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# FACTORIAL DESIGNS WITH MULTIPLE LEVELS OF RANDOMIZATION

Derek Bingham<sup>1</sup>, Randy Sitter<sup>1</sup>, Elizabeth Kelly<sup>2</sup>, Leslie Moore<sup>2</sup>

and J. David Olivas<sup>2</sup>

<sup>1</sup>Simon Fraser University and <sup>2</sup>Los Alamos National Labs

Abstract: Design and analysis of factorial experiments with randomization restrictions has received considerable attention in recent years; motivated by studies of multi-stage processes or systems. This has given rise to seemingly unrelated methods of design construction, specific to the layout (e.g., split-plot, split-lot, strip-plot designs). We develop a general approach to this problem that includes most approaches in the literature as special cases, and is easily adaptable to designs which are combinations of different layouts.

Key words and phrases: Blocking, orthogonal array, split-lot, split-plot, strip-plot.

# 1. Introduction

Factorial and fractional factorial designs are commonly used as experiment plans to study the impact of several factors on a process. Complete randomization of the experiment trials is frequently impractical when it is difficult or costly to change the level settings of some of the factors. Being cognizant of the nature of the system, one may instead choose a layout which imposes restrictions on the randomization of the runs.

Recently, there has been considerable attention given to fractional factorial designs with such randomization restrictions. Experimenters have adapted familiar plans such as split-plot (Addelman (1964), Huang, Chen and Voelkel (1998), Bingham and Sitter (1999, 2001) and Bisgaard (2000)), strip-plot (Miller (1997)), split-lot (Mee and Bates (1998)) and blocked designs (Bisgaard (1994), Sitter, Chen and Feder (1997), Sun, Wu and Chen (1997) and Cheng, Li and Ye (2004)) to the fractional factorial treatment structure. However, there is no unified approach to the construction of such designs with randomization restrictions. For instance, Miller (1997) requires the use of a *Latin square fraction* to construct a fractional factorial strip-plot design, whereas for split-plot designs, simple rules for the number of sub-plot factors in a fractional generator are given (e.g., see Bisgaard (2000) and Bingham and Sitter (1999, 2001)).

In this article, we develop a general method for the construction of fractional factorial designs with randomization restrictions that considers the randomization structure and treatment structure separately. By examining the randomization structure first, we can determine which factorial effects are impacted by the error term at each stage of randomization. In addition, we can easily determine the allowable fractional generators for the desired randomization structure. The approach is simple and adaptable to combinations of several design structures.

This research was motivated by a study at Los Alamos National Laboratory (LANL) to produce a plutonium alloy with high decay rate (Freibert, Olivas and Coonley (2002)). The nature of the process and cost/time restrictions made it advantageous to consider what one might term a split-plot/split-lot experiment with four stages. The plutonium application is described in Section 2. Section 3 proposes a framework for the construction of full factorial designs with randomization restrictions, and Section 4 shows how to adapt the approach to fractional factorial designs. We conclude with some remarks and discussion in Section 5.

### 2. Motivating Application

Researchers at LANL are interested in studying a process that creates a plutonium alloy with a high decay rate for eventual use in accelerated testing (see Freibert, Olivas and Coonley (2002)). The current interest is in performing a designed experiment to determine which factors most impact the alloy properties and should be subsequently studied to optimize the process.

The process consists of four stages, each with one or more factors, described below. Though the process seems simple, keep in mind that the experimenters are working with a highly toxic material and even a simple task such as cutting the material must be done while keeping the material in isolation.

**Stage 1.** Molten material is poured into a cast that yields ten "cookies" with roughly the dimensions of a hockey puck. A casting of ten cookies will be done at each of the high and low levels of factor 1 (Composition), however, only two cookies from each casting will be available for the study.

Stage 2. The material undergoes a type of heat treatment which can be run at two possible settings of factor 2 (Heat Treat 1), high and low. To do so, each of the four cookies are cut in half to form eight half-cookies. The heat treatment is applied to a half-cookie (four at the high level of factor 1 and four at the low level). The two halves of a cookie are randomly assigned one of the two levels of factor 2 and run through the first heat treatment process. Following the heat treatment, each half-cookie is cut into five coupons, one of which is held back in case of run failures at subsequent stages, leaving four coupons available for experimentation.

**Stage 3.** Another heat treatment is applied to coupons at either the high or low level of factor 3 (Heat Treat 2). For practical reasons, it is necessary for four coupons to undergo the heat treatment simultaneously.

**Stage 4.** The coupons undergo a final heat treatment at the four possible high and low settings of factors 4 (HT-Hot) and 5 (HT-Cold). Similar to the previous stage, it is necessary to process several coupons at the same time. The measured density of the fully processed coupons is the characteristic of interest.

In this experiment, subsequent stages of processing begin only after all materials have been processed at a given stage. For example, Stage 3 can begin only after all half-cookies have undergone Stage 2 heat treatments. While this appears to complicate matters, it can be an advantage as it allows us to combine coupons from different half-cookies in the same application of a heat treatment.

We wish to explore the impact of 5 factors, each at 2 levels, in 32 runs. Thus, a  $2^5$  full factorial plan can be used. There are, however, randomization restrictions at each of the four stages of the process. There are also costs associated with the number of applications of each heat treatment, forcing one to group coupons together at various stages of the experiment.

So, how should the experiment be run? Facing this question and more specific issues such as how to form groups of experimental units to impact effect estimates as little as possible, and how to maintain a reasonably simple analysis strategy, led us to consider the general problem of designing experiments with multiple stages, various randomization restrictions, and batch-size restrictions; eg., blocked designs, split-plot designs, split-split-plot designs, blocked split-plot designs, split-lot designs, strip-plot designs, and combinations and generalizations of all of the above. We attempt to develop a general methodology for doing so, and return to the plutonium experiment to demonstrate the approach.

# 3. Full Factorial Designs

# 3.1. A Framework for Randomization Restrictions

We consider the design of full factorial experiments with randomization restrictions and delay discussion of fractional factorial designs to Section 4. Ours is an attempt to develop a unified approach for using columns of the full factorial design matrix to define the randomization structure of an experiment in a similar way to determining the treatment structure of a fractional factorial design.

A  $2^k$  full factorial design has k factors, each with 2 levels, and  $n = 2^k$  runs consisting of all level combinations of the k factors. More formally, let **P** be the  $k \times (2^k - 1)$  matrix whose columns consist of the vector space spanned by the columns of  $I_k$  over the finite field GF(2), excluding the identity column of 0's. All vectors of the k-dimensional vector space generated by the rows of **P** correspond

to an  $n \times (n-1)$  matrix, X. The full factorial design is an assignment of k factors to basis columns of X. Without loss of generality, we can write the columns of Xas  $X = \{c_1, \ldots, c_k, c_{k+1}, \ldots, c_{n-1}\}$ , with the basis columns labelled  $c_1, \ldots, c_k$ . From a linear model standpoint, columns  $c_1, \ldots, c_k$  represent the main effect columns and the remaining columns are for interactions obtained via additions of subsets of  $c_1, \ldots, c_k$  modulo 2.

The first k columns of  $\boldsymbol{X}$  define the treatment structure of the design (i.e., which treatments are applied to experimental units), but not the randomization structure. The randomization structure of the experiment defines the grouping of the experiment runs at each stage of randomization. For example, in Section 2 the grouping of trials refers to coupons which are processed together at each stage of the plutonium application.

Let there be S stages of randomization. This implies that there are S-1stages with randomization restrictions, with the final stage of randomization being the final unit to unit variability. For the s-th stage of restricted randomization, we use  $r_s$  linearly independent columns of X to group the trials of a  $2^k$ design into  $G_s = 2^{r_s}$  sets of size  $2^{k-r_s} = 2^k/G_s$  (the linear independence refers only to the current stage of randomization and not necessarily to that between stages). Define  $\boldsymbol{\delta}_{i}^{(s)}$  to be the *i*<sup>th</sup> randomization restriction factor for  $i = 1, \ldots, r_s$ at the s-th stage of randomization  $(s = 1, \dots, S-1)$ , and let  $\boldsymbol{\delta}_i^{(s)}$  be assigned to a column of X and no other  $\delta_j^{(s)}$  be assigned to this column. Together,  $\delta_1^{(s)}, \ldots, \delta_{r_s}^{(s)}$ define the randomization restrictions at the s-th stage. That is, the  $2^{r_s}$  unique combinations of the randomization restrictions in the rows of X are used to form the  $G_s$  sets of trials for this stage of randomization. Note that we are using the term "randomization restriction factor" to parallel terminology used in the literature for special cases, even though the  $\delta$ 's are not really factors but merely constructs to formalize the randomization structure. Examples include blocking factors (Sitter, Chen and Feder (1997) and Sun, Wu and Chen (1997)) and splitting factors (Bingham, Schoen and Sitter (2003)).

Similar to blocking factorial designs (Sun, Wu and Chen (1997), this can be viewed as a special case of fractionation. The assignment of randomization restriction factors to columns of  $\boldsymbol{X}$  implies other restrictions. Thus, if  $\boldsymbol{\delta}_i^{(s)}$  and  $\boldsymbol{\delta}_j^{(s)}$  are two randomization restriction columns in the full factorial design matrix at the *s*-th stage of randomization, then not only will the levels of these columns be constant for the set of trials, but so will their sum (over GF(2)).

Let  $\mathcal{L}_s = \{l_{si}\}_{i=1}^{r_s}$  be the index set of columns used for assignment of randomization restriction factors at stage s, so that  $\boldsymbol{\delta}_i^{(s)} = \boldsymbol{c}_{l_{si}}$  or, equivalently,  $\Delta^{(s)} = \boldsymbol{c}_{l_{si}} \boldsymbol{\delta}_i^{(s)}$  for  $i = 1, \ldots, r_s$ , where  $\Delta^{(s)}$  is a column of 0's. Call the  $r_s$  words of this type, randomization defining words. Then, similar to fractional factorial

designs, taking all possible sets of sums (over GF(2)) of these defining words creates the randomization defining contrast sub-group (RDCSG) for the s-th stage of randomization. This amounts to associating the sub-space spanned by the  $r_s$ randomization restriction columns with randomization restrictions at this stage.

One way to view the RDCSG is that it contains the list of columns of X whose elements are not allowed to vary within each of the unique settings in the columns corresponding to the randomization defining words. Consequently, when the current stage of randomization, s, is nested within another stage, each of the randomization restrictions from the previous stage which describe the nesting must be included as randomization restrictions in the current stage.

The randomization restrictions impact the analysis of the experiment. The multiple linear regression model is assumed to be the model of interest. Each stage of randomization induces a new random error term, with runs in the same group receiving the same error term and thus being correlated. The model is

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \sum_{s=1}^{S-1} \boldsymbol{E}^{(s)} + \boldsymbol{\epsilon}, \qquad (1)$$

where  $\boldsymbol{y} = (y_1, \ldots, y_n)', \ \boldsymbol{\beta} = (\beta_0, \ldots, \beta_k)', \ \boldsymbol{\epsilon} = (\epsilon_1, \ldots, \epsilon_n)' \sim N(\boldsymbol{0}, \boldsymbol{I}\sigma_{\boldsymbol{\epsilon}}^2)$  and  $\boldsymbol{E}^{(s)} = (E_1^{(s)}, \ldots, E_n^{(s)})'$ . We define  $E_j^{(s)} = e_{k(j)}^{(s)}$ , where  $k(j) = 1 + \sum_{i=1}^{r_s} c_{l_sij} 2^{i-1}$ ,  $c_{l_sij}$  is the *j*-th element of  $\boldsymbol{c}_{l_{si}}$  and  $e_1^{(s)}, \ldots, e_{G_s}^{(s)}$  are iid  $N(0, \sigma_s^2)$  and independent of  $\boldsymbol{\epsilon}$ . Note that, for the *s*-th stage, there are only  $G_s$  different  $e_{k(j)}^{(s)}$ 's, and thus only  $G_s$  unique  $E_j^{(s)}$ 's corresponding to the  $G_s$  groups.

Under this model, the factorial effects resulting from performing the experiment design  $\mathbf{X}$  will have an error variance which is a linear combination of the  $\sigma_s^2$ 's and  $\sigma_\epsilon^2$ . Specifically, the effects which are confounded with randomization restrictions at the s-th stage of randomization have an error variance which contains a multiple of  $\sigma_s^2$  in the sum of variance components. The effects which are orthogonal to the randomization restrictions at the s-th stage have error variances which do not depend on  $\sigma_s^2$ . We illustrate via two examples.

**Example 1.** Consider the  $2^4$  design (factors labeled 1-4) in  $2^2$  blocks. Let  $\delta_1^{(1)} = 14$  and  $\delta_2^{(1)} = 123$ , where 14 represents the sum of columns 1 and 4 and 123 of columns 1, 2 and 3, of X modulo 2, respectively. The RDCSG, which Sun, Wu and Chen (1997) call the block defining contrast sub-group, is

$$\Delta^{(1)} = 14\boldsymbol{\delta}_1^{(1)} = 123\boldsymbol{\delta}_2^{(1)} = 234\boldsymbol{\delta}_1^{(1)}\boldsymbol{\delta}_2^{(1)}$$

Rather than beginning the RDCSG with the mean I, which is traditional for the defining contrast sub-group of a fractional factorial design, we use  $\Delta^{(1)}$ .

						$oldsymbol{\delta}_1^{(1)}$	$oldsymbol{\delta}_2^{(1)}$	$oldsymbol{\delta}_1^{(1)}oldsymbol{\delta}_2^{(1)}$
		1	2	3	4	14	$1\bar{2}3$	234
$E_1 = e_1$	$\epsilon_1$	1	0	1	1	0	0	0
$E_2 = e_1$	$\epsilon_2$	1	1	0	1	0	0	0
$E_3 = e_1$	$\epsilon_3$	0	1	1	0	0	0	0
$E_4 = e_1$	$\epsilon_4$	0	0	0	0	0	0	0
$E_5 = e_2$	$\epsilon_5$	0	0	0	1	1	0	1
$E_6 = e_2$	$\epsilon_6$	1	0	1	0	1	0	1
$E_7 = e_2$	$\epsilon_7$	1	1	0	0	1	0	1
$E_8 = e_2$	$\epsilon_8$	0	1	1	1	1	0	1
$E_{9} = e_{3}$	$\epsilon_9$	1	1	1	1	0	1	1
$E_{10} = e_3$	$\epsilon_{10}$	1	0	0	1	0	1	1
$E_{11} = e_3$	$\epsilon_{11}$	0	1	0	0	0	1	1
$E_{12} = e_3$	$\epsilon_{12}$	0	0	1	0	0	1	1
$E_{13} = e_4$	$\epsilon_{13}$	1	0	0	0	1	1	0
$E_{14} = e_4$	$\epsilon_{14}$	0	0	1	1	1	1	0
$E_{15} = e_4$	$\epsilon_{15}$	0	1	0	1	1	1	0
$E_{16} = e_4$	$\epsilon_{16}$	1	1	1	0	1	1	0

Table 1. Design for Example 1.

This is done for two reasons. First, it avoids confusion with fractional factorial designs where effects appearing in the defining contrast sub-group are aliased with the mean. Second, it allows us to easily see which effects are confounded with a randomization restriction, or sum thereof. The importance of this latter fact is emphasized shortly.

To see how the experiment would be run, and the impact on the variance of the effect estimates, consider Table 1 (we suppress the superscript (1) on  $E_j^{(1)}$ and  $e_{k(j)}^{(1)}$  for simplicity). The first two columns contain the block and replication errors, respectively. Columns labeled 1-4 represent the settings of the four factors in the full factorial design. Observe that the experiment is run in four blocks of four units according to the values of  $\delta_1^{(1)}$  and  $\delta_2^{(1)}$ . Furthermore see that the error terms  $(e_1, \ldots, e_4)$  are associated with the values of  $\delta_1^{(1)}$  and  $\delta_2^{(1)}$ , 00, 01, 10, 11, respectively, yielding k(j) values  $1, \ldots, 4$  (i.e., the four blocks). Since all columns not associated with  $\Delta^{(1)}$  are orthogonal to the four level column of e's, they cancel out of the effect estimates and the error variance of these effects depends only on  $\sigma_{\epsilon}^2$ . Whereas, for the three columns 14, 123 and 234 this is not so, and their variance will be a linear combination of  $\sigma_{\epsilon}^2$  and  $\sigma_1^2$ .

While this representation of the randomization structure for blocked designs is well known, our abstraction describes a much wider class of randomization restricted designs. For designs with multiple stages of randomization (S > 1), where trials are performed in groups of size  $2^{r_s}$ , a separate RDCSG is required for each s = 1, ..., S - 1. For nested designs, randomization restrictions from previous stages are included in subsequent stages to identify the final grouping of trials. When this is not done, it implies that no nesting is occurring and that the design is crossed in some sense. We illustrate these features in the next example.

**Example 2.** Consider the 2<sup>5</sup> split-split-plot design, with factors  $\{1, 2\}$ ,  $\{3, 4\}$ , and  $\{5\}$  labeling whole-plot, sub-plot and sub-sub-plot factors, respectively. To begin, factors 1 and 2 group trials within whole-plot settings, via the restrictions  $\boldsymbol{\delta}_1^{(1)} = 1$  and  $\boldsymbol{\delta}_2^{(1)} = 2$ . Within each whole-plot setting, one randomly selects a level setting of factors 3 and 4 and performs two trials, varying only factor 5. To group the experimental trials into 16 sets of size 2 where only factor 5 can change levels, set  $\boldsymbol{\delta}_1^{(2)} = 1$ ,  $\boldsymbol{\delta}_2^{(2)} = 2$ ,  $\boldsymbol{\delta}_3^{(2)} = 3$  and  $\boldsymbol{\delta}_4^{(2)} = 4$ . Thus,

$$\begin{split} \Delta^{(1)} &= 1\boldsymbol{\delta}_{1}^{(1)} = 2\boldsymbol{\delta}_{2}^{(1)} = 12\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{2}^{(1)},\\ \Delta^{(2)} &= 1\boldsymbol{\delta}_{1}^{(2)} = 2\boldsymbol{\delta}_{2}^{(2)} = 3\boldsymbol{\delta}_{3}^{(2)} = 4\boldsymbol{\delta}_{4}^{(2)} = 12\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{2}^{(2)} = 13\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{3}^{(2)} = 14\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{4}^{(2)} \\ &= 23\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{3}^{(2)} = 24\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{4}^{(2)} = 34\boldsymbol{\delta}_{3}^{(2)}\boldsymbol{\delta}_{4}^{(2)} = 123\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{3}^{(2)} = 124\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{4}^{(2)} \\ &= 134\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{3}^{(2)}\boldsymbol{\delta}_{4}^{(2)} = 234\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{3}^{(2)}\boldsymbol{\delta}_{4}^{(2)} = 1234\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{3}^{(2)}\boldsymbol{\delta}_{4}^{(2)}. \end{split}$$

Suppose instead that the first two randomization restrictions at the second stage were not included. The corresponding RDCSG would then be  $\Delta^{(2)} = 3\delta_1^{(2)} = 4\delta_2^{(2)} = 34\delta_1^{(2)}\delta_2^{(2)}$ . This would imply that factors 3 and 4 are not nested within level settings of factors 1 and 2. Instead, the levels of factors 1 and 2 would be allowed to vary within level settings of factors 3 and 4. In this case, one randomly chooses one of the four setting combinations of factors 1 and 2, and then processes eight units in random order. Then one randomly chooses a second setting combination of factors 1 and 2, and so on. After this first stage is completed one randomly chooses one of the four setting combinations of factors 3 and 4. This is an example of a split-lot design, and we revisit it in Example 3.

#### 3.2. Implications of analysis on design

One can use the columns of X to design experiments with randomization restrictions, and the RDCSG's show which effects are impacted by each stage of randomization. This is important as this approach shows how to both construct randomization restricted designs and evaluate the impact of confounding at each stage of randomization.

From a design perspective, the randomization restrictions pose an important challenge. The experiment design should be chosen so that the estimated factorial effects are impacted as little as possible by the additional error terms. So, by using the columns of the design matrix to determine the grouping of runs for

Effect	Variance	Degrees of Freedom
1, 2, 12	$\sigma_1^2 + \frac{1}{8}\sigma_\epsilon^2$	3
3, 4, 34	$\sigma_2^2 + \frac{1}{8}\sigma_\epsilon^2$	3
5,13,14,15,23,24,25,35,45 and 16 others	$\frac{1}{8}\sigma_{\epsilon}^2$	25

Table 2. Effect Variances for the Split-Lot Example.

each stage of randomization, we should make as many of the factorial effects orthogonal to the randomization error terms as possible, thereby eliminating these random effects from the variance of these factorial effects. In addition, the analysis method is impacted by the grouping of factorial effects into those with common variance. For example, in unreplicated factorial experiments, separate half-normal plots of effects with the same variance is a common analysis strategy.

Viewing Examples 1 and 2, there does not appear to be a design issue. However, this is not the case once we consider how we might analyze the experiment. We illustrate by re-visiting the split-lot design given at the end of Example 2.

**Example 3. Split-lot Reconsidered.** Suppose the split-lot design introduced at the end of Example 2 is unreplicated. In light of model (1), the two RDCSG's group effect estimates into three sets with different variances as depicted in Table 2. The traditional way to analyze such an unreplicated factorial experiment is to construct a separate half-normal plot for each group of effects that have the same error variance (Daniels (1959)). One is left with almost no way to analyze effects 1, 2, and 12, or 3, 4, and 34, because there are very few degrees of freedom within each of the first two groups.

To avoid this difficulty, one can introduce two additional randomization restriction factors  $\boldsymbol{\delta}_3^{(1)}$  and  $\boldsymbol{\delta}_3^{(2)}$ , one at each stage of randomization. This has the effect of grouping the trials into 8 sets of 4 runs instead of 4 sets of 8 runs. Care must be taken in how  $\boldsymbol{\delta}_3^{(1)}$  and  $\boldsymbol{\delta}_3^{(2)}$  are assigned to interaction columns. For example, if we assign  $\boldsymbol{\delta}_3^{(1)} = 13$ , then  $3 = \boldsymbol{\delta}_1^{(1)} \boldsymbol{\delta}_3^{(1)}$ . As a consequence factor 3 will also be the same as a first stage factor, thereby destroying the desired randomization structure. We call this assignment ineligible (we shall be clearer on this shortly). An example of eligible assignments are  $\boldsymbol{\delta}_3^{(1)} = 1345$  and  $\boldsymbol{\delta}_3^{(2)} = 1245$ , and the two RDCSG's become

$$\begin{split} \Delta^{(1)} &= 1\boldsymbol{\delta}_{1}^{(1)} = 2\boldsymbol{\delta}_{2}^{(1)} = 12\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{2}^{(1)} = 345\boldsymbol{\delta}_{3}^{(1)} = 1345\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{3}^{(1)} = 2345\boldsymbol{\delta}_{2}^{(1)}\boldsymbol{\delta}_{3}^{(1)} \\ &= 12345\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{2}^{(1)}\boldsymbol{\delta}_{3}^{(1)} \\ \Delta^{(2)} &= 3\boldsymbol{\delta}_{1}^{(2)} = 4\boldsymbol{\delta}_{2}^{(2)} = 34\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{2}^{(2)} = 125\boldsymbol{\delta}_{3}^{(2)} = 1245\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{3}^{(2)} = 1235\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{3}^{(2)} \\ &= 12345\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{3}^{(2)}. \end{split}$$

### DESIGNS WITH MULTI-LEVEL RANDOMIZATION

Effect	Variance	Degrees of Freedom
1, 2, 12, 345, 1345, 2345	$\frac{1}{2}\sigma_1^2 + \frac{1}{8}\sigma_\epsilon^2$	6
3, 4, 34, 125, 1245, 1235	$\frac{1}{2}\sigma_2^2 + \frac{1}{8}\sigma_\epsilon^2$	6
5,13,14,15,23,24,25,35,45 and 9 others	$\frac{1}{8}\sigma_{\epsilon}^2$	18
12345	$\tfrac{1}{2}(\sigma_1^2+\sigma_2^2)+\tfrac{1}{8}\sigma_\epsilon^2$	1

Table 3. New Effect Variances for Example 3.

Notice that effect 12, 345 appears in both  $\Delta^{(1)}$  and  $\Delta^{(2)}$ , and thus picks up both  $\sigma_1^2$  and  $\sigma_2^2$ . The distribution of degrees of freedom for this randomization structure is as depicted in Table 3. Now one has sacrificed the ability to consider 12345, but can do separate half-normal plots for the other three groups that have some validity under the usual assumptions of effect sparsity and effect hierarchy. To see that there are different choices with varying desirability, consider instead choosing  $\boldsymbol{\delta}_3^{(1)} = 1,234$  and  $\boldsymbol{\delta}_3^{(2)} = 1,345$ . In this case, the common effect in  $\Delta^{(1)}$ and  $\Delta^{(2)}$  would be 34 and the design could not be used to test for this effect.

# 3.3. Searching for Designs

In this section, the problem of searching for full factorial experiment designs with randomization restrictions is considered. We describe an algorithm to do so as a series of steps and use Example 3 to aid in the explanation of each step.

Step 1. Initial Restrictions. To set up the design selection problem, one must first decide upon the basic desired structure: number of stages of randomization restriction, S; which factors are at each stage; the number of groups at each stage of randomization; split or lot (i.e., nested or crossed) structure at each stage.

The grouping of experimental units at each stage of randomization can then be achieved by using the columns of X to construct an RDCSG for each stage of randomization that maintains the desired structure. To do so, the framework developed in the previous section can be applied with combinations of randomization restrictions, as long as some rules are followed: (i) the  $r_s$  randomization restrictions must form a sub-group of columns of X of size  $2^{r_s} - 1$ ; (ii) when the current stage of randomization, s, is nested within another stage, s'(< s), each of the randomization restrictions from the previous stage which describe the nesting must be included as randomization restrictions in the current stage; (iii) the choice of generators must not change which factors are at which stage.

The above eligibility requirements bear resemblance to rules used for splitplot or blocked designs (Bisgaard (1994, 2000) and Bingham and Sitter (1999, 2001)). If we look at a particular stage of randomization in isolation, main effects

and interactions that are fixed act like whole-plot or blocking factors. The eligibility rules do not allow other main effects to be confounded with these blocks or whole-plots. Overall, when effects appear in multiple RDCSG's, these effects are confounded with randomization restriction factors at multiple stages of randomization. The spirit here, akin to blocked designs, is to have the confounding, when possible, occur with higher-order rather than lower-order interactions.

The rules have implications on the selection of randomization restrictions. First, when one is assigning a randomization restriction to a column of X, the column cannot be a linear combination of other randomization restrictions at the same stage, otherwise rule (i) would be violated. Second, rule (ii) implies that in nested designs such as split-split-plot designs one must carry forward the randomization restrictions from previous stages and some of these randomization restrictions can apply to main effects. Third, a main effect cannot be confounded with a randomization restriction factor or product of randomization restriction factors from a different stage than its own. Any design satisfying the three rules will be termed *eligible* as it has the desired structure.

To illustrate, consider Example 3. There are S = 3 stages of randomization and we wish to run both stages 1 and 2 in eight groups of four. Factors 1 and 2 are necessarily at stage 1 and factors 3 and 4 at stage 2. Since S = 3, we need S - 1 = 2 RDCSG's. In addition, the desired structure predetermines part of each RDCSG so that

$$\Delta^{(1)} = 1\boldsymbol{\delta}_{1}^{(1)} = 2\boldsymbol{\delta}_{2}^{(1)} = 12\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{2}^{(1)} = w_{1}\boldsymbol{\delta}_{3}^{(1)} = 1w_{1}\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{3}^{(1)} = 2w_{1}\boldsymbol{\delta}_{2}^{(1)}\boldsymbol{\delta}_{3}^{(1)}$$

$$= 12w_{1}\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{2}^{(1)}\boldsymbol{\delta}_{3}^{(1)}, \qquad (2)$$

$$\Delta^{(2)} = 3\boldsymbol{\delta}_{1}^{(2)} = 4\boldsymbol{\delta}_{2}^{(2)} = 34\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{2}^{(2)} = w_{2}\boldsymbol{\delta}_{3}^{(2)} = 3w_{2}\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{3}^{(2)} = 4w_{2}\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{3}^{(2)}$$

$$= 34w_{2}\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{3}^{(2)}, \qquad (3)$$

and the problem reduces to finding good generators  $\boldsymbol{\delta}_3^{(1)} = w_1$  and  $\boldsymbol{\delta}_3^{(2)} = w_2$ .

Step 2. Constructing a Search Table. Similar to the algorithm of Franklin and Bailey (1977) for finding fractional factorial designs (see also, Bingham and Sitter (1999)), a search table can be constructed to aid the design search process. The column headers of the search table represent the randomization restrictions that are not already set by the initial structure, ordered by the stage of randomization. The row headers of the search table are the interactions that can potentially be confounded with a randomization factor. The elements of the search table are the interaction between the row and column headers. The search table for Example 3 is given in Table 4.

Step 3. Obtaining an Eligible Design. Finding a design amounts to finding an eligible randomization restriction assignment in each of the columns in the

search table. This can be done systematically by stepping down Column 1 until an eligible effect is obtained for the first restriction. This would then be what we termed  $\delta_3^{(1)} = w_1$  in (2). Then keeping the eligible effect in Column 1 fixed, step down Column 2 until an eligible effect is obtained;  $w_2$  in (3). If there are additional columns, one would hold the two chosen effects in Columns 1 and 2 fixed and step down Column 3 and so on. Once a generator from each column is obtained, we have an eligible design. (1) Note that one must take into account all effects in  $\Delta^{(s)}$  for  $s = 1, \ldots, S - 1$  when using rules (i), (ii) and (iii) to determine whether an effect in Column 2 is eligible. For example, in Example 3 in Column 1, all 2fi's containing a 1 or 2, and all 3fi's containing both 1 and 2, are ineligible, and choosing  $123\delta_3^{(1)}$  (ie.,  $w_1 = 123$ ), implies  $12w_1\delta_1^{(1)}\delta_2^{(1)}\delta_3^{(1)} = 3\delta_1^{(1)}\delta_2^{(1)}\delta_3^{(1)}$ , which violates rule (iii). (2) Within a stage of randomization one need only consider effects below the current effect from previous columns within that stage of randomization. But, when one moves to a new stage of randomization, one must start at the top of the column.

Step 4. Checking Isomorphism. Once an eligible design is obtained, it need only be kept if it is non-isomorphic to the current collection of *eligible designs*, say  $\mathcal{D}$ . Thus one must check the isomorphism of the eligible design to each design in the current collection. Here, two designs are isomorphic if one can be obtained from the other via a sequence of row exchanges, re-labeling of 0's as 1's and vice versa within a column, and re-labeling of factors within each stage of randomization. If one is not too concerned with missing non-isomorphic choices that have the same value of a particular design criterion, the search can be made much quicker by declaring two designs isomorphic if they have the same value of this criterion. We discuss the choice of a good design subsequently.

Step 5. Repeat Steps 3 and 4 until all designs have been considered; i.e., keep all but the previous choice in the last column fixed, step down to the next effect, etc.

### 3.4. Design criterion

One can use the above approach to obtain all non-isomorphic designs, and then, in principle, choose the design which best suits the specific situation. In practice, one would rather have a simple "measure" that ranks design choices in some reasonable way, and then more closely view the top ten designs, say.

There is not going to be a globally best criterion for all situations. However, we can consider what is trying to be achieved in this complicated setting. As was alluded to in Example 3, we would like to have as few effects in common between RDCSG's at differing stages, as these effects will inherit variances from both stages. We would also like to have a few main effects and 2fi's at each stage,

Table 4. Search Table				
	Level 1	Level 2		
	$oldsymbol{\delta}_3^{(1)}$	$oldsymbol{\delta}_3^{(2)}$		
12	$12\boldsymbol{\delta}_2^{(1)}$	$12\boldsymbol{\delta}_2^{(3)}$		
13	$13\boldsymbol{\delta}_2^{(1)}$	$13\boldsymbol{\delta}_2^{(3)}$		
14	$14\boldsymbol{\delta}_2^{(1)}$	$14\boldsymbol{\delta}_2^{(3)}$		
15	$15\boldsymbol{\delta}_2^{(1)}$	$15\boldsymbol{\delta}_2^{(3)}$		
23	$23\boldsymbol{\delta}_2^{(1)}$	$23\boldsymbol{\delta}_2^{(3)}$		
24	$24\boldsymbol{\delta}_2^{(1)}$	$24\boldsymbol{\delta}_2^{(3)}$		
25	$25 \boldsymbol{\delta}_2^{(1)}$	$25 \boldsymbol{\delta}_2^{(3)}$		
34	$34\boldsymbol{\delta}_2^{(1)}$	$34\boldsymbol{\delta}_2^{(3)}$		
35	$35 \boldsymbol{\delta}_2^{(1)}$	$35 \boldsymbol{\delta}_2^{(3)}$		
45	$45\boldsymbol{\delta}_2^{(1)}$	$45\boldsymbol{\delta}_2^{(3)}$		
123	$123\boldsymbol{\delta}_2^{(1)}$	$123\boldsymbol{\delta}_2^{(3)}$		
•	:	•		
2345	$2345\boldsymbol{\delta}_{2}^{(1)}$	$2345\boldsymbol{\delta}_2^{(3)}$		
12345	$12345\boldsymbol{\delta}_2^{(1)}$	$12345 \delta_2^{(3)}$		

Table 4. Search Table

and the rest of the effects at that stage to be higher-order interactions, so that half-normal plots or pooling of higher-order effects is a viable analysis strategy. That is, we would like to uniformly spread out our ability to consider main effects and lower-order effects at each stage of randomization. This allows us to avoid placing all potentially active effects at the same stage of randomization.

With these ideas in mind, we introduce a simple 3-step criterion to rank the set of eligible designs. Order designs first on number of effects which are common to multiple stages, with fewer being better, and then sequentially minimize the number of such words of each length to ensure that as few lower order terms as possible appear in multiple RDCSG's. Lastly, for designs of equal rank, order on

$$V = \sum_{s=1}^{S-1} (p_s - \bar{p})^2, \tag{4}$$

where  $p_s$  is the proportion of degrees of freedom at the s-th stage that are associated with main effects or 2fi's and  $\bar{p} = \sum_s p_s/(S-1)$ . Designs with a small V are regarded as better. Being cognizant that the effect sparsity principle refers to the entire experiment design and not the individual stages of randomization, the criterion in (4) aims to evenly spread the number of potentially active effects across stages of the analysis.

As an example, in Table 3 of Example 3, only one effect is common to multiple stages, and  $p_1 = 3/6 = 0.5$ ,  $p_2 = 3/6 = 0.5$ , and  $p_3 = 9/18 = 0.5$ , so that V = 0.

#### 3.5. The plutonium processing example

We now reconsider the motivating plutonium application of Section 2 as a further illustration of applying the search strategy of Sections 3.3 and 3.4.

Step 1. There are S = 5 stages of randomization. It was desirable to use only four cookies at the first stage, each consisting of eight coupons. As such, Stage 1, consisting of settings of factor 1, must necessarily be run in four groups of eight coupons. Following this stage, each cookie is cut in half. Next, factor 2 is set and the heat treatment is applied to a half-cookie. The levels of factor 2 are set within fixed settings of factor 1, (i.e., a split-plot structure between Stage 1 and Stage 2). As each half-cookie consists of four useable coupons, the second stage is run as eight groups of four coupons. After Stage 2, the half-cookies are cut into coupons. Due to the time it takes to do each of the heat treatments in Stages 3 and 4 it was desired to run at most eight groups in each of these stages. Suppose we first chose to consider running eight groups of four coupons in Stages 3 and 4 and then four groups of eight in Stage 5. Here, none of the stages are nested within any of the previous stages.

Since S = 5, we need 4 RDCSG's. As before, the above desired structure predetermines part of each RDCSG. Thus we have

$$\begin{aligned} \Delta^{(1)} \mathbf{1} \boldsymbol{\delta}_{1}^{(1)} &= w_{1} \boldsymbol{\delta}_{2}^{(1)} = 1 w_{1} \boldsymbol{\delta}_{1}^{(1)} \boldsymbol{\delta}_{2}^{(1)}, \\ \Delta^{(2)} &= \mathbf{1} \boldsymbol{\delta}_{1}^{(2)} = w_{1} \boldsymbol{\delta}_{2}^{(2)} = 1 w_{1} \boldsymbol{\delta}_{1}^{(2)} \boldsymbol{\delta}_{2}^{(2)} = 2 \boldsymbol{\delta}_{3}^{(2)} = \mathbf{1} 2 \boldsymbol{\delta}_{1}^{(2)} \boldsymbol{\delta}_{3}^{(2)} = w_{1} 2 \boldsymbol{\delta}_{2}^{(2)} \boldsymbol{\delta}_{3}^{(2)} \\ &= \mathbf{1} 2 w_{1} \boldsymbol{\delta}_{1}^{(2)} \boldsymbol{\delta}_{2}^{(2)} \boldsymbol{\delta}_{3}^{(2)}, \\ \Delta^{(3)} &= \mathbf{3} \boldsymbol{\delta}_{1}^{(3)} = w_{2} \boldsymbol{\delta}_{2}^{(3)} = w_{3} \boldsymbol{\delta}_{3}^{(3)} = 3 w_{2} \boldsymbol{\delta}_{1}^{(3)} \boldsymbol{\delta}_{2}^{(3)} = 3 w_{3} \boldsymbol{\delta}_{1}^{(3)} \boldsymbol{\delta}_{3}^{(3)} = w_{2} w_{3} \boldsymbol{\delta}_{2}^{(3)} \boldsymbol{\delta}_{3}^{(3)} \\ &= 3 w_{2} w_{3} \boldsymbol{\delta}_{1}^{(3)} \boldsymbol{\delta}_{2}^{(3)} \boldsymbol{\delta}_{3}^{(3)}, \end{aligned} \tag{6} \end{aligned}$$

Note that the fact that 1,  $w_1$  and  $1w_1$  appear in both  $\Delta^{(1)}$  and  $\Delta^{(2)}$  implies the first two stages have a split-plot structure. This design might be termed a split-split-lot experiment in five stages. Within this structure we must search for a good set of four generators;  $\boldsymbol{\delta}_2^{(1)} = \boldsymbol{\delta}_2^{(2)} = w_1$ ,  $\boldsymbol{\delta}_2^{(3)} = w_2$ ,  $\boldsymbol{\delta}_3^{(3)} = w_3$  and  $\boldsymbol{\delta}_3^{(4)} = w_4$ .

Step 2. With the desired randomization structure set, the search table is constructed for the four remaining randomization restrictions, in Table 5. The entries in Column 1 are the possible products of the randomization restrictions,  $\delta_2^{(1)} = \delta_2^{(2)}$ , and the interactions,  $w_1$ . Similarly for Columns 2-4 and the respective randomization restrictions. For illustration purposes, we have grouped the columns by stage of randomization.

Step 3. To choose  $w_1, \ldots, w_4$  that result in eligible designs, systematically search through the entries in Table 5. Beginning at the top of Column 1 for  $w_1$ , we first consider  $w_1 = 12$  (i.e.,  $12\delta_2^{(1)}$ ). Since by rule (i) the three randomization restrictions must form a group of size  $2^3 - 1$ ,  $w_1 = 12$  will not produce an eligible design. Stepping down the column, the next choice is  $w_1 = 13$ . Notice that the RDCSG in (5) contains the term  $1w_1\delta_1^{(2)}\delta_2^{(2)}$ , meaning that  $w_1 = 13$  gives a product of  $3\delta_1^{(2)}\delta_2^{(2)}$ . This assignment results in factor 3 being present at the second stage of randomization, thereby violating rule (iii). Continuing in this manner, the first assignment that produces an eligible design is  $w_1 = 34$ .

Next, the first of two randomization restrictions for the third stage is selected. Beginning at the top of Column 2, we step down the column until an assignment for  $w_2$  that gives an eligible design is found. The first such choice is  $w_2 = 14$ . Moving to the next randomization restriction at this stage,  $w_3$  must be selected. There is no need to ever consider a choice of  $w_3$  above  $w_2$  in the search table because these assignments have already been considered by  $w_2$ . We emphasize this by placing a "-" at the top of Column 3 since this assignment need never be considered. Starting with  $w_3 = 15$ , we step down Column 3 until a choice of  $w_3$ is found which produces an eligible design. Notice that  $w_3 = 15$  is such a choice.

Finally,  $w_4$  is chosen for the final stage of randomization. Beginning at the top of Column 4, we step down the column until a  $w_4$  is found that yields an eligible design. The first such assignment is  $w_4 = 13$ . Thus, the first elegible design has  $w_1 = 34$ ,  $w_2 = 14$ ,  $w_3 = 15$  and  $w_4 = 13$ .

The next design is found by keeping  $w_1 - w_3$  fixed and continuing to step down Column 4, searching for eligible choices of  $w_4$ . When every choice of  $w_4$  has been entertained, we step back to the third column and consider the next eligible choice of  $w_3$ , keeping  $w_1$  and  $w_2$  fixed, and repeat the procedure as before for Column 4. Continue in this manner for all columns until all choices for  $w_1 - w_4$ have been considered and all eligible designs have been identified.

Steps 4 and 5. To check isomorphism we use the complete definition given in Step 4 of Section 3.3. We step through every choice and obtain the set of nonisomorphic eligible designs. We ranked designs by first minimizing the number of effects which appear in multiple RDCSG's, then sequentially minimizing the number of effects of each length appearing in multiple RDCSG's, and lastly minimizing (4). Following this strategy, the best design has  $w_1 = 12,345, w_2 = 235$ ,

	Level 1 & 2	Lev	el 3	Level 4
	$m{\delta}_{2}^{(1)}=m{\delta}_{2}^{(2)}$	$\boldsymbol{\delta}_2^{(3)}$	$\delta_3^{(3)}$	$\boldsymbol{\delta}_3^{(4)}$
12	$12\boldsymbol{\delta}_2^{(1)}$	$12\boldsymbol{\delta}_2^{(3)}$	-	$12\delta_{3}^{(4)}$
13	$13\delta_{2}^{(1)}$	$13 \boldsymbol{\delta}_2^{(3)}$	$13\delta_{3}^{(3)}$	$13oldsymbol{\delta}_3^{(4)}$
14	$14 \delta_{2}^{(1)}$	$14\boldsymbol{\delta}_2^{(3)}$	$14 \delta_{3}^{(3)}$	$14\boldsymbol{\delta}_3^{(4)}$
15	$15\delta_{2}^{(1)}$	$15\delta_{2}^{(3)}$	$15oldsymbol{\delta}_3^{(3)}$	$15\delta_{3}^{(4)}$
23	$23\boldsymbol{\delta}_2^{(1)}$	$23\boldsymbol{\delta}_2^{(3)}$	$23\boldsymbol{\delta}_{3}^{(3)}$	$23oldsymbol{\delta}_3^{(4)}$
24	$24\boldsymbol{\delta}_{2}^{(1)}$	$24\delta_{2}^{(3)}$	$24 \delta_{3}^{(3)}$	$24 \boldsymbol{\delta}_3^{(4)}$
25	$25 \boldsymbol{\delta}_2^{(1)}$	$25 \boldsymbol{\delta}_2^{(3)}$	$25 \boldsymbol{\delta}_3^{(3)}$	$25oldsymbol{\delta}_3^{(4)}$
34	$34 oldsymbol{\delta}_2^{(1)}$	$34\boldsymbol{\delta}_2^{(3)}$	$34\boldsymbol{\delta}_{3}^{(3)}$	$34 oldsymbol{\delta}_3^{(4)}$
35	$35 oldsymbol{\delta}_2^{(1)}$	$35oldsymbol{\delta}_2^{\overline{(3)}}$	$35 oldsymbol{\delta}_3^{(3)}$	$35 oldsymbol{\delta}_3^{(4)}$
45	$45\boldsymbol{\delta}_{2}^{(1)}$	$45 \overline{\boldsymbol{\delta}}_2^{\overline{(3)}}$	$45\boldsymbol{\delta}_3^{(3)}$	$45 \boldsymbol{\delta}_3^{(4)}$
123	$123\boldsymbol{\delta}_2^{(1)}$	$123\boldsymbol{\delta}_{2}^{\overline{(3)}}$	$123\boldsymbol{\delta}_3^{(3)}$	$123\boldsymbol{\delta}_{3}^{(4)}$
:		•	:	:
2345	$2345 \delta_2^{(1)}$	$2345\boldsymbol{\delta}_2^{(3)}$	$2345 \delta_{3}^{(3)}$	$2345 \delta_{3}^{(4)}$
12345	$12345 \delta_2^{(1)}$	$12345 \delta_2^{(3)}$	$12345\delta_{3}^{(3)}$	$12345\delta_{3}^{(4)}$

Table 5. Search Table

 $w_3 = 134$  and  $w_4 = 1,235$ , with V = 0. There are some features of this design, which we shall call  $D_1$ , worth noting. First, each of the four defining contrast subgroups (DCSG) contain the 12,345 interaction. Therefore, the variance of the estimator of the 5-factor interaction is a linear combination of each of the variance components and cannot be evaluated without replication. Further,  $D_1$ has 2, 4, 6, 6 and 12 degrees of freedom for effect estimation at the five stages of randomization, respectively. At each stage, half of the degrees of freedom correspond to main effects or two-factor interactions. The effects associated with each stage of randomization for this design are summarized in column  $D_1$  of Table 6.

Of course, the optimal design is not the only eligible design. For instance, if one ranks the designs by first minimizing the number of effects which appear in multiple RDCSG's, then sequentially minimizes the number of effects of each length appearing in multiple RDCSG's, then the second best design  $(D_2)$ , in terms of (4) has  $w_1 = 345$ ,  $w_2 = 14$ ,  $w_3 = 25$  and  $w_4 = 123$ , with V = 0.0139. Again, there is only one effect 12,345 which appears in multiple RDCSG's, but unlike the first design, this effect does not appear in each of the RDCSG's. Instead, the common effect appears only in the RDCSG's associated with Stages 2-4 of the randomization. The effects associated with each stage of randomization for this design are summarized in the  $D_2$  column of Table 6.

Comparing the designs  $D_1$  and  $D_2$ , we see that they have essentially the same properties with respect to Stages 3-5 of randomization. The main differences are

Randomization Stage	$D_1$	$D_2$	$D_3$
1	1,2345	1,345,1345	1,145
2	2, 12, 345, 1345	2, 12, 2345	2, 12, 245, 1245
3	3, 14, 25, 134,	3, 14, 25, 134,	3, 14, 15, 134,
	235, 1245	235, 1245	135,  345
4	4, 5, 45, 123,	4, 5, 45, 123,	4, 5, 23, 234,
	1234, 1235	1234, 1235	235, 2345
5	13, 15, 23, 24,	13, 15, 23, 24,	13, 23, 24, 25, 35,
	34,  35,  124,  125,	34,  35,  124,  125,	123, 124, 125, 1235,
	135, 145, 234, 245	135, 145, 234, 245	1345, 2345, 12345
Multiple	12345	12345	45

Table 6. Distribution of effects across levels of randomization

in the number of effects associated with the first two stages of randomization. There are 6 degrees of freedom in total at these stages, with  $D_1$  having 2 and  $D_2$  having 3 degrees of freedom at the first stage of randomization, respectively. Since the second stage of randomization is nested within the first, the first stage effects will have estimators whose variance is a linear combination of two variance components. In contrast, the second stage effects will have a variance which is a function of only one variance component and is smaller than the first stage effect variance. While we would not want to argue that one design is vastly superior to the other,  $D_1$  can be viewed as better than  $D_2$  in the sense that it has one more 2fi with a smaller variance than  $D_2$ , and has smaller V.

If one ranked the designs only using (4), there are other designs to consider. For example, consider  $D_3$  with  $w_1 = 45$ ,  $w_2 = 14$ ,  $w_3 = 15$ ,  $w_4 = 23$ , and V = 0.0014. Looking at V alone, this design is almost optimal. However, a quick glance at the  $D_3$  column in Table 6 shows that the 45 interaction will have a variance component from multiple stages of randomization. Therefore this design will have less power for estimating 2fi's than either  $D_1$  or  $D_2$ 

The methodology presented was used above to construct a multi-stage design for the plutonium processing experiment. There were some practical disadvantages to this design however. For instance, see that there are at most three degrees of freedom associated with the first stage of randomization. Since the experiment was unreplicated, it is difficult to assess the significance of these effects using half-normal plots. Indeed, this is true for the first two stages of randomization.

The obvious first thought is to use more cookies at Stage 1 to obtain some form of replication. This was undesirable for various economic reasons. After some discussion with the scientists, we learned of one feature of the process that could be exploited. There was considerable experience and knowledge with the first two stages of the process, and the experimenters felt that the unit-to-unit variability at the first casting stage was essentially zero. This fact allowed us to view the first two stages of randomization as one.

The experiment then reduces to a four stage split-lot design, with factors 1 and 2 at Stage 1, factor 3 at Stage 2 and factors 4 and 5 at Stage 3. We could consider running eight (half-cookies) groups of four at Stage 1, at Stage 2 and again at Stage 3. Since S = 4, we need three RDCSG's. This desired structure again predetermines part of each RDCSG. Thus we have

$$\begin{split} \Delta^{(1)} &= 1\boldsymbol{\delta}_{1}^{(1)} = 2\boldsymbol{\delta}_{2}^{(1)} = w_{1}\boldsymbol{\delta}_{3}^{(1)} = 12\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{2}^{(1)} = 1w_{1}\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{3}^{(1)} = 2w_{1}\boldsymbol{\delta}_{2}^{(1)}\boldsymbol{\delta}_{3}^{(1)} \\ &= 12w_{1}\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{2}^{(1)}\boldsymbol{\delta}_{3}^{(1)}, \\ \Delta^{(2)} &= 3\boldsymbol{\delta}_{1}^{(2)} = w_{2}\boldsymbol{\delta}_{2}^{(2)} = w_{3}\boldsymbol{\delta}_{3}^{(2)} = 3w_{2}\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{2}^{(2)} = 3w_{3}\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{3}^{(2)} = w_{2}w_{3}\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{3}^{(2)} \\ &= 3w_{2}w_{3}\boldsymbol{\delta}_{1}^{(2)}\boldsymbol{\delta}_{2}^{(2)}\boldsymbol{\delta}_{3}^{(2)}, \\ \Delta^{(3)} &= 4\boldsymbol{\delta}_{1}^{(3)} = 5\boldsymbol{\delta}_{2}^{(3)} = w_{4}\boldsymbol{\delta}_{3}^{(3)} = 45\boldsymbol{\delta}_{1}^{(3)}\boldsymbol{\delta}_{2}^{(3)} = 4w_{4}\boldsymbol{\delta}_{1}^{(3)}\boldsymbol{\delta}_{3}^{(3)} = 5w_{4}\boldsymbol{\delta}_{2}^{(3)}\boldsymbol{\delta}_{3}^{(3)} \\ &= 45w_{4}\boldsymbol{\delta}_{1}^{(3)}\boldsymbol{\delta}_{2}^{(3)}\boldsymbol{\delta}_{3}^{(3)}, \end{split}$$

and the problem reduces to finding a good set of four generators;  $\boldsymbol{\delta}_3^{(1)} = w_1$ ,  $\boldsymbol{\delta}_2^{(2)} = w_2$ ,  $\boldsymbol{\delta}_3^{(2)} = w_3$  and  $\boldsymbol{\delta}_3^{(3)} = w_4$ , within this structure.

The search table approach was applied and the suggested criterion used to rank designs. The best design has  $w_1 = 345$ ,  $w_2 = 14$ ,  $w_3 = 25$  and  $w_4 = 123$ . The effects associated with each stage of randomization and their respective variances are shown in Table 7. Note that  $p_1 = p_2 = p_3 = p_4 = 0.5$ , and V = 0.

There are other designs with V > 0 that have similar properties. For instance, the next best set of designs in terms of the proportion of effects equally distributed across the RDCSG's have V = 0.0017. One such design has  $w_1 = 1,245$ ,  $w_2 = 234$ ,  $w_3 = 235$ , and  $w_4 = 1,345$ . Similar to the above design, there is one effect which appears in each of the RDCSG's. However, unlike the best design, this effect is a 2fi (the 23 interaction). Clearly, one would prefer to assess the importance of this interaction and thus the previous design is superior.

### 4. Fractional Factorial Designs with Randomization Restrictions

The construction of fractional factorial designs with randomization restrictions can be a challenging problem. The reasons for this are related to the impact of fractionation on the alias structure and also the requirements to maintain the desired randomization structure (see Bisgaard (2000) or Bingham and Sitter (2001)). However, in the framework of the previous sections, it does not change the procedure. One merely sets up the desired randomization structure, the number of stages of randomization restriction, S, which factors are at each stage, the number of groups at each stage of randomization, and the split or lot structure at each stage. Once this is done, one places the randomization restriction

Effect	Variance	Degrees of Freedom
1, 2, 12, 345, 1345, 2345	$\frac{1}{2}\sigma_1^2 + \frac{1}{8}\sigma_\epsilon^2$	6
3, 14, 25, 134, 235, 1245	$\frac{1}{2}\sigma_2^2 + \frac{1}{8}\sigma_\epsilon^2$	6
4, 5, 45, 123, 1235, 1234	$\frac{1}{2}\sigma_3^2 + \frac{1}{8}\sigma_\epsilon^2$	6
13,14,15,23,24,35 and 6 others	$b\sigma_{\epsilon}^2$	12
12345	$\frac{1}{2}(\sigma_{1}^{2}+\sigma_{2}^{2}+\sigma_{3}^{2})+\frac{1}{8}\sigma_{\epsilon}^{2}$	1

Table 7. Effect variances for final plutonium design.

factors and the fractionation factors at the top of columns of the search table and, as before, searches for all eligible designs. For common smaller designs, all non-isomorphic fractional factorial (FF) designs are available in the literature (see Chen, Sun and Wu (1993)). Thus one can take an approach more akin to Huang, Chen and Voelkel (1998) whereby, for a particular fractionation, one begins with the minimum aberration (MA) design. Next apply the searchtable approach to the randomization restriction structure, but including the alias structure of the MA design when viewing the rules for eligibility. If there are no eligible designs, go to the next best design according to the aberration criterion.

This approach first ranks designs using a criterion which captures the ability to estimate as many of the effects of interest as possible (e.g., MA or clear effects). Thus, an eligible resolution IV design would be preferred to an eligible resolution III design. Next, designs are ranked by (4) in an attempt to make the effect sparsity principle hold for each level of randomization.

A special case worth commenting on is blocked fractional factorial designs. It is common to consider the effects that are confounded with blocks as not interpretable. The reason is that block effects are viewed as fixed effects. If blocks are random effects, then interactions confounded with blocks are simply effects with a different error variance than the other effects, and the significance of these can be assessed using a separate half-normal plot. If instead one prefers to use a criterion (Sitter, Chen and Feder (1997), Sun, Wu and Chen (1997) Bisgaard (2000) and Chen and Chen (1999)) with different types of words in the defining contrast sub-group (words that contain blocks and those that do not), one would first rank designs using the criterion and then by (4).

If the situation with multiple design choices arises, a criterion, such as was done for the full factorial case, to choose between the eligible designs can be used. For example, we could still use V, but when counting the proportion of main effects and 2fi's at a particular stage of the design we would include all effects within each alias string. We illustrate via the following example.

