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SOME RECENT RESULTS IN LINEAR ESTIMATION

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SUMMARY. Some recent work of the author on 'Unified Theory of Linear Estimation' is described. The general Gauss-Markoff (GM) model $(Y, X\beta, \sigma^2V)$ is considered, where $V = E[(Y - X\beta)(Y - X\beta)']$ is possibly singular and X possibly deficient in rank. Aitken's procedure of least squares is not applicable when V is singular. The object of the paper is to lay down procedures which are valid in all situations and which do not require prior examination of the ranks of V and X . Two unified methods are suggested. One is a numerical approach called the Inverse Partitioned Matrix (IPM) method. Another is an analogue of the least squares theory, called the Unified Least Squares (ULS) method.

It has been pointed out that singularity of V imposes some restriction on the parameter β , which has to be taken into account in constructing unbiased estimators.

In a series of papers (Rao, 1971, 1972a, 1972b, 1973), the author developed two approaches towards a unified treatment of the General Gauss-Markoff (GM) linear model $(Y, X\beta, \sigma^2V)$ where V , the dispersion matrix of Y , may be singular and X may be deficient in rank. One is called the Inverse Partition Matrix (IPM) method, which depends on the numerical evaluation of a g -inverse of a partitioned matrix (see Rao, 1971, 1972b). Another is an analogue of least squares theory and is called unified least square (ULS) method (see Rao, 1971, 1973). It may be noted that Aitken's approach (which is called generalized least squares) is applicable only when V is non-singular. The object of the present paper is to bring out the salient features of these two methods and to point out some interesting features of linear unbiased estimation when the dispersion matrix of the observations is singular.

2. CONDITION OF CONSISTENCY

Consider the triplet

$$(Y, X\beta, \sigma^2V) \quad \dots \quad (2.1)$$

where Y is the vector of random variables, $E(Y) = X\beta$ and $D(Y) = \sigma^2V$, β and σ^2 being unknown. We refer to the set-up (2.1) as the General Gauss-Markoff (GM) model when no assumption is made about $R(V)$ and $R(X)$, where $R(\cdot)$ denotes the rank of the matrix argument.

It may be noted that the Gauss-Markoff model with restrictions on the parameter β

$$(Y, X\beta, \sigma^2V), c = R\beta. \quad \dots (2.2)$$

can be written as the GOM model

$$(Y_e, X_e\beta, \sigma^2V_e) \quad \dots (2.3)$$

where

$$Y_e = \begin{pmatrix} Y \\ c \end{pmatrix}, X_e = \begin{pmatrix} X \\ R \end{pmatrix}, V_e = \begin{pmatrix} V & 0 \\ 0 & 0 \end{pmatrix}. \quad \dots (2.4)$$

When V is singular in (2.1), there are some natural restrictions on the random vector Y and possibly on the parameter vector β . One such restriction on Y is

$$L'X = 0, L'V = 0 \implies L'Y = 0 \quad \text{with probability 1,} \quad \dots (2.5)$$

which implies that $Y \in \mathcal{L}(V \cup X)$, the linear manifold generated by the columns of V and X . Further if K is a matrix such that $K'V = 0$, then $K'Y$ is a constant which is known when Y is known. In such a case

$$K'Y = K'X\beta \quad \dots (2.6)$$

is a natural restriction on β unless $K'X = 0$, or in other words, the random vector Y and the parameter β are such that $(Y - X\beta) \in \mathcal{L}(V)$.

Let V be of order n and rank k . Then there exists a $n \times (n-k)$ matrix N of rank $n-k$ or $n-k-1$ such that $N'Y = 0$ which implies

$$N'X\beta = 0. \quad \dots (2.7)$$

The restrictions $N'Y = 0$ and $N'X\beta = 0$ imply that Y and β are confined to subspaces which can be specified when V and a sample observation on Y are known.

3. UNBIASEDNESS OF A LINEAR ESTIMATOR

Let us consider the model (2.1) and find the condition for a linear function $L'Y$ to be unbiased for $p'\beta$.

$$E(L'Y) = L'X\beta = p'\beta \quad \dots (3.1)$$

which must hold for all β such that $N'X\beta = 0$. Then there exists a vector λ such that

$$L'X - p' = \lambda'N'X \text{ or } p = X'(L - N\lambda).$$

Thus we have the following lemmas.

