

FURTHER RESULTS ON INVARIANCE AND RANDOMIZATION IN FRACTIONAL REPLICATION¹

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The partitioning of the complete parametric vector from the experimenter's viewpoint for the general mixed factorial gives rise to the usual four exhaustive cases, (i), (ii), (iii) and (iv). Cases (i) and (iv) may be viewed as special cases of cases (ii) and (iii) respectively in connection with the problem of spectrum invariance under the group of level permutations and the problem of unbiased estimation under a uniform randomized design. Srivastava, Raktoe and Pesotan (1976) resolved these problems for case (ii) and this paper does the same for case (iii) so that the study is now complete.

1. Introduction. Ehrenfeld and Zacks (1961), Zacks (1963, 1964) and Paik and Federer (1970) have dealt with the problems of invariance and randomization for regular and irregular fractions of the symmetrical factorial. Subsequently, Srivastava, Raktoe and Pesotan (1976) generalized these results to arbitrary fractions from the general mixed factorial. All of the above results considered one specific partitioning of the parametric vector, the odd resolution case being a special case of this. In this paper we provide a more general partitioning of the parametric vector which gives rise to four exhaustive cases. Two of these cases are special cases of the other two. Since Srivastava, et al., (1976), solved one of the cases the remaining case is dealt with in this paper, which includes the even resolution case as a special case. Hence the problem of spectrum invariance under the group of level permutations and the associated problem of unbiased estimation under uniform randomization is completely resolved.

Section 2 presents the basic setting and the partitioning of the complete parametric vector from the experimenter's viewpoint. Expressions for BLUEs are provided in the resulting four cases for the parametric vector of interest and of linear functions. In Section 3 the invariance and randomization theorems are recalled for the case which is resolved by Srivastava, et al., (1976). These results are used in Section 4, to establish the two theorems for the remaining case. Section 5 provides applications and an example on resolution IV designs.

2. Partitioning of factorial effects from the experimenter's viewpoint. In this paper the notation of Srivastava, et al., (1976), and Raktoe, et al., (1978), will be adopted. Consider the general $s_1 \times s_2 \times \dots \times s_m$ factorial, $s_i \geq 2$, where the i th factor has s_i levels from the set $S_i = \{0, 1, 2, \dots, s_i - 1\}$. Let $S = S_1 \times S_2 \times \dots \times S_m$ be the Cartesian product of the sets S_i . With a treatment (i_1, i_2, \dots, i_m) in S associate an observation $y(i_1, i_2, \dots, i_m)$. A factorial effect will be indicated $A_1^{i_1} A_2^{i_2} \dots A_m^{i_m}$ with at least one of the $i_j \neq 0$, and $i_j \in S_j$ ($j = 1, 2, \dots, m$). The mean will be denoted by $A_1^0 A_2^0 \dots A_m^0$. Let Y_0 be the set of all observations associated with the full replicate S and P_0 the set of effects (including the

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mean). Let $X = X_1 \otimes X_2 \otimes \dots \otimes X_m$ be the Kronecker product of real orthogonal matrices X_i of order s_i with first column all $1/\sqrt{s_i}$. Then X is a real orthogonal matrix of order $s = \prod_{i=1}^m s_i$, with each first column entry equal to $1/\sqrt{s}$. It follows that the sum of the entries of each column of X_i and of X besides the first is equal to zero. Associate with the observation vector Y_0 and the column vector P_0 of parameters the well-known linear model

$$(2.1) \quad E(Y_0) = XP_0, \text{Cov}(Y_0) = \sigma^2 I_s.$$

From the experimenter's viewpoint the complete parametric vector P_0 can be partitioned as

$$(2.2) \quad P'_0 = (P'_1 : P'_2 : P'_3)$$

where P_1 is a $t_1 \times 1$ vector to be estimated, P_2 is a $t_2 \times 1$ vector not of interest and not assumed to be known, and P_3 is a $t_3 \times 1$ vector of parameters assumed to be known (which, without loss of generality, can be taken to be zero), such that $1 \leq t_1 \leq s$, $0 \leq t_2 \leq s - 1$, and $0 \leq t_3 \leq s - t_1 - t_2 \leq s - 1$. Explicitly the following cases occur:

- (i) $t_1 = s, t_2 = t_3 = 0$;
- (ii) $t_2 = 0, t_3 \neq 0$;
- (iii) $t_2 \neq 0, t_3 \neq 0$;

and

- (iv) $t_2 \neq 0, t_3 = 0$.

By the degree of a factorial effect $A_1^{i_1} A_2^{i_2} \dots A_m^{i_m}$ is meant the number of nonzero exponents among the i_1, i_2, \dots, i_m . This concept may be connected up with the concept of a resolution of a design. A *design* or a *fractional factorial arrangement* (FFA) is a collection of treatment combinations from S . A design is said to be of resolution R if all factorial effects up to degree k are estimable, where k is the greatest integer less than $R/2$, under the assumption that all factorial effects of degree $R-k$ and higher are zero. The designs of resolution R have been divided into two types in the literature, namely

- (a) $R = 2r$, known as designs of even resolution, and
- (b) $R = 2r + 1$, known as designs of odd resolution.

It follows that an even resolution design is a special case of (iii) and an odd resolution design is a special case of (ii) above.

The observation vector of an FFA will be denoted by Y and the model for Y and a given parametric vector P is read off from the full model (2.1). Specifically the models for the observation vector Y in the above four cases are

- (i) $E(Y) = X(Y, P_0)P_0, \text{Cov}(Y) = \sigma^2 I_n,$
- (ii) $E(Y) = X(Y, P_1)P_1, \text{Cov}(Y) = \sigma^2 I_n,$
- (iii) $E(Y) = X(Y, P_1)P_1 + X(Y, P_2)P_2, \text{Cov}(Y) = \sigma^2 I_n,$ where P_1 and P_2 do not exhaust P_0 , and
- (iv) $E(Y) = X(Y, P_1)P_1 + X(Y, P_2)P_2, \text{Cov}(Y) = \sigma^2 I_n,$ where P_1 and P_2 exhaust P_0 .

In the above four equations the observation vector Y is assumed to be coming from an FFA with n treatment combinations, that is, $|Y| = n$.

Consider the partition of P_0 given in (2.2) and let

$$M_{ij} = M_{ij}(Y) = X'(Y, P_i)X(Y, P_j),$$

where $i = 1, 2, 3$ and $j = 1, 2, 3$, and let $M_{ij}^-(Y)$ be a generalized inverse of M_{ij} . In particular note that $M_{ii}(Y)$ is the information matrix of the observation vector Y relative to the parametric vector P_i . For an unbiased design the best linear unbiased estimates (BLUEs) for P_1 in the above four cases are obtained by

- (i) $\hat{P}_1 = \hat{P}_0 = [X'(Y, P_0)X(Y, P_0)]^{-1}X'(Y, P_0) Y;$
- (ii) $\hat{P}_1 = M_{11}^{-1} X'(Y, P_1) Y;$
- (iii) $\hat{P}_1 = [M_{11} - M_{12}M_{22}M_{21}]^{-1}[X'(Y, P_1) - M_{12}M_{22}X'(Y, P_2)]Y;$
- (iv) \hat{P}_1 is identical to (iii), with the understanding that P_1 and P_2 exhaust P_0 .

Instead of pursuing the BLUEs of P_1 in these four cases, the BLUEs of linear functions of P_1 may be considered. If $\mu'P_1$ is a linear function of P_1 then it is estimable if and only if μ' is in the row space of the underlying design matrix which is different in each of the four cases. The BLUEs of $\mu'P_1$ can be obtained by standard formulae via the normal equations. These are as follows in the four cases

- (i) $\mu'P_1 = \mu'P_0 = \mu'(X'(Y, P_0)X(Y, P_0))^{-1}X'(Y, P_0)Y;$
- (ii) $\mu'P_1 = \mu'M_{11}^{-1}X'(Y, P_1)Y;$
- (iii) $\mu'P_1 = \mu'[M_{11} - M_{12}M_{22}^{-1}M_{21}]^{-1}[X'(Y, P_1) - M_{12}M_{22}^{-1}X'(Y, P_2)]Y;$
- (iv) same as in (iii), with the understanding that P_1 and P_2 exhaust P_0 .

