

ON A RANDOMIZED PROCEDURE FOR SATURATED FRACTIONAL REPLICATES IN A 2^n -FACTORIAL

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The authors previously presented a randomized procedure for non-orthogonal saturated main effect fractional replicates in an s^n -factorial and presented an unbiased estimator of the main effect parameter vector. However, the explicit expression of the variance of the estimator remained an unsolved problem. In this paper our attention is restricted to a 2^n -factorial, and the randomized procedure is extended to any preassigned parameters in a 2^n -factorial system. An explicit expression of the variances of unbiased estimators of the parameters is presented. Also, in a 2^n -factorial, some invariant properties of the information matrices and variances of the estimators in the randomized fractional replicates and a semi-invariant property of alias schemes of the fractional replicates are obtained.

0. Introduction and summary. Paik and Federer [4] presented a randomized procedure and defined an invariance property for nonorthogonal saturated main effect fractional replicates from an s^n -factorial; also, an unbiased estimator of the main effect parameter vector was obtained but the variance of the estimator was not. In the present paper we shall limit ourselves to the 2^n -factorial; after some preliminary definitions and notations, a property for any saturated fractional replicate from the 2^n -factorial is described in Section 2, and a lemma is stated to bring together some of the results. In the third section of the paper, an invariant property of the information matrix of a saturated fractional replicate and a semi-invariant property of the aliasing matrix are developed and are summarized in Theorem 1. A randomized procedure, an unbiased estimator of the parameter vector, and the corresponding covariance matrix have been derived and are presented in the second theorem.

1. Basic notations and statistical model. In a 2^n -factorial system, the space of treatment combinations, Z , is represented by the set $Z = \{(i_1, i_2, \dots, i_n): i_h = 0 \text{ or } 1 \text{ for all } h = 1, 2, \dots, n\}$ which contains 2^n points, say $N = 2^n$. A standard ordering of points in Z is given by the relationship between the coordinate of a point $z_v = (i_1, i_2, \dots, i_n)$, $v = 0, 1, \dots, N - 1$, and order subscript $v = \sum_{h=1}^n i_h 2^{n-h}$.

The addition operation $+$ and multiplication operation \cdot of any of two treatment combinations z_v and $z_{v'}$ are defined as addition and inner product of two row vectors of $z_v = (i_1, i_2, \dots, i_n)$ and $z_{v'} = (i'_1, i'_2, \dots, i'_n)$, modulo 2, respectively. It follows immediately that the set Z is a group with respect to addition.

The expected value of the random vector $y(Z)$ associated with the space of

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treatment combinations Z is given by

$$E[y(Z)] = X\mathbf{B},$$

where X is a $2^n \times 2^n$ matrix with orthogonal column vectors such that $X'X = 2^n I$, \mathbf{B} is the $N \times 1$ column vector of single degrees of freedom parameters $\beta_0, \beta_1, \dots, \beta_{N-1}$ and $y(Z)$ is the $N \times 1$ column vector of observations, with covariance matrix $\sigma^2 I$. The parameters β_u have the usual interpretation of main effects and interactions of n factors. We further describe the structure of N parameters, β_u , $u = 0, 1, \dots, N-1$, by considering the space B of N points where $B = \{(\alpha_1, \alpha_2, \dots, \alpha_n): \alpha_h = 0 \text{ or } 1 \text{ for all } h = 1, 2, \dots, n\}$. The correspondence between the parameters and the points of B is given by the order relation specified by $u = \sum_{h=1}^n \alpha_h 2^{n-h}$. We also introduce addition and the inner product of any of two row vectors $\beta_u = (\alpha_1, \alpha_2, \dots, \alpha_n)$ and $\beta_u' = (\alpha_1', \alpha_2', \dots, \alpha_n')$ or between z_v and β_u . The unit element of this parameter group in addition, $\beta_0 = (0, 0, \dots, 0)$, is the mean response of all the treatment combinations. The parameter point β_u in which the k th position is 1 and all other positions are zero, corresponds to the k th factor first degree main effect. Interactions correspond to points where coordinates are zero or nonzero with at least two nonzero coordinates. The matrix X can be defined as

$$X = X^{(2)} \otimes \dots \otimes X^{(2)},$$

where $X^{(2)} = \begin{pmatrix} 1 & -1 \end{pmatrix}$ and \otimes denotes Kronecker product.

