〈Research Paper〉

Journal of the Korean
Statistical Society
Vol. 18, No.1, 1989

An Efficient Method for Computing MINQUE Estimators in the Mixed Models

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ABSTRACT

An efficient method for computing minimum norm quadratic unbiased estimates (MINQUE) of variance components in the mixed model is developed. This computing algorithm which used W-matrix saves both storage usage and computing time.

1. Introduction

An important procedure, minimum norm quadratic unbiased estimation (MINQUE) developed by Rao, C.R.(1973) provides a unified approach to variance component estimation in the mixed model. His principle of MINQUE is formulated through justifiable theoretical and applied considerations. The universality of the MINQUE method as described in Rao and Kleffe (1980) and in this article arises from the following advantages:

(a) It involves no normality assumptions as do maximum likelihood (ML) method and restricted maximum likelihood(REML) method.

(b) The equations that yield MINQUE do not have to be solved iteratively.

(c) It offers a wide scope in the choice of the norm depending on the nature of the model and prior information available.

(d) The method is applicable in situations where ML and REML fail.

(e) The ML and REML estimators can be exhibited as iterated versions of MINQUE's.

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(f) For a suitable choice of the norm, the MINQUE estimators provide minimum variance estimators when y is normally distributed.

However, MINQUE users may have hesitation because it contains numerous multipliations and inversions on N × N matrix, where N is the number of observations. For the general mixed model, Liu and Senturia(1977) reduced the computational load to the problem which requires the inversion of a smaller m × m matrix, where m is the total number of random levels in the mixed model. Also Wansbeek(1980) proved that the MINQUE computation in the mixed model can be computed in O(N) time by using the regression interpretation. His interpretation of the intermediate steps as regression residuals suggested that a computation procedure that was more straightforward and simpler to program than Liu and Senturia's method. Later, Giesbrecht(1983) handled this difficulty as modification of the W transformation which requires a series of sweep operations. In the case in which cell replications exists, Kaplan(1983) further demonstrated potential improvement. While these articles may be an appