

## Chapter 8. Supplemental Text Material

### 8-1. Yates' Method for the Analysis of Fractional Factorials

Computer programs are almost always used for the analysis of fractional factorial. However, we may use Yates' algorithm for the analysis of a  $2^{k-1}$  fractional factorial design by initially considering the data as having been obtained from a full factorial in  $k - 1$  variables. The treatment combinations for this full factorial are listed in standard order, and then an additional letter (or letters) is added in parentheses to these treatment combinations to produce the actual treatment combinations run. Yates' algorithm then proceeds as usual. The actual effects estimated are identified by multiplying the effects associated with the treatment combinations in the full  $2^{k-1}$  design by the defining relation of the  $2^{k-1}$  fractional factorial.

The procedure is demonstrated in Table 1 below using the data from Example 8-1. This is a  $2^{4-1}$  fractional. The data are arranged as a full  $2^3$  design in the factors  $A$ ,  $B$ , and  $C$ . Then the letter  $d$  is added in parentheses to yield the actual treatment combinations that were performed. The effect estimated by, say, the second row in this table is  $A + BCD$  since  $A$  and  $BCD$  are aliases.

**Table 1.** Yates' Algorithm for the  $2^{4-1}_{IV}$  Fractional Factorial in Example 8-1

Treatment Combination	Response	(1)	(2)	(3)	Effect	Effect Estimate $2 \times (3) / N$
(1)	45	145	255	566	-	-
$a(d)$	100	110	311	76	$A+BCD$	19.00
$b(d)$	45	135	75	6	$B+ACD$	1.5
$ab$	65	176	1	-4	$AB+CD$	-1.00
$c(d)$	75	55	-35	56	$C+ABD$	14.00
$ac$	60	20	41	-74	$AC+BD$	-18.50
$bc$	80	-15	-15	76	$BC+AD$	19.00
$abc(d)$	96	16	16	66	$ABC+D$	16.50

### 8-2. Fold-Over and Partial Fold-Over of Fractional Factorials

In the textbook, we illustrate how a fractional factorial design can be augmented with additional runs to separate effects that are aliased. A fold-over is another design that is the same size as the original fraction. So if the original experiment has 16 runs, the fold-over will require another 16 runs.

Sometimes it is possible to augment a  $2^{k-p}$  fractional factorial with fewer than an additional  $2^{k-p}$  runs. For example, consider the  $2^{5-2}$  design shown in Table 2. The alias structure for this design is shown below the table.

**Table 2.** A  $2^{5-2}$  Design

Std ord	Run ord	Block	Factor A:A	Factor B:B	Factor C:C	Factor D:D	Factor E:E
2	1	Block 1	1	-1	-1	-1	-1
6	2	Block 1	1	-1	1	-1	1
3	3	Block 1	-1	1	-1	-1	1
1	4	Block 1	-1	-1	-1	1	1
8	5	Block 1	1	1	1	1	1
5	6	Block 1	-1	-1	1	1	-1
4	7	Block 1	1	1	-1	1	-1
7	8	Block 1	-1	1	1	-1	-1

$$[A] = A + BD + CE$$

$$[B] = B + AD + CDE$$

$$[C] = C + AE + BDE$$

$$[D] = D + AB + BCE$$

$$[E] = E + AC + BCD$$

$$[BC] = BC + DE + ABE + ACD$$

$$[BE] = BE + CD + ABC + ADE$$

Now suppose that after running the eight trials in Table 2, the largest effects are the main effects  $A$ ,  $B$ , and  $D$ , and the  $BC + DE$  interaction. The experimenter believes that all other effects are negligible. Now this is a situation where fold-over of the original design is not an attractive alternative. Recall that when a resolution III design is folded over by reversing all the signs in the test matrix, the combined design is resolution IV. Consequently, the  $BC$  and  $DE$  interactions will still be aliased in the combined design. One could alternatively consider reversing signs in individual columns, but these approaches will essentially require that another eight runs be performed.

The experimenter wants to fit the model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_4 x_4 + \beta_{23} x_2 x_3 + \beta_{45} x_4 x_5 + \varepsilon$$

where  $x_1 = A, x_2 = B, x_3 = C, x_4 = D$ , and  $x_5 = E$ . A **partial fold-over** is a design containing fewer than eight runs that can be used to augment the original design and will allow the experimenter to fit this model. One way to select the runs for the partial fold-over is to select points from the remaining unused portion of the  $2^5$  such that the variances of the model coefficients in the above regression equation are minimized. This augmentation strategy is based on the idea of a **D-optimal design**, discussed in Chapter 11.

