FRACTIONAL FACTORIAL TREATMENT DESIGN

by

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Abstract

An expository treatment of fractional replication is presented. The concepts follow a somewhat more general approach than is given in textbook literature. Types of treatment designs and general fractions are considered. Various types of fractional replicate designs are discussed. It is shown how to construct various types of fractional replicates. Some properties of fractional replicates are discussed.

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1. Introduction

The single entities included in an experiment are often called treatments. A treatment may be a variety of corn, a brand of soup, a temperature of 25°C, 300 pounds of nitrogen fertilizer per acre, two milligrams of a drug, a high protein diet, a recreational program, etc. A set of treatments in an experiment may be different levels of one factor (e.g., humidity), different levels of several factors, or combinations of levels of two or more factors, where factors are independent variables, such as the above, whose levels are selected by the experimenter. The selection of treatments to be included in an experiment is denoted as treatment design, whereas the arrangement of treatments in an experiment is denoted as the experiment design. Treatments are selected by the experimenter to achieve specified goals. Since many goals are involved in experimentation, there are many treatment designs. It is useful to classify treatments as follows:

(i) Levels of a factor are discrete (e.g., brands of a product, number of applications, days to maturity, etc.),

(ii) Levels of a factor are continuous (e.g., temperature, amount of fertilizer, amount of a drug, etc.),

(iii) A single level of one factor is combined with a single level of a second factor in a fixed ratio (e.g., a genetic cross of two lines, a game in a tournament, a 50:50 mixture of two cultivars, etc.), and

(iv) Controls, standards, placebos (points of reference such as a standard medical treatment, the adapted variety or fertilizer, product brand, etc., need to be included).

The selection of treatments from one or more of the above categories constitutes the treatment design.

In most of the literature a factorial treatment design has been defined to be all possible combinations of two or more levels of two or more factors. Some literature implies that the combinations appear equally often in the experiment. One reference (Raktoe, Hedayat, and Federer (1980)) uses "one or more levels of one or more factors" in the definition, as this is a useful one in a mathematical presentation of the subject. Also, the literature is confused with regard to discrete or continuous levels of factors. We restrict ourselves to discrete levels of factors for a factorial treatment design. When the levels of factors are continuous, the treatment designs are known as regression treatment designs or response surface treatment designs. When only one level of a factor is involved and when combinations of single levels of factors are involved, the treatment design is defined to be a fixed-ratio mixture treatment design (Federer (1979), Federer and Wijesinha (1979)).

Since the population of interest, the parameters to be estimated, the form of the statistical analysis, and the statistical inferences to be made, differ considerably for the discrete, continuous, and single-level cases, it is in the interest of clarity to keep them separate. It should be noted that in a given set of experiments, the treatment design used in the experiment may be of the same nature for all three cases, but this does not imply that statistical analyses and inferences will be the same. The type of treatment design used in an experiment is dictated by the goals of the experimenter.

The levels of a discrete-level factor in the population may be sampled or all levels may be used. The population represented by a given factorial treatment design of n factors is an n-dimensional lattice of points formed by combinations of one level of each of n factors. The factorial treatment design is all combinations of the selected levels of n factors. Let k_i be the number of levels for factor i . Then, the total number of combinations of n factors is $N = k_1 \times k_2 \times \cdots \times k_n$ and each combination is denoted as (j1, j2, ⋯, jn), where ji = 1, 2, ⋯, k_i . Note that ji = 1 could mean absence of a factor, or the zero level. For example, consider three brands of soup, two types of preparation, and two different seasonings in all combinations. This would be a $3 \times 2 \times 2$ factorial with the following combinations:

Brand of Soup	Seasoning 1 Preparation		Seasoning 2 Preparation	
	1	2	1	2
1	111	121	112	122
2	211	221	212	222
3	311	321	312	322

There are 12 combinations of levels of the three factors.