Lemma 3.1: *A necessary and sufficient condition that $p'\beta$ admits a linear unbiased estimator is that $p \in \mathcal{L}(X')$.*

Lemma 3.2: *If $L'Y$ is unbiased for $p'\beta$ then it is necessary and sufficient that there exists a vector λ such that*

$$X'(L - N\lambda) = p. \quad \dots (3.2)$$

Note that when V is of full rank or when the observation Y is unknown, the condition for unbiasedness is $X'L = p$, which is usually given in text books. This is not true in general as (3.2) shows.

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Lemma 3.3: If $L'Y$ is an unbiased estimator of $p'\beta$, then there exists a vector M such that $X'M = p$ and $L'Y = M'Y$.

Lemma 3.3 shows, however, that the entire class of unbiased estimators of an estimable function $p'\beta$ can be generated by $M'Y$ where M satisfies the condition $X'M = p$. Thus to find the minimum variance unbiased estimator of $p'\beta$ we need determine M such that $M'Y$ is a minimum subject to the condition $X'M = p$.

Note 1: The result of Lemma 3.2 is based on the knowledge of the matrix N , which can be computed if V and a sample observation on the random variable Y are known. However, if we want $L'Y$ to be unbiased for $p'\beta$ irrespective of the subspace to which Y may belong, then the condition is $X'L = p$. Fortunately, in view of Lemma 3.3, the formulae we develop for the BLUE of $p'\beta$ and for the estimation of σ^2 are valid to whichever particular subspace Y may belong.

4. THE IPM METHOD

The Inverse Partition Matrix (IPM) method, needs the computation of a g -inverse of the partitioned matrix

$$\begin{pmatrix} V & X \\ X' & 0 \end{pmatrix}^{-1} = \begin{pmatrix} C_1 & C_2 \\ C_3 & -C_4 \end{pmatrix} \quad \dots (4.1)$$

as the basic step. The inverse matrix (4.1) is like a Pandora Box which gives all that is necessary for drawing inference on the β parameters. We state the results in Theorem 4.1 which gives the use of the submatrices in (4.1).

Theorem 4.1: Let C_1, C_2, C_3, C_4 be as defined in (4.1) Then :

- (i) The BLUE of an estimable function $p'\beta$ is $p'\hat{\beta}$ where

$$\hat{\beta} = C_2'Y \text{ or } C_3'Y. \quad \dots (4.2)$$

- (ii) $V(p'\beta) = \sigma^2 p' C_4 p$, $\text{cov}(p'\hat{\beta}, q'\hat{\beta}) = \sigma^2 p' C_4 q$ (4.3)

- (iii) An unbiased estimator of σ^2 is

$$\hat{\sigma}^2 = Y' C_1 Y / f, \quad f = R(Y : X) - R(X). \quad \dots (4.4)$$

Theorem 4.2: Let C_1, C_2, C_3, C_4 be as defined in (4.1) and $P'\beta = u$ be a set of linear hypotheses to be tested. Then

- (i) the hypothesis is consistent if

$$DD^{-1}u = u \quad \dots (4.5)$$

where $u = P'\hat{\beta} - u$, $D = P'C_4P$, and D^{-1} is any g -inverse of D .

- (ii) If (4.6) is satisfied and Y has an n -variate normal distribution with mean $N'\beta$ and dispersion matrix σ^2V , then

$$F = \frac{u'D^{-1}u}{h} \div \frac{Y'C_1Y}{f} \quad \dots (4.6)$$

has a central F distribution on h and f degrees of freedom where f is as in (4.4) and $h = R(D)$.

Proofs of Theorems 4.1 and 4.2 are given in detail in Rao (1971, 1972b).

Note 1. In (4.1) we have not made any assumption about the ranks of V and X . Thus the $1RM$ method is applicable to the most general situation where V is possibly singular and X may be deficient in rank. The inverse in (4.1) will be a regular inverse iff V and X are both of full rank. In all other situations the partitioned matrix on the left hand side of (4.1) is singular and we need compute any g -inverse. For definition of g -inverse and its properties the reader is referred to a recent book by Rao and Mitra (1971). Suitable computer programs have been developed for obtaining a g -inverse, (see Golub and Kahan, 1965; Bhimasankaram and Rao, 1972, and Shinozaki, Sibuya and Tanabe, 1972). The author (Rao, 1972b) has also given explicit algebraic expressions for C_1, C_2, C_3, C_4 , which may also be useful in computing the g -inverse (4.1). Thus we have provided a numerical solution to problems of inference on parameters in the $oovt$ model through the $1RM$ method. Further refinements have to be sought only in computing a g -inverse through a computer program.

Note 2: Theorem 4.2 lays down the procedure for testing the linear hypothesis $P'\beta = \tau_0$, and consequently for obtaining simultaneous confidence intervals for the linear parametric function $P'\beta$. The test for consistency (4.5) ensures that the null hypothesis does not contradict the natural restrictions (2.6) on the β parameters imposed by the singularity of V . If (4.5) is not satisfied the null hypothesis of course stands rejected. If (4.5) is satisfied, then we proceed to the F test as in (4.6), which examines that part of the null hypothesis which does not directly depend on the restrictions (2.6). Large values of F indicate departure from the null hypothesis.

5. THE ULS METHOD

When V is nonsingular, the current theory of least squares as formulated by Aitken (1934) lays down the following procedure :

- (i) Obtain $\hat{\beta}$ which minimises the quadratic form

$$(Y - X\beta)'V^{-1}(Y - X\beta) \quad \dots (5.1)$$

and estimate $p'\beta$ by $p'\hat{\beta}$ provided $p'\beta$ is estimable.

- (ii) The unknown parameter σ^2 is estimated by

$$\hat{\sigma}^2 = (Y - X\hat{\beta})'V^{-1}(Y - X\hat{\beta}) \div f, \quad \dots (5.2)$$

$$f = R(V) - R(X) = R(V : X) - R(X).$$

The Aitken procedure is not available when V is singular.

We raise the following question. Whether V is nonsingular or not, what is the most general form of symmetric matrix M such that the following hold.

- (i) The BLUE of an estimable function $p'\beta$ is $p'\hat{\beta}$ where $\hat{\beta}$ is a stationary point of

$$(Y - X\beta)'M(Y - X\beta) \quad \dots (5.3)$$

i.e., where its derivative with respect to β vanishes.

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(ii) An unbiased estimator σ^2 is obtained as

$$\hat{\sigma}^2 = (Y - X\beta)'M(Y - X\beta) \div f \quad \dots (5.4)$$

$$f = R(V : X) - R(X)$$

which is the same as (4.4).

It is shown (Rao, 1973) that the most general form of M , whether V is non-singular or not and whether X is deficient in rank or not is

$$M = (V + XU'X)^- \quad \dots (5.5)$$

for any symmetric g -inverse, where U is any symmetric matrix such that

$$\mathcal{A}(V : X) = \mathcal{A}(V + XU'X) \text{ or } R(V : X) = R(V + XU'X). \quad \dots (5.6)$$

We note that U always exists such that (5.6) is satisfied. For instance $U = k^2I$ is one choice. The main results are stated in Theorem 5.1.

Theorem 5.1: Let U be any symmetric matrix such that $R(V + XU'X) = R(V : X)$ and $M = (V + XU'X)^-$ be any g -inverse (symmetric or not). Then :

(i) The quadratic form

$$(Y - X\beta)'M(Y - X\beta) \quad \dots (5.7)$$

has stationary values. Let $\hat{\beta}$ be a stationary point. Then the BLUE of an estimable function $p'\beta$ is $p'\hat{\beta}$.

(ii) The same estimate of σ^2 as in (4.4) is given by the formula

$$\hat{\sigma}^2 = (Y - X\hat{\beta})'M(Y - X\hat{\beta}) \div f \quad \dots (5.8)$$

$$f = R(V : X) - R(X).$$

(iii) The variances and covariances of BLUE's are obtained as follows :

$$V(p'\hat{\beta}) = \sigma^2 p'[(X'MX)^- - U]p. \quad \dots (5.9)$$

$$\text{cov}(p'\hat{\beta}, q'\hat{\beta}) = \sigma^2 p'[(X'MX)^- - U]q$$

where $(X'MX)^-$ is any g -inverse.

