ON MEASURING BIAS DUE TO CONFOUNDING OF EFFECTS

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A. Hedayat, B. L. Raktoe, and W. T. Federer Cornell University and University of Guelph

BU-408-M January 1972

ABSTRACT

Relatively little has been accomplished to date in constructing general aliasing schemes in fractional replication and in developing a measure for comparing the relative amount of bias (or confounding) in two fractional replicates. Thus if we are given two arbitrary fractions from a t-way classification, one possible criterion to use in choosing between the fractions would be to select the one with the "least contamination or bias" from the effects aliased with those being estimated. If additional criteria are desired, the one proposed here could easily be combined with presently used criteria. Given that the criterion of the "least amount of contamination" of estimated effects is desired, a measure of bias is required. Such a measure is proposed in this paper. Various theorems are proved in connection with the proposed measure. These results are of a fundamental nature in that a new property of treatments is defined and a new measure for quantifying the amount of biassing is presented.

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O. Introduction. The actual treatment design constituting the fractional replicate may occur by design, by accident, or by the impossibility or inadmissibility of certain treatment combinations. Although fractional replication frequently occurred in experimentation, it was first formally treated in various forms by Yates [1936], Fisher [1942], Finney [1945, 1946, 1947], Plackett and Burman [1946], Kempthorne [1947], Kishen [1947, 1948], Banerjee [1950], and perhaps others. Since that time there has been considerable activity in this area but despite this the major problems are far from being resolved. Many problems are of a complex combinatorial nature while others are of an analytic nature.

One of the major analytic problems in fractional replication involves the confounding of an estimated set of effects with an unestimated set. Thus, the estimated set of effects is biased by the amount of confounding present between the effects in the t-way classification which are estimated and those which are not. The untenable assumption that non-estimated effects are zero simply because they were not or could not be estimated, is not of infrequent usage in statistical literature. Since only a composite of several effects may be estimable in any given situation, this should always be stated in any application of statistics.

¹ Research supported in part by NRC Grant No. 99157543 and NIH Grant No. 5-R01-GM-05900.

² Visiting Professor of Biological Statistics, Cornell University, Sept. 1, 1971 - Sept. 1, 1972.

Key words and phrases: Treatment design, factorial experiment, fractional replicate, aliasing, bias, confounding, measure of bias, regression.

Unfortunately, it is not and only the effects most interesting or considered most likely are discussed. Ignoring the remaining effects does not change the situation in any way. One cannot assume away the difficulties in an experiment. Cochran and Cox [1957], section 6A.11, and Federer [1955], section IX-3.5, warn the reader about possible misinterpretations in the presence of confounding of effects.

Except for the easy to derive results concerning aliasing in regular fractions (fractions in which only complete confounding of effects is present) in s^m factorials, for s a prime power, and results by Raktoe and Federer [1965] on the generalized defining contrast in the 2^m case, by Paik and Federer [1971a] on a semi-invariance property of the aliasing matrix in the 2^m case, and by Paik and Federer [1971b] on the need for studying the alias matrix, little has been accomplished in constructing general aliasing schemes and nothing has been done in developing a measure for comparing the relative amount of bias (or conforunding) in two fractional replicates. Thus if we are given two arbitrary fractions from a t-way classification, one possible criterion to use in choosing between the fractions would be to select the one with the "least contamination or bias" from the effects aliased with those we are estimating. If additional criteria are desired this criterion could easily be combined with well-known criteria based on the characteristic roots of the information matrix.

Given that the criterion of the "least amount of bias or contamination" of estimated effects is desired, a measure of bias is needed. Such a measure is proposed in this paper after precisely defining the analytic concepts involved. Various theorems are proved in connection with the proposed measure. The results herein, then, are of a fundamental nature in that a new property of treatment

designs is defined and a new measure for quantifying the amount of biasing is presented. We hope that the results of this paper will encourage further research in this area. Several open problems are stated in section 7.

1. Preliminaries and notation. Let there be t factors, the ith one having k_i levels. The total number of treatment combinations in the full factorial is is equal to $N = \prod_{i=1}^{t} k_i$. Let T denote the set of all treatment combinations. A collection C of treatment combinations is said to be an (m,n,r_1,r_2,\cdots,r_n) fractional replicate (or fraction) if the cardinality of C is m and the number of distinct combinations in C is n < N. In the special case m = n the fraction is referred to as a proper fraction. Let Y(T) be the $N \times l$ vector of observations corresponding to the treatment combinations in T, written out in some fixed order. The equation system associated with Y(T) is:

$$(1.1) Y(T) = X(T)\beta + \epsilon(T),$$

where X(T) is an N × N orthogonal matrix (i.e. X'(T)X(T) = I), β is an N × l vector of linear parametric contrasts and ϵ (T) is an N × l random error vector. We assume that

(1.2)
$$\mathbb{E}[\epsilon(T)] = 0, \ \mathbb{E}[\epsilon(T)\epsilon'(T)] = \sigma^{2}I$$

and that the observation vector Y(T) was obtained from a properly randomized experiment design.

Corresponding to C there is an observational system induced by (1.1), namely,

$$(1.3) Y(C) = X(C)\beta + \epsilon(C)$$

where Y(C) is the m \times l vector of observations associated with treatment combinations in C. The m \times N matrix X(C) is simply read off from X(T) taking repetitions of treatment combinations in C into account. The m \times l random error vector ε (C) is assumed to be a homoscedastic vector in the sense of (1.2).

