ESTIMATES OF EFFECTS FOR FRACTIONAL REPLICATES[1]

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0. Summary. Given any fraction of a factorial experiment in which the treatments either occur zero or one time, previous results were obtained on augmentation of the treatment design matrix, X, such that the product of the transpose and of the augmented matrix, $X_1 = [X' \vdots X'\lambda]'$, resulted in a diagonal matrix, and on a transformation of X_1 to another matrix $X_2 = FX_1$. In the present paper results are obtained on the evaluation of the variances of estimated effects under augmentation, on the existence and evaluation of F and λ, on the determination of aliases of effects, and on the calculation of inverses for $[X'X]$ and for the information matrix $[X'_{22}X_{22}]$ for the deleted treatments.

1. Introduction. In a recent paper by the authors (1963) it was shown how to adjust the treatment design matrix to furnish estimates of effects as orthogonal linear functions of stochastic variates for any fractional replicate of a complete factorial. (The fractional replicate is such that any combination occurs zero or one time.) Such an adjustment for fractions greater than one-half reduces the required calculations by inverting a smaller matrix than the original treatment design matrix X. In the present paper results are presented on the evaluation of variances of the estimated effects, on the existence and evaluation of matrices λ and F used in the adjustment or augmentation of X, on the determination of aliases of effects, and on the calculation of the inverse of the information matrix $[X'X]$ and of the information matrix $[X'_{22}X_{22}]$ for the deleted treatments.

The notation and some results of the previous paper are reproduced below for completeness. The n observational equations are $Y = X\mathbf{B} + e$, where Y is an $n \times 1$ random vector of observations with elements y_i, X is the $n \times p$ treatment design matrix with rank $p \leqq n$, $\mathbf{B}$ is the $p \times 1$ vector of effect parameters, and e is an $n \times 1$ random vector of errors with $E(ee') = \sigma^2 I$. Then the least squares estimates of $\mathbf{B}$ are given by $\mathbf{B}^+ = [X'X]^{-1}X'Y$ with variance-covariance matrix cov $(\mathbf{B}^+) = \sigma^2[X'X]^{-1}$. When $p = n$, $\mathbf{B}^+ = X^{-1}Y$.

Since $[X'X]$ is not diagonal for all X, the proposed adjustment involves finding a matrix λ such that the matrix X and the vector Y are augmented to become $X_1 = [X' \vdots X'\lambda]'$ and $Y_1 = [Y' \vdots Y'\lambda]'$ in such a way that $[X'_1X_1]$ is a diagonal matrix. Then it was shown (Theorem 1 below) that the estimates with augmentation were identical to those without augmentation.

Let the treatment design matrix X be augmented with m additional rows of p columns each; these m additional rows correspond to m additional stochastic variates $Y'\lambda = Y'_m = [y'_1, y'_2, \cdots, y'_m]$. Denote the augmented part of X as

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$X_m = \lambda' X$. X_1 is a $(p + m) \times p$ matrix; Y_1 is a $(p + m) \times 1$ vector. Denote the rows of X by $\alpha_1, \alpha_2, \cdots, \alpha_p$ and those of X_1 by $\alpha_1, \alpha_2, \cdots, \alpha_p, \beta_1, \beta_2, \cdots, \beta_m$. The least squares estimates corresponding to the $p + m$ observational equations $Y_1 = X_1\mathbf{B}_1 + e_1$ are $\mathbf{B}_1^+ = [X_1'X_1]^{-1}X_1'Y_1$. Then we have:

THEOREM 1. *If* $\beta_k = \sum_{i=1}^{p} \lambda_{ik}\alpha_i$ and $y_k' = \sum_{i=1}^{p} \lambda_{ik}y_i$, *where* $k = 1, 2, \cdots, m$ *and* λ_{ik} *are scalars, then* $\mathbf{B}^+ = \mathbf{B}_1^+$.

Let the square matrix X of rank p be transformed to X_2 in such a manner that the rows of X_2 are dependent on the rows of X, and such that the vector space generated by the row vectors of X_2 is the same as that generated by the row vectors of X; both X and X_2 will have rank p. Let $X_2 = FX$, where F is the square matrix required to transform X to X_2 and involves only addition or subtraction of rows. Then we have:

THEOREM 2. *If the treatment design matrix* X *and the stochastic vector* Y *be transformed to* X_2 *and* Y_2, *respectively, in such a manner that* $X_2 = FX$ *and* $Y_2 = FY$, *where the matrices are as defined above, then the least squares estimates* $\mathbf{B}_2^+$ *from the observational equations* $Y_2 = X_2\mathbf{B}_2 + e_2$ *will be the same as* $\mathbf{B}^+$ *from the observational equations* $Y = X\mathbf{B} + e$.

2. Variance of the estimated effects under adjustment of Theorem 1. Let $e_1 = [e' \vdots e'\lambda]'$ corresponding to $Y_1 = [Y' \vdots Y'\lambda]'$. Then,

$$E(e_1e_1') = E\begin{bmatrix} ee' & ee'\lambda \\ \lambda'ee' & \lambda'ee'\lambda \end{bmatrix} = \sigma^2\begin{bmatrix} I_p & \lambda \\ \lambda' & \lambda'\lambda \end{bmatrix},$$

where I_p is the $p \times p$ identity matrix and $\lambda'\lambda$ has dimensions $m \times m$. The covariance matrix of $\mathbf{B}_1^+$ is

$$\operatorname{cov}(\mathbf{B}_1^+) = E[(\mathbf{B}_1^+ - \mathbf{B}_1)(\mathbf{B}_1^+ - \mathbf{B}_1)']$$
$$= E[(S_1^{-1}X_1'Y_1 - \mathbf{B}_1)(S_1^{-1}X_1'Y_1 - \mathbf{B}_1)'],$$

where $S_1 = [X_1'X_1]$. Substitution of $X_1\mathbf{B}_1 + e_1$ for Y_1 reduces the covariance matrix to

$$(1) \qquad \operatorname{cov}(\mathbf{B}_1^+) = E(S_1^{-1}X_1'e_1 e_1'X_1 S_1^{-1}) = S_1^{-1}X_1'\begin{bmatrix} I_p & \lambda \\ \lambda' & \lambda'\lambda \end{bmatrix}X_1S_1^{-1}\sigma^2.$$

It can further be shown that

$$(2) \qquad X_1'\begin{bmatrix} I_p & \lambda \\ \lambda' & \lambda'\lambda \end{bmatrix}X_1 = X'(I_p + \lambda\lambda')^2X;$$

$$S_1^{-1} = [X'(I_p + \lambda\lambda')X]^{-1} = X^{-1}(I_p + \lambda\lambda')^{-1}X'^{-1}.$$

Substituting (2) and for S_1^{-1} in (1) we have

$$\operatorname{cov}(\mathbf{B}_1^+) = [X^{-1}(I_p + \lambda\lambda')^{-1}X'^{-1}X'(I_p + \lambda\lambda')^2XX^{-1}(I_p + \lambda\lambda')^{-1}X'^{-1}]$$
$$= \sigma^2[X'X]^{-1}.$$

Hence, the estimates of the variances remain unchanged.

3. Variance of the estimated effects under adjustment of Theorem 2. Let $e_2 = Fe$ corresponding to $Y_2 = FY$. Then, $E(e_2e_2') = \sigma^2FF'$ and

$$\text{cov}(\mathbf{B}_2^+) = E[\mathbf{B}_2^+ - \mathbf{B}_2)(\mathbf{B}_2^+ - \mathbf{B}_2)']$$
$$= E[(S_2^{-1}X_2'Y_2 - \mathbf{B}_2)(S_2^{-1}X_2'Y_2 - \mathbf{B}_2)'],$$

where $S_2 = [X_2'X_2]$. Substitution of $X_2\mathbf{B}_2 + e_2$ for Y_2 reduces the covariance matrix to

$$\text{cov}(\mathbf{B}_2^+) = E[\{(X_2'X_2)^{-1}X_2'e_2\}\{(X_2'X_2)^{-1}X_2'e_2\}'] = \sigma^2(X'X)^{-1}.$$

Here also the estimates of the variances remain unchanged under the procedure of adjustment as in Theorem 2.

The results above and those in Theorem 1 are related to those of Leech and Healy (1959).

4. On the existence of the matrix λ of Theorem 1. The full design matrix X may be partitioned as

$$X = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} = [X_1 \vdots X_2], \tag{3}$$

where the matrix X_{11} corresponds to the design matrix for the fractional replicate retained. X_{11} and X_{21} would respectively be the same as X and X_m of Theorem 1, and in terms of the conditions of Theorem 1, the dimensions of X_{11} are $p \times p$ and those of X_{22} are $m \times m$. The corresponding partitions of the full vector of observations Y_a may be taken as $[Y' \vdots Y_m']'$, where Y is the Y of Theorem 1, and Y_m represents the remaining m observations.

