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EQUALITY OF TWO BLUES AND RIDGE-TYPE ESTIMATES

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ABSTRACT

Equality is shown of the g-inverse and Moore-Penrose inverse representation of the BLUE in the general linear model. The proof is based on a matrix identity which allows also to establish a functional relationship between the BLUE and Ridge-type estimates.

1. INTRODUCTION

The present communication focuses on some computational properties of the matrices that appear in BLUE and Ridge-type estimation in linear model theory. In Section 3 we shortly define what now we loosely call Ridge-type estimates, for its statistical import, however, the reader is referred to Hoerl & Kennard (1970), Rao (1973, p.306), or Rolph (1976), the latter including many additional references. Procedures for mean estimation are also useful for the estimation of variance components, see Pukelsheim (1976).

Consider the general linear model

$$\mathfrak{E}Y = Xb, \quad \mathfrak{D}Y = \sigma^2 V^2, \tag{1}$$

where Y is an $\mathbb{R}^n$-valued random vector, X is a known real- $n \times p$ matrix, and V^2 is a known dispersion matrix written as the square of its unique nonnegative definite symmetric square root V. Interest concentrates on linear estimators $\hat{b}Y$ for the vector parameter b, and on appropriate justifications which $p \times n$ matrix $\hat{b}$ that is determining the estimator is to be chosen.

Section 2 deals with the g-inverse and the Moore-Penrose inverse representation of the BLUE. The class of all those matrices $\hat{b}$ leading to BLUEs $q'\hat{b}Y$ for all estimable linear forms $q'b$, $q \in \mathbb{R}^p$, has been given two different representations by Albert (1973, p.184):

$$X^+(I - V(MV)^+) + Z(M - MV(MV)^+), \quad M=I-XX^+, \tag{2}$$

and by Mitra & Moore (1973, p.141):

$$(X'(V^2 + XX')^- X)^- X'(V^2 + XX')^-. \tag{3}$$

The multiplicity is generated in (2) by the arbitrariness of the $p \times n$ matrix Z, and in (3) by the choice of the g-inverses. Mitra & Moore (1973, p.142) proved that

$$B := X^+(I - V(MV)^+) \tag{4}$$

is in the class (3); Proposition 1 below states more exactly that B is equal to the Moore-Penrose version in (3). Thus the naturally distinguished matrices in (2) and (3) coincide.

Section 3 turns to Ridge-type estimates since the term $X'(V^2 + XX')$ not only arises in BLUE theory as in (3) but is even more important for Ridge-type estimation, see Hoerl & Kennard (1970, p.57), Rao (1973, p.306), Rolph (1976, p.794). Proposition 2 shows how to compute the BLUE from Ridge-type estimates and vice versa; as a corollary we obtain various representations for Ridge-type estimates whose derivations follow easily from BLUE theory.

All proofs are collected in Section 4.

2. EQUALITY OF TWO BLUES

Proposition 1 proposes an answer to Albert's (1973, p.183) "question concerning the relationship between the matrices in (2) and (3)": Put Z = 0 in (2) and choose Moore-Penrose inverses in (3), and the resulting matrices are equal.

Proposition 1: $B = (X'(V^2 + XX')^+X)^+X'(V^2 + XX')^+$.

The proof is given in Section 4; its crucial step is the following matrix identity which follows from Cline's (1965, p.100) inverse for the sum of nonnegative definite matrices.

Lemma: $X'(V^2 + XX')^+ = (I + BV^2B')^{-1}B$.

Since the two terms in (2) are orthogonal with respect to the trace inner product of matrices, B is the shortest matrix in (2) and Proposition 1 has the

Corollary 1: $(X'(V^2 + XX')^+X)^+X'(V^2 + XX')^+$ is of minimum norm in the class (3) with respect to the Euclidean matrix norm.

In model (1) the variance component σ^2 is unknown; since, however, in $X^+(I - \sigma V(\sigma MV)^+)$ the σ cancels out, Proposition 1 gives rise to the further

Corollary 2: $B = (X'(\sigma^2V^2 + XX')^+X)^+(\ {}^2V^2 + XX')^+$ for all $\sigma^2>0$.

It is obvious from (2) that the BLUE admits a unique linear representation if and only if $Z(M - MV(MV)^*) = 0$ for all Z. But $M - MV(MV)^+$ orthogonally projects onto the intersection of the nullspaces of X' and V^2, which is the orthogonal complement of range X + range V^2, where range means column space. Thus we finally get the

Corollary 3: $B = (X'(V^2 + XX')^-X')^-X'(V^2 + XX')^-$ for all choices of g-inverses if and only if $V + XX'$ is nonsingular. In this case $(V^2 + XX')^- = (V^2 + XX')^{-1}$.

Corollary 3 rather states that in (3) the versions of the g-inverses are not, in general, negligible in order to have equality with B.

While the estimator $q'\hat{b}Y$ for $q'b$, with $\widehat{b}$ from (2), need not be unbiased for all $q\in\mathbb{R}^p$, it is always the minimum variance - minimum bias - linear estimator (MV-MB-LE) for $q'b$, see Rao (1973, p.307). Particularly when unbiasedness is not possible, one is interested in alternative estimation procedures.

3. RIDGE-TYPE ESTIMATES

In model (1) the mean square error of a linear estimator $\hat{q}'Y$ for $q'b$ is $\sigma^2\|V\hat{q}\|^2 + \|(X'\hat{q} - q)'b\|^2$, with maximum value $\sigma^2\|V\hat{q}\|^2 + \beta^2\|X'\hat{q} - q\|^2$ when the vector parameter b

varies subject to $\|b\| \leq \beta$. Minimizing the maximal mean square error on the ball $\|b\| \leq \beta$ thus leads to the problem of minimizing

$$k\|V\hat{q}\|^2 + \|X'\hat{q} - q\|^2, \quad k>0. \tag{5}$$

The resulting estimators are $q'b_k{*}Y$, where the defining equality for the p x n matrix $b_k{*}$ is, see Rao (1973, p.306),

$$b_k{*} \cdot (kV^2 + XX') = X'. \tag{6}$$

In the present communication we call, per definition, $b_k{*}Y$ Ridge-type estimate for b whenever $b_k{*}$ solves (6).