Let the combinations (j1, j2, ⋯, jn) be numbered from h = 1, 2, ⋯, $N = \prod_{i=1}^{n} k_i$ and let r_h be the number of times the <u>hth</u> combination appears in the experiment. In a factorial, or a complete factorial, design, all $r_h > 0$. Some of the literature implies that all r_h must equal a constant r in order to have a factorial design. This is not true, and one may consider a factorial as an n-way classification with or without disproportionate numbers in the subclasses. Whenever one or more of the $r_h = 0$, a <u>fractional replicate of a complete factorial</u> results. Thus, an n-way classification with missing subclasses and discrete-level factors is a fractional replicate of a factorial (see, e.g., Paik and Federer (1974)). In a complete factorial, there are N - 1 single-degree-of-freedom parameters involving main effects and interactions of the n factors. In addition, there is the overall mean, resulting in N parameters. If there are k of the r_h equal to zero, then it is possible to estimate only $N-k$ linear combinations of the N parameters. Whenever a linear combination of parameters involves more than one of the N parameters we say that the parameters are aliases (see, e.g., Kempthorne (1952), Hedayat et al. (1974), Raktoe et al. (1978, 1980)). For example, in a $2 \times 2 = 2^2$ factorial with combinations 00, 01, 10, and 11, and with the four parameters mean, A, B, and AB, suppose only combinations 00 and 01 were available. Then, the mean and -A are completely aliased (confounded) and B and -AB are aliased. The linear combinations of parameters estimated are mean -A and B - AB . If combinations 00, 01, and 10 were available, then the linear combinations of parameters one can estimate are: mean - AB, A - AB, and B - AB . As a second example, consider a 2^3 factorial with the eight combinations: 000, 001, 010, 011, 100, 101, 110, and 111 and parameters mean, A, B, C, AB, AC, BC, and ABC . If one has the fractional replicate consisting of observations for combinations 000, 011, 101, and 110, the aliasing scheme is: mean - ABC, A - BC, B - AC, and C - AB, where the main effects A, B, and C are aliased with two-factor interactions. The three-factor interaction ABC is aliased with the mean. In general matrix form, suppose that we have a vector of response means $\underline{Y}_{p\times 1}$, $p < N$, and the responses are for p different treatments, then for a complete factorial, we have

$$X\underline{\beta} = \begin{bmatrix} X_{11,p\times p} & X_{12,p\times(N-p)} \\ X_{21,(N-p)\times p} & X_{22,(N-p)\times(N-p)} \end{bmatrix} \begin{bmatrix} \underline{\beta}_{1,p\times 1} \\ \underline{\beta}_{2,(N-p)\times 1} \end{bmatrix} = \begin{bmatrix} \underline{Y}_{1,p\times 1} \\ \underline{Y}_{2,(N-p)\times 1} \end{bmatrix} = \underline{Y} \quad ,$$

where $\underline{Y}$ is the vector of N means.

For a fractional replicate, we have

$$[X_{11} \quad X_{12}] \begin{bmatrix} \underline{\beta}_1 \\ \underline{\beta}_2 \end{bmatrix} = \underline{Y}_1 \quad .$$

The normal equations are

$$X'_{11}X_{11}\underline{\beta}_1 + X'_{11}X_{12}\underline{\beta}_2 = X'_{11}\underline{Y}_1 \quad ,$$

or

$$\underline{\beta}_1 + (X'_{11}X_{11})^{-1}X'_{11}X_{12}\underline{\beta}_2 = (X'_{11}X_{11})^{-1}X'_{11}\underline{Y}_1$$

where $(\ )^{-1}$ denotes an inverse. Note that rank of $X'_{11}X_{11}$ could be less than p, and hence there would be aliasing among $\underline{\beta}_1$ parameters. Also, in the above, X_{11} is a square matrix and then we may write:

$$\underline{\beta}_1 + X_{11}^{-1}X_{12}\underline{\beta}_2 = X_{11}^{-1}\underline{Y}_1 \quad .$$

The matrix $(X'_{11}X_{11})^{-1}X'_{11}X_{12} = A$ or $X_{11}^{-1}X_{12} = A$ is called the aliasing matrix. The goals of fractional replicate plan construction are:

(i) To minimize the variance of $\underline{\beta}_1 + X_{11}^{-1}X_{12}\underline{\beta}_2$, e.g., by selecting X_{11} such that **determinant of** $X'_{11}X_{11}$ is maximum, and

(ii) To put parameters in $\underline{\beta}_2$ which are negligible and which minimize the bias, $A\underline{\beta}_2$, in estimating $\underline{\beta}_1$.

If $\underline{\beta}_2 = \underline{0}$, then an unbiased estimate of $\hat{\underline{\beta}}_1$ is $X_{11}^{-1}\underline{Y}_1$, and variance of $\hat{\underline{\beta}}_1$ is $X_{11}^{-1}\sigma^2$, where σ^2 is the error variance under **homoscedasticity.** When $\underline{\beta}_2 \neq 0$, the variance of $\hat{\underline{\beta}}_1 + A\hat{\underline{\beta}}_2$ is $X_{11}^{-1}\sigma^2$ and the mean square error of $\hat{\underline{\beta}}_1$ is $X_{11}^{-1}\sigma2$ $+ A\underline{\beta}_2\underline{\beta}_2'A'$. Unless one has prior knowledge about $\underline{\beta}_2$, the bias term $A\underline{\beta}_2\underline{\beta}_2'A'$ could be anything. There are situations wherein the experimenter has reason to believe that the parameters in $\underline{\beta}_2$ are negligible. When such is the case, a fractional replicate design is appropriate.

