	1
15	1	0	0	0	0	0	0	0	0

$$Z_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad Z_2 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

where the structure of Z_1 corresponds to the restrictions on randomizing HTC factor X_1 and Z_2 corresponds to the restrictions on randomizing HTC factor X_2 . Therefore, $Z = [Z_1 \ Z_2]$.

To analyze a mixed model with this structure, it is necessary for a statistical package to:

- Be able to estimate the fixed effects and regression coefficients.
- Be able to estimate the variance components associated with the split-plotting created by the HTC factors.
- Use the estimated variance components so that the proper F -statistics with approximate (Satterthwaite) degrees of freedom [46] are generated.

The *Proc Mixed* procedure in SAS [52] is capable of doing all of this.

The SAS code for the analysis of the bond strength data is:

```
TITLE 'BOND STRENGTH ANALYSIS';
DATA IN; INPUT SPACING SPEED TEMP STRENGTH
B_SPACE B_SPEED @@; CARDS;
  0  1 -1  .005  1  1
  0  1  1  4.17  1  1
  0  0  0  4.235  1  2
  1  0  1  3.45  2  2
  1  0 -1  .11  2  2
  1 -1  0  4.155  2  3
  1  1  0  .01  2  4
 -1  1  0  .80  3  4
 -1 -1  0  5.885  3  5
 -1  0 -1  .94  3  6
 -1  0  1  4.11  3  6
  0  0  0  3.09  4  6
  0 -1 -1  4.10  4  7
  0 -1  1  5.15  4  7
  0  0  0  3.195  4  8
;
PROC MIXED DATA=IN;
  CLASS B_SPACE B_SPEED;
  MODEL STRENGTH = SPACING|SPEED|TEMP^2
  SPACING*SPACING SPEED*SPEED TEMP*TEMP / DDFM=SATTERTH;
  RANDOM B_SPACE B_SPEED;
RUN;
```

The two variables,

B_SPACE

and

B_SPEED

correspond to the random block effects in the mixed model associated with HTC factors spacing and speed. The default variance component estimation procedure in *Proc Mixed* is the REML procedure, which was the recommended procedure from Chapter 6. Portions of the results contained in the SAS output follow.

Covariance Parameter Estimates (REML)

Cov Parm	Estimate
B_SPACE	1.08011103
B_SPEED	0.00000000
Residual	0.15624008

Solution for Fixed Effects

Effect	Estimate	Std Error	DF	t	Pr > t
INTERCEPT	3.74437098	0.77177613	1.08	4.85	0.1162
SPACING	-0.50125000	0.74805449	0.95	-0.67	0.6287
SPEED	-2.14468147	0.16556394	4.14	-12.95	0.0002
TEMP	1.46562500	0.13974981	4.00	10.49	0.0005
SPACING*SPEED	0.23500000	0.19763608	4.00	1.19	0.3002
SPACING*TEMP	0.04250000	0.19763608	4.00	0.22	0.8403
SPEED*TEMP	0.77875000	0.19763608	4.00	3.94	0.0170
SPACING*SPACING	-1.11781049	1.05985931	0.96	-1.05	0.4889
SPEED*SPEED	0.08593951	0.20782381	4.01	0.41	0.7004
TEMP*TEMP	-0.47406049	0.20782381	4.01	-2.28	0.0845

Once again, the analysis indicates that the two main effects, speed and temperature, are significant. But, the mixed model analysis also reveals the significant interaction, speed*temp. This interaction was considered non-significant in the traditional analysis which assumed complete randomization. Optimization of this procedure depends upon speed, temperature, and their interaction, not just the main effects as was previously thought. The mixed model analysis also provides variance component estimates: $\sigma^2 = .1562$, $\sigma_1^2 = 1.080$, and $\sigma_2^2 = 0$. This is informative because it indicates that the variance component estimate associated with the HTC factor speed is zero. This implies that speed need not be reset from run to run when it is held at the same level in future experimentation. But, the resetting of spacing is very important because its variance component is relatively large when compared to the overall error.