(iv) The dispersion matrix of a number of estimates $P'\hat{\beta}$ is $\sigma^2 D$ where

$$D = P'[(X'MX)^- - U]P. \quad \dots (5.10)$$

Tests of significance can be carried out as in Theorem (4.2) with D as computed in (5.10) and $u = P'\hat{\beta} - u_0$.

Note 3 : The ULS theory leads us to differentiate the quadratic form

$$(Y - X\beta)'(V + XU'X)^-(Y - X\beta)$$

in all situations. The rest of the method is nearly the same as in the current theory of least squares except that we have slightly different expressions for variances and covariances of estimators. The results of Theorem 5.1 are independent of the choice of U subject only to the condition $R(V + XU'X) = R(V : X)$. This condition is always satisfied if $U = k^2I$ where k is any nonzero scalar. It may be noted that Aitken's

procedure is valid only for $|V| \neq 0$. The results of Theorem 5.1 hold good whether V is nonsingular or not and X is deficient in rank or not and thus constitute a unified theory of least squares.

We shall now examine whether it is possible to compute $u'D^{-1}u$ which occurs in the numerator of the F statistic (4.6) as the difference, $(R_1^2 - R_0^2)$, where

$$R_0^2 = \min_{\beta} (Y - X\beta)' M (Y - X\beta) \quad \dots (5.11)$$

$$R_1^2 = \min_{P\beta = u} (Y - X\beta)' M (Y - X\beta) \quad \dots (5.12)$$

as in the usual theory of least squares.

The following theorem is of interest in this connection.

Theorem 5.2: Let $M = (V + XU'X)^{-}$ and $R(V + XU'X) = R(V : X)$, $\hat{\beta}$ is of the value of β which minimises (5.11), $\tilde{\beta}$ is the value of β which minimises (5.12) and $u = P' \tilde{\beta} - u$. Then

$$\tilde{\beta} = \hat{\beta} + (X'MX)^{-} P \{ P'(X'MX)^{-} P \}^{-1} u \quad \dots (5.13)$$

$$R_1 - R_0^2 = u \{ P'(X'MX)^{-} P \}^{-1} u \quad \dots (5.14)$$

The results (5.13) and (5.14) follow on standard lines as in the usual least squares theory.

The expression (5.14) is not the same as

$$u'D^{-1}u = u \{ P'(X'MX)^{-} P - P'UP \}^{-1} u$$

for all testable linear hypotheses (i.e., for all P of the form $X'Q$) however U is chosen, unless $XUX' = 0 \implies \mathcal{A}(X) \subset \mathcal{A}(V)$. So the answer to the question raised is in the negative if $\mathcal{A}(X)$ is not a subspace of $\mathcal{A}(V)$. In the general case, Theorems 5.3 and 5.4 provide the answer.

Theorem 5.3: Let V^{-} be any g -inverse of V , N be a matrix of maximum rank such that $N'V = 0$, and

$$R_0^2 = \min_{N'\beta = N'Y} (Y - X\beta)' V^{-} (Y - X\beta) \quad \dots (5.15)$$

$$R_1^2 = \min_{\substack{N'\beta = N'Y \\ P\beta = u}} (Y - X\beta)' V^{-} (Y - X\beta) \quad \dots (5.16)$$

Then $R_1^2 - R_0^2 = u'D^{-1}u$ and the F statistic in (4.6) can be written

$$F = \frac{R_1^2 - R_0^2}{h} \frac{R_0^2}{f} \quad \dots (5.17)$$

Theorem 5.3 is proved in Rao and Mitra (1971).

We shall now consider n.n.d. matrices of the form $V + XGG'X'$. It is easy to show that there exists a matrix G such that $R(V + XGG'X) = R(V : X)$, and $\mathcal{A}(V)$ and $\mathcal{A}(XG)$ are virtually disjoint. For such a choice of G and any g -inverse,

$$M = (V + XGG'X)^{-} \quad \dots (5.18)$$

is also a g -inverse of V .

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Given a testable hypothesis $P'\beta = v$, we can write it in the equivalent form

$$Q'\beta = v \quad \dots (5.19)$$

where $Q' = P' - KN'X$ and $v = v - KN'Y$, and K is chosen such that

$$(P' - KN'X)G = 0. \quad \dots (5.20)$$

K exists in view of the particular choice of G .

Theorem 5.4: Let M be as in (5.18) and $Q'\beta = v$ be the hypothesis as in (5.19) equivalent to $P'\beta = v$. Further let

$$R_0^2 = \min_{\beta} (Y - X\beta)'M(Y - X\beta), \quad \dots (5.21)$$

$$R_1^2 = \min_{Q'\beta = v} (Y - X\beta)'M(Y - X\beta). \quad \dots (5.22)$$

Then $R_1^2 - R_0^2 = u'D^{-1}u$, and the F statistic (4.6) can be computed as in (5.17).

Theorem 5.4 is proved by using Theorem 5.2 which gives an explicit expression for the difference (5.22)-(5.21), by observing

$$\begin{aligned} Q'(X'MX)Q - Q'GG'Q &= Q'(X'MX)Q \\ &= P'(X'MX)P - P'GG'P. \dots (5.23) \end{aligned}$$

Indeed it can be shown that if $M = (V + XGG'X)^{-1}$ and G is such that $R(V + XUX) = R(V; X)$, then for the result of Theorem 5.4 to be true for all testable hypotheses it is necessary and sufficient that $\mathcal{A}(V)$ and $\mathcal{A}(XG)$ are virtually disjoint. Theorems 5.2, 5.3 and 5.4 are more of theoretical interest than of practical use in computations. Theorem 5.1 provides the basic results in the unified theory of least squares.

6. BEST LINEAR ESTIMATION (BLE)

Not much work is done on BLE compared to that on BLUE. References to earlier work on BLE can be found in papers by Hoerl and Kennard (1970a, 1970b) who introduced what are called ridge regression estimators, which do not satisfy the criterion of unbiasedness. In this section we approach the problem of BLE in a direct manner.

Let $L'Y$ be an estimator of $p'\beta$. The mean square error of $L'Y$ for given β is

$$E(L'Y - p'\beta)^2 = \sigma^2 L'VL + (X'L - p)'\beta\beta'(X'L - p) \quad \dots (6.1)$$

which involves both the unknown parameters σ^2 and β , and as it stands is not a practical criterion for minimising. Then we have the following possibilities:

(i) Choose an a priori value of $\sigma^{-2}\beta$, say b , based on previous knowledge and set-up the criterion as

$$S = L'VL + (X'L - p)'W(X'L - p) \quad \dots (6.2)$$

where $W = bb'$.

(ii) If β is considered to have an a priori distribution with $E(\beta\beta') = \sigma^2W$ where W is known, then, on taking expectation of the right hand side of (6.1) considering β as a random variable, the criterion for minimising is of the same form as (6.2) with a different definition of W .

For a given choice of W , we can minimise S to obtain L and compute the BLE of $p'\beta$. Theorem 6.1 contains the basic result. We shall denote the BLE of $p'\beta$, in the sense of minimising (6.2) by BLE (w).

Theorem 6.1: The BLE (W) of $p'\beta$ is $p'\tilde{\beta}$ where

$$\tilde{\beta} = W'X'(V+XW'X')^{-1}Y \quad \dots (6.3)$$

for any choice of the g -inverse.

The minimum value of S is attained when L satisfies the equation

$$(V+XW'X')L = XW'p$$

so that the optimum choice of L is $\{(V+XW'X')^{-1}XW'p\}$ giving the BLE (w)

$$LY = p'W'X'(V+XW'X')^{-1}Y = p'\tilde{\beta}$$

where $\tilde{\beta}$ is as defined in (6.3).

It may be noted that there is no restriction on the parametric function $p'\beta$ to be estimated in the case of BLE (w), while p must belong to $\mathcal{A}(X')$ in the case of BLUE.

It is of some interest to compare the mean square errors of BLE (w) and BLUE of estimable parametric functions. For this purpose we assume $R(V+XW'X') = R(V: X)$. Then from Theorem 5.1 it follows that the BLUE of $p'\beta$, when estimable is $p'\hat{\beta}$, where

$$\hat{\beta} = (X'T^{-1}X)^{-1}X'T^{-1}Y, \quad T = V+XW'X'. \quad \dots (6.4)$$

In fact, we have the interesting relationship

$$\tilde{\beta} = G\hat{\beta}, \quad \text{where } G = W'X'T^{-1}X. \quad \dots (6.5)$$