Since the rank of X(C) = n, it follows that the experimenter can estimate $p \le n$ independent linear functions of the components of β . Let $L\beta$ be a vector of linear functions suct that L has rank p. Let $\beta' = [B'_1 : \beta'_2]$, where β_1 is a $p \times 1$ subvector of β , and suppose that the experimenter is interested in estimating v linear functions of β which are functions of β_1 alone, i.e. given that

$$(1.4) L = [L_1 + L_2 = 0]$$

where L is $v \times N$. Note that the partitioning of β induces the following partitioned system on (1.3):

(1.5)
$$Y(C) = [X_1(C) : X_2(C)][\beta_1' : \beta_2']' + \epsilon(C)$$

where $X_1(C)$ is the m x p matrix determined by β_1 and $X_2(C)$ is the m x (N-p) matrix determined by the complementary vector β_2 . It follows that the rank of $X_1(C) \leq p$. Hereafter we shall drop the C in the notations above.

Now, for the vector $L\beta$ to be estimable it is well-known that a necessary and sufficient condition is that there exists a $v \times N$ matrix K such that

$$(1.6) L = KX$$

If L is as in (1.4) then the condition (1.6) together with (1.5) results in:

$$(1.7) L_1 = K_1 X_1$$

where K_1 is a v x p matrix determined by L_1 .

Applying the least squares procedure to (1.5) together with (1.7), we obtain the following estimator for $L_1\beta_1$:

$$\widehat{\mathbf{L}_{1}\boldsymbol{\beta}_{1}} = \mathbf{L}_{1}(\mathbf{X}_{1}^{\prime}\mathbf{X}_{1})^{\mathsf{T}}\mathbf{X}_{1}^{\prime}\mathbf{Y}$$

where $(X_1'X_1)^-$ is a generalized inverse of $X_1'X_1$. The expected value of $\widehat{L_1\beta_1}$ is:

$$(1.9) E\{\widehat{L_1\beta_1}\} = L_1\beta_1 + A\beta_2$$

where $A = K_1 X_1 (X_1 X_1)^T X_1 X_2$.

A problem of fractional replication is to choose for a given $L_1\beta_1$, a fraction satisfying certain desirable criteria such as:

- (i) The expected value of the components of $\widehat{L_1\beta_1}$ should have a minimum amount of contamination or bias from the elements of β_2 .
- (ii) The components of β_1 should be estimable if the experimenter is interested in estimating each one rather than linear functions of them.
- (iii) If the experimenter is also interested in estimating σ^2 then m-p should be of a desirable magnitude.
- (iv) The total number of treatment combinations m should not be too large, otherwise the design might become cumbersome and costly.
- (v) The fraction should be "balanced" in some meaningful sense, so that the analysis and inference can be facilitated.

(vi) The fraction should satisfy some optimality criterion on the variance-covariance matrix of the estimator of $L_1\beta_1$.

This paper concerns itself with the first criterion i.e. we shall explore the various aspects of aliasing in fractional replication. As stated in the introduction, not much attention has been paid to this topic, perhaps because many researchers have unrealistically equated β_2 to zero or assumed it be negligible. From both theoretical and practical viewpoints there is, then, a need to develop the aliasing concepts rigorously without resorting to unrealistic assumptions.

2. Some measures of contamination or bias for comparing different aliasing structures. In this section we introduce various measures of bias and discuss a selected one more deeply. Referring to equations (1.7) the matrix

(2.1)
$$A = K_1 X_1 (X_1' X_1)^{-1} X_1' X_2$$

will be defined to be the alias matrix of a given fraction C and given vector $L_1\beta_1$. Note that even though $(X_1'X_1)^-$ is not unique the matrix $X_1(X_1'X_1)^-X_1'$ is symmetric and invariant for any choice of $(X_1'X_1)^-$. Hence for the given fraction C and K_1 the matrix A in (2.1) is unique.

Of the various measures which can be introduced those which take into account all the entries of A and their magnitudes are the appealing ones. The following measures are of this nature and are also norms of A in the mathematical sense:

$$m_2(A) = \max_{i} \sum_{j} |a_{ij}|$$

$$(2.4) m3(A) = Max |aij|$$

$$m_{\mu}(A) = \sum_{i} \sum_{j} |a_{ij}|$$

where $|a_{ij}|$ indicates the absolute value of a_{ij} . All these measures are indeed matrix norms because they satisfy the following properties:

- (a) $m_i(A) \ge 0$
- (b) $m_i(\alpha A) = |\alpha| m_i(A)$
- (c) $m_i(A + B) \le m_i(A) + m_i(B)$ if A + B is defined
- (d) $m_{i}(AB) \leq m_{i}(A)m_{i}(B)$ if AB is defined
- (e) $m_i(A) = 1$ if A has a 1 in the (i,j) cell and zero elsewhere.

There are no relations between these measures except that $m_{\downarrow}(A) \ge m_{j}(A)$, j=1,2,3. The first measure $m_{\downarrow}(A)$ enjoys some desirable properties which the others do not possess, namely:

- (i) $m_1(A)$ is orthogonally invariant, i.e. $m_1(PA) = m_1(AQ) = m_1(A)$ if P and Q are orthogonal matrices.
- (ii) $m_1(A) = (\text{trace A'A})^{\frac{1}{2}}$, which implies that $m_1(A)$ is the positive square root of the sum of the eigen-values of A'A. In particular, if A is a square matrix, then $m_1(A) = \text{trace } (A'A)^{\frac{1}{2}} = (\text{trace AA'})^{\frac{1}{2}} = (\sum \lambda_1^2)^{\frac{1}{2}}$, where the λ 's are the eigen-values of A.

Because of the properties (a) through (c) together with (i) and (ii) above we will take $m_1(A)$ to be our measure of contamination or bias of $L_1\beta_1$ by $A\beta_2$ as indicated in (1.9). Note that in fractional replication, as we have defined it in this paper, the matrix A is never equal to zero. This implies that $m_1(A)$ (and any other measure in the list) is never equal to zero in fractional factorials. Or, to put it in another way, fractional factorials can be characterized and thus classified by the amount of contamination or bias $m_1(A)$ associated with their alias matrices.

