The Annals of Mathematical Statistics
1968, Vol. 39, No. 2, 657–663

ON THE STRUCTURE AND ANALYSIS OF SINGULAR FRACTIONAL REPLICATES[1]

By K. S. Banerjee[2] and W. T. Federer

Development and Planning Department, West Bengal, and Cornell University

1. Summary and introduction. In a recent paper [1], the authors presented a procedure showing how the treatment design matrix for an irregular fractional replicate of an N treatment factorial might be adjusted to furnish estimates of the effect parameters as orthogonal linear functions of the observations. The procedure may be summarized as follows: If the $N \times N$ design matrix X of the complete factorial is partitioned into four submatrices X_{11}, X_{12}, X_{21}, X_{22} having dimension $(p + m_1) \times p$, $(p + m_1) \times m$, $m_2 \times p$ and $m_2 \times m$ respectively, with $m_1 + m_2 = m$ and $p + m = N$, X_{11} would correspond to the design matrix of an irregular fractional replicate consisting of p effect parameters. With the help of an auxiliary design matrix Λ, the design matrix X_{11} and the corresponding observation vector Y_{p+m_1} of $(p + m_1)$ components were then augmented to become $X_1 = [X'_{11}:X'_{11}\Lambda]'$ of dimensions $(p + m_1 + m_2) \times p$, and $Y_1 = [Y':Y'\Lambda]'$ of dimensions $(p + m_1 + m_2) \times 1$ in such a way that $[X_1'X_1]$ reduced to a diagonal matrix. The success of the procedure depended on being able to find least squares estimates for *each* of m_2 omitted observations, and this, in turn, was possible because it was possible to have least squares estimates for *each* of the effect parameters retained. In other words, this meant that both $(X'_{11}X_{11})^{-1}$ and $(X_{22}X'_{22})^{-1}$ existed. The structural relationship between the effect parameters retained and the observations omitted was such that existence of one of the inverses implied the existence of the other.

If the rank of $(X'_{11}X_{11})$ is not full, either as a result of defective or intentional construction of the fractional replicate, the rank of $(X_{22}X'_{22})$ will be less than full, and, as a result, it will not be possible to have unique least squares estimates for *each* of the omitted observations. When this is the case, the corresponding fractional replicate would be what might be characterized as a singular fractional replicate. A question then arises as to how the results presented in [1] would be affected by this singularity. The question has been resolved and analogous results have been obtained through use of generalized inverses (referred to as g-inverses) in the present paper. By way of an aid to the derivation of the analogues, a few additional results on the ranks of the associated submatrices have also been obtained.

2. Notation and the preliminaries. A set of $\nu = p + m_1$ observational equations is denoted by $Y = X\mathbf{B}_p + e$, where Y is a $\nu \times 1$ random vector of observa-

Received 1 February 1967.
[1] Supported in part by N.S.F. Grant No. GP-6129 and N.I.H. Grant No. GM-05900.
[2] Formerly at Kansas State University.

tions with elements y_i, X is the $\nu \times p$ treatment design matrix with rank $p \leqq \nu$, $\mathbf{B}_p$ is a $p \times 1$ vector of effect parameters, and e is a $\nu \times 1$ random vector of errors with $E(ee') = \sigma^2 I_\nu$. When the design matrix X is of full rank, $(X'X)$ is non-singular, and the least squares estimates of $\mathbf{B}_p$ are given by $\mathbf{B}_p^+ = [X'X]^{-1}X'Y$ with the covariance matrix as cov $(\mathbf{B}_p^+) = [X'X]^{-1}\sigma^2$. When, however, X is not of full rank, that is, when $[X'X]$ is singular, we have the solutions for $\mathbf{B}_p^+$ as given by $\mathbf{B}_p^+ = S^-X'Y + (I_p - H)Z$, where $S = X'X$, S^- is a g-inverse of S, $H = S^-S$ and has a special form; and Z is an arbitrary column vector. A particular solution would be given by $\mathbf{B}_p^+ = S^-X'Y$. Whatever form of a g-inverse we adopt, either a unique one as defined and developed by Penrose in [3], or a non-unique one as discussed by Rao in [5], or the one as referred to by Banerjee in [2], we would have the following identity: [The interested reader may also refer to the work of Price [4] and Zelen [6] in this context].