3. Invariance and randomization theorems for cases (i) and (ii). In the sequel the following concepts from Srivastava, et al., (1976), will be needed. A set of effects will be called *admissible* if only if whenever $A_1^{i_1}A_2^{i_2} \dots A_m^{i_m}$ belongs to the set and $i_j \neq 0$ ($1 \leq j \leq m$) then $A_1^{j-1}A_2^{i_2} \dots A_j^{i_j}A_{j+1}^{i_{j+1}} \dots A_m^{i_m}$ belongs to the set for all $l \neq 0$ in S_j . Since P_0 , the set of all effects, is admissible, it follows that if P is an admissible set of effects that so is $P_0 - P$.

Let Ω_i be the symmetric group of all permutations on S_i and let Ω be the direct product of these groups. Then $\Omega = \{\omega: \omega = (\omega_1, \omega_2, \dots, \omega_m), \omega_j \in \Omega_j\}$. If Y is any observation vector corresponding to an FFA and ω in Ω is any *level* permutation then $\omega(Y)$ will denote the observation vector obtained from Y wherein each component $y(k_1, k_2, \dots, k_m)$ in Y is replaced by $y(\omega_1(k_1), \omega_2(k_2), \dots, \omega_m(k_m))$.

In Srivastava, et al., (1976), case (ii) has been resolved with respect to spectrum invariance and unbiased estimation of a linear function using a uniform randomized design. Specifically, these authors proved the following two theorems which will be used subsequently.

THEOREM 3.1. *For each level permutation ω in Ω , an admissible vector P_1 , and, any observation vector Y , there exists an orthogonal matrix $U(P_1, \omega)$ such that*

$$X(Y, P_1)U(P_1, \omega) = X(\omega(Y), P_1).$$

Further,

$$\begin{aligned} \frac{1}{\prod (s_i!)} \sum_{\omega \in \Omega} U(P_1, \omega) &= 0, \quad \text{if } P_1 \neq (A_1^0 A_2^0 \dots A_m^0) \\ &= I, \quad \text{if } P_1 = (A_1^0 A_2^0 \dots A_m^0) \end{aligned}$$

where 0 is the zero matrix and I is the one by one identity matrix.

Note that this theorem implies that all matrices in the set of information matrices $\{X'(\omega(Y), P_1)X(\omega(Y), P_1): \omega \in \Omega\}$ have the same characteristic roots.

THEOREM 3.2. *Let Y be a given observation vector and consider the class of observation vectors $\omega(Y)$ generated by ω in Ω . Select a permutation η in Ω with probability $(\prod_{i=1}^m s_i!)^{-1}$. If μ is a column vector such that $\mu' = \lambda'_\omega X(\omega(Y), P_1)$ for each ω in Ω , where P_1 is an admissible vector, then $E_\Omega(\mu'P_\eta^0) = \mu'P_1$, where P_η^0 is a solution to the equation $\eta(Y) = X(\eta(Y), P_1)P_1$.*

In case (i), the assumption of P_1 being admissible is not necessary since in this case $P_1 = P_0$ and the complete vector P_0 is already admissible. Hence case (i) may be viewed as a special case of (ii) so that both theorems are applicable in this case. The reader should note that in case (i) the design matrix has the dimension $n \times s$ for the invariance theorem and in the randomization theorem the linear function is a function of the total parametric vector, while in case (ii) the design matrix is a $n \times |P_1|$ matrix and the linear function is a function of a subset of the parameters.

4. Invariance and randomization theorems for cases (iii) and (iv). Let Y be an observation vector corresponding to a given FFA and $\omega(Y)$ for ω in Ω be the corresponding observation vector for the permuted design. Assume that P_1 and P_2 are admissible vectors of effects. Then we have the following theorem for case (iii):

THEOREM 4.1. *There exists an orthogonal matrix U such that*

$$X(Y, P)U = X(\omega(Y), P),$$

where $P' = [P_1' : P_2']$.