**Example 4.** Consider an example based on the final 4-stage split-lot version of the plutonium example. Suppose there was one more factor at the second stage of randomization (factor 6). Let the desired structure remain the same, so that

$$\begin{split} \Delta^{(1)} &= 1 \boldsymbol{\delta}_{1}^{(1)} = 2 \boldsymbol{\delta}_{2}^{(1)} = w_{1} \boldsymbol{\delta}_{3}^{(1)} = 12 \boldsymbol{\delta}_{1}^{(1)} \boldsymbol{\delta}_{2}^{(1)} = 1 w_{1} \boldsymbol{\delta}_{1}^{(1)} \boldsymbol{\delta}_{3}^{(1)} = 2 w_{1} \boldsymbol{\delta}_{2}^{(1)} \boldsymbol{\delta}_{3}^{(1)} \\ &= 12 w_{1} \boldsymbol{\delta}_{1}^{(1)} \boldsymbol{\delta}_{2}^{(1)} \boldsymbol{\delta}_{3}^{(1)}, \\ \Delta^{(2)} &= 3 \boldsymbol{\delta}_{1}^{(2)} = 6 \boldsymbol{\delta}_{2}^{(2)} = w_{2} \boldsymbol{\delta}_{3}^{(2)} = 36 \boldsymbol{\delta}_{1}^{(2)} \boldsymbol{\delta}_{2}^{(2)} = 3 w_{2} \boldsymbol{\delta}_{1}^{(2)} \boldsymbol{\delta}_{3}^{(2)} = 6 w_{2} \boldsymbol{\delta}_{2}^{(2)} \boldsymbol{\delta}_{3}^{(2)} \\ &= 36 w_{2} \boldsymbol{\delta}_{1}^{(2)} \boldsymbol{\delta}_{2}^{(2)} \boldsymbol{\delta}_{3}^{(2)}, \\ \Delta^{(3)} &= 4 \boldsymbol{\delta}_{1}^{(3)} = 5 \boldsymbol{\delta}_{2}^{(3)} = w_{3} \boldsymbol{\delta}_{3}^{(3)} = 45 \boldsymbol{\delta}_{1}^{(3)} \boldsymbol{\delta}_{2}^{(3)} = 4 w_{3} \boldsymbol{\delta}_{1}^{(3)} \boldsymbol{\delta}_{3}^{(3)} = 5 w_{3} \boldsymbol{\delta}_{2}^{(3)} \boldsymbol{\delta}_{3}^{(3)} \\ &= 45 w_{3} \boldsymbol{\delta}_{1}^{(3)} \boldsymbol{\delta}_{2}^{(3)} \boldsymbol{\delta}_{3}^{(3)}. \end{split}$$

The DCSG for the MA FF design is I = 123,456. If we view the known words in  $\Delta^{(1)}$ ,  $\Delta^{(2)}$  and  $\Delta^{(3)}$ , there are no obvious problems. For example,  $36\delta_1^{(2)}\delta_2^{(2)}$  when combined with the DCSG implies that 1,245 picks up  $\sigma_2^2$ , but no main effect is inadvertently moved to a different stage of randomization. Strictly speaking, one should combine the DCSG with the RDCSG's,

$$\Delta^{(1)} = 1\boldsymbol{\delta}_{1}^{(1)} = 2\boldsymbol{\delta}_{2}^{(1)} = w_{1}\boldsymbol{\delta}_{3}^{(1)} = 12\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{2}^{(1)} = 1w_{1}\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{3}^{(1)} = 2w_{1}\boldsymbol{\delta}_{2}^{(1)}\boldsymbol{\delta}_{3}^{(1)}$$
  
$$= 12w_{1}\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{2}^{(1)}\boldsymbol{\delta}_{3}^{(1)} = 23456\boldsymbol{\delta}_{1}^{(1)} = 13456\boldsymbol{\delta}_{2}^{(1)} = 123456w_{1}\boldsymbol{\delta}_{3}^{(1)} = 3456\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{2}^{(1)}$$
  
$$= 23456w_{1}\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{3}^{(1)} = 13456w_{1}\boldsymbol{\delta}_{2}^{(1)}\boldsymbol{\delta}_{3}^{(1)} = 3456w_{1}\boldsymbol{\delta}_{1}^{(1)}\boldsymbol{\delta}_{2}^{(1)}\boldsymbol{\delta}_{3}^{(1)} = 123456.$$
(8)

In (8),  $w_1$  must be chosen to heed rules (i), (ii) and (iii) from Section 3.3. One proceeds similarly for the subsequent stages of randomization. We do not give the full  $\Delta^{(2)}$  and  $\Delta^{(3)}$  to save space. Construction of  $\Delta^{(2)}$  and  $\Delta^{(3)}$  merely amounts to adding each word in the DCSG to the words in the RDCSG, modulo 2.

The choice of  $w_1$ ,  $w_2$  and  $w_3$  must be done with care. To illustrate, consider the MA design with the following two choices:  $D_1$  with  $w_1 = 345$ ,  $w_2 = 14$ ,  $w_3 =$ 123; and  $D_2$  with  $w_1 = 34$ ,  $w_2 = 14$ ,  $w_3 = 13$ . To compare the designs, the RD-CSG's must be constructed and crossed with the FF DCSG (i.e., I = 123, 456). We do not present these here, and instead discuss the results. For  $D_1$ , for instance, notice that 12, 345 is contained in  $\Delta^{(1)}$ . Thus, when crossing the DCSG with the RDCSG, the term  $6\delta_1^{(1)}\delta_2^{(1)}\delta_3^{(1)}$  appears. This means that factor 6 is also a factor at the first stage of randomization, violating rule (ii) in Section 3.3. So,  $D_1$  is not an eligible design. On the other hand,  $D_2$  is eligible and has 5 main effects or 2fi's at each of the first three stages of randomization. The last stage of randomization (with effects getting only replication error) has six 2fi's to be assessed. It turns out that there is only one value of V for eligible designs (V = 0.0033).

Now suppose that instead one prefers a design which is not MA, say I = 12346, and consider  $D_3$  with  $w_1 = 34$ ,  $w_2 = 14$  and  $w_3 = 13$ . This design has V = 0.013 and thus would be viewed as inferior by both the MA and the V criteria. However, this design has some desirable properties. First, this design has resolution V and still has main effects and 2fi's aliased only with negligible interactions. Second,  $D_3$  has 5, 4 and 4 main effects or 2fi's, respectively at each of the first three stages of randomization. Furthermore  $D_3$  has eight 2fi's at the final stage of randomization. As a consequence,  $D_3$  has more effects with an error variance that is only a multiple of replication error, and thus has more power to detect significant effects of interest.

When there are more factors at a stage of randomization than randomization restriction factors, one proceeds by assigning the first  $r_s$  of these factors to the randomization restriction factors. The only eligible fractional generators for the remaining factors at this stage will be interactions in the RDCSG associated with the  $r_s$  factors. Once the RDCSG and DCSG have been constructed, they can be combined to verify that the design obeys rules (i), (ii) and (iii) from Section 3.3.

## 5. Concluding Remarks

Factorial and fractional factorial designs with randomization restrictions are frequently used in industrial applications. Here, we have developed a general framework for constructing and evaluating such experiment plans so as to search for a "good" design. We do so by introducing the randomization defining contrast subgroup and using the defining generators to form sets of experiment units that will be processed together.

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Department of Statistics and Actuarial Science, Simon Fraser University, Burnaby, BC V5A-1S6, Canada.

E-mail: dbingham@stat.sfu.ca

Department of Statistics and Actuarial Science, Simon Fraser University, Burnaby, BC V5A-1S6, Canada.

E-mail: sitter@stat.sfu.ca

Statistical Sciences Group, Los Alamos National Laboratory, Los Alamos, NM, USA 87545. E-mail: ekelly@lanl.gov

Statistical Sciences Group, Los Alamos National Laboratory, Los Alamos, NM, USA 87545. E-mail: lmoore@lanl.gov

Process Science and Technology, Los Alamos National Laboratory, Los Alamos, NM, USA 87545.

E-mail: dolivas@lanl.gov

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