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A RANDOMIZED PROCEDURE OF SATURATED MAIN EFFECT FRACTIONAL REPLICATES[1]

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0. Introduction and summary. Ehrenfeld and Zacks [2] presented randomized procedures for regular fractions and Zacks [3], [4] 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. In this paper, a similar method to the Randomized Procedure I in their paper is given for the saturated irregular main effect fractional replicates and an unbiased estimator of the main effect parameter vector is presented. Prior to this presentation, an invariant property of the information matrix is investigated. The explicit expression of the variance of the estimator is a remaining problem.

1. Basic notation and statistical model. In an s^n-factorial system (s is a prime or a power of a prime), the space of treatment combinations, Z, is represented by the set $Z = \{(i_1, i_2, \cdots, i_n): i_h = 0, 1, \cdots, s-1 \text{ for all } h = 1, 2, \cdots, n\}$ which contains s^n points. The addition operator $+$ between any two treatment combinations z and z' is defined as follows: If $z = (i_1, i_2, \cdots, i_n)$ and $z' = (i_1', i_2', \cdots, i_n')$ then $z + z' = (i_1'', i_2'', \cdots, i_n'')$, where $i_h'' = i_h + i_h' \pmod s$ for all $h = 1, 2, \cdots, n$. The expected value of the random vector $y(Z)$ associated with the space of treatment combinations Z is given by

$$E[y(Z)] = X\mathbf{B}, \tag{1.1}$$

where X is an $s^n \times s^n$ matrix with orthogonal column vectors. If $X'X = D$, a diagonal matrix, and $\Lambda = D^{\frac{1}{2}}$ then $H = X\Lambda^{-1}$ is orthogonal. $\mathbf{B}$ is the $s^n \times 1$ column vector of single degree of freedom parameters, and $y(Z)$ is the $s^n \times 1$ column vector of observations with covariance matrix $\sigma^2 I$.

Let $X^{(s)}$ be the matrix of coefficients of orthogonal polynomials of order s, where the elements of the first columns are all 1 and the inner product of any two different column vectors of $X^{(s)}$ is zero. This matrix $X^{(s)}$ corresponds to a factor level vector $(0, 1, \cdots, s-1)'$. The matrix X can be defined as

$$X = X^{(s^n)} = X^{(s)} \otimes \cdots \otimes X^{(s)},$$

where $\otimes$ denotes Kronecker product.

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As an example, consider the 3^2-factorial system. In this case, the matrix $X^{(3)}$ corresponding to a factor level vector $(0, 1, 2)'$ is

$$X^{(3)} = \begin{bmatrix} 1 & -1 & 1 \\ 1 & 0 & -2 \\ 1 & 1 & 1 \end{bmatrix}.$$

Hence, the matrix X is written as:

$$X = X^{(3^2)} = X^{(3)} \otimes X^{(3)} = \begin{bmatrix} 1 & -1 & 1 \\ 1 & 0 & -2 \\ 1 & 1 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & -1 & 1 \\ 1 & 0 & -2 \\ 1 & 1 & 1 \end{bmatrix},$$

i.e., the matrix of coefficients is

	Parameters								
treatments	M	A	A^2	B	AB	A^2B	B^2	AB^2	A^2B^2
(0, 0)	1	−1	1	−1	1	−1	1	−1	1
(1, 0)	1	0	−2	−1	0	2	1	0	−2
(2, 0)	1	1	1	−1	−1	−1	1	1	1
(0, 1)	1	−1	1	0	0	0	−2	2	−2
(1, 1)	1	0	−2	0	0	0	−2	0	4
(2, 1)	1	1	1	0	0	0	−2	−2	−2
(0, 2)	1	−1	1	1	−1	1	1	−1	1
(1, 2)	1	0	−2	1	0	−2	1	0	−2
(2, 2)	1	1	1	1	1	1	1	1	1

Suppose that the vectors $y(Z)$ and $\mathbf{B}$ are rearranged and partitioned as follows: $y(Z^*)' = (y(Z_p)', \; y(Z_{N-p})')$, $\mathbf{B}^{*\prime} = (\mathbf{B}_p', \mathbf{B}_{N-p}')$, where $y(Z_p)$ and $\mathbf{B}_p$ are $p \times 1 = (n(s-1)+1) \times 1$ observation and main effect parameter vectors, respectively, with the mean parameter as the first element of $\mathbf{B}_p$ and $N = s^n$. We shall write $\mathbf{y}_p$ and $\mathbf{y}_{N-p}$ for $y(Z_p)$ and $y(Z_{N-p})$, respectively.