Our aim in this paper is to put the concept of contamination or bias on a rigorous foundation, so that a meaningful theory can be developed. This will be in complete agreement with the development of fractional factorial designs from the viewpoint of measures associated with the information matrix $X_1^*X_1^*$.

3. <u>Basic definitions and examples</u>. We will need the following two definitions:

Definition 3.1. A fractional factorial design C is to be contamination or bias balanced if $(\sum_j a_{ij}^2)^{\frac{1}{2}}$ is constant for all i.

Note that this definition implies that in a bias balanced design the bias associated with each element of $L_1\beta_1$ is equal to:

$$(3.1)$$
 $m_1(A)/c$

where c is a positive constant. We say that the ith component of $L_1\beta_1$ is estimated with less bias than the ith component of $L_1\beta_1$ if:

(3.2)
$$\left(\sum_{j} a_{ij}^{2}\right)^{\frac{1}{2}} < \left(\sum_{j} a_{i,j}^{2}\right)^{\frac{1}{2}}$$

Definition 3.2. Let C_1 and C_2 be two competing fractional factorial designs from the same π_k factorial with the aim to estimate the fixed vector $L_1\beta_1$. Then C_1 is said to be (bias) better than C_2 if:

$$(3.3)$$
 $m_1(A_1) - m_1(A_2) < 0$ or

$$(3.4)$$
 $m_1(A_1) / m_1(A_2) < 1$

We will define C_1 and C_2 to be bias equivalent if $m_1(A_1) = m_1(A_2)$.

Before proceeding further we illustrate the concepts developed so far with an example.

Let t = 3 and $k_i = 2$ levels denoted by 0 and 1. Then $N = 2^3 = 8$, so that (1.1) will be equal to:

Let C be the following fraction from the above factorial:

$$C = \{(000), (000), (010), (011), (011)\}$$

where $(x_1x_2x_3)$ refers to the treatment combination with the ith factor being at the x_i level, i = 1,2,3. Note that m = 5 and n = 3 in this case. The equation system (1.3) for this fraction is:

Suppose now that the experimenter is interested in obtaining information regarding p=3 parameters specified by $\beta_1'=[\alpha_1,\alpha_2,\alpha_3]$. The partitioned system (1.5) corresponding to this choice of β_1 is then:

(3.8)
$$Y(C) = \frac{1}{\sqrt{8}} \begin{bmatrix} + - - & - + - + + \\ + - - & - + - + + \\ + - + & + - - + - \\ + - - & + - + - + \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_8 \\ \vdots \\ \alpha_7 \end{bmatrix} + \epsilon(C)$$

The rank of $X_1(C)$ in this example is clearly equal to 2, so that separate information for each component of β_1 is not available. This implies that at most 2 independent linear functions of β_1 can be estimated. Let these two linear functions be:

(3.9)
$$\gamma_1 = \beta_1 - \beta_2 - \beta_8$$

$$\gamma_2 = \beta_8$$

These two functions specify the matrices L_1 and L_2 respectively:

(3.10)
$$L = [L_1; L_2] = \begin{bmatrix} 1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The functions Y_1 and Y_2 are estimable because $L = K_1 X_1$, where:

(3.11)
$$K_{1} = \sqrt{8} \begin{bmatrix} 1 & -1 & 0 & -1 & 2 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -1 \end{bmatrix}$$

Now, in order to calculate the alias matrix A in (2.1) we use the following generalized inverse of $X_1^{\dagger}X_1$:

$$(3.12) \qquad (x'_1 x_1)^{-} = \frac{1}{2} \begin{bmatrix} 5 & 0 & 3 \\ 0 & 0 & 0 \\ 3 & 0 & 5 \end{bmatrix}$$

Hence for the above $\mathbf{K}_{\mathbf{l}}$ the alias matrix is:

(3.13)
$$A = \frac{\sqrt{8}}{32\sqrt{2}} \begin{bmatrix} 15 & -15 & -15 & 15 & 133 \\ -1 & 1 & 1 & -1 & -43 \end{bmatrix}$$

The amount of bias or contamination as measured by $\mathbf{m}_1(\mathbf{A})$ for this example equals:

$$(3.14) m1(A) = \left(\frac{10721}{128}\right)^{\frac{1}{2}} = 9.15$$

Note that in this fractional factorial design Y_2 is estimated with less bias than Y_1 and hence it follows from definition 3.1 that this fraction is not bias balanced.

Next, consider the competing fraction

$$C^* = \{(000), (110), (101), (001)\}$$

The corresponding matrices X_1^* , $X_1^{*_1}X_1^*$ and $(X_1^{*_1}X_1^*)^-$ are respectively:

$$(3.16) \quad X_{1}^{*} = \frac{1}{\sqrt{8}} \begin{bmatrix} 1 & -1 & -1 \\ 1 & 1 & -1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix}, \quad X_{1}^{*} \cdot X_{1}^{*} = \frac{1}{8} \begin{bmatrix} 4 & 0 & -2 \\ 0 & 4 & -2 \\ -2 & -2 & 4 \end{bmatrix}, \quad (X_{1}^{*} \cdot X_{1}^{*})^{-} = \begin{bmatrix} 3 & 1 & 2 \\ 1 & 3 & 2 \\ 2 & 2 & 4 \end{bmatrix}$$

Hence we have:

(3.17)
$$X_{1}^{*}(X_{1}^{*}, X_{1}^{*})^{T}X_{1}^{*} = \frac{1}{2} \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}$$

Clearly $\mathbf{L}_1 \boldsymbol{\beta}_1$ as defined earlier is estimable by this fraction. In this case:

(3.18)
$$K_1^* = \sqrt{8} \begin{bmatrix} 1 & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

Therefore the alias matrix associated with C* is:

(3.19)
$$A^* = \frac{1}{2} \begin{bmatrix} -1 & 1 & -1 & 1 & 1 \\ 2 & 0 & 0 & -2 & -2 \end{bmatrix}$$

Hence the amount of bias for C* is equal to:

(3.20)
$$m_1(A^*) = \frac{1}{2}(17)^{\frac{1}{2}} = 2.06.$$

Again, C^* is not bias balanced and clearly C^* is better than C from the viewpoint of bias.