7.2 A Second Box-Behnken design

A Box-Behnken experiment was conducted at E.I. Du Pont de Nemours and Co [7]. The experiment was used to examine a polymer used in the production of under-the-hood automobile parts, such as gaskets. The viscosity of the polymer was of principle interest. Three process factors which potentially impact polymer viscosity were included in the experiment. These factors are:

1. Amount of additive, which will be referred to as ADDITIVE (X_1).
2. Temperature, which will be referred to as TEMP (X_2).
3. Add time, which will be referred to as ADDTIME (X_3).

The Box-Behnken design matrix is as follows:

$$X = \begin{array}{cc} & \text{Run} \\ & \begin{bmatrix} X_1 & X_2 & X_3 \end{bmatrix} \\ \begin{matrix} 1 - 4 \\ 5 - 8 \\ 9 - 12 \\ 13 - 15 \end{matrix} & \begin{bmatrix} \pm 1 & \pm 1 & 0 \\ \pm 1 & 0 & \pm 1 \\ 0 & \pm 1 & \pm 1 \\ 0 & 0 & 0 \end{bmatrix} \end{array},$$

where the vector, $0\ 0\ 0\ 0$, corresponds to three runs at the center of the design space. A fourth variable, process time, was not controlled but was monitored and recorded during the experiment. Process time will be referred to as PROCTIME (X_4).

The experiment was conducted with a randomized run order. The viscosity of the polymer was measured at the middle of each run and at the end of each run. The two values for each run were averaged and the average was used as the response in the analysis. The observed values for PROCTIME were centered and scaled. The

randomized run order and data are as follows:

Run	ADDITIVE	TEMP	ADDTIME	PROCTIME	VISCOSITY
1	-1	1	0	1.000	31.80
2	1	0	-1	-0.333	34.40
3	0	0	0	0.667	35.25
4	0	-1	-1	-0.333	31.95
5	-1	0	1	0.560	30.45
6	1	1	0	-0.333	32.55
7	0	1	1	0.000	31.45
8	0	0	0	-1.000	27.50
9	0	-1	1	-0.227	30.50
10	-1	-1	0	-0.333	28.05
11	0	1	-1	0.333	36.65
12	-1	0	-1	-0.560	34.65
13	1	-1	0	-1.000	30.50
14	0	0	0	-0.227	35.80
15	1	0	1	1.000	36.25

The experiment was carried out and analyzed using the following model:

$$y = X\beta + \epsilon,$$

where the typical assumption of independent and identical error structure, $E[\epsilon] = 0$ and $\text{Var}[\epsilon] = \sigma^2 I_n$, was made. The initial analysis did not take make use of the data for PROCTIME. The full quadratic model was fit and portions of the results are as follows:

POLYMER ANALYSIS

Covariance Parameter Estimates (REML)

Cov Parm	Estimate
Residual	9.21787500

Tests of Fixed Effects

Source	NDF	DDF	Type III F	Pr > F
ADDITIVE	1	5	1.04	0.3550
TEMP	1	5	1.78	0.2399
ADDITIVE*TEMP	1	5	0.08	0.7907
ADDTIME	1	5	1.10	0.3426
ADDITIVE*ADDTIME	1	5	0.99	0.3648
TEMP*ADDTIME	1	5	0.38	0.5639
ADDITIVE*ADDITIVE	1	5	0.07	0.8045
TEMP*TEMP	1	5	1.17	0.3279
ADDTIME*ADDTIME	1	5	0.90	0.3860

The results revealed nothing significant and the estimate of 9.218 for σ^2 is very large.