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 arranging the column order in X and 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 nonsingular $p \times p$ 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:

$$E\begin{bmatrix} \mathbf{y}_p \\ \\ \mathbf{y}_{N-p} \end{bmatrix} = \begin{bmatrix} X_{11} & X_{12} \\ \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} \mathbf{B}_p \\ \\ \mathbf{B}_{N-p} \end{bmatrix} \tag{1.2}$$

such that X_{11} is a nonsingular $p \times p$ matrix. From (1.2), we obtain

$$E[\mathbf{y}_p] = [X_{11}, X_{12}][\mathbf{B}_p{}', \mathbf{B}'_{N-p}]' \tag{1.3}$$

and the observations in $\mathbf{y}_p$ yield a saturated fractional replicate for the given parameter vector $\mathbf{B}_p$.

Using the least squares method we obtain the following solution (Banerjee and Federer [1], Zacks [3]),

$$\hat{\mathbf{B}}_p + X_{11}^{-1} X_{12} \hat{\mathbf{B}}_{N-p} = X_{11}^{-1} \mathbf{y}_p. \tag{1.4}$$

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. An invariant property of $|X'_{11} X_{11}|$. First we shall prove the following lemma.

LEMMA 1. *In an s^n-factorial, if $X^{(s)}$ is the corresponding matrix of coefficients of orthogonal polynomials of order s to a factor level vector* $(0, 1, \cdots, s-1)'$ *and $X_1{}^{(s)}$ is the matrix corresponding to* $(1, 2, \cdots, s-1, 0)' = (0, 1, \cdots, s-1)' + (1, 1 \cdots, 1)'$, (mod s), *and $X_i^{(s)}$ is the matrix corresponding to* $(i, i+1, \cdots, i-1)' = (0, 1, \cdots, s-i)' + (i, i, \cdots, i)'$, (mod s), *then*

(i) *there exist $s \times s$ matrices A and B such that*

$$X_1{}^{(s)} = AX^{(s)}, \qquad X_i^{(s)} = A^i X^{(s)}$$

$$X_1{}^{(s)} = X^{(s)}B, \quad \textit{and} \quad X_i^{(s)} = X^{(s)}B^i,$$

(ii) $A^s = I_{s \times s}$, $B^s = I_{s \times s}$, $|A| = 1$, *and* $|B| = 1$,

(iii) *the matrix B has the form*

$$\begin{bmatrix} 1 & 0 \cdots 0 \\ 0 & \vdots \cdots\cdots \\ \vdots & \vdots \quad C \\ 0 & \vdots \end{bmatrix} \tag{2.1}$$

and $C^s = I_{(s-1)\times(s-1)}$ *and* $|C| = 1$.

PROOF. Let

$$A = \begin{bmatrix} 0 & 1 & 0 \cdots 0 \\ 0 & 0 & 1 \cdots 0 \\ & \cdots & \\ 0 & 0 & 0 \cdots 1 \\ 1 & 0 & 0 \cdots 0 \end{bmatrix},$$

then, clearly $A^s = I$, $X_1{}^{(s)} = AX^{(s)}$, and $X_i^{(s)} = A^i X^{(s)}$. $|A| = 1$ as can be immediately verified. Next, letting $X_1{}^{(s)} = X^{(s)}B$, $B = (X^{(s)})^{-1} X_1{}^{(s)}$ since $X^{(s)}$ is a nonsingular matrix. Also, since $B = (X^{(s)})^{-1}AX^{(s)}$, $B^i = (X^{(s)})^{-1}A^iX^{(s)} = (X^{(s)})^{-1}X_i^{(s)}$. Hence $X_i^{(s)} = X^{(s)}B^i$ and $B^s = I_{s\times s}$. We may write B as $(X^{(s)\prime}X^{(s)})^{-1}X^{(s)\prime}X_1^{(s)}$ and since $X^{(s)\prime}X^{(s)}$ is a diagonal matrix and $X^{(s)\prime}X_1^{(s)}$ has the form