When the number of omitted treatments is the same as the number of interactions set equal to zero, estimates of the omitted treatments may be obtained in a manner similar to what has been done by Tocher (1952), that is, by equating the observations for these interactions to zero. Estimability of the omitted treatments on this basis is related to the existence of λ, the conditions for which are embodied in the following two theorems.

THEOREM 3. *If solutions Y_m^+ to the equations $X_{22}'Y_m^+ = -X_{12}'Y$ exist, X_{22}' will be non-singular.*

PROOF. If solutions to the linear equations $X_{22}'Y_m^+ = -X_{12}'Y$ exist, we must have Rank $[X_{22}']$ = Rank $[X_{22}' \vdots X_{12}']$. Since the m columns of X_2 are linearly independent, the rank of X_{22}' is equal to m. Hence X_{22}' is non-singular.

THEOREM 4. *If solutions to the equations $X_{22}'Y_m^+ = -X_{12}'Y$ exist, it is always possible to find the matrix $\lambda = -X_{12}[X_{22}]^{-1}$.*

PROOF. Since $X'X$ is diagonal, then $X_{12}'X_{11} + X_{22}'X_{21} = 0$, or $X_{21} = -[X_{22}']^{-1}X_{12}'X_{11}$. If X_{22}' has an inverse as in Theorem 3, then λ' may be taken as $-[X_{22}']^{-1}X_{12}'$ and always exists.

5. On the existence of the matrix F of Theorem 2. What may be achievable on the basis of Theorem 1 can also be achieved by Theorem 2. We can always have a matrix F given by

$$F = \begin{bmatrix} I_p & 0 \\ 0 & m^{-\frac{1}{2}}X'_{22} \end{bmatrix},$$

where I_p is the $p \times p$ identity matrix. Premultiplying X by F, we have

$$FX = \begin{bmatrix} I_p & 0 \\ 0 & m^{-\frac{1}{2}}X'_{22} \end{bmatrix} \cdot \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} = \begin{bmatrix} X_{11} & X_{12} \\ m^{-\frac{1}{2}}X'_{22}\,X_{21} & m^{-\frac{1}{2}}X'_{22}\,X_{22} \end{bmatrix};$$

$$FX \begin{bmatrix} \mathbf{B}_1 \\ 0 \end{bmatrix} = \begin{bmatrix} X_{11} & X_{12} \\ m^{-\frac{1}{2}}X'_{22}\,X_{21} & m^{-\frac{1}{2}}X'_{22}\,X_{22} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{B}_1 \\ 0 \end{bmatrix} = \begin{bmatrix} X_{11} \\ m^{-\frac{1}{2}}X'_{22}\,X_{21} \end{bmatrix} \mathbf{B}_1,$$

where $\mathbf{B}_1$ is the $p \times 1$ column vector in Theorem 1. Similarly,

$$F[Y' \vdots Y'\lambda]' = [Y' \vdots -m^{-\frac{1}{2}}Y'X_{12}]'. \tag{5}$$

From the above, it will be clear that application of Theorem 2 gives us the same set of observational equations, $[X'_{11} \vdots X'_{21}]'\mathbf{B}_1 = [Y' \vdots Y'\lambda]'$ as obtained for Theorem 1. It may be noted from Equation (5) that the last m rows may be obtained by reversing the signs of X'_{12} as was pointed out for 2^n series in the original paper.

6. Aliasing in fractional replication. In a full replicate of a complete factorial with $m + p$ treatments we may write the observational equations as:

$$\begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} \mathbf{B} \\ \mathbf{B}_0 \end{bmatrix} = Y_a,$$

where $\mathbf{B}$ is the $p \times 1$ vector of effect parameters not equated to zero in the fractional replicate and $\mathbf{B}_0$ is the $m \times 1$ vector of effect parameters equated to zero. Then, in the fractional replicate the observational equations may be written as:

$$[X_{11} \vdots X_{12}][\mathbf{B}' \vdots \mathbf{B}'_0]' = [X_{11}\mathbf{B} + X_{12}\mathbf{B}_0] = Y,$$

or

$$X_{11}\mathbf{B} = [Y - X_{12}\mathbf{B}_0].$$

The last equation may be solved directly, or we may utilize the adjustment in Theorem 1 as $[X'_{11} \vdots X'_{11}\lambda]'\mathbf{B}_1 = [[Y - X_{12}\mathbf{B}_0]' \vdots [Y - X_{12}\mathbf{B}_0]'\lambda]'$. Solution of either form of the observational equations yields the effects which are completely or partially aliased with the effect parameters in $\mathbf{B}$.