Now let $p = X'q$ in which case, the mean square error of $p'\tilde{\beta}$ is

$$E(q'X\tilde{\beta} - q'X\beta)^2 = E(q'XG\hat{\beta} - q'X\beta)^2 = q'Fq$$

where

$$F = XGDG'X' + X(G-I)\beta\beta'(G-I)X'$$

$$D = E(\hat{\beta} - \beta)(\hat{\beta} - \beta)'$$

Then mean square error of the BLUE of $p'\beta$ is

$$E(q'X\hat{\beta} - q'X\beta)^2 = q'XDX'q.$$

It is easily shown that the matrix $D - GDG'$ is n.n.d. in which case $XDX' - F$ is n.n.d. for a certain range of β depending on W . Thus if we have some knowledge of the domain in which β lies, we may be able to choose W in such a way that the BLE (w) is uniformly better than the BLUE for any estimable function. Further investigation in this direction such as the comparison of BLE (w) with ridge estimators of Hoerl and Kennard (1970a, 1970b) will be useful.

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7. BEST LINEAR MINIMUM BIAS ESTIMATION (BLIMBE)

Let us consider the GOM model $(Y, Y\beta, \sigma^2V)$. If there is deficiency in $R(X)$, then not all linear functions of β are unbiasedly estimable. Then we raise the following two questions.

- (i) What is the minimum restriction to be put on β so that every linear parametric function admits a LUE (linear unbiased estimator) and hence the BLUE?
- (ii) In what sense can we find the best linear minimum bias estimator (BLIMBE) of $p'\beta$ if it does not admit a LUE?

The answer to the first question is contained in Theorem 7.1.

Theorem 7.1. Let $R(X) = r < m$, the number of components of β . The minimum restriction on β can be expressed in the following alternative forms:

- (i) $R\beta = c$, $R(R) = m - r$, $R(X' : R') = m$.
- (ii) $\beta = \beta_0 + AY$, where A is any matrix such that $R(A) = R(X) = R(XA)$, and Y is arbitrary.
- (iii) $\beta = \beta_0 + TX'\delta$, where T is any matrix such that $R(XTX') = R(X)$ and δ is arbitrary.

The first restriction is obvious and the others can be deduced from the first. All these restrictions imply that β is confined to a hyperplane of dimension r .

To answer the second question we proceed as follows. The bias in $L'Y$ as an estimator of $p'\beta$ is $(L'X - p')\beta$. We say that $L'Y$ is a linear minimum bias estimator (LIMBE) of $p'\beta$ if L is such that $\|L'X - p'\|$, a suitably defined norm or semi-norm of the deviation $L'X - p'$ in E_m , m -dimensional Eutlidian space, is a minimum.

Theorem 7.2: Let the norm or semi-norm of vector u in E_m be defined by $\|u\| = (u'Mu)^{1/2}$ where M is n.n.d. Then $L'Y$ is a LIMBE of $p'\beta$ iff L satisfies the equation

$$XMX'L = XMp. \quad \dots (7.1)$$

The proof consists in equating the derivative of

$$(L'X - p')M(X'L - p) \quad \dots (7.2)$$

with respect to L to the null vector.

The LIMBE may not be unique, in which case we may choose L such that $V(L'Y) = \sigma^2L'VL$ is a minimum subject to the condition (7.1). The estimator $L'Y$ with such a choice of L is called BLIMBE.

Theorem 7.3: (a) Let

$$\begin{pmatrix} V & XMX' \\ XMX' & 0 \end{pmatrix}^{-1} = \begin{pmatrix} G_1 & G_2 \\ G_3 & G_4 \end{pmatrix}$$

Then the BLIMBE of $p'\beta$ is $p'\bar{\beta}$ where

$$\bar{\beta} = MX'G_4^{-1}Y. \quad \dots (7.3)$$

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(b) Let $(X')_{M}^{\dagger}$ be a V -norm M -least squares inverse of X' as defined in Rao and Mitra (1971). Then the BLUE of β' is $\beta' \bar{\beta}$ where

$$\bar{\beta} = \{(X')_{M}^{\dagger}\}' Y. \quad \dots (7.4)$$

The result (7.3) follows on the same lines as in Rao (1971, 1972b) and (7.4) by definition.

It may be noted that in Theorem 7.3, we have not made any assumption about the ranks of V , M and X .

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