$$\begin{bmatrix} s & 0 \cdots 0 \\ 0 & \vdots \cdots\cdots \\ \vdots & \vdots \quad W \\ 0 & \vdots \end{bmatrix},$$

B has the form (2.1) and $B^s = I$; thus, $C^s = I_{(s-1)\times(s-1)}$. Finally, from the facts $|B^s| = 1$ and $|C^s| = 1$, we have $|B| = 1$ and $|C| = 1$. □

The matrix B may be more useful than the matrix A in our application. For example, in the above lemma, suppose the second row vector in $X^{(s)}$ is $(x^{(0)}, x^{(1)}, \cdots, x^{(s-1)})$ and the corresponding second row vector in $X_i^{(s)}$ is $(x_i^{(0)}, x_i^{(1)}, \cdots, x_i^{(s-1)})$, then $(x_i^{(0)}, x_i^{(1)}, \cdots, x_i^{(s-1)}) = (x^{(0)}, x^{(1)}, \cdots, x^{(s-1)})B^i$.

Let $Z_p(s^n)$ be a saturated main effect plan; write this as Z_p, represented by a submatrix of Z such as a $p\times n$ matrix in an s^n-factorial and X_{11} by a $p\times p$ coefficient matrix of the main effect parameters corresponding to the plan Z_p, and let $J(i_1, i_2, \cdots, i_n)$ be a $p\times n$ matrix such that

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

where $i_h = 0, 1, \cdots, s-1$ for all $h = 1, 2, \cdots, n$, and $X_{11,v}$ be a $p\times p$ coefficient matrix of the main effect parameters corresponding to the plan $Z_{p,v} = Z_p + J(i_1, i_2, \cdots, i_n)$, (mod s), where the order subscript $v = \sum_{h=1}^{n} i_h s^{n-h}$. To illustrate consider the following example. In a 3^2-factorial a main effect plan is $Z_p = \{(0,0), (1,0), (2,0), (0,1), (0,2)\}$ with a corresponding

$$X_{11} = \begin{bmatrix} 1 & -1 & 1 & -1 & 1 \\ 1 & 0 & -2 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 0 & -2 \\ 1 & -1 & 1 & 1 & 1 \end{bmatrix}.$$

Let $v = 2$. This index corresponds to $i = 0$, $i = 2$. Hence, $Z_p + J(0, 2) = \{(0,2), (1,2), (2,2), (0,0), (0,1)\}$ with corresponding matrix

$$X_{11,2} = \begin{bmatrix} 1 & -1 & 1 & 1 & 1 \\ 1 & 0 & -2 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 0 & -2 \end{bmatrix}.$$

It is easy to verify that:

$$X_{11,2} = X_{11}\left[\begin{array}{c|cc|cc} 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & -\frac{1}{2} & -\frac{3}{2} \\ 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} \end{array}\right].$$

Thus, $C^{i_1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ with $|C^{i_1}| = 1$, and $C^{i_2} = \begin{bmatrix} -\frac{1}{2} & -\frac{3}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{bmatrix}$ with $|C^{i_2}| = 1$.

We now present the following theorem:

THEOREM 1. *If Z_p is a saturated main effect plan, then $Z_{p,v}$ also is a saturated main effect plan and* $|X'_{11,v}X_{11,v}| = |X'_{11}X_{11}|$.