Design-Expert can utilize this strategy to find a partial fold-over. The design produced by the computer program is shown in Table 3. This design completely dealiases the  $BC$  and  $DE$  interactions.

**Table 3.** The Partially-Folded Fractional Design

Std ord	Run ord	Block	Factor A:A	Factor B:B	Factor C:C	Factor D:D	Factor E:E
2	1	Block 1	1	-1	-1	-1	-1
6	2	Block 1	1	-1	1	-1	1
3	3	Block 1	-1	1	-1	-1	1
1	4	Block 1	-1	-1	-1	1	1
8	5	Block 1	1	1	1	1	1
5	6	Block 1	-1	-1	1	1	-1
4	7	Block 1	1	1	-1	1	-1
7	8	Block 1	-1	1	1	-1	-1
9	9	Block 2	-1	-1	-1	-1	1
10	10	Block 2	1	1	1	1	-1
11	11	Block 2	-1	-1	1	-1	-1
12	12	Block 2	1	1	-1	1	1

Notice that the partial fold-over design requires four additional trials. Furthermore, these trials are arranged in a second block that is orthogonal to the first block of eight trials.

This strategy is very useful in 16-run resolution IV designs, situations in which a full fold-over would require another 16 trials. Often a partial fold-over with four or eight runs can be used as an alternative.

As a second example, consider the  $2^{6-2}$  resolution IV design shown in Table 4. The alias structure for the design is shown below the table.

**Table 4.** A  $2^{6-2}$  Resolution IV Design

Std ord	Run ord	Block	Factor A:A	Factor B:B	Factor C:C	Factor D:D	Factor E:E	Factor F:F
10	1	Block 1	1	-1	-1	1	1	1
11	2	Block 1	-1	1	-1	1	1	-1
2	3	Block 1	1	-1	-1	-1	1	-1
12	4	Block 1	1	1	-1	1	-1	-1
16	5	Block 1	1	1	1	1	1	1
15	6	Block 1	-1	1	1	1	-1	1
8	7	Block 1	1	1	1	-1	1	-1
7	8	Block 1	-1	1	1	-1	-1	-1
5	9	Block 1	-1	-1	1	-1	1	1
1	10	Block 1	-1	-1	-1	-1	-1	-1
6	11	Block 1	1	-1	1	-1	-1	1
4	12	Block 1	1	1	-1	-1	-1	1
14	13	Block 1	1	-1	1	1	-1	-1
13	14	Block 1	-1	-1	1	1	1	-1
9	15	Block 1	-1	-1	-1	1	-1	1
3	16	Block 1	-1	1	-1	-1	1	1

$$\begin{aligned}
[A] &= A + BCE + DEF \\
[B] &= B + ACE + CDF \\
[C] &= C + ABE + BDF \\
[D] &= D + AEF + BCF \\
[E] &= E + ABC + ADF \\
[F] &= F + ADE + BCD \\
[AB] &= AB + CE \\
[AC] &= AC + BE \\
[AD] &= AD + EF \\
[AE] &= AE + BC + DF \\
[AF] &= AF + DE \\
[BD] &= BD + CF \\
[BF] &= BF + CD \\
[ABD] &= ABD + ACF + BEF + CDE \\
[ABF] &= ABF + ACD + BDE + CEF
\end{aligned}$$

Suppose that the main effects of factors  $A$ ,  $B$ ,  $C$ , and  $E$  are large, along with the  $AB + CE$  interaction chain. A full fold-over of this design would involve reversing the signs in columns  $B$ ,  $C$ ,  $D$ ,  $E$ , and  $F$ . This would, of course, require another 16 trials. The D-optimal partial fold-over approach requires only four additional runs. The augmented design, obtained from Design-Expert, is shown in Table 5. These four runs form a second block that is orthogonal to the first block of 16 runs, and allows the interactions of interest in the original alias chain be separately estimated.

**Table 5.** The Partial Fold-Over

Std	Run	Block	Factor A:A	Factor B:B	Factor C:C	Factor D:D	Factor E:E	Factor F:F
12	1	Block 1	1	1	-1	1	-1	-1
15	2	Block 1	-1	1	1	1	-1	1
2	3	Block 1	1	-1	-1	-1	1	-1
9	4	Block 1	-1	-1	-1	1	-1	1
5	5	Block 1	-1	-1	1	-1	1	1
8	6	Block 1	1	1	1	-1	1	-1
11	7	Block 1	-1	1	-1	1	1	-1
14	8	Block 1	1	-1	1	1	-1	-1
13	9	Block 1	-1	-1	1	1	1	-1
4	10	Block 1	1	1	-1	-1	-1	1
10	11	Block 1	1	-1	-1	1	1	1
6	12	Block 1	1	-1	1	-1	-1	1
7	13	Block 1	-1	1	1	-1	-1	-1
16	14	Block 1	1	1	1	1	1	1
3	15	Block 1	-1	1	-1	-1	1	1
1	16	Block 1	-1	-1	-1	-1	-1	-1
17	17	Block 2	1	-1	1	-1	-1	-1
18	18	Block 2	-1	1	-1	-1	-1	-1
19	19	Block 2	-1	-1	1	1	1	1
20	20	Block 2	1	1	-1	1	1	1