2. Types of Fractional Replicate Designs

Various classification schemes for fractional replicates of an n-factor factorial are possible. One procedure is to classify the types of factorial effects and their parameters which can be estimated from a given design under the condition that all remaining parameters are zero. In a complete factorial with n factors, there is one parameter for the mean, $\sum_{i=1}^{n}(k_i - 1) = N_1$ main effect parameters for the n factors with the ith factor having k_i levels,

$$\sum_{\substack{i=1 \\ i<j}}^{n-1} \sum_{j=2}^{n} (k_i - 1)(k_j - 1) = N_2$$ two-factor interaction parameters,

$$\sum_{\substack{h=1 \\ h<i<j}}^{n-2} \sum_{i=2}^{n-1} \sum_{j=3}^{n} (k_h - 1)(k_i - 1)(k_j - 1) = N_3$$ three-factor interaction parameters, etc.

Let $\underline{\beta}_1$ be an $(N_1 + 1) \times 1$ vector of the mean and the N_1 main effect parameters. If $\underline{\beta}_1$ is estimable, this is denoted as a main effect plan and is called a Resolution III design. Let the vector of parameters in a complete factorial be partitioned as follows $\underline{\beta}' = (\underline{\beta}_1', \underline{\beta}_2', \underline{\beta}_3')'$ where $\underline{\beta}_1$ is as above; $\underline{\beta}_2'$ is $N_2 \times 1$ and consists of the two-factor interaction parameters; $\underline{\beta}_3$ consists of the remaining parameters. If $\underline{\beta}_1$ is estimable and if the parameters in $\underline{\beta}_1$ are not aliased with those in $\underline{\beta}_2$, we denote this main effect plan as a Resolution IV design. Now if parameters in both $\underline{\beta}_1$ and $\underline{\beta}_2$ can be estimated under the condition that $\underline{\beta}_3 = \underline{0}$, this is denoted as a Resolution V design. One can extend the idea of Resolution as given by Box and Hunter (1961) in an obvious way to Resolution VI, VII, $\cdots$ designs.

Another scheme (see Raktoe et al. (1980)) is to divide all fractional factorial designs into odd and even Resolution designs. Still another scheme is to divide these designs into regular (complete confounding among aliases in $\underline{\beta}_2$ and parameters in $\underline{\beta}_1$; see Raktoe et al. (1978)) and irregular fractional replicate designs. Another scheme would be to consider all designs for which $X_{11}'X_{11}$ was a diagonal matrix and denote these as orthogonal designs with all others being nonorthogonal designs. Finally, one could classify these designs on the basis of the lengths of the $\underline{\beta}_1$ and $\underline{Y}_1$ vectors. Let $\underline{\beta}_1$ be a $p \times 1$ vector and $\underline{Y}_1$ be a $k \times 1$ vector. If $p = k$, we would have a saturated fractional replicate design; if $p < k$, this would be an unsaturated fractional replicate design; and if $p > k$, we could call this a super-saturated fractional replicate design.

A regular and an irregular one-half replicate of a 2^3 factorial are:

Regular Fraction

Aliases	Treatments
Mean + ABC	111
A + BC	001
B + AC	010
C + AB	100

$$\hat{\underline{\beta}}_1 + A\hat{\underline{\beta}}_2 = \underline{Y}_1$$

$$\begin{bmatrix} \text{Mean} \\ A \\ B \\ C \end{bmatrix} + \begin{bmatrix} 0001 \\ 0010 \\ 0100 \\ 1000 \end{bmatrix} \begin{bmatrix} AB \\ AC \\ BC \\ ABC \end{bmatrix} = \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \end{bmatrix} \begin{bmatrix} Y_{111} \\ Y_{001} \\ Y_{010} \\ Y_{100} \end{bmatrix}$$

Irregular Fraction

Treatments
000
100
010
001

$$\hat{\underline{\beta}}_1 + A\hat{\underline{\beta}}_2 = \underline{Y}_1$$

$$\begin{bmatrix} \text{Mean} \\ A \\ B \\ C \end{bmatrix} + \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} AB \\ AC \\ BC \\ ABC \end{bmatrix} = X_{11}^{-1}\underline{Y}_1$$

$$= \begin{bmatrix} \text{Mean} \\ A \\ B \\ \end{bmatrix} + \begin{bmatrix} -1 & -1 & -1 & 2 \\ -1 & -1 & 0 & 1 \\ -1 & 0 & -1 & 1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} AB \\ AC \\ BC \\ ABC \end{bmatrix} = \frac{1}{2} \begin{bmatrix} -1 & 1 & 1 & 1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} Y_{000} \\ Y_{100} \\ Y_{010} \\ Y_{001} \end{bmatrix}$$