PROOF. From Lemma 1, we may obtain $X_{11,v} = X_{11}\cdot \operatorname{diag}(1, C^{i_1}, C^{i_2}, \cdots, C^{i_n})$ where

$$\operatorname{diag}(1, C^{i_1}, \cdots, C^{i_n}) = \begin{bmatrix} 1 & & & 0 \\ & C^{i_1} & & \\ & & \ddots & \\ 0 & & & C^{i_n} \end{bmatrix}$$

and C^i is the submatrix of B^i, in

$$B^i = \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & C^i \end{array}\right].$$

Since $|C^{i_h}| = 1$ for $i_h = 0, 1, \cdots, s-1$, $|X_{11,v}| = |X_{11}|$, $|X'_{11,v}X_{11,v}| = |X'_{11}X_{11}|$, and since $|X_{11}| \neq 0$, $Z_{p,v}$ also is a saturated main effect plan. □

The meaning of this theorem is that if Z_p is not a subgroup (in the algebraic sense) of Z in an s^n-factorial, $Z_p + J(i_1, i_2, \cdots, i_n)$, $i_h = 0, 1, \cdots, s-1$ for all $h = 1, 2, \cdots, n$, may produce s^n different main effect plans, but determinants of the information matrices have the same value.

3. A randomized procedure for saturated main effect fractional replicates. A main effect plan $Z_{p,v}$ in an s^n-factorial is said to be *independent* of a main effect plan Z_p if $Z_{p,v}$ cannot be constructed by the procedure $Z_p + J(i_1, i_2, \cdots, i_n)$, $i_h = 0, 1, \cdots, s-1$ for all $h = 1, 2, \cdots, n$. If $Z_{p,v}$ and Z_p are not independent then the plan $Z_{p,v}$ is an element of the set, $S(Z_p) = \{Z_p + J(i_1, i_2, \cdots, i_n)\colon i_h = 0, 1, \cdots, s-1$ for all $h = 1, 2, \cdots, n\}$. The set $S(Z_p)$ is said to be the main effect plan set *generated* by Z_p. The following two examples illustrate the types of independent saturated main effect plans for two cases:

Saturated main effect plans in a 2^4-factorial. In this case, every $|X'_{11}X_{11}|$ has one of the four values, i.e. 2304, 1024, 256, or 0. The set generated by a plan (0000, 0111, 1011, 1101, 1110) has the value 2304.

Saturated main effect plans in a 3^3-factorial. In this case, every $|X'_{11}X_{11}|$ has one of the five values, i.e. 746496, 419904, 186624, 46656, or 0. The sets generated by the following 9 plans have the maximum value 746496.

000	000	000	000	000	000	000	000	000
021	012	012	011	011	012	011	022	022
101	102	021	101	102	101	101	202	202
112	110	102	112	110	110	110	220	220
120	121	110	120	201	211	122	211	011
202	201	211	210	121	021	212	121	101
210	220	220	222	222	222	221	112	110

Suppose a plan $Z_{p,v}$ was chosen at random from the set $S(Z_p)$, then it is easy to verify that $E_v[X'_{11,v}X_{11,v}] = s^{-n}pX_1'X_1$ and $E_v[X'_{11,v}X_{12,v}] = 0$, where $X_1 = [X'_{11}, X'_{12}]'$.

LEMMA 2. *Under the randomized procedure, the following relationship holds:*

$$E_v X_{11,v}^{-1} X_{12,v} = 0. \tag{3.1}$$

PROOF. Let $X_2 = [X'_{12}, X'_{22}]' = ||x_{fg}||, f = 1, 2, \cdots, N;\ g = 1, 2, \cdots, N-p$ in (1.2) and $(x_{fg} \mid i_h)$ denotes that elements in the gth column in X_2 given the level i_h of the hth factor in an s^n-factorial. Then

$$\textstyle\sum_f (x_{fg} \mid i_h) = 0 \tag{3.2}$$

for $i_h = 0, 1, \cdots, s-1$. Let $X_{11}^{-1} = ||w_{ij}||$, $i, j = 1, 2, \cdots, p$, and $X_{12,v} = ||x_{ij}(v)||$, $i = 1, 2, \cdots, p; j = 1, 2, \cdots, N-p$. Suppose

$$X_{11,v} = X_{11} \cdot \text{diag}(1, C^{i_1}, \cdots, C^{i_n}), \qquad \text{then}$$