A relatively simple procedure for determining which effects can appear in $\mathbf{B}$ and which in $\mathbf{B}_0$ is to construct the complete set of observational equations; then, for each treatment combination deleted, the associated effect from that observational equation is also deleted, i.e., the effect is allocated to $\mathbf{B}_0$.

7. On the calculation of the inverse. A straightforward solution for the effect parameters in $\mathbf{B}$ for a fractional replicate involves inversion of the matrix $[X'_{11}X_{11}]$. This matrix is not in diagonal form for the so-called irregular fractions of a complete factorial, and hence some tedious calculations may result. In order to simplify the inversion X_{11} was augmented to become $[X'_{11} \vdots X'_{21}]' = X_1$ and then X'_1X_1 becomes a diagonal matrix and its inverse offers no problem. However, in order to obtain a λ for fractional replicates of complete factorials under Theorem 1 it is necessary to invert the matrix X_{22} of dimensions $m \times m$. Less labor is involved in inverting X_{22} than in inverting X_{11} for all $m < p$.

The variances for the estimated effects may be obtained from Equation (1) in the following form:

$$\begin{aligned}\text{cov}\,(\mathbf{B}^+) &= \sigma^2 S_1^{-1}[X'_{11} \vdots X'_{21}][I'_p \vdots \lambda]'[I'_p \vdots \lambda][X'_{11} \vdots X'_{21}]' S_1^{-1} \\ &= \sigma^2 S_1^{-1}[X_{11} - X_{12}X_{22}^{-1}X_{21}]'[X_{11} - X_{12}X_{22}^{-1}X_{21}]S_1^{-1},\end{aligned}$$

where S_1 is diagonal and $X_{12}X_{22}^{-1}X_{21}$ would need the inversion of the matrix X_{22}.

If it is desired to invert X_{11} (or X_{22}) this can be done rather simply by partitioning X_{11} as follows:

$$X_{11} = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix}.$$

If we premultiply both sides of the observational equations $X_{11}\mathbf{B} = Y = [Y'_f \vdots Y'_r]'$ as follows:

$$\begin{aligned}\begin{bmatrix} A'_{00} & 0 \\ 0 & A'_{11} \end{bmatrix} X_{11}\,\mathbf{B} &= \begin{bmatrix} A'_{00}A_{00} & A'_{00}A_{01} \\ A'_{11}A_{10} & A'_{11}A_{11} \end{bmatrix} \begin{bmatrix} \mathbf{B}_f \\ \mathbf{B}_r \end{bmatrix} = \begin{bmatrix} A'_{00}Y_f \\ A'_{11}Y_r \end{bmatrix} \\ &= \begin{bmatrix} A'_{00} & 0 \\ 0 & A'_{11} \end{bmatrix} Y\end{aligned}$$

and if $A_{00}\mathbf{B}_f = Y_f$ represents a regular fraction of a factorial, then $A'_{00}A_{00}$ is a diagonal matrix; if $A_{11}\mathbf{B}_r = Y_r$ forms a regular fraction then $A'_{11}A_{11}$ is also a diagonal matrix. The inverse of

$$\begin{bmatrix} A'_{00} & 0 \\ 0 & A'_{11} \end{bmatrix} X_{11}$$

involves the inverse of a matrix of the same dimensions as A_{11} and the inverse of the diagonal matrix $A'_{00}A_{00}$; since $A_{00}\mathbf{B}_f = Y_f$ represents the largest regular fraction in X_{11}, the required inverse of non-diagonal matrices will have small dimensions for many fractional replicates.

The above scheme would be useful if observations and effect parameters were to be added sequentially. Here the inverse of $A'_{00}A_{00}$ would have been obtained from previous steps and it would be necessary to invert a matrix of the same dimensions as A_{11}.

REFERENCES

[1] Banerjee, K. S. and Federer, W. T. (1963). On estimates for fractions of a complete factorial experiment as orthogonal linear combinations of the observations. *Ann. Math. Statist.* **34** 1068–1078.

[2] Leech, F. B. and Healy, M. J. R. (1959). The analysis of experiments on growth rate. *Biometrics* **15** 98–106.

[3] Tocher, K. D. (1952). The design and analysis of block experiments. *J. Roy. Statist. Soc. Ser. B* **14** 45–100.