The experiment was then analyzed again using PROCTIME as a covariate in the analysis. The linear and quadratic PROCTIME terms were added to the model. No interactions between PROCTIME and any other factors in the model were considered. The results for this subsequent analysis are as follows:

POLYMER ANALYSIS

Covariance Parameter Estimates (REML)

Cov Parm	Estimate
Residual	0.97931148

Tests of Fixed Effects

Source	NDF	DDF	Type III F	Pr > F
ADDITIVE	1	3	26.31	0.0143
TEMP	1	3	1.06	0.3799
ADDITIVE*TEMP	1	3	11.90	0.0409
ADDTIME	1	3	11.75	0.0416
ADDITIVE*ADDTIME	1	3	22.11	0.0182
TEMP*ADDTIME	1	3	2.06	0.2469
ADDITIVE*ADDITIVE	1	3	0.73	0.4566
TEMP*TEMP	1	3	18.02	0.0239
ADDTIME*ADDTIME	1	3	1.36	0.3277
PROCTIME	1	3	24.95	0.0154
PROCTIME*PROCTIME	1	3	21.79	0.0186

The use of PROCTIME as a covariate dramatically improved the model. The estimate of σ^2 dropped from 9.218 to 0.979. The better fitting model also revealed that the terms ADDITIVE, ADDTIME, PROCTIME, ADDITIVE*TEMP, ADDITIVE*ADDTIME, TEMP*TEMP, and PROCTIME*PROCTIME are significant at the $\alpha = .05$ level.

A more complete analysis of this data should include the restrictions on randomization which occurred during the experiment. The factor TEMP (X_2) is a HTC factor and should be treated as such in the analysis. Using results from the previous chapters, the correct model is;

$$y = X\beta + Zu + \epsilon,$$

where

$\mathbf{X} =$

run	X_1	X_2	X_3	X_{12}	X_{13}	X_{23}	X_1^2	X_2^2	X_3^2	X_4	X_4^2	
1	1	-1	1	0	-1	0	0	1	1	0	1.000	1.000
2	1	1	0	-1	0	-1	0	1	0	1	-0.333	0.111
3	1	0	0	0	0	0	0	0	0	0	0.667	0.445
4	1	0	-1	-1	0	0	1	0	1	1	-0.333	0.111
5	1	-1	0	1	0	-1	0	1	0	1	0.560	0.314
6	1	1	1	0	1	0	0	1	1	0	-0.333	0.111
7	1	0	1	1	0	0	1	0	1	1	0.000	0.000
8	1	0	0	0	0	0	0	0	0	0	-1.000	1.000
9	1	0	-1	1	0	0	-1	0	1	1	-0.227	0.052
10	1	-1	-1	0	1	0	0	1	1	0	-0.333	0.111
11	1	0	1	-1	0	0	-1	0	1	1	0.333	0.111
12	1	-1	0	-1	0	1	0	1	0	1	-0.560	0.314
13	1	1	-1	0	-1	0	0	1	1	0	-1.000	1.000
14	1	0	0	0	0	0	0	0	0	0	-0.227	0.052
15	1	1	0	1	0	1	0	1	0	1	1.000	1.000

and

$$Z = Z_2 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

where the horizontal lines in the design matrix X represent restrictions on randomization due to the HTC factor TEMP. The structure of Z_2 follows from the structure of X and the restrictions on randomization due to HTC factor TEMP.

The SAS code for the analysis of this mixed model is as follows:

```
TITLE 'POLYMER ANALYSIS';
DATA IN; INPUT ADDITIVE TEMP ADDTIME
PROCTIME MID END TEMP_B @@;
CARDS;
-1 1 0 1.000 32.6 31.0 1
1 0 -1 -0.333 32.2 36.6 2
0 0 0 0.667 35.7 34.8 2
0 -1 -1 -0.333 31.9 32.0 3
-1 0 1 0.560 32.1 28.8 4
1 1 0 -0.333 32.0 33.1 5
0 1 1 0.000 31.1 31.8 5
0 0 0 -1.000 28.0 27.0 6
0 -1 1 -0.227 29.0 32.0 7
```

```

-1 -1 0 -0.333 27.3 28.8 7
0 1 -1 0.333 35.5 37.8 8
-1 0 -1 -0.560 34.6 34.7 9
1 -1 0 -1.000 29.9 31.1 10
0 0 0 -0.227 34.5 37.1 11
1 0 1 1.000 36.5 36.0 11