$$SS^-S = S. \tag{2.1}$$

In this context, we also note that when the full factorial is partitioned into N orthogonal contrasts, $X'X$ will be a diagonal matrix D. In case of a 2^n experiment, we shall have $X'X = NI_N = XX'$, where $2^n = N$. This will not be true, in general, for other factorial design matrices X, since they are only columnwise orthogonal. However, we may introduce an analogous situation in the general case by transforming the design matrix and the parameters as $X\mathbf{B} = (XD^{-\frac{1}{2}})\cdot(D^{\frac{1}{2}}\mathbf{B}) = W\mathbf{C}$, where $W = XD^{-\frac{1}{2}}$, $\mathbf{C} = D^{\frac{1}{2}}\mathbf{B}$, $D^{\frac{1}{2}}$ is an $N \times N$ diagonal matrix with diagonal elements $d_i^{\frac{1}{2}}$, d_i $(i = 1, 2, \cdots, N)$ being the ith diagonal element of D. With this transformation, we shall have, in the general case, $W'W = I_N = WW'$, restoring the required orthogonality. We also note that the following relations will hold good for the transformed design matrix W, in general:

$$\begin{bmatrix} W'_{11} & W'_{21} \\ W'_{12} & W'_{22} \end{bmatrix} \cdot \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix} = \begin{bmatrix} W'_{11}W_{11} + W'_{21}W_{21} & W'_{11}W_{12} + W'_{21}W_{22} \\ W'_{12}W_{11} + W'_{22}W_{21} & W'_{12}W_{12} + W'_{22}W_{22} \end{bmatrix} = \begin{bmatrix} I_p & 0 \\ 0 & I_m \end{bmatrix},$$

(2.2)

$$\begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \cdot \begin{bmatrix} W'_{11} & W'_{21} \\ W'_{12} & W'_{22} \end{bmatrix} = \begin{bmatrix} W_{11}W'_{11} + W_{12}W'_{12} & W_{11}W'_{21} + W_{12}W'_{22} \\ W_{21}W'_{11} + W_{22}W'_{12} & W_{21}W'_{21} + W_{22}W'_{22} \end{bmatrix} = \begin{bmatrix} I_{p+m_1} & 0 \\ 0 & I_{m_2} \end{bmatrix}$$

where I_p, I_m, I_{p+m_1}, I_{m_2} are identity matrices of dimensions $p \times p$, $m \times m$, $(p + m_1) \times (p + m_1)$ and $m_2 \times m_2$ respectively.

It may also be noted here that the rank of the matrix X is not altered by post-multiplication with the non-singular matrix $D^{-\frac{1}{2}}$.

3. Structure and analysis of a singular fractional replicate. It was proved in [1] that if, the rank of X'_{22} is m_2, or in other words, if X'_{22} is of full rank, the rank of X_{11} is also full, and *vice versa.* From this theorem, it can be inferred that, if X'_{22} is not of full rank, the rank of X_{11} will also be less than the full. We would therefore need to determine the rank of X_{11} with reference to the deficiency in the rank of X_{22}, and for this purpose, we need the following lemmas.

LEMMA 1. *If Rank* $[X_{22}X'_{22}]$ *is* $m_2 - s$, *then Rank* $[X_{21}X'_{21}] \geqq s$ *and* $\leqq m_2$.

We shall prove this result and subsequently, some similar ones with reference to the corresponding W-submatrices, as the ranks will remain unaltered.

PROOF. Rank $[W_{21}W'_{21}]$ cannot exceed m_2, and we have

$$I_{m_2} = [W_{21}W'_{21} + W_{22}W'_{22}].$$

Hence, $m_2 \leqq$ Rank $[W_{21}W'_{21}]$ + Rank $[W_{22}W'_{22}]$ or, $m_2 \leqq$ Rank $[W_{21}W'_{21}] + m_2 - s$ or, Rank $[W_{21}W'_{21}] \geqq s$. Hence, the lemma.

We shall show that the rows of $W_{21}W'_{21}$ corresponding to the dependent rows of $W_{22}W'_{22}$ are independent. That is to say, if the last s rows of $W_{22}W'_{22}$ are dependent on its first $m_2 - s$ rows, the last s rows of $W_{21}W'_{21}$ will be independent. In order to demonstrate this result, we need the help of the following lemma:

LEMMA 2. *Matrices* $[W_{21}W'_{21}]$ *and* $[W_{22}W'_{22}]$ *are commutative.*

PROOF. We have, by (2.2),

$$\begin{aligned}[W_{21}W'_{21}][W_{22}W'_{22}] &= -[W_{21}W'_{11}W_{12}W'_{22}] \\ &= -[W_{22}W'_{12}W_{11}W'_{21}] = [W_{22}W'_{22}][W_{21}W'_{21}].\end{aligned}$$

We have now obtained the auxiliary results to prove the following theorem.

THEOREM 1. *The rows of* $W_{21}W'_{21}$ *corresponding to the s dependent rows of* $W_{22}W'_{22}$ *will be independent.*

PROOF. Since $W_{21}W'_{21} + W_{22}W'_{22} = I_{m_2}$, $W_{21}W'_{21}$ and $W_{22}W'_{22}$ will be of the following form:

$$[W_{22}W'_{22}] = mN^{-1}I_{m_2} + A, \qquad [W_{21}W'_{21}] = pN^{-1}I_{m_2} - A.$$

By Lemma 2, $W_{22}W'_{22}$ and $W_{21}W'_{21}$ commute; there exist orthogonal matrices, say P' and P, which will simultaneously diagonalize these matrices. Let it be possible to arrange the rows of W_{22} or of $W_{22}W'_{22}$ in such a manner that the $(m_2 - s)$ independent rows occupy the first $(m_2 - s)$ positions, and let μ_i $(i = 1, 2, \cdots, m_2 - s)$ be the diagonal elements of $W_{22}W'_{22}$ when reduced. Then, we shall have

$$P'W_{21}W'_{21}P + P'W_{22}W'_{22}P = I_{m_2},$$

where $P'W_{22}W'_{22}P$ will be of the form:

$$P'W_{22}\,W_{22}'\,P = mN^{-1}I_{m_2} + \begin{bmatrix} (\mu_1 - m/N) & & & & & & \\ & \cdot & & & & 0 & \\ & & \cdot & & & & \\ & & & (\mu_{m_2-s} - m/N) & & & \\ & & & & - m/N & & \\ & 0 & & & & \cdot & \\ & & & & & & -m/N \end{bmatrix},$$

and $P'W_{21}W_{21}'P$ will be of the form:

$$P'W_{21}\,W_{21}'\,P = pN^{-1}I_{m_2} + \begin{bmatrix} -(\mu_1 - m/N) & & & & & & \\ & \cdot & & & & 0 & \\ & & \cdot & & & & \\ & & & -(\mu_{m_2-s} - m/N) & & & \\ & & & & m/N & & \\ & 0 & & & & \cdot & \\ & & & & & & m/N \end{bmatrix}.$$

The preceding would show that the last s rows of $W_{21}W_{21}'$ are independent. Incidentally, it may be pointed out here that if the rank of $W_{21}W_{21}'$ is $r = s + t$, $0 \leqq t \leqq m_2 - s$, then $(m_2 - s - t)$ of the diagonal elements of $W_{22}W_{22}'$ will be unities.