PROOF. By Theorem 3.1, there exist orthogonal matrices $U_1(P_1, \omega)$ and $U_2(P_2, \omega)$ such that $X(Y, P_i)U_i(P_i, \omega) = X(\omega(Y), P_i)$, $i = 1, 2$. Let U be the block diagonal matrix

$$U = \begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix}.$$

Then, clearly $X(Y, P)U = X(\omega(Y), P)$ thereby establishing the result.

Now consider the entire class of observation vectors generated by the action of Ω on the $n \times 1$ observation vector Y corresponding to a given FFA. Let the total parametric vector P_0 be partitioned as in (2.2) and let μ be a $|P_1| \times 1$ column vector such that

$$\mu'P_1 = [\mu' | O'] \begin{bmatrix} P_1 \\ P_2 \end{bmatrix}.$$

Then a necessary and sufficient condition for the estimability of $\mu'P_1$ is that the vector $[\mu' | O']$ be in the row space of the design matrix $[X(\omega(Y), P_1) | X(\omega(Y), P_2)]$. For each ω in Ω , define

$$A(\omega(Y)) = M_{11}(\omega(Y)) - M_{12}(\omega(Y))M_{22}^{-1}(\omega(Y))M_{21}(\omega(Y)).$$

It is known that the estimability of $\mu'P_1$ is then equivalent to the condition that μ' is in the row space of the matrix $A(Y)$. The following lemmas will be useful in establishing the randomization theorem for case (iii).

LEMMA 4.1.

$$\frac{1}{\prod (s_i!)} \sum_{\omega \in \Omega} \mu' A^{-1}(\omega(Y)) A(\omega(Y)) P_1 = \mu' P_1,$$

where for each ω in Ω , the vector $[\mu' | O']$ lies in the row space of the design matrix $[X(\omega(Y), P_1) | X(\omega(Y), P_2)]$.

PROOF. From the facts noted above, it follows that for each ω in Ω , the vector μ' lies in the row space of $A(\omega(Y))$. Hence $\mu' = \lambda'_\omega A(\omega(Y))$ for each ω in Ω . Substituting $\lambda'_\omega A(\omega(Y))$ for μ' in the expression given in the lemma, since $AA^{-1}A = A$, the lemma follows.

LEMMA 4.2. *If P_1 and P_2 are admissible vectors, then*

$$\sum_{\omega \in \Omega} A^{-1}(\omega(Y)) [M_{13}(\omega(Y)) - M_{12}(\omega(Y))M_{22}^{-1}(\omega(Y))M_{23}(\omega(Y))] = 0,$$

where 0 is the zero matrix.

PROOF. Since P_1 and P_2 are admissible vectors then so is the vector P_3 . By theorem 4.1, there exist orthogonal matrices $U(P_i, \omega)$ such that $X(\omega(Y), P_i) = X(Y, P_i)U(P_i, \omega)$ for $i = 1, 2, 3$. Substituting these equations in the expression given in the lemma it follows that

$$\begin{aligned} \sum_{\omega \in \Omega} A^{-1}(\omega(Y)) [M_{13}(\omega(Y)) - M_{12}(\omega(Y))M_{22}^{-1}(\omega(Y))M_{23}(\omega(Y))] \\ = \sum_{\omega \in \Omega} U'(\omega, P_1) L U(\omega, P_3), \end{aligned}$$

where $L = [M_{11}(Y) - M_{12}(Y) M_{22}^{-1}(Y) M_{21}(Y)]^{-1} [M_{13}(Y) - M_{12}(Y) M_{22}^{-1}(Y) M_{23}(Y)]$ is a fixed matrix independent of ω in Ω . The proof may now be completed by using the same argument as that given for Lemma 4.2 of Srivastava, et al., (1976).