4. Invariance of the amount of bias $m_1(A)$ under various operations. In this section we shall characterize some operations which leave the amount of bias $m_1(A)$ invariant. These operations arise naturally in practical and theoretical considerations.

A. Replication operation. Let C be an (m,n,r_1,r_2,\cdots,r_n) fraction and $C(\alpha)$ be the fraction obtained from C simply by taking each (distinct or not) element of C α times. The process of obtaining $C(\alpha)$ from C will be referred to in this paper as the replication operation. With respect to this operation the following theorem can be easily verified:

Theorem 4.1. The amount of bias m₁(A) associated with the fraction C is invariant under the replication operation, i.e.

$$(4.1) m1(AC) = m1(AC(\alpha))$$

Definition 4.1. Let $C(m,n,r_1,r_2,\cdots,r_n)$ be a fraction and let the greatest common divisor of r_1,r_2,\cdots,r_n be d. Then the fraction $C'(m',n,r_1',\cdots,r_n')$ where m'=m/d and $r_1'=r_1/d$ is said to be the reduced form of C if C and C' are based on the same set of treatment combinations. This definition then leads us to the following:

Corollary 4.1. The amount of bias $m_1(A)$ associated with the fraction C is the same as the amount of bias associated with the reduced fraction C.

This corollary states that as far as bias is concerned the experimenter can reduce the fraction to a reduced form in order to facilitate calculations. Note that no amount of replication of a multiple of the given set changes the amount of bias.

Now, let $D_1 = C(m,n,r_1,\cdots,r_n)$ be an arbitrary fraction. The theorem below establishes a relation between the amount of bias of this fraction and the amount of bias of the minimal proper fraction $D_0 = C(n,n,1,\cdots,1)$ associated with D_1 .

Let $[B_1:B_2]$ be the partitioned design matrix of D_0 with respect to $L_1\beta_1$. By corollary 4.1 we equivalently measure the amount of bias of D_1 by calculating the amount of bias of $D_1' = C(m',n,r_1',\cdots,r_n')$ where m' = m/d and $r_1' = r_1/d$, $i = 1,2,\cdots,n$ and d is the greatest common divisor of (r_1,r_2,\cdots,r_n) . With no loss of generality we may assume that $r_1' \geq r_2' \cdots \geq r_n'$.

Theorem 4.2. The amounts of bias of the fractions D_0 and D_1' are related though the replication matrix $R = diag(r_1', \dots, r_n')$ by:

$$(4.2)$$
 $m_1(A_{D_1^i}) = m_1[K_1B_1(B_1^iRB_1)^-B_1^iRB_2]$

$$(4.3)$$
 $m_1(A_{D_0}) = m_1[K_1B_1(B_1'B_1)^-B_1'B_2]$

<u>Proof:</u> Let $[X_1 : X_2]$ be the partitioned design matrix of D_1 . It follows from the \mathbf{r}_i^{\prime} 's, that the matrices X_1 and X_2 can be written explicitly as:

(4.4)
$$X_{1} = \begin{bmatrix} G_{r_{1}^{1}}B_{1} \\ G_{r_{2}^{1}}B_{1} \\ \vdots \\ G_{r_{n}^{1}}B_{1} \end{bmatrix}$$
, and, $X_{2} = \begin{bmatrix} G_{r_{1}^{1}}B_{2} \\ G_{r_{2}^{1}}B_{2} \\ \vdots \\ G_{r_{n}^{1}}B_{2} \end{bmatrix}$

where the matrix G_i is an n x n diagonal indicator matrix with entries equal to one if treatment combinations corresponding to the rows of B_l are present and zero otherwise. This implies that:

(4.5)
$$X_{1}'X_{1} = B_{1}'\sum_{i=1}^{r_{n}} G_{i}B_{1} = B_{1}'RB_{1}$$

Furthermore, the estimability condition on $L_1\beta_1$ using design D_0 implies that there exists a K_1 such that $L_1 = K_1B_1$. Clearly if L_1 is estimable by D_0 then it is also estimable by design D_1 , since $L_1 = K_1^*X_1$ where $K_1^* = [K_1 : 0]$. The proof of the theorem then follows using the definitions of the alias matrices of D_0 and D_1 .

Before proceeding further we quote the following well-known lemma:

Lemma 4.1. If P_1 has full column rank and P_2 has full row rank and A is any matrix, then $(P_1A_1P_2)^{-} = P_2A^{-}P_1^{-}$, where "=" indicates the unique Penrose generalized inverse.

Using this lemma and the fact that $P_2P_2^- = I$ and $P_1^-P_1^- = I$, the following corollary can be easily established:

Corollary 4.2. The amount of bias of a design $C(m,n,r_1,\cdots,r_n)$ is equal to the amount of bias of the minimal proper fraction associated with the given design if the design matrix B_1 has full rank.

This corollary indicates that with respect to bias or contamination the effect of replication is of no consequence if the design is "nonsingular", i.e. the amount of bias is invariant under replication as long as the design is of full rank. The practical consequence of this corollary is that the experimenter is economically better off using the proper minimal fraction in this situation. This result, by the way, also shows the unimportance of the classical notion of unbalanced (unequal numbers) designs as far as bias is concerned. Unequal numbers designs do affect analysis problems and variance considerations.

B. Permutation operation. In typical applications the experimenter has to adopt a coding system of the levels of the factors. If his aims are realistic then it is natural to expect that the coding system will have no bearing whatsoever on the total information obtained in the experiment. The aim of this section is to establish the invariance of the amount of contamination or bias, when the levels of the factors are permuted, i.e. when the levels of the factors are recoded.