### 8-3. Alias Structures in Fractional Factorials and Other Designs

In this chapter we show how to find the alias relationships in a  $2^{k-p}$  fractional factorial design by use of the complete defining relation. This method works well in simple designs, such as the regular fractions we use most frequently, but it does not work as well in more complex settings. Furthermore, there are some fractional factorials that do not have defining relations, such as Plackett-Burman designs, so the defining relation method will not work for these types of designs at all.

Fortunately, there is a general method available that works satisfactorily in many situations. The method uses the polynomial or regression model representation of the model, say

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \boldsymbol{\varepsilon}$$

where  $\mathbf{y}$  is an  $n \times 1$  vector of the responses,  $\mathbf{X}_1$  is an  $n \times p_1$  matrix containing the design matrix expanded to the form of the model that the experimenter is fitting,  $\boldsymbol{\beta}_1$  is an  $p_1 \times 1$  vector of the model parameters, and  $\boldsymbol{\varepsilon}$  is an  $n \times 1$  vector of errors. The least squares estimate of  $\boldsymbol{\beta}_1$  is

$$\hat{\boldsymbol{\beta}}_1 = (\mathbf{X}'_1\mathbf{X}_1)^{-1}\mathbf{X}'_1\mathbf{y}$$

Suppose that the **true** model is

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\varepsilon}$$

where  $\mathbf{X}_2$  is an  $n \times p_2$  matrix containing additional variables that are not in the fitted model and  $\boldsymbol{\beta}_2$  is a  $p_2 \times 1$  vector of the parameters associated with these variables. It can be easily shown that

$$\begin{aligned} E(\hat{\boldsymbol{\beta}}_1) &= \boldsymbol{\beta}_1 + (\mathbf{X}'_1\mathbf{X}_1)^{-1}\mathbf{X}'_1\mathbf{X}_2\boldsymbol{\beta}_2 \\ &= \boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2 \end{aligned}$$

where  $\mathbf{A} = (\mathbf{X}'_1\mathbf{X}_1)^{-1}\mathbf{X}'_1\mathbf{X}_2$  is called the **alias matrix**. The elements of this matrix operating on  $\boldsymbol{\beta}_2$  identify the alias relationships for the parameters in the vector  $\boldsymbol{\beta}_1$ .

We illustrate the application of this procedure with a familiar example. Suppose that we have conducted a  $2^{3-1}$  design with defining relation  $I = ABC$  or  $I = x_1x_2x_3$ . The model that the experimenter plans to fit is the main-effects-only model

$$y = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \boldsymbol{\varepsilon}$$

In the notation defined above,

$$\boldsymbol{\beta}_1 = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}, \text{ and } \mathbf{X}_1 = \begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

Suppose that the true model contains all the two-factor interactions, so that

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \varepsilon$$

and

$$\beta_2 = \begin{bmatrix} \beta_{12} \\ \beta_{13} \\ \beta_{23} \end{bmatrix}, \text{ and } \mathbf{X}_2 = \begin{bmatrix} 1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \end{bmatrix}$$

Now

$$(\mathbf{X}'_1 \mathbf{X}_1)^{-1} = \frac{1}{4} \mathbf{I}_4 \text{ and } \mathbf{X}'_1 \mathbf{X}_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 4 \\ 0 & 4 & 0 \\ 4 & 0 & 0 \end{bmatrix}$$

Therefore

$$\begin{aligned} E(\hat{\beta}_1) &= \beta_1 + (\mathbf{X}'_1 \mathbf{X}_1)^{-1} \mathbf{X}'_1 \mathbf{X}_2 \beta_2 \\ E \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_3 \end{bmatrix} &= \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} + \frac{1}{4} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 4 \\ 0 & 4 & 0 \\ 4 & 0 & 0 \end{bmatrix} \begin{bmatrix} \beta_{12} \\ \beta_{13} \\ \beta_{23} \end{bmatrix} \\ &= \begin{bmatrix} \beta_0 \\ \beta_1 + \beta_{23} \\ \beta_2 + \beta_{13} \\ \beta_3 + \beta_{12} \end{bmatrix} \end{aligned}$$

The interpretation of this, of course, is that each of the main effects is aliased with one of the two-factor interactions, which we know to be the case for this design. While this is a very simple example, the method is very general and can be applied to much more complex designs.