Suppose that the vectors of $y(Z)$ and \mathbf{B} are rearranged and partitioned as follows: $y(Z^*)' = (y(Z_p)', y(Z_{N-p})')$, $\mathbf{B}^{*'} = (\mathbf{B}_p', \mathbf{B}_{N-p}')$, where $y(Z_p)$ and \mathbf{B}_p are $p \times 1$ observation and $p \times 1$ interesting parameter vectors, respectively, with the mean parameter as the first element of \mathbf{B}_p . We shall write \mathbf{y}_p and \mathbf{y}_{N-p} for $y(Z_p)$ and $(y(Z_{N-p}))$, respectively, and also we shall use a new notation for the rearranged parameters in vectors \mathbf{B}_p and \mathbf{B}_{N-p} such that $\mathbf{B}_p = (b_0, b_1, \dots, b_{p-1})'$ and $\mathbf{B}_{N-p} = (b_1^*, b_2^*, \dots, b_{N-p}^*)'$.

Consider the expression $E[y(Z)] = [X_1, X_2][\mathbf{B}_p', \mathbf{B}_{N-p}']'$ where X_1 is an $N \times p$ matrix and X_2 is an $N \times (N-p)$ matrix. The matrix $[X_1, X_2]$ is obtained by rearranging the column order in X and the partitioning of that matrix. Since X is an $N \times N$ matrix with orthogonal column vectors, $r(X_1) = p$. Hence, there exists at least one non-singular $p \times p$ matrix X_{11} in the matrix X_1 .

After rearranging the order of the elements in $y(Z)$ and the row order in $[X_1, X_2]$, respectively, we obtain the following expression:

$$E[\mathbf{y}_p] = [X_{11}, X_{12}][\mathbf{B}_p', \mathbf{B}_{N-p}']'$$

such that X_{11} is a non-singular $p \times p$ matrix, the observations in \mathbf{y}_p yield a saturated fractional replicate for the given parameter vector \mathbf{B}_p .

Using the least squares procedure we obtain the solution (Banerjee and Federer [1], Zacks [7]),

$$\hat{\mathbf{B}}_p = X_{11}^{-1} \mathbf{y}_p.$$

Hence, $X_{11}^{-1} \mathbf{y}_p$ is the best linear unbiased estimator of $\mathbf{B}_p + X_{11}^{-1} X_{12} \mathbf{B}_{N-p}$.

2. A property of matrices X_{11} and X_{12} . Let Z_p be a saturated fractional replicate plan given a parameter vector \mathbf{B}_p represented by a submatrix of Z such as a $p \times n$ matrix in a 2^n -factorial and X_{11} by a $p \times p$ coefficient matrix of \mathbf{B}_p and X_{12} by a $p \times (N - p)$ coefficient matrix of \mathbf{B}_{N-p} corresponding to the plan Z_p , and let $J(i_1, i_2, \dots, i_n)$ be a $p \times n$ matrix such that

$$J(i_1, i_2, \dots, i_n) = \begin{bmatrix} i_1, i_2, \dots, i_n \\ \cdot \cdot \cdot \cdot \cdot \cdot \\ i_1, i_2, \dots, i_n \end{bmatrix}$$

where $i_h = 0$ or 1 for all $h = 1, 2, \dots, n$, and $X_{11,v}$ and $X_{12,v}$ be a $p \times p$ coefficient matrix of \mathbf{B}_p and a $p \times (N - p)$ coefficient matrix of \mathbf{B}_{N-p} corresponding to the plan $Z_{p,v} = Z_p + J(i_1, i_2, \dots, i_n) \bmod 2$, where the order subscript $v = \sum_{h=1}^n i_h 2^{n-h}$. Note that the effect of adding a J matrix to the Z matrix is to modify the design by changing the levels of some factors; if $i_h = 0$ the levels of the h th factor are the same in the new design as they were in the old one; if $i_h = 1$ we change the levels of the h th factor at every point, which amounts to a relabelling of the levels of the factor and clearly does not affect the resolution of the design.