$$X_{11,v}^{-1} = \text{diag}(1, C^{j_1}, \cdots, C^{j_n})X_{11}^{-1},$$

where $j_h = s - i_h$. Let $\text{diag}(1, C^{j_1}, \cdots, C^{j_n}) = ||c_{ij}(v)||$, $i, j = 1, 2, \cdots, p$, and let $X_{11,v}^{-1}X_{12,v} = ||\alpha_{ut}(v)||$, $u = 1, 2, \cdots, p$; $t = 1, 2, \cdots, N-p$, then

$$\alpha_{ut}(v) = \textstyle\sum_r c_{ur}(v) \sum_k w_{rk} x_{kt}(v). \tag{3.3}$$

Further define

$$C^{j_h} = ||c_{mn}^{(j_h)}||, \qquad m, n = 1, 2, \cdots, s-1. \tag{3.4}$$

If $u = 1$, from (3.3) $\alpha_{1t}(v) = \sum_k w_{1k} x_{kt}(v)$, then $E_v \alpha_{1t}(v) = \sum_k w_{1k} E_v[x_{kt}(v)] = 0$. If $2 \leqq u \leqq p$,

$$\alpha_{ut}(v) = c_{u1}(v) \textstyle\sum_k w_{1k} x_{kt}(v) + \cdots + c_{up}(v) \sum_k w_{pk} x_{kt}(v). \tag{3.5}$$

Consider the ith term in (3.5):

$$c_{ui}(v)\sum_k w_{ik}x_{kt}(v) = w_{i1}[c_{ui}(v)x_{1t}(v)] + \cdots + w_{up}[c_{ui}(v)x_{pt}(v)].$$

We shall show that $E_v[c_{ui}(v)x_{gt}(v)] = 0$ for $g = 1, 2, \cdots, p$. If $c_{ui}(v)$ is not an element of any C^{j_h} then $c_{ui}(v) = 0$ and if $c_{ui}(v)$ is an element of any C^{j_h} then we may write $c_{mn}^{(j_h)}$ as $c_{ui}(v)$ using the notation (3.4), where $u = (h-1)(s-1)+m+1$ and $i = (h-1)(s-1)+n+1$. Then

$$E_v[c_{ui}(v)x_{gt}(v)] = s^{-n}[\textstyle\sum_{j_h=0}^{s-1} c_{mn}^{(j_h)} \sum_f (x_{ft}\,|\,j_h)] = 0 \quad \text{from (3.2)},$$

then $E_v[c_{ui}(v)\sum_k w_{ik}x_{kt}(v)] = 0$, and hence $E_v[\alpha_{ut}(v)] = 0$ for all u and t. Hence, $E_v[X_{11,v}^{-1}X_{12,v}] = 0$. ∎

THEOREM 2. *Suppose a saturated main effect plan $Z_{p,v}$ is chosen at random from a set generated by a plan Z_p, then, given plan $Z_{p,v}$, the least squares estimator $\hat{\mathbf{B}}_{p,v}^* = X_{11,v}^{-1}y(Z_{p,v})$ of $\mathbf{B}_{p,v}^* = \mathbf{B}_p + X_{11,v}^{-1}X_{12,v}\mathbf{B}_{N-p}$ is an unbiased estimator of B_p.*

PROOF.
$$\begin{aligned} E\hat{\mathbf{B}}_{p,v}^* &= E_v\{E[\hat{\mathbf{B}}_{p,v}^*\,|\,X_{11,v}]\} \\ &= E_v\{E[X_{11,v}^{-1}\mathbf{y}_{p,v}\,|\,X_{11,v}]\} \\ &= E_v[X_{11,v}^{-1}(X_{11,v}\mathbf{B}_p + X_{12,v}\mathbf{B}_{N-p})] \\ &= \mathbf{B}_p + (E_v[X_{11,v}^{-1}X_{12,v}])\mathbf{B}_{N-p} \\ &= \mathbf{B}_p \quad \text{by Lemma 2.} \quad ∎ \end{aligned}$$

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