Formally, let the k_1 levels of the factor F_1 be coded as $\{0,1,2,\cdots,k_1-1\}$, $i=1,2,\cdots,t$. Let Ω be the set of permutations of the form $\omega=(\omega_1,\omega_2,\cdots,\omega_t)$ where ω_i is a permutation acting on the levels of the i^{th} factor. A realistic choice of $\{L_1,\beta_1,C\}$ implies that the design C should be capable of providing the desired statistical information on $L_1\beta_1$. However, not all realistic choices of $\{L_1,\beta_1,C\}$ guarantee the invariance of information and amount of bias under a permutation ω . (This may sound strange but a later example will clarify the point.) An interesting and open problem is to characterize the set $\{L_1,\beta_1\}$ such that a permutation ω leaves the information and/or amount of bias invariant. A partial solution to this problem is provided by theorem 4.3 below.

Before proceeding to theorem 4.3 let us first introduce some necessary conditions. Denote an element of β by the symbol $A_1^{X_1}A_2^{X_2}\cdots A_t^{X_t}$, where $x_i\in\{0,1,2,\cdots,k_i-1\}$. Note that in this notation the mean $\mu=A_1^0A_2^0\cdots A_t^0$ and $\{A_1^0A_2^0\cdots A_{i-1}^0A_i^1A_{i+1}^0\cdots A_t^0,\ A_1^0A_2^0\cdots A_{i-1}^0A_i^1A_{i+1}^0\cdots A_t^0,\ A_1^0A_2^0\cdots A_{i-1}^0A_i^0A_1^0\cdots A_{i-1}^0A_{i+1}^0\cdots A_t^0\}$ represents the set of k_i -1 normalized orthogonal parametric contrasts associated with the i^{th} factor. Define β_1 to be admissable if and only if whenever $A_1^{X_1}A_2^{X_2}\cdots A_i^{X_i}\cdots A_t^{X_t}$ belongs to β_1 and $x_i\neq 0$ ($1\leq i\leq t$), then $A_1^{X_1}A_2^{X_2}\cdots A_i^1\cdots A_t^{X_t}$ belongs to β_1 for all $z\neq 0$. The following lemma can be obtained from the paper by Srivastava, Raktoe, and Pesotan (1971).

Lemma 4.2. If C is an arbitrary fraction and C_{ω} is the fraction corresponding to $\omega \in \Omega$ and β_1 is admissable then there exist orthogonal matrices $P_{1\omega}$ and $P_{2\omega}$ such that:

(4.6)
$$X_1 P_{1\omega} = X_{1\omega}, X_2 P_{2\omega} = X_{2\omega}$$

where X_1 and X_{lw} respectively are the design matrices corresponding to $\{C,\beta_1\}$ and $\{C_w,\beta_1\}$; X_2 and X_{2w} are the corresponding matrices as defined in (1.5).

We next have:

Theorem 4.3. The amount of bias or contamination $m_1(A)$ is invariant under Ω if β_1 is admissable.

Proof:
$$m_1(A_w) = m_1(K_1X_1P_{1w}[(X_1P_{1w})'(X_1P_{1w})]^*(X_1P_{1w})'X_2P_{2w})$$

$$= m_1(K_1X_1(X_1'X_1)^*X_1'X_2P_{2w}), \text{ by a property of generalized inverse}$$

$$= m_1(A) \text{ by property (i) of section 2.}$$

We conclude this section with some examples to illustrate some of the findings.

C. Examples. Consider a 3×3 factorial with the full model written out as:

$$\begin{bmatrix} Y_{00} \\ Y_{10} \\ Y_{20} \\ \end{bmatrix} = \begin{bmatrix} \frac{1}{3} & -\frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & -\frac{1}{\sqrt{6}} & \frac{1}{2} & -\frac{1}{2\sqrt{3}} & \frac{1}{3\sqrt{2}} & -\frac{1}{2\sqrt{3}} & \frac{1}{6} \\ \frac{1}{3} & 0 & -\frac{2}{3\sqrt{2}} & -\frac{1}{\sqrt{6}} & 0 & \frac{2}{2\sqrt{3}} & \frac{1}{3\sqrt{2}} & 0 & -\frac{2}{6} \\ \frac{1}{3} & \frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & -\frac{1}{\sqrt{6}} & -\frac{1}{2} & -\frac{1}{2\sqrt{3}} & \frac{1}{3\sqrt{2}} & \frac{1}{2\sqrt{3}} & \frac{1}{6} \\ Y_{01} & \frac{1}{3} & -\frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & 0 & 0 & 0 & -\frac{2}{3\sqrt{2}} & \frac{2}{2\sqrt{3}} & -\frac{2}{6} \\ Y_{11} & \frac{1}{3} & 0 & -\frac{2}{3\sqrt{2}} & 0 & 0 & 0 & -\frac{2}{3\sqrt{2}} & \frac{2}{2\sqrt{3}} & -\frac{2}{6} \\ Y_{21} & \frac{1}{3} & \frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & 0 & 0 & 0 & -\frac{2}{3\sqrt{2}} & -\frac{2}{2\sqrt{3}} & -\frac{2}{6} \\ Y_{21} & \frac{1}{3} & -\frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & 0 & 0 & 0 & -\frac{2}{3\sqrt{2}} & -\frac{2}{2\sqrt{3}} & -\frac{2}{6} \\ Y_{12} & \frac{1}{3} & -\frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & \frac{1}{\sqrt{6}} & -\frac{1}{2} & \frac{1}{2\sqrt{3}} & \frac{1}{3\sqrt{2}} & -\frac{1}{2\sqrt{3}} & \frac{1}{6} \\ Y_{12} & \frac{1}{3} & 0 & -\frac{2}{3\sqrt{2}} & \frac{1}{\sqrt{6}} & 0 & -\frac{2}{2\sqrt{3}} & \frac{1}{3\sqrt{2}} & 0 & -\frac{2}{6} \\ Y_{12} & \frac{1}{3} & \frac{1}{\sqrt{6}} & \frac{1}{3\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{2} & \frac{1}{2\sqrt{3}} & \frac{1}{3\sqrt{2}} & \frac{1}{2\sqrt{3}} & \frac{1}{6} \end{bmatrix} \begin{pmatrix} A_1^0 A_2^0 \\ A_1^1 A_2^0 \\ A_1^2 A_2^0 \\ A_1^2 A_2^0 \\ A_1^2 A_2^0 \\ A_1^2 A_2^0 \end{pmatrix}$$