#### 8-4. Irregular Fractions

Occasionally experimenters encounter a situation where a “standard” or **regular** fractional factorial design may not be entire appropriate. In these situations, an irregular fraction should be considered. For example, suppose that an engineer at a semiconductor manufacturer is studying  $k = 4$  factors and he or she is concerned about the four main effects and all two-factor interactions. Now the standard fraction, a  $2^{4-1}$ , is inappropriate since it is a resolution IV design and the two-factor interactions are aliased in pairs. The experimenter could employ a full factorial with 16 runs, but suppose that runs are expensive and time consuming, so a smaller design would be desirable if one can be found.

The 12-run irregular resolution V fraction shown in Table 6 will allow all main effects and two-factor interactions to be estimated. Several of these designs are available in the Design-Expert software package.

**Table 6.** An Irregular Fraction

Std	Run	Block	Factor 1 A:A	Factor 2 B:B	Factor 3 C:C	Factor 4 D:D
1	12	Block 1	-1	-1	-1	-1
2	6	Block 1	1	1	-1	-1
3	7	Block 1	-1	-1	1	-1
4	2	Block 1	1	-1	1	-1
5	3	Block 1	-1	1	1	-1
6	8	Block 1	1	1	1	-1
7	9	Block 1	-1	-1	-1	1
8	4	Block 1	1	-1	-1	1
9	1	Block 1	-1	1	-1	1
10	11	Block 1	1	1	-1	1
11	10	Block 1	1	-1	1	1
12	5	Block 1	-1	1	1	1

The alias relationships associated with the irregular fractional factorial in Table 6 are

- [A] = A - ACD
- [B] = B - BCD
- [C] = C - ABCD
- [D] = D - ABCD
- [AB] = AB - ABCD
- [AC] = AC - BCD
- [AD] = AD - BCD
- [BC] = BC - ACD
- [BD] = BD - ACD
- [CD] = CD - 0.5 \* ABC - 0.5 \* ABD

Notice that all effects are estimated free of two-factor interactions, and that the two-factor interactions are aliased with higher-order interactions. Thus, the same information about these effects has been obtained from this design as would be found with a full  $2^4$ .

If a full  $2^4$  had been used, all factor effects would be orthogonal, and the standard error of each effect would be  $\sigma / \sqrt{16} = \sigma / 4 = 0.25\sigma$ . In the irregular fraction, the standard errors of the model regression coefficients are larger, therefore the model parameters are not estimated as precisely as they would be by using a full factorial. Specifically the standard errors from the irregular fraction are

Term	StdErr
A	0.35
B	0.35
C	0.35
D	0.35
AB	0.35
AC	0.35
AD	0.35
BC	0.35
BD	0.35
CD	0.31

Furthermore, these model coefficients are correlated. Generally, this will be the price an experimenter will pay for using an irregular fraction; correlated effect estimates and larger standard errors than would result from the more complete design.

### 8-5. Supersaturated Designs

In recent years, there has been considerable interest in developing and using **supersaturated designs** for factor screening experiments. Now in the textbook a saturated design is defined as a fractional factorial in which the number of factors or design variables is exactly equal to the number of runs. A supersaturated design contains more variables than runs. The idea of using supersaturated designs was first proposed by Satterthwaite (1959). He proposed random balanced experiments to determine the important factors. In an extensive discussion of this paper, Youden, Box, Hunter, Cochran, Tukey, Kempthorne, and Anscombe criticized these ideas. These individuals are eminent authorities in designed experiments, so supersaturated designs received little attention for the next 30 years. A notable exception to this is the systematic supersaturated designs developed by Booth and Cox (1962). Their designs were not randomly generated. This is a significant departure from the proposal of Satterthwaite. They generated their designs with elementary computer search methods. They also developed the basic criteria by which supersaturated designs are judged.

Many authors have proposed methods to construct supersaturated designs. Most are limited computer search techniques based on simple heuristics [Booth and Cox (1962), Lin (1995), and Li and Wu (1995)]. Others have proposed methods based on optimal design construction techniques (we will discuss some of these techniques in Chapter 11).