```

```

;
PROC MIXED DATA=IN;
  CLASS TEMP_B;
  MODEL AVG = ADDITIVE|TEMP|ADDTIME@2 ADDITIVE*ADDITIVE TEMP*TEMP
    ADDTIME*ADDTIME PROCTIME PROCTIME*PROCTIME / DDFM=SATTERTH;
  RANDOM TEMP_B;
RUN;

```

The variable,

TEMP_B

corresponds to the random effect in the mixed model associated with the HTC factor TEMP. The default variance component estimation procedure in *Proc Mixed* is the REML procedure, which was the recommended procedure from Chapter 6. Portions of the results from the SAS output follow.

POLYMER ANALYSIS

Covariance Parameter Estimates (REML)

Cov Parm	Estimate
TEMP_B	1.02675602
Residual	0.00000001

Tests of Fixed Effects

Source	NDF	DDF	Type III F	Pr > F
ADDITIVE	1	3	21.57	0.0188
TEMP	1	3	0.45	0.5515
ADDITIVE*TEMP	1	3	15.40	0.0295
ADDTIME	1	3	11.47	0.0429
ADDITIVE*ADDTIME	1	3	21.46	0.0190
TEMP*ADDTIME	1	3	2.18	0.2359
ADDITIVE*ADDITIVE	1	3	0.81	0.4338
TEMP*TEMP	1	3	11.85	0.0412

ADDTIME*ADDTIME	1	3	6.29	0.0871
PROCTIME	1	3	28.80	0.0127
PROCTIME*PROCTIME	1	3	27.76	0.0133

Once again, the analysis indicates that the terms ADDITIVE, ADDTIME, PROCTIME, ADDITIVE*TEMP, ADDITIVE*ADDTIME, TEMP*TEMP, and PROCTIME*PROCTIME are significant at the $\alpha = .05$ level. Including the presence of the HTC factor, TEMP, into the analysis does not reveal any other factors to be significant at the $\alpha = .05$ level. But, the quadratic term for ADDTIME is marginally non-significant with a p-value of 0.0871. This term might be of interest to the experimenter in order to quantify the process more completely.

The mixed model analysis also gives variance component estimates of: $\sigma^2 = 1 \times 10^{-8}$ and $\sigma_1^2 = 1.0268$. This is very informative in that the variance component associated with the HTC factor TEMP is extremely large compared to the overall error, σ^2 . Although the analysis with TEMP treated as a HTC factor did not differ very much from the conventional analysis, care should be taken with future experimentation. The resetting of TEMP from run to run is very important because its variance component is quite substantial when compared to the overall error. This should be taken into consideration with all future experimentation on this process.

7.3 A Factorial Experiment

The following example was presented in an article on restricting randomization by Anderson and McLean [4]. An experiment was conducted at General Mills, Inc. in Minneapolis to investigate peel strength of package liners. Engineers choose three factors to study: temperature (X_1), pressure (X_2), and time of heating (X_3). The factors and levels investigated are listed below:

Factor	Level
Temperature(X_1)	-1, 1
Pressure(X_2)	-1, 0, 1
Time of Heating(X_3)	-1, 0, 1

Based on the levels of interest, a $2 \times 3 \times 3$ factorial experiment was run. Eighteen sheets of package liner were used in the experiment. One sheet of package liner was subjected to each of the 18 factor combinations. The sheet was then cut into 5 pieces and the peel strength was measured on each piece. Temperature and pressure were difficult to reset in this experiment and are considered HTC factors. Temperature was only set up twice and Pressure was set up 6 times. The data and run order in which the experiment was carried out are:

Run	Temp.	Pres.	Heating	Peel Strength Reps				
			Time	1	2	3	4	5
1	-1	-1	-1	7.0	6.9	6.5	6.0	5.5
2	-1	-1	0	6.5	6.1	6.7	7.3	6.9
3	-1	-1	1	5.5	5.5	5.5	5.3	5.9
4	-1	0	-1	6.1	6.0	6.3	5.7	4.3
5	-1	0	0	3.7	5.3	6.0	5.3	5.7
6	-1	0	1	6.6	5.7	5.3	5.1	5.5
7	-1	1	-1	5.3	4.5	5.1	6.3	6.4
8	-1	1	0	4.3	6.5	6.0	5.3	6.2
9	-1	1	1	4.1	5.9	6.0	5.9	5.7
10	1	-1	-1	5.7	5.0	6.1	6.2	6.9
11	1	-1	0	5.3	5.7	4.7	5.9	5.7
12	1	-1	1	5.5	5.3	5.0	6.0	5.3
13	1	0	-1	5.5	5.3	5.9	5.7	6.1
14	1	0	0	5.3	5.3	5.3	5.7	5.5
15	1	0	1	5.5	5.7	4.7	6.0	5.5
16	1	1	-1	5.3	4.5	5.7	5.7	5.3
17	1	1	0	5.1	5.5	5.9	5.7	6.1
18	1	1	1	6.2	6.4	6.0	6.2	4.7

It is obvious that there are restrictions in randomization due to temperature and pressure. Another restriction on randomization is due to the fact that each sheet of package liner was subjected to a treatment combination, then cut into 5 pieces. The third factor in the experiment, time of heating, was run in a systematic fashion, but was reset at the beginning of each run because it was at a different level.

For comparison, the experiment was analyzed assuming that there were no restrictions on randomization. The model used was:

$$y = X\beta + \epsilon,$$

where the typical assumption of independent and identical error structure, $E[\epsilon] = 0$ and $\text{Var}[\epsilon] = \sigma^2 I_n$, was made. All main effects, two factor interactions, and quadratic terms for PRES and TIME were fit. The results are:

Tests of Fixed Effects

Source	NDF	DDF	Type III F	Pr > F
TEMP	1	81	1.73	0.1917
PRES	1	81	4.15	0.0449
TEMP*PRES	1	81	4.15	0.0449
TIME	1	81	1.26	0.2641
TEMP*TIME	1	81	0.55	0.4599
PRES*TIME	1	81	6.75	0.0111
PRES*PRES	1	81	2.94	0.0902
TIME*TIME	1	81	0.01	0.9319

PRES is significant at the $\alpha = .05$ level. The two factor interactions of TEMP*PRES and PRES*TIME are also significant.

An appropriate analysis of this experiment should include the restrictions on randomization which occurred during the experiment. Using results from the previous chapters, the correct model for examining main effects and two factor interactions is;

$$y = X\beta + Zu + \epsilon,$$

where

$$\mathbf{X} = \begin{array}{c|cccccc} \text{run} & X_1 & X_2 & X_3 & X_{12} & X_{13} & X_{23} \\ \hline 1 & \mathbf{1} & \mathbf{-1} & \mathbf{-1} & \mathbf{-1} & \mathbf{1} & \mathbf{1} & \mathbf{1} \\ 2 & \mathbf{1} & \mathbf{-1} & \mathbf{-1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\ 3 & \mathbf{1} & \mathbf{-1} & \mathbf{-1} & \mathbf{1} & \mathbf{1} & \mathbf{-1} & \mathbf{-1} \\ 4 & \mathbf{1} & \mathbf{-1} & \mathbf{0} & \mathbf{-1} & \mathbf{0} & \mathbf{1} & \mathbf{0} \\ 5 & \mathbf{1} & \mathbf{-1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ 6 & \mathbf{1} & \mathbf{-1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{-1} & \mathbf{0} \\ 7 & \mathbf{1} & \mathbf{-1} & \mathbf{1} & \mathbf{-1} & \mathbf{-1} & \mathbf{1} & \mathbf{-1} \\ 8 & \mathbf{1} & \mathbf{-1} & \mathbf{1} & \mathbf{0} & \mathbf{-1} & \mathbf{0} & \mathbf{0} \\ 9 & \mathbf{1} & \mathbf{-1} & \mathbf{1} & \mathbf{1} & \mathbf{-1} & \mathbf{-1} & \mathbf{1} \\ 10 & \mathbf{1} & \mathbf{1} & \mathbf{-1} & \mathbf{-1} & \mathbf{-1} & \mathbf{-1} & \mathbf{1} \\ 11 & \mathbf{1} & \mathbf{1} & \mathbf{-1} & \mathbf{0} & \mathbf{-1} & \mathbf{0} & \mathbf{0} \\ 12 & \mathbf{1} & \mathbf{1} & \mathbf{-1} & \mathbf{1} & \mathbf{-1} & \mathbf{1} & \mathbf{-1} \\ 13 & \mathbf{1} & \mathbf{1} & \mathbf{0} & \mathbf{-1} & \mathbf{0} & \mathbf{-1} & \mathbf{0} \\ 14 & \mathbf{1} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ 15 & \mathbf{1} & \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} \\ 16 & \mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{-1} & \mathbf{1} & \mathbf{-1} & \mathbf{-1} \\ 17 & \mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\ 18 & \mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{1} \end{array}$$