The following points illustrate some of the concepts developed in this section:

(1) The triple $\{L_1, \beta_1, C\}$, where

(4.8)
$$L_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
, $\beta_1 = \begin{bmatrix} A_1^0 & A_2^0 \\ A_1^1 & A_2^0 \\ A_1^0 & A_2^1 \end{bmatrix}$ and $C = \{00, 10, 20\}$

is not realistic, because C is incapable of providing an estimate of $A_1^0A_2^1$. Note that $A_1^0A_2^1$ measures the linearity associated with the second factor. In conventional language the fraction is such that $A_1^0A_2^1$ is completely confounded will $A_1^0A_2^0$.

(2) The triple $\{L_1^*, \beta_1^*, C^*\}$, where

(4.9)
$$L_1^* = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$
, $\beta_1^* = \begin{bmatrix} A_1^1 & A_2^0 \\ A_1^0 & A_2^1 \end{bmatrix}$ and $C = \{01, 12\}$

is realistic. However the reader can check for himself that the bias measure will not be invariant under the permutation

because β_1^* is not admissible.

- (3) The examples discussed in section 3 illustrate the invariance of the bias measure under any permutation ω , since they satisfy the condition of theorem 4.3.
- D. Remarks. Let us explore now the behavior of the bias measure of two rank equivalent designs. More specifically consider two fractions C and C* from the same factorial such that (i) they have the same cardinality, (ii) the corresponding design matrices X_1 and X_1^* have the same rank, and (iii) the complementary matrices X_2 and X_2^* have the same rank. We assume here that L_1 and β_1 are the same for both designs. From elementary matrix algebra we know that:

$$(4.11)$$
 $X_1^* = E_1 X_1 F_1$, $X_2^* = E_2 X_2 F_2$

where E_1 , E_2 , F_1 and F_2 are nonsingular square matrices of appropriate dimensions. This leads us to the following expression for the bias measure of design C^* :

$$(4.12) m_1(A^*) = m_1(K_1E_1X_1F_1[(E_1X_1F_1)'(E_1X_1F_1)]^{-1}(E_1X_1F_1)'E_2X_2F_2)$$

If E, and E, are orthogonal and

$$[(X_1F_1)^{\dagger}(X_1F_1)]^{-1} = F_1^{-1}(X_1^{\dagger}X_2)^{-1}F_1^{\dagger}$$

then:

$$(4.14) m_1(A^{**}) = m_1(K_1X_1(X_1, X_1) X_1 X_2 F_2)$$

Finally, if F_2 is also orthogonal we then have that $m_1(A^*) = m_1(A)$.

Note that theorem 4.3 is a special case of this, i.e. $E_1 = E_2 = I$, and, F_1 and F_2 are orthogonal.

Further characterization of E_1 , E_2 , F_1 and F_2 is needed which describes the relation between $m_1(A)$ and $m_1(A^*)$ under various settings.

5. Biasses of a design and its complement. This section explores some relations between the bias measures of a design and its complement. Consider the fraction $C^*(m^*, N, r_1, \dots, r_N)$, then we can easily establish:

(5.1)
$$X'(C^*)X(C^*) = \sum_{i=1}^{N} r_i^* x_i x_i'$$

where x_i is the ith row of X(T) in (1.1) corresponding to the ith treatment combination in C^* . Note that $x_i x_i'$ is an idempotent matrix of rank unity, since x_i is an orthonormal vector. In the case $r_i = r$ for all $i = 1, 2, \dots, N$, then obviously:

$$(5.2) X'(C^*)X(C^*) = rI$$

Corresponding to the fraction $C(m,n,r_1,r_2,\cdots,r_n)$ and the partitioned vector $\beta'=(\beta_1':\beta_2')$ we have the following partitioning of $X(C^*)$:

$$(5.3) X(c^*) = \begin{bmatrix} \mathbf{1}_{r_1} & \mathbf{x}'_{11} & \mathbf{1}_{r_1} & \mathbf{x}'_{12} \\ \mathbf{1}_{r_2} & \mathbf{x}'_{21} & \mathbf{1}_{r_2} & \mathbf{x}'_{22} \\ \vdots & \vdots & \vdots \\ \mathbf{1}_{r_n} & \mathbf{x}'_{n1} & \mathbf{1}_{r_n} & \mathbf{x}'_{n2} \\ \mathbf{1}_{r_{n+1}} & \mathbf{x}'_{n+11} & \mathbf{1}_{r_{n+1}} & \mathbf{x}'_{n+12} \\ \mathbf{1}_{r_{n+2}} & \mathbf{x}'_{n+21} & \mathbf{1}_{r_{n+3}} & \mathbf{x}'_{n+22} \\ \vdots & \vdots & \vdots \\ \mathbf{1}_{r_n} & \mathbf{x}'_{N1} & \mathbf{1}_{r_n} & \mathbf{x}'_{N2} \end{bmatrix} = \begin{bmatrix} X_{11}(c^*) & X_{12}(c^*) \\ X_{21}(c^*) & X_{22}(c^*) \end{bmatrix}$$