Aliases

Mean - AB - AC - BC + 2ABC
A - AB - AC + ABC
B - AB - BC + ABC
C - AC - BC + ABC

3. Construction of Fractional Replicate Designs

Several methods for constructing fractional replicates are available (see, e.g. Addelman (1963)). Some of these are confounding, single-degree-of-freedom contrasts, orthogonal matrices, weighing designs, orthogonal arrays, orthogonal Latin squares, balanced incomplete block designs, augmentation of existing fractions, one-factor at a time, Galois Field Theory, etc. A considerable theory and literature has evolved for constructing s^{m-k} fractions of an s^m factorial; a lot is known for s a prime power, but for s not a prime power not much is known. Likewise for fractions of the general asymmetrical factorial $\prod_{i=1}^{n} k_i$ not much is known and most that is relates to $k_i = 2$ or 3 (see, e.g., Margolin (1967)). For $s = 2$ and for 2^{n-k}, fractions, there is a voluminous literature, but for $p/2^n$ fractions of a 2^n factorial there is little literature and there are many unsolved problems (see, e.g., Anderson and Federer (1975)).

Perhaps the simplest and most general method of construction of fractional replicates is the so-called one-at-a-time procedure. Unfortunately, it produces the most inefficient main effect designs (see Anderson and Federer (1974, 1975)). To illustrate, suppose $k_1 = 2$, $k_2 = 3$, and $k_3 = 4$ for A, B, and C, respectively. Then, a main effect plan would be either plan I or plan II below:

plan I	plan II
000	000
100	100
010	110
020	120
001	121
002	122
003	123

Note that in plan I, all levels are held constant at zero while the levels of a given factor change. In going down a column in plan II, only one number is changed from the previous row. Fractional factorial main effect designs of the plan I type are the least efficient designs possible, but they are the easiest to construct. Adding the combinations 110 and 120 to the plan would allow estimation of the $A \times B$ interaction effects, and adding combinations 011, 012, 013, 021, 022, and 023 would allow estimation of the $B \times C$ interaction effects. An individual combination can be added to plan I, and it is easy to determine the contrast represented by the additional observations. Any combination of main effects and interactions may be obtained using the plan I scheme. Also, note that as the fraction approaches 100%, it approaches the optimal design, that is, the complete factorial.

To construct a Resolution IV design, one can use a technique known as a "fold-over" (see, e.g., Addelman (1963) and Raktoe and Federer (1968)). One starts with a main effect plan, e.g., 0000, 1110, 1101, 1011, and 0111 for four factors each at two levels. Then, one replaces the ones with zeros and the zeros with ones to obtain the additional five treatments 1111, 0001, 0010, 0100, and 1000 . Now we can obtain another Resolution IV design for five factors from this design as follows:

Main effect plan	Fold-over plan
0000:0	1111:1
1110:0	0001:1
1101:0	0010:1
1011:0	0100:1
0111:0	1000:0

That is, we append zeros to the first one-half and ones to the second one-half to obtain a Resolution IV plan for five factors. For $s > 2$, see Raktoe and Federer (1968).

As a third illustration, consider the following Resolution V fractional replicate design for five factors. The 16 treatments are: 00001, 00010, 00100, 01000, 10000, 11100, 11010, 11001, 10110, 10101, 10011, 00111, 01110, 01101, 01011, and 11111 . (The other 16 treatments of a 2^5 factorial could have been used equally well.) The aliasing scheme for this fraction is

Mean + ABCDE	AD + BCE
A + BCDE	AE + BCD
B + ACDE	BC + ADE
C + ABDE	BD + ACE
D + ABCE	BE + ACD
E + ABCD	CD + ABE
AB + CDE	CE + ABD
AC + BDE	DE + ABC

The mean, the 5 main effects, and the 10 two-factor interactions can be estimated free of each other. The mean is completely confounded with a five-factor interaction, the main effects with four-factor interactions, and the two-factor intereactions are confounded with three-factor interactions.