Every row in the $\mathbf{X}$ matrix is in boldface because it represents 5 replicated rows, one

for each sheet of package liner being cut into 5 pieces.

$$Z_1 = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}, \quad Z_2 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \text{ and}$$

$$Z_3 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Every row in the Z_1 , Z_2 , and Z_3 matrices is in boldface because it represents 5 replicated rows, one for each sheet of package liner being cut into 5 pieces. The structure of Z_1 corresponds to the restrictions on randomizing HTC factor X_1 , the structure of Z_2 corresponds to the restrictions on randomizing HTC factor X_2 , and the structure of Z_3 corresponds to the restrictions on randomization caused by each sheet of plastic liner being cut into 5 pieces. Therefore, $Z = [Z_1 \ Z_2 \ Z_3]$.

The SAS code for the analysis of this mixed model is as follows:

```
TITLE 'PEEL STRENGTH ANALYSIS';
DATA IN; INPUT TEMP PRES TIME STRENGTH
TEMP_B PRES_B REP_B @@;
CARDS;
-1 -1 -1 7.0 1 1 1
```

-1	-1	-1	6.9	1	1	1
-1	-1	-1	6.5	1	1	1
-1	-1	-1	6.0	1	1	1
-1	-1	-1	5.5	1	1	1
-1	-1	0	6.5	1	1	2
-1	-1	0	6.1	1	1	2
-1	-1	0	6.7	1	1	2
-1	-1	0	7.3	1	1	2
-1	-1	0	6.9	1	1	2
-1	-1	1	5.5	1	1	3
-1	-1	1	5.5	1	1	3
-1	-1	1	5.5	1	1	3
-1	-1	1	5.3	1	1	3
-1	-1	1	5.9	1	1	3
-1	0	-1	6.1	1	2	4
-1	0	-1	6.0	1	2	4
-1	0	-1	6.3	1	2	4
-1	0	-1	5.7	1	2	4
-1	0	-1	4.3	1	2	4
-1	0	0	3.7	1	2	5
-1	0	0	5.3	1	2	5
-1	0	0	6.0	1	2	5
-1	0	0	5.3	1	2	5
-1	0	0	5.7	1	2	5
-1	0	1	6.6	1	2	6
-1	0	1	5.7	1	2	6
-1	0	1	5.3	1	2	6
-1	0	1	5.1	1	2	6
-1	0	1	5.5	1	2	6
-1	1	-1	5.3	1	3	7
-1	1	-1	4.5	1	3	7
-1	1	-1	5.1	1	3	7
-1	1	-1	6.3	1	3	7
-1	1	-1	6.4	1	3	7
-1	1	0	4.3	1	3	8
-1	1	0	6.5	1	3	8
-1	1	0	6.0	1	3	8
-1	1	0	5.3	1	3	8
-1	1	0	6.2	1	3	8
-1	1	1	4.1	1	3	9
-1	1	1	5.9	1	3	9
-1	1	1	6.0	1	3	9