A saturated fractional replicate plan $Z_{p,v}$ of \mathbf{B}_p in a 2^n -factorial is said to be *independent* of a saturated fractional replicate plan Z_p if $Z_{p,v}$ cannot be constructed by the procedure $Z_p + J(i_1, i_2, \dots, i_n)$, $i_h = 0$ or 1 for all $h = 1, 2, \dots, n$. If $Z_{p,v}$ and Z_p are not independent then the plan $Z_{p,v}$ is an element of the set, $S(Z) = \{Z_p + J(i_1, i_2, \dots, i_n): i_h = 0 \text{ or } 1 \text{ for all } h = 1, 2, \dots, n\}$. The set $S(Z_p)$ is said to be the saturated fractional replicate plan set of \mathbf{B}_p generated by Z_p . Paik and Federer [5] presented a complete list of the generators of the saturated main effect plans in the cases for 2^2 , 2^3 and 2^4 factorials, and Raktoe and Federer [6] obtained a formula for the number of generators of saturated main effect fractional replicates for s^n -factorials.

Let $G_{p,v}$ and $G_{N-p,v}$ be a $p \times p$ diagonal matrix and an $(N - p) \times (N - p)$ diagonal matrix, respectively, such that the $(1 + u)$ th diagonal element of $G_{p,v}$ is $d_v(u) = (-1)^{z_v b_u}$ and the r th diagonal element of G_{N-p} is $d_v^*(r) = (-1)^{z_v b_r^*}$. Then, since each diagonal element of $G_{p,v}$ and $G_{N-p,v}$ is -1 or 1 , $G_{p,v}^{-1} = G_{p,v}$ and $G_{N-p,v}^{-1} = G_{N-p,v}$ for all $v = 0, 1, \dots, N - 1$ and the lemma presented below may be easily verified.

LEMMA.

- (i) $X_{11,v} = X_{11} G_{p,v}$, $X_{12,v} = X_{12} G_{N-p,v}$.
- (ii) $\sum_{v=0}^{N-1} d_v(u) = 0$ for all $u = 1, 2, \dots, p - 1$, and $\sum_{v=0}^{N-1} d_v^*(r) = 0$ for all $r = 1, 2, \dots, N - p$.
- (iii) $\sum_{v=0}^{N-1} d_v(u) d_v(u') = N$ if $u = u'$; or 0 otherwise,
 $\sum_{v=0}^{N-1} d_v^*(r) d_v^*(r') = N$ if $r = r'$; or 0 otherwise.
- (iv) $\sum_{v=0}^{N-1} d_v(u) d_v^*(r) = 0$ for all $u = 0, 1, \dots, p - 1$; $r = 1, 2, \dots, N - p$.
- (v) $\sum_{v=0}^{N-1} d_v(u) d_v(u') d_v^*(r) d_v^*(r') = N$ if $u = u'$ and $r = r'$ or if $u \neq u'$ and $r \neq r'$ but $b_u + b_{u'} + b_r^* + b_{r'}^* = b_0$; or 0 otherwise.

3. An invariant property of $|X'_{11}X_{11}|$ and a semi-invariant property of $X'_{11}X_{11}$ and $X_{11}^{-1}X_{12}\mathbf{B}_{N-p}$. Paik and Federer [5] presented some patterns of $X_{11}^{-1}X_{12}$ in irregular fractional replicates in a 2^n -factorial as this gives the aliasing scheme for the fractional replicate. Now, we define a *semi-invariant* property of $X_{11}^{-1}X_{12}$ such that if the matrix $X_{11}^{-1}X_{12}$ remains unchanged, except the sign of each element under the procedure $Z_p + J(i_1, i_2, \dots, i_n)$ where $i_h = 0$ or 1 for all $h = 1, 2, \dots, n$, we say that the matrix $X_{11}^{-1}X_{12}$ is *semi-invariant* under such a procedure. Also, we define a notation $\text{abs}(A)$ such that if $A = ||a_{ij}||$, $i = 1, 2, \dots, m$; $j = 1, 2, \dots, n$, $\text{abs}(A) = |||a_{ij}|||$, $i = 1, 2, \dots, m$; $j = 1, 2, \dots, n$, where $|a_{ij}|$ denotes the absolute value of the element a_{ij} .

Since $X_{11,v} = X_{11}G_{p,v}$, $|G_{p,v}| = 1$, $X_{12,v} = X_{12}G_{N-p,v}$, and all elements of the diagonal matrices $G_{p,v}$ and $G_{N-p,v}$ are -1 or 1 , the following theorem may be easily verified.