As the number of factors becomes large, the number of treatments (also called assemblies, rows, combinations, etc.) increases much faster. Much of the work on fractional replicate designs is concerned with an s^{-k} fraction of an s^n factorial. This limits the number of treatments to specific powers of s . Some papers consider adding different powers of s until the desired number of combinations is obtained; that is, $s^{k_1} + s^{k_2} + s^{k_3} + s^{k_4} + \cdots$ is less than s^{n-k} . This procedure does not always insure that the minimum number of observations possible is attained. The one-at-a-time procedure does assure the minimal number. To illustrate, consider the following for 2^n and 3^n factorials for Resolution V designs:

n	2^n	Minimal 2^{n-k}	Minimal $2^{k_1} + 2^{k_2} + 2^{k_3} + \cdots$	Minimal fraction
2	4	4	$4 = 2^2$	4
3	8	8	$8 = 2^3$	7
4	16	16	$12 = 2^3 + 2^2$	11
5	32	16	$16 = 2^4$	16
6	64	32	$22 = 2^4 + 2^2 + 2$	21
7	128	32	$28 = 2^4 + 2^3 + 2^2$	28
8	256	64	$36 = 2^5 + 2^2$	36
9	512	64	$46 = 2^5 + 2^3 + 2^2 + 2$	45

n	3^n	Minimal 3^k	Minimal $3^{k_1} + 3^{k_2} + 3^{k_3} + \cdots$	Minimal fraction
2	9	9	$9 = 3^2$	9
3	27	27	$21 = 3^2 + 3^2 + 3$	19
4	81	81	$33 = 3^3 + 3 + 3$	33
5	243	81	$51 = 3^3 + 3^2 + 3^2 + 3 + 3$	51
6	729	81	$75 = 3^3 + 3^3 + 3^2 + 3^2 + 3$	73
7	2187	243	$99 = 3^4 + 3^2 + 3^2$	99
8	6561	243	$129 = 3^4 + 3^3 + 3^2 + 3^2 + 3$	129

The minimal fraction design can be formed using the one-at-a-time or other procedures.

4. Mathematical and Statistical Properties of Fractional Replicate Designs

The mathematical and statistical properties and theory of fractional replicate designs can become rather complicated (see, e.g., Fisher (1942), Bose (1947), Pesotan et al. (1975), and Raktoe et al. (1980)). Fractional replication theory is a combinatorial method of mathematics in a manner similar to orthogonal latin squares and balanced incomplete block designs. As in combinatorial mathematics, considerable theory exists for s^n factorials when s is a prime power and when fractions of s^{-k} are being considered. Thus, there are many unsolved problems here of considerable mathematical and statistical interest. It is a fruitful area of research as evidenced by the large number of papers on the topic listed in Federer and Balaam (1972), for example.

One property of statistical interest is that of variance optimality. Other properties are minimal bias, most economic, invariance, similarity, etc. In considering variance optimal designs, it is usually assumed that $\underset{\sim}{\beta}_2 = \underset{\sim}{0}$ and that $\hat{\underset{\sim}{\beta}}_1$ is an unbiased estimator. If $\underset{\sim}{\beta}_2 \neq \underset{\sim}{0}$ then it is necessary to consider the bias term $A\underset{\sim}{\beta}_2\underset{\sim}{\beta}_2'A'$ and properties of this (see, e.g., Hedayat et al. (1974)). In considering variance optimality, one considers properties of X_{11} or of $X_{11}'X_{11}$. For D-optimality one considers X_{11} or $X_{11}'X_{11}$ with maximal absolute value of the determinant, resulting in a minimal X_{11}^{-1} or $(X_{11}'X_{11})^{-1}$ as a criterion of variance optimality. For example, consider the main effect plans 000, 110, 101, and 011 and 000, 100, 010, and 001 . The absolute values of their determinants are:

$$\left\|\begin{matrix}1000\\1110\\1101\\1011\end{matrix}\right\| = 2 \qquad \text{and} \qquad \left\|\begin{matrix}1000\\1100\\1010\\1001\end{matrix}\right\| = 1 \quad .$$

The first plan is the better plan and the second plan is the poorer plan. Consider the following two plans 0000, 1000, 0100, 0010, and 0001 and 0000, 0110, 0011, 1101, and 1010 . The absolute value of the determinant of the first plan is one while that for the second plan is three. As Anderson and Federer (1974, 1975) have shown, the problem of enumerating all possible values of the determinants is unsolved. They have upper and lower bounds for the maximal value but do not have a procedure for finding the design producing this value. They show how to construct the least efficient design as well as many in between the extremes. For the user of fractional replicates, plans can be developed and their determinant values compared with the upper and lower bounds of the maximal one. A plan that is above or near the lower bound may be sufficiently good for the purposes at hand.

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