-1 1 1 5.9 1 3 9
-1 1 1 5.7 1 3 9
1 -1 -1 5.7 2 4 10
1 -1 -1 5.0 2 4 10
1 -1 -1 6.1 2 4 10
1 -1 -1 6.2 2 4 10
1 -1 -1 6.9 2 4 10
1 -1 0 5.3 2 4 11
1 -1 0 5.7 2 4 11
1 -1 0 4.7 2 4 11
1 -1 0 5.9 2 4 11
1 -1 0 5.7 2 4 11
1 -1 1 5.5 2 4 12
1 -1 1 5.3 2 4 12
1 -1 1 5.0 2 4 12
1 -1 1 6.0 2 4 12
1 -1 1 5.3 2 4 12
1 0 -1 5.5 2 5 13
1 0 -1 5.3 2 5 13
1 0 -1 5.9 2 5 13
1 0 -1 5.7 2 5 13
1 0 -1 6.1 2 5 13
1 0 0 5.3 2 5 14
1 0 0 5.3 2 5 14
1 0 0 5.3 2 5 14
1 0 0 5.7 2 5 14
1 0 0 5.5 2 5 14
1 0 1 5.5 2 5 15
1 0 1 5.7 2 5 15
1 0 1 4.7 2 5 15
1 0 1 6.0 2 5 15
1 0 1 5.5 2 5 15
1 1 -1 5.3 2 6 16
1 1 -1 4.5 2 6 16
1 1 -1 5.7 2 6 16
1 1 -1 5.7 2 6 16
1 1 -1 5.3 2 6 16
1 1 0 5.1 2 6 17
1 1 0 5.5 2 6 17
1 1 0 5.9 2 6 17
1 1 0 5.7 2 6 17
1 1 0 6.1 2 6 17

```

1 1 1 6.2 2 6 18
1 1 1 6.4 2 6 18
1 1 1 6.0 2 6 18
1 1 1 6.2 2 6 18
1 1 1 4.7 2 6 18
;
PROC MIXED DATA=IN;
  CLASS TEMP_B PRES_B REP_B;
  MODEL STRENGTH = TEMP|PRES|TIME@2
  PRES*PRES TIME*TIME / DDFM=SATTERTH;
  RANDOM TEMP_B PRES_B REP_B;
RUN;

```

The variable,

TEMP_B

corresponds to the random effect in the mixed model associated with the HTC factor TEMP, the variable

PRES_B

corresponds to the random effect in the model associated with the HTC factor PRES, and the variable

REP_B

corresponds to the random effect in the model associated with each sheet of package liner being cut into 5 pieces. The default variance component estimation procedure in *Proc Mixed* is the REML procedure, which was the recommended procedure from Chapter 6. Portions of the results from the SAS output follow.

Covariance Parameter Estimates (REML)

Cov Parm	Estimate
TEMP_B	0.00000000
PRES_B	0.00122917
REP_B	0.00940139
Residual	0.36477778

Tests of Fixed Effects

Source	NDF	DDF	Type III F	Pr > F
TEMP	1	1	1.49	0.4368
PRES	1	1	3.57	0.3099
TEMP*PRES	1	1	3.57	0.3099
TIME	1	8	1.14	0.3174
TEMP*TIME	1	8	0.50	0.5013
PRES*TIME	1	8	6.07	0.0391
PRES*PRES	1	1	2.53	0.3572
TIME*TIME	1	8	0.01	0.9372

This analysis, where randomization restrictions are accounted for, is quite different than the traditional analysis. Now, PRES and TEMP*PRES are very non-significant. The two factor interaction, PRES*TIME, is still significant at the $\alpha = .05$ level.

The mixed model analysis also gives variance component estimates of: $\sigma^2 = 0.36478$, $\sigma_1^2 = 0.0$, $\sigma_2^2 = .00123$, and $\sigma_3^2 = .00940$. This is very informative in that the variance component associated with the HTC factor TEMP is zero, and the two variance components associated with PRES and REP are also very small compared to the overall error, σ^2 . Even though the variance components are either zero or very small, the analysis differs markedly from the more traditional analysis.

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