We now prove a theorem on the rank of $[X_{11}'X_{11}]$ as compared to the rank of $[X_{22}X_{22}']$.

THEOREM 2. *If Rank* $[X_{22}X_{22}'] = m_2 - s$, *then Rank* $[X_{11}'X_{11}] = p - s$.

PROOF. It has been proved in [1] that when Rank $[X_{22}W_{22}']$ is full, that is, when Rank $[W_{22}W_{22}'] = m_2$, Rank $[W_{11}'W_{11}]$ is also full, that is, Rank $[W_{11}'W_{11}] = p$. The converse has also been proved in [1]. That is to say, that when Rank $[W_{11}'W_{11}]$ is full, Rank $[W_{22}W_{22}']$ is also full. This result may be utilized to argue that when $[W_{22}W_{22}']$ is singular, $[W_{11}'W_{11}]$ will also be singular.

Arrange the rows of W_{22} in such a manner that its independent rows, $m_2 - s$ in number, occupy the last positions, and its s dependent rows are pushed up. A corresponding change of rows is also made in W_{21}. With such a change, and by virtue of Theorem 1, the uppermost s rows of W_{21} will be mutually independent. These s rows of W_{21} may now be added to the rows of W_{11} to form the new W_{11}. By the theorem proved in [1], the new W_{11} will now have full rank. We thus note that addition of s rows, which are mutually independent, raises the rank of the old W_{11} to p. Hence, Rank $[W_{11}]$ was equal to $p - s$, or Rank $[W'_{11}W_{11}] = p - s$.

The following theorem was also proved in [1]: If X'_{22} is of rank m_2, then the least squares estimates $Y^+_{m_2}$ obtained from the observational equations $X'_{22}Y^+_{m_2} = - X'_{12}Y_{p+m_1}$ (the error part not indicated) and expressed as $\Lambda' Y_{p+m_1}$, are such that $X_{21} = \Lambda' X_{11}$. [The observational equations were obtained by equating the omitted effect parameters to zero.] In the altered situation, however, that is, when $[X_{22}X'_{22}]$ is singular, $\Lambda' X_{11}$ will not be equal to X_{21}. The problem starts from this point. However, in this case, a "particular solution" for the estimates of $Y^+_{m_2}$ will be given by

$$Y^+_{m_2} = -S_2^- X_{22}X'_{12}Y_{p+m_2},$$

where $S_2 = [X_{22}X'_{22}]$, and S_2^- is a g-inverse of S_2. Λ' will have the form as given by $\Lambda' = -S_2^- X_{22}X'_{12}$, and $\Lambda' X_{11} = -S_2^- X_{22}X'_{12}X_{11} = S_2^-[X_{22}X'_{22}]X_{21} = H_2X_{21}$ where $S_2^- S_2 = H_2$.

If we change from X-submatrices to W-submatrices, there will be no structural change in the above relations except that H_2 will then be equal to $[W_{22}W'_{22}]^- \cdot [W_{22}W'_{22}]$ with the corresponding change in S_2, Λ, etc.

We make a special note of the fact that in the altered situation, premultiplication of X_{11} by Λ' gives us H_2X_{21} instead of X_{21}. This calls for a reexamination of of the results proved in [1], where $[X_{22}X'_{22}]$ was considered to be of full rank.

We prove below two theorems to indicate that the previous results would, formally, still hold in the altered context.

THEOREM 3. *If X_{11}, Y_{p+m_1}, and e_{p+m_1} are augmented respectively by $\Lambda' X_{11}$, $\Lambda' Y_{p+m_1}$ and $\Lambda' e_{p+m_1}$ to become X_1, Y_1, and e_1, then the least squares estimates $\mathbf{B}_p^*$, obtained from the observational equations $Y_1 = X_1\mathbf{B}_p + e_1$, are algebraically the same as the least squares estimates, $\mathbf{B}_p^+$, obtained from the observational equations $Y_{p+m_1} = X_{11}\mathbf{B}_p + e_{p+m_1}$.*