The general solution to (6) is $b_k{*} = X'(kV^2 + XX')^-$, and it follows from (3) that then $(b_k{*}X)^- b_k{*}Y$ is the MV-MB-LE for b, irrespective of the value of k. In particular, if $b_k{*} = X'(kV^2 + XX')^+$, then $(b_k{*}X)^+ b_k{*} = B$, by Proposition 1. Thus the MV-MB-LE may be computed when a Ridge-type estimate is given; Proposition 2 solves the converse problem.

<u>Proposition 2:</u> If $\hat{b}Y$ is a MV-MB-LE for b, i.e., $\hat{b}$ is representable as in (2), and if $k>0$, then $(I + k\hat{b}V^2\hat{b}')^{-1}\hat{b}Y$ is a Ridge-type estimator.

The proof follows from the Lemma and is given in Section 4. The functional relationship of $\hat{b}$ and $b_k{*}$ may be used to derive alternative representations for $b_k{*}$. The Aitken estimator $(X'V^{2+}X)^+X'V^{2+}Y$ is a MV-MB-LE if and only if range $X \subset$ range V^2, see Zyskind (1975, p.658). The reader will then easily verify the

<u>Corollary 4:</u> $(kI + (X'V^{2+}X)^{-1}X'V^{2+}Y$ is a Ridge-type estimate if and only if range X c range V^2.

The simple least squares estimator X^+Y is a MV-MB-LE if and only if range $V^2X \subset$ range X, see Zyskind (1975, p.684), hence

Corollary 5: $(I + kX^+V^2X^{+\prime})X^+Y$ is a Ridge-type estimate if and only if range $V^2X \subset$ range X.

If $V^2 = I$ then Corollaries 4 and 5 apply and yield the representations (2.1) and (2.3) in Hoerl & Kennard (1970, p.57). We are now left with proving the Lemma and Propositions 1 and 2.

4. PROOFS

First, we prove the Lemma. Inverting the sum $V^2 + XX'$ with Cline's formula (1965, p.100) and some computation yield

$$X'(V^2 + XX')^+ = (I - BVKVX^{+\prime})\cdot B \;, \quad K = (I + VB'BV)^{-1}. \quad (7)$$

Now, $BVK = (I + BV^2B')^{-1}BV$, and $BV^2(VM)^+ = X^+V(I - (MV)^+MV)\cdot VM(VM)^+ = 0$. Hence

$$\begin{aligned} I - BVK\cdot VX^{+\prime} &= I - (I + BV^2B')^{-1}BV\cdot V\cdot(I - (VM)^+V + (VM)^+V)\cdot X^{+\prime} \\ &= I - (I + BV^2B')^{-1}(BV^2B' + 0 + I - I) \\ &= (I + BV^2B')^{-1}. \end{aligned} \quad (8)$$

The Lemma is then established by inserting (8) into (7).

Next, we prove Proposition 1. Clearly, $BX = X^+X$, and $B=X^+XB$. Using the Lemma, we obtain

$$\begin{aligned} &(X'(V^2 + XX')^+X)^+X'(V^2 + XX')^+ \\ &\quad = ((I + BV^2B')^{-1}BX)^+(I + BV^2B')^{-1}B \\ &\quad = ((I + BV^2B')^{-1}X^+X)^+((I + BV^2B')^{-1}X^+X)\cdot B. \end{aligned}$$

Since the ranges of $X^+X(I + BV^2B')^{-1}$ and X^+X coincide, so do their projectors. Thus the last equalities may be continued $= X^+XB = B$, establishing Proposition 1.

Finally, we prove Proposition 2. The Lemma implies

$$(I + k\,\hat{b}V^2\hat{b}')^{-1}\hat{b} = (I + k\,BV^2B')^{-1}B + Z(M - MV(MV)^+)$$
$$= X'(k\,V^2 + XX')^+ + Z(M - MV(MV)^+),$$

and postmultiplication with $kV^2 + XX'$ yields X', and Proposition 2 is established.

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BIBLIOGRAPHY

Albert, A. (1973). The Gauss-Markov theorem for regression models with possibly singular covariances. SIAM J. Appl. Math. 24, 182–87.

Cline, R.E. (1965). Representations for the generalized inverse of sums of matrices. SIAM J. Numer. Anal. 2, 99–114.

Hoerl, A.E. and Kennard, R.W. (1970). Ridge regression: biased estimation for nonorthogonal problems. Technometrics 12, 55–67.

Mitra, S.K. and Moore, B.J. (1973). Gauss-Markov estimation with an incorrect dispersion matrix. Sankhyā A 35, 139–52.

Pukelsheim, F. (1976). Estimating variance components in linear models. J. Multivariate Anal. 6, 626–29.

Rao, C.R. (1973). Linear Statistical Inference and Its Applications (2nd ed.). New York: John Wiley and Sons, Inc.

Rolph, J.E. (1976). Choosing shrinkage estimators for regression problems. Commun. Statist. A 5, 789–802.

Zyskind, G. (1975). Error structures, projections and conditional inverses in linear model theory. In A Survey of Statistical Design and Linear Models (J.N. Srivastava, Ed.). Amsterdam: North-Holland Publ. Co., pp. 647–63.

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