THEOREM 1. *If Z_p is a saturated fractional replicate plan in a 2^n -factorial system given \mathbf{B}_p , then $Z_{p,v}$ also is a saturated fractional replicate plan of \mathbf{B}_p and $|X'_{11,v}X_{11,v}| = |X'_{11}X_{11}|$, $\text{abs}(X'_{11,v}X_{11,v}) = \text{abs}(X'_{11}X_{11})$, and $\text{abs}(X_{11,v}^{-1}X_{12,v}) = \text{abs}(X_{11}^{-1}X_{12})$.*

The meaning of this theorem is that if Z_p is not a subgroup of Z in a 2^n -factorial, $Z_p + J(i_1, i_2, \dots, i_n)$, $i_h = 0$ or 1 for all $h = 1, 2, \dots, n$, may produce 2^n different saturated fractional replicate plans of \mathbf{B}_p , but the determinants of the information matrices have the same value. Furthermore, the information matrices and the aliasing matrices have the semi-invariant property.

4. A randomized procedure for saturated fractional replicates. Ehrenfeld and Zacks [2, 3] presented randomized procedures for regular fractions, and Zacks [7] showed that an unbiased estimator of a given parameter vector in the saturated fractional replicate case exists only if one randomizes over all possible designs of a certain structure. Paik and Federer [4] give a method similar to the Randomized Procedure I in the above papers and present an unbiased estimator of the main effect parameter vector for irregular saturated fractional replicates. As an extension of the authors' results, an unbiased estimator and the corresponding variances are given below for any saturated fractional replicate for the 2^n -factorial.

Let

$$X_{11}^{-1} = ||x_{ij}||, \quad i = 0, 1, \dots, p-1; j = 0, 1, \dots, p-1, \quad \text{and} \\ X_{11}^{-1}X_{12} = ||w_{st}||, \quad s = 1, 2, \dots, p; t = 1, 2, \dots, N-p.$$

THEOREM 2. *Suppose a saturated fractional replicate plan $Z_{p,v}$ of \mathbf{B}_p is chosen at random from a set generated by a plan Z_p in a 2^n -factorial, then, given plan $Z_{p,v}$, the least squares estimator $\hat{\mathbf{B}}_{p,v} = X_{11,v}^{-1}\mathbf{y}_p$ of $\mathbf{B}_p + X_{11,v}^{-1}X_{12,v}\mathbf{B}_{N-p}$ is an unbiased estimator of \mathbf{B}_p and for $i = 0, 1, \dots, p-1$*

$$V(\hat{b}_i) = \sum_{k=0}^{p-1} x_{ki}^2 \sigma^2 + \sum_{t=1}^{N-p} w_{it}^2 b_t^{*2}.$$

Note that the variance vector $(V(\hat{b}_0), V(\hat{b}_1), \dots, V(\hat{b}_{p-1}))$ is invariant under the procedure $Z_p + J(i_1, i_2, \dots, i_n)$, $i_h = 0$ or 1 for all $h = 1, 2, \dots, n$.

PROOF.

$$\begin{aligned} E_v[X_{11,v}^{-1} X_{12,v}] &= E_v[G_{p,v}(X_{11}^{-1} X_{12}) G_{N-p,v}] \\ &= E_v[|d_v(s-1) d_v^*(t) w_{st}|], \\ &\quad \text{where } s = 1, 2, \dots, p; t = 1, 2, \dots, N-p, \\ &= 0 \quad \text{by the Lemma (iv).} \end{aligned}$$

Then

$$\begin{aligned} E\hat{\mathbf{B}}_{p,v} &= E_v\{E[\hat{\mathbf{B}}_{p,v} | X_{11,v}]\} \\ &= E_v\{X_{11,v}^{-1}(X_{11,v} \mathbf{B}_p + X_{12,v} \mathbf{B}_{N-p})\} \\ &= \mathbf{B}_p + (E[X_{11,v}^{-1} X_{12,v}]) \mathbf{B}_{N-p} = \mathbf{B}_p. \end{aligned}$$

Next,

$$\begin{aligned} \text{Cov}(\hat{\mathbf{B}}_{p,v}) &= E_v\{\text{Cov}(\hat{\mathbf{B}}_{p,v} | X_{11,v})\} + \text{Cov}_v\{E(\hat{\mathbf{B}}_{p,v} | X_{11,v})\} \\ &= E_v(X'_{11,v} X_{11,v})^{-1} \sigma^2 + \text{Cov}_v(\mathbf{B}_p, v). \\ E_v(X'_{11,v} X_{11,v})^{-1} &= E_v(G_{p,v} X'_{11} X_{11} G_{p,v})^{-1} \\ &= E_v[G_{p,v}(X'_{11} X_{11})^{-1} G_{p,v}] \\ &= E_v[|d_v(i) d_v(j) \sum_{k=0}^{p-1} x_{ki} x_{kj}|], \\ &\quad \text{where } i, j = 0, 1, \dots, p-1. \end{aligned}$$