PROOF. We have to show that $\mathbf{B}_p^+$ as obtained from $[X'_{11}X_{11}]\mathbf{B}_p^+ = X'_{11}Y_{p+m_1}$ is the same as $\mathbf{B}_p^*$ obtained from

$$[X'_{11}X_{11} + X'_{11}\Lambda\Lambda' X_{11}]\mathbf{B}_p^* = [X'_{11} + X'_{11}\Lambda\Lambda']Y_{p+m_1}.$$

We may transform the design matrix and the parameters such that $X\mathbf{B} = W\mathbf{C}$, and after we have proved the corresponding results in terms of $\mathbf{C}_p^+$ and $\mathbf{C}_p^*$, we may go back to $\mathbf{B}_p^+$ and $\mathbf{B}_p^*$ by the inverse of the same non-singular transformations to prove the required theorem. The theorem will therefore be proved, if we can show that $\mathbf{C}_p^+$ as obtained from

$$[W'_{11}W_{11}]\mathbf{C}_p^+ = W'_{11}Y_{p+m_1} \tag{3.1}$$

is the same as $\mathbf{C}_p^*$, obtained from

$$[W'_{11}W_{11} + W'_{11}\Lambda\Lambda' W_{11}]\mathbf{C}_p^* = [W'_{11} + W'_{11}\Lambda\Lambda']Y_{p+m_1}, \tag{3.2}$$

where Λ is the corresponding expression in terms of W-submatrices.

We shall prove this theorem by substituting $[W'_{11}W_{11}]^{-}W'_{11}Y_{p+m_1}$ [which is a particular solution of $\mathbf{C}_p^+$ obtained from (3.1)] for $\mathbf{C}_p^*$ in the expression on the left hand side of (3.2) and show that equations (3.1) and (3.2) are consistent.

Substituting the above expression for $\mathbf{C}_p^*$ in (3.2), we get, by repeated application of the identities in (2.2),

$$\begin{aligned}
&[W'_{11}W_{11} + W'_{11}\Lambda\Lambda' W_{11}][W'_{11}W_{11}]^{-}W'_{11}Y_{p+m_1} \\
&\quad = [W'_{11}W_{11}][W'_{11}W_{11}]^{-}[W'_{11}W_{11}]\mathbf{C}_p^+ + W'_{11}W_{12}W'_{22}[W_{22}W'_{22}]^{-}[W_{22}W'_{22}]^{-} \\
&\qquad \cdot W_{22}W'_{12}W_{11}[W'_{11}W_{11}]^{-}[W'_{11}W_{11}]\mathbf{C}_p^+ \\
&\quad = [W'_{11}W_{11}]\mathbf{C}_p^+ - W'_{11}W_{12}W'_{22}[W_{22}W'_{22}]^{-}[W_{22}W'_{22}]^{-}W_{21}[W'_{11}W_{11}] \\
&\qquad \cdot [W'_{11}W_{11}]^{-}[W'_{11}W_{11}]\mathbf{C}_p^+ \\
&\quad = W'_{11}Y_{p+m_1} + W'_{11}W_{12}W'_{22}[W_{22}W'_{22}]^{-}[W_{22}W'_{22}]^{-}W_{22}W'_{12}Y_{p+m_1} \\
&\quad = [W'_{11} + W'_{11}\Lambda\Lambda']Y_{p+m_1}.
\end{aligned}$$

We now need to show that $\operatorname{cov}(\mathbf{C}_p^+) = \operatorname{cov}(\mathbf{C}_p^*)$. In order to demonstrate this result, we need the help of the following identity.

Lemma 3. $[W'_{11}W_{11}]T^{-}[W'_{11} + W'_{11}\Lambda\Lambda'] = W'_{11}$, *where* $T^{-} = [W'_{11}W_{11} + W'_{11}\Lambda\Lambda' W_{11}]^{-}$.