Another construction method for supersaturated designs is based on the structure of existing orthogonal designs. These include using the half-fraction of Hadamard matrices [Lin (1993)] and enumerating the two-factor interactions of certain Hadamard matrices [Wu (1995)]. When the number of factors in the experiment exceeds the number of runs, the design matrix cannot be orthogonal. Consequently the effect estimates of the factors are not independent. An experiment with one dominant factor may contaminate and

obscure the contribution of another factor. Supersaturated designs are created to minimize this amount of non-orthogonality between factors.

In a supersaturated design the number of factors ( $k$ , or columns) exceeds the number of runs or experiments ( $n$ , rows). The goal is to find a design matrix,  $\mathbf{X}$ , that is as close as possible to orthogonal. The covariance matrix ( $\mathbf{X}'\mathbf{X}$ ) of the design will have non-zero off-diagonal terms. Making these off-diagonal elements as small as possible makes the design as close to orthogonal as possible.

Consider the shape of a design matrix for a supersaturated design. The design matrix will have more columns than rows. Recall that  $n$  is the number of experiments. Initially, we will restrict  $n$  to be even. Each column of  $\mathbf{X}$  is composed of half  $+1$ 's and half  $-1$ 's, so the

possible columns of  $\mathbf{X}$  are all possible combinations,  $n/2 +1$ 's and  $n/2 -1$ 's.  $\mathbf{X}$  has  $\binom{n}{n/2}$

candidate columns. Let  $r$  be the near-orthogonality parameter. When  $r$  is zero, the design is orthogonal. Let  $t$  be the value of the off-diagonal covariance elements of  $\mathbf{X}'\mathbf{X}$ . The value of  $t$  may vary from  $-n \leq t < n$ . The off-diagonal elements are not continuous, since the entries of the design matrix are  $-1$  or  $+1$ . The off-diagonal elements take on integer values in steps of 4. For a given number of rows,  $n$ , the covariance between rows is given by  $\mathbf{c}'_i\mathbf{c}_j$  (the dot or inner product of columns  $\mathbf{c}_i$  and  $\mathbf{c}_j$ ). The covariance minus  $n \bmod 4$  is zero; that is,  $(\mathbf{c}'_i\mathbf{c}_j - n) \bmod(4) = 0$ . The goal is to find the greatest number of columns for a given degree of non-orthogonality.

When  $n$  is odd, the number of  $+1$ 's may be selected as one more than the number of  $-1$ 's.

The number of candidate columns becomes  $\binom{n}{(n-1)/2}$ . The rest of the discussion for  $n$  even applies to  $n$  odd also.

Lin (1995) has proposed a relatively straightforward algorithm for constructing supersaturated designs. His procedure essentially generates all possible columns. Then a master set of near-orthogonal columns is formed by checking all candidate columns, one at a time, against the columns in the existing master set. If a column is not nearly orthogonal to exactly one column that is already in the existing master set, it is stored for possible later addition to the master set. When two columns are found that are near-orthogonal and that are also near orthogonal to all but one column that are members of the master set, they are swapped with these columns. Due to the random nature of this search, Lin suggests that it be conducted several times in order to find better designs.

No secondary criteria are evaluated with Lin's algorithm. A secondary criterion [proposed by Booth and Cox (1962)] discussed in the Lin paper is the average amount of near-orthogonality in the  $\mathbf{X}'\mathbf{X}$  matrix. This measure utilizes the off-diagonal terms,  $s_{ij}$  of the matrix. These elements are squared, summed and standardized by dividing by the number of off-diagonal terms. Computationally, this criterion is

$$\rho = \sum s_{ij}^2 / \binom{k}{2},$$

where  $k$  is the number of columns in  $\mathbf{X}'\mathbf{X}$ . Another paper by Wu (1995) also generates supersaturated designs and evaluates them with this criterion. Wu uses a D-optimal column-swapping scheme as the generating method. The run times to find designs that Wu reported were very long. Wu produced design with many fewer columns than Lin. Wu claims that the designs that his algorithm generated are superior based on the secondary criterion, the  $\rho$  statistic. Recently Balkin and Lin [1998] have introduced additional secondary criteria for evaluating and comparing supersaturated design generation methods. The methods involve evaluating the design projectivity and a criterion similar to the trace of the  $\mathbf{X}'\mathbf{X}$  matrix, a design-optimality criterion that we will discuss in Chapter 11.

Supersaturated designs are typically analyzed by regression model-fitting methods, such as forward selection. This is a procedure in which variables are selected one-at-a-time for inclusion in the model until no other variables appear useful in explaining the response. These designs have not had widespread use, but they are an interesting and potentially useful method for experimentation with systems where there are many variables and only a very few of these are expected to produce large effects.

### Supplemental References

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