From (iii) of the Lemma, $E[d_v(i) d_v(j)] = 0$ for $i \neq j$. Hence, $E_v(X'_{11,v} X_{11,v})^{-1}$ is a diagonal matrix whose diagonal elements are $\sum_{k=0}^{p-1} x_{ki}^2$ for $i = 0, 1, \dots, p-1$.

$$\begin{aligned} \text{Cov}_v(\mathbf{B}_p, v) &= E_v(X_{11,v}^{-1} X_{12,v} \mathbf{B}_{N-p})(X_{11,v}^{-1} X_{12,v} \mathbf{B}_{N-p})' \\ &= E_v(G_{p,v} X_{11}^{-1} X_{12} G_{N-p} \mathbf{B}_{N-p} \mathbf{B}_{N-p}' G_{N-p,v} X_{12}' X_{11}^{-1} G_{p,v}) \\ &= E_v[|d_v(i) d_v(j) \sum_{t=1}^{N-p} \sum_{r=1}^{N-p} w_{it} w_{jr} d_v^*(r) d_v^*(t) b_r^* b_t^*|], \\ &\quad \text{where } i, j = 0, 1, \dots, p-1, \\ &= E_v[|\sum_{t=1}^{N-p} \sum_{r=1}^{N-p} d_v(i) d_v(j) d_v^*(r) d_v^*(t) w_{it} w_{jr} b_r^* b_t^*|], \\ &\quad \text{where } i, j = 0, 1, \dots, p-1. \end{aligned}$$

Hence,

$$\begin{aligned} \text{Cov}(\hat{\mathbf{B}}_{p,v}) &= |E_v[d_v(i) d_v(j) \sum_{k=0}^{p-1} x_{ki} x_{kj}]| \sigma^2 \\ &\quad + |\sum_{t=1}^{N-p} \sum_{r=1}^{N-p} E_v[d_v(i) d_v(j) d_v^*(r) d_v^*(t) w_{it} w_{jr} b_r^* b_t^*]| \\ &\quad \text{where } i = 0, 1, \dots, p-1; j = 0, 1, \dots, p-1. \end{aligned}$$

Using the Lemma (v), for $i = 0, 1, \dots, p-1$,

$$V(\hat{b}_i) = \sum_{k=0}^{p-1} x_{ki}^2 \sigma^2 + \sum_{t=1}^{N-p} w_{it}^2 b_t^{*2}$$

and this completes the proof of Theorem 2.

The following consequences of the above may be noted:

(i) Since $d_v(i) d_v(j) d_v^*(r) d_v^*(t) = (-1)^{z_v(b_i + b_j + b_r^* + b_t^*)}$ and $b_i + b_j + b_r^* + b_t^*$ could be b_0 , the estimators $\hat{b}_0, \hat{b}_1, \dots, \hat{b}_{p-1}$ are not always uncorrelated, i.e., the off diagonal elements of $\text{Cov}_v(\mathbf{B}_{p,v}^*)$ are not always zero; these depend upon the

choice of a generator of non-orthogonal fractions and choice of parameter vector \mathbf{B}_p in a 2^n -factorial.

(ii) $E_v[d_v(i)d_v(j)d_v^*(r)d_v^*(t)]$ only depends upon the choice of parameter vector \mathbf{B}_p and not on the choice of a generator. Hence, $\text{Cov}(\hat{\mathbf{B}}_{p,v})$ is invariant under the procedure $Z_p + J(i_1, i_2, \dots, i_n)$, $i_h = 0$ or 1 for all $h = 1, 2, \dots, n$.

(iii) Suppose that k saturated fractional replicate plans Z_{p,v_i} , $i = 1, 2, \dots, k$, $1 \leq k \leq N$, of \mathbf{B}_p are chosen at random, and without replacement, then an unbiased estimator of \mathbf{B}_p is given by

$$\hat{\mathbf{B}}_p = \frac{1}{k} \sum_{i=1}^k \hat{\mathbf{B}}_{p,v_i},$$

and from sampling theory, we obtain:

$$\text{Cov}(\hat{\mathbf{B}}_p) = \left(1 - \frac{k-1}{N-1}\right) \frac{1}{k} \text{Cov}(\hat{\mathbf{B}}_{p,v}).$$

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