Proof. Since equations (3.1) and (3.2) are consistent, we shall have

$$[W'_{11}W_{11}]T^{-}[W'_{11} + W'_{11}\Lambda\Lambda']Y_{p+m_1} = W'_{11}Y_{p+m_1}$$

for *all values* of Y_{p+m_1}. Hence, $[W'_{11}W_{11}]T^{-}[W'_{11} + W'_{11}\Lambda\Lambda'] = W'_{11}$.

Theorem 4. $\operatorname{cov}(\mathbf{B}_p^+) = \operatorname{cov}(\mathbf{B}_p^*)$.

Proof. The theorem will be proved, if we can show $\operatorname{cov}(\mathbf{C}_p^+) = \operatorname{cov}(\mathbf{C}_p^*)$. We have $\operatorname{cov}(\mathbf{C}_p^+) = [W'_{11}W_{11}]^{-}\sigma^2$. Now, $\operatorname{cov}(\mathbf{C}_p^*)$ will be given (see [1]) by $\operatorname{cov}(\mathbf{C}_p^*) = T^{-}W'_{11}[I + \Lambda\Lambda']^2 W_{11}T^{-}\sigma^2$.

By Lemma 3, we have $W'_{11}W_{11}T^{-}W'_{11}[I + \Lambda\Lambda'] = W'_{11}$. By postmultiplying both sides of the above by the transpose of W'_{11} and its equivalent, we shall have

$$W'_{11}W_{11}[T^{-}W'_{11}[I + \Lambda\Lambda'][I + \Lambda\Lambda'][W_{11}T^{-}][W'_{11}W_{11}]] = W'_{11}W_{11}.$$

Thus, by (2.1), we shall have

$$[W'_{11}W_{11}]^{-} = [T^{-}W'_{11}[I + \Lambda\Lambda']^2 W_{11}T^{-}].$$

This would follow from the following reasoning: Let

$$F = T^{-}W'_{11}[I + \Lambda\Lambda']^2 W_{11}T^{-}.$$

Then, we shall have, by (2.1),

$$SS^{-}S = SFS, \tag{3.3}$$

where $S = [W'_{11}W_{11}]$. From (3.3), we have $S(F - S^{-})S = 0$. Hence, since $S \neq 0$, we shall have either $F - S^{-} = 0$, i.e. $F = S^{-}$, or, $(F - S^{-})S = 0$, otherwise, (i.e. by both $(F - S^{-})$ and S being appropriately singular). In the latter case also, we must have $FS = S^{-}S = H$ (say). Now, any matrix, which would reduce S to the form of an H by premultiplication, will, by definition (see [2] and [5]), be a g-inverse, although it may not be unique. Hence, the theorem.

It is thus noted that the main theorems proved in [1] hold good even when the fractional replicates are "singular."

The above results form the basis for analysis of a singular fractional replicate and bring out the relationship between the effect parameters that are retained as against the observations that are omitted.

REFERENCES

[1] BANERJEE, K. S. and FEDERER, W. T. (1966). On estimation and construction in fractional replication. *Ann. Math. Statist.* **37** 1021–1032.

[2] BANERJEE, K. S. (1966). Singularity in Hotelling's weighing designs and a generalized inverse. *Ann. Math. Statist.* **37** 1033–1039.

[3] PENROSE, R. A. (1955). A generalized inverse for matrices. *Proc. Cambridge Phil. Soc.* **51** 406–413.

[4] PRICE, C. M. (1964). The matrix pseudo-inverse and minimal variance estimates. *SIAM Rev.* **6** 2, 115–120.

[5] RAO, C. R. (1962). A note on a generalized inverse of a matrix with applications to problems in Mathematical Statistics. *J. Roy. Stat. Soc. Ser. B* **24** 152–158.

[6] ZELEN, M. (1962). The role of constraints in the theory of least squares. Technical Summary Report, No. 314, Math. Res. Center, U.S. Army, University of Wisconsin.