Select a permutation η in Ω with probability $(\prod (s_i!))^{-1}$. Then we have the following theorem:

THEOREM 4.2. *Let $P_{1, \eta}^0$ be a solution to the equation $\eta(Y) = X(\eta(Y), P) P$, where $P = [P_1 | P_2]$ and P_1, P_2 are admissible vectors of effects. Then $E_{\Omega}(\mu' P_{1, \eta}^0) = \mu' P_1$, where*

$$E_{\Omega}(\mu' P_{1, \eta}^0) = \frac{1}{\prod (s_i!)} \sum_{\omega \in \Omega} E_G(\mu' P_{1, \omega}^0 | \omega(Y)),$$

G is the probability distribution of the random variable $\omega(Y)$, and μ is a $|P_1| \times 1$ column vector such that $[\mu' | 0']$ lies in the row space of the design matrix $[X(\omega(Y), P_1) | X(\omega(Y), P_2)]$ for each ω in Ω .

PROOF. Now

$$\begin{aligned} E_{\Omega}(\mu' P_{1, \eta}^0) &= \frac{1}{\prod (s_i!)} \sum_{\omega \in \Omega} E_G(\mu' P_{1, \omega}^0 | \omega(Y)) \\ &= \frac{1}{\prod (s_i!)} \mu' [A^{-}(\omega(Y)) A(\omega(Y)) P_1 + A^{-}(\omega(Y)) (M_{12}(\omega(Y)) \\ &\quad - M_{12}(\omega(Y)) M_{22}^{-1}(\omega(Y)) M_{22}(\omega(Y)) P_2 + A^{-}(\omega(Y)) (M_{13}(\omega(Y)) \\ &\quad - M_{12}(\omega(Y)) M_{22}^{-1}(\omega(Y)) M_{23}(\omega(Y)) P_3]. \end{aligned}$$

By a property of generalized inverse the second term in the above expression is the zero matrix for each ω in Ω . By Lemma 4.2 the sum of the third term in the above expression is the zero matrix and by Lemma 4.1 the sum of the first term is $\mu' P_1$, completing the proof.

In case (iv) since $t_3 = 0$, the vector P_3 does not appear at all so that P_1 and P_2 exhaust P_0 . Hence this case may be viewed as a special case of case (iii) in the sense that the third term in the randomization Theorem 4.2 does not appear, and, thus both the theorems of this section apply in this case.

5. Applications and an example. In the paper by Srivastava, et al., (1976), it is indicated that the results obtained for case (ii) (and hence also on the trivial case (i)) have wide applications in odd resolution problems, where the interest lies on the vector P_1 rather than on linear functions. The full column rank condition of the design matrix of an initial design implies the preservation of rank under the group of level permutations. Similar observations can also be made on even resolution designs belonging to case (iii) (and hence also to the special case (iv)). Srivastava, et al., (1976), presented an explicit example of the use of the results on a class of determinant optimal resolution III designs of the 2^4 factorial. Here we shall present an example of a class of resolution IV designs of the 2^3 factorial. Let the initial resolution IV design be $D_1 = \{(100), (010), (001), (011), (101), (110)\}$. Under the action of the group of level permutations Ω , a class of 4 designs is produced. The initial design is already listed and the others are $D_2 = \{(000), (110), (101), (111), (001), (010)\}$, $D_3 = \{(110), (000), (011), (001), (111), (100)\}$, and $D_4 = \{(000), (011), (101), (111), (100), (010)\}$. In the terminology of Pesotan, et al., (1975), the design D_1 is an unfaithful design and therefore produces fewer than $8 = 2! \times 2! \times 2!$ designs under Ω . The above class of four designs are such that the information matrices have the same spectrum. In order for the results to be unbiased by P_3 (if the assumption of negligibility is in doubt) a uniform randomized design may be selected. Another approach which may be adopted

is to introduce a cost function on the designs and pick one which minimizes the cost. The initial design used above is a minimal full column rank design (e.g., see Margolin (1969)) and since the action of Ω preserves the rank all the four designs are of full column rank. One could have imposed an optimality criterion on the spectrum of the information matrix (e.g., d -optimality) and starting out with an initial optimal design produce a class of optimal designs on which a cost function can be imposed to select a minimum cost optimal design.

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