Hence:

$$(5.4) \quad X'(C^*)X(C^*) = \begin{bmatrix} n & N & n & N \\ \sum_{i=1}^{n} r_i x_{i1} x_{i1}' + \sum_{i=1}^{n} r_i x_{i1} x_{i1}' & \sum_{i=1}^{n} r_i x_{i1} x_{i2}' + \sum_{i=n+1}^{n} r_i x_{i1} x_{i2}' \\ \vdots = 1 & i = n+1 & i = 1 & i = n+1 \end{bmatrix}$$

$$\begin{bmatrix} n & N & n & N \\ \sum_{i=1}^{n} r_i x_{i2} x_{i1}' + \sum_{i=1}^{n} r_i x_{i2} x_{i1}' & \sum_{i=1}^{n} r_i x_{i2} x_{i2}' + \sum_{i=n+1}^{n} r_i x_{i2} x_{i2}' \\ \vdots = 1 & i = n+1 & i = 1 & i = n+1 \end{bmatrix}$$

$$= \begin{bmatrix} x^{15}(c_*)x^{11}(c_*) + x_1^{55}(c_*)x^{51}(c_*) & x^{15}(c_*)x^{15}(c_*) + x_1^{55}(c_*)x^{55}(c_*) \\ & x^{11}(c_*)x^{11}(c_*) + x_1^{51}(c_*)x^{51}(c_*) & x^{11}(c_*)x^{15}(c_*) + x_1^{51}(c_*)x^{55}(c_*) \end{bmatrix}$$

Clearly, in the case $r_i = r$, $i = 1, 2, \dots, N$, we obtain the following equations:

(5.5)
$$X'_{11}(C^*)X_{11}(C^*) + X'_{21}(C^*)X_{21}(C^*) = I_n$$

$$(5.6) X'_{11}(C^*)X_{12}(C^*) + X'_{21}(C^*)X_{22}(C^*) = 0$$

$$(5.7) X'_{12}(C^*)X_{11}(C^*) + X'_{22}(C^*)X_{21}(C^*) = 0$$

(5.8)
$$X_{12}^{i}(C^{*})X_{12}(C^{*}) + X_{22}^{i}(C^{*})X_{22}(C^{*}) = I_{N-n}$$

Similar relations can be established by considering the product $X(C^*)X'(C^*)$, as for example, was done in Banerjee and Federer [1966].

For the case $r_i = r$, $i = 1, 2, \cdots, N$, without loss of generality we may consider the fraction $C(n,n,l,l,\cdots,l)$. Assume further that β_l has n elements and the problem is to estimate this vector. Finally suppose that the design is variance balanced and orthogonal, i.e. $X_{ll}^t X_{ll} = k_l I$, where X_{ll} is the design matrix of C. For given β_l and C let X be partitioned as:

where X_{11} is the design matrix of C. Hence X_{22} is the design matrix of $\bar{C}(N-n, N-n, 1, 1, \cdots, 1)$ for $\beta_2 = \bar{\beta}_1$ (- indicates set theoretic complement). Whenever \bar{C} is also a variance balanced orthogonal fraction, i.e. $X_{22}^{\bullet}X_{22} = k_2I$, then, under these assumptions the bias measures of C and \bar{C} are respectively:

(5.10)
$$m_{1}(A_{1}) = m_{1}(x_{11}^{-1}x_{12})$$

$$= \left\{ trace \left(x_{12}^{\prime} x_{11}^{-1} x_{12}^{-1} \right) \right\}^{\frac{1}{2}}$$

$$= \left\{ \text{trace } \left(X_{12}' \frac{1}{k_1} X_{11} X_{12} X_{12} \right) \right\}^{\frac{1}{2}}$$

$$= \left\{ \text{trace } \left[\frac{1}{k_1} \left(X_{12}' X_{12} \right) \right] \right\}^{\frac{1}{2}}$$

$$= \left\{ \text{trace } \left[\frac{1}{k_1} \left(I_{N-n}^{-k_2} I_{N-n} \right) \right] \right\}^{\frac{1}{2}}$$

$$= \left\{ \frac{(N-n)(1-k_2)}{k_1} \right\}^{\frac{1}{2}}$$
and,
$$m_1(A_2) = m_1 \left(X_{22}^{-1} X_{21} \right)$$

$$= \left\{ \text{trace } \left(X_{21}' X_{22}^{-1} X_{22}^{-1} X_{21} \right) \right\}^{\frac{1}{2}}$$

$$= \left\{ \text{trace } \left(\frac{X_{21}' X_{22}}{k_2} \frac{X_{22}' X_{21}}{k_2} \right) \right\}^{\frac{1}{2}}$$

$$= \left\{ \text{trace } \left[\frac{1}{k_2} \left(X_{21}' X_{21} \right) \right] \right\}^{\frac{1}{2}}$$

$$= \left\{ \text{trace } \left[\frac{1}{k_2} \left(1-k_1 \right) I_n \right] \right\}^{\frac{1}{2}}$$

$$= \left\{ \frac{n(1-k_1)}{k_2} \right\}^{\frac{1}{2}}.$$

Since det $X'_{11}X_{11} = k_1^n$ it is clear that $|\det X_{11}| = k_1^{n/2}$. Similarly $|\det X_{22}| = k_2^{(N-n)/2}$, but, from a theorem in Muir and Metzler [1933] we know that $|\det X_{11}| = |\det X_{22}|$, so that $k_1^{n/2} = k_2^{(N-n)/2}$. Hence, $k_1^n = k_2^{N-n}$. We thus have established:

Theorem 5.1. Let C and \bar{C} be balanced orthogonal fractions, then knowledge of the amount of bias in C implies knowledge of the amount of bias in \bar{C} . Further, if C has cardinality $\frac{N}{2}$ then C and \bar{C} have equal amounts of bias or contamination.

Writing
$$m_1(A_2) = \left\{\frac{n(1-k_1)}{k_2}\right\}^{\frac{1}{2}} = \frac{n(1-k_1)}{k_1^{n/(N-n)}}$$
 we see that $m_1(A_1) = (N-n)(1-k_1^{n/(N-n)})$

so that $m_1(A_1) \longrightarrow 0$ as $n \longrightarrow \mathbb{N}$ as intuitively expected.

Further exploration of relations between the biasses of C and $\bar{\text{C}}$ is desirable in less restricted fractions.

6. Orthogonality and bias balance. Characterization of bias balanced designs is an important topic. However this is not an easy task at all. We characterize only a subfamily of bias balanced designs below.

Let C be an (m,n,r_1,\cdots,r_n) fraction from the $\prod_{r=1}^k$ factorial with cardinality

of β_1 equal to n. Let X_1 be the corresponding design matrix of C. Assume $r_1 = r$ and C to be an orthogonal fraction, i.e.

(6.1)
$$X_1'X_1 = Diagonal matrix = D.$$

An unsolved problem is to find conditions on C and β_1 such that the design is bias balanced. (To solve this problem one must show that the lengths of the rows of $A = X_1(X_1'X_1)^{-1}X_1'X_2 = X_1D^{-1}X_1X_2 \text{ are the same.})$

To make some headway let us restrict ourselves to the subclass of variance balanced orthogonal designs satisfying:

(6.2)
$$X_1'X_1 = k_1I$$
, and $X_2'X_2 = k_2I$;

then we prove the following:

Theorem 6.1. The fraction C is also bias balanced if condition (6.2) is satisfied.

<u>Proof:</u> The alias matrix $A = X_1(X_1^{\dagger}X_1)^{-1}X_1^{\dagger}X_2 = k_1^{-1}X_1X_1^{\dagger}X_2$. The proof is complete if we can show that A'A has equal diagonal elements. But,

Since $X_1 X_1' + X_2 X_2' = I$, we have $X_1 X_1' = (1-k_2)$ I from (6.2). Therefore:

(6.4)
$$A'A = \frac{(1-k_3)}{k_1} X_2' X_2$$
$$= \frac{k_3(1-k_3)}{k_1} I$$

which proves the theorem.

Example. As an example consider the fraction C(4,4,1,1,1,1) of the 2^3 factorial consisting of:

(6.5)
$$C = \{(000), (110), (101), (011)\}$$

with the desire to estimate $\beta_1' = (\mu,A,B,C)$. The matrices required here are:

Clearly C satisfies condition (6.2), since $X_1^{\dagger}X_1 = \frac{1}{2}$ I and $X_2X_2^{\dagger} = \frac{1}{2}$ I. Here $k_1 = k_2 = \frac{1}{2}$. The alias matrix $A = X_1(X_1^{\dagger}X_1)^{\top}X_2 = 2X_1X_1^{\dagger}X_2 = X_2$. The length of a row of X_2 is $\sqrt{1/2}$, so that C is bias balanced. Using theorem 6.1, we see that is true, since $A^{\dagger}A = \frac{k_2(1-k_2)}{k_1}$ I = $\frac{1}{2}$ I, so that the length of a row is $\sqrt{1/2}$.

In this section we have explored the relation between certain orthogonal fractions and the concept of bias balance. There is a classical concept in fractional replication which is also related to bias balance, namely the concept of regular fractions in symmetrical prime powered factorials. A fraction of cardinality $s^{m-\mu}$ of the $\mathbb{R}_i = s^m$ (s is a prime or a power of a prime) factorial is said to be regular if it is such that the mean and $(s^{\mu}-1)/(s-1)$ effects confounded with it form a subgroup of the Abelian group associated with the s^m factorial. It is well-known that every set of (s-1) single degree of freedom parameters is confounded with $(s^{\mu}-1)/(s-1)$ sets of (s-1) single degree of freedom parameters. In this framework all regular fractions are bias balanced.

7. Some comments. The richness of research on factorial treatment designs is again allustrated by the results in this paper for quantifying bias in fractional replicates and in which the concept of measuring bias due to aliasing in fractional replication has been introduced. The measuring device selected was the matrix norm obtained from the trace of A'A where A is the alias matrix of a fractional replicate. Many extensions of our results are possible. For example, an easy and straight-forward extension is to the case of polynomial regression for a pth degree polynomial and for N possible parameters. Another extension possible in multiple regression for given values of the b independent variables would be

to measure the bias due to higher degree polynomials and cross products not considered. Other extensions could involve the development of different measures of bias to characterize the alias matrix. Finally, an unsolved problem of considerable complexity is to find the precise range of the bias measure for a given class of fractional replicates, e.g. saturated main effect plans.

8. A background note. The authors' interest in measuring bias due to aliasing and in characterizing the alias matrix has been in a twenty year incubation period for one of us (Federer) and for about eight for another (Raktoe). During the 1950's, A. E. Brandt often stressed the importance of always writing down the aliases for any incomplete factorial, several authors routinely equated alias effects to zero, students had difficulties understanding situations wherein only a sum of effects was estimable, and research problems which required nonregular fractional replicates were encountered under several different situations. All these had their effect in bringing to light the importance of studying aliases. Also, during the early 1960's when an Associate Editor of the Annals of Mathematical Statistics suggested that the study of variance optimality may be unimportant in fractional replication, M. Zelen and W. T. Federer were led to the conclusion that he was correct and that the nature of the aliasing may be the criterion to use in such cases. The study of nonregular fractions of a factorial led W. T. Federer and B. L. Raktoe, and consequently U. B. Paik, directly to a study of aliasing. In searching for methods of measuring the amount of aliasing, the number or proportion of zeros in the alias matrix A was considered. Since the main and perhaps only property of this measure was ease of computation, the present authors decided to find a measure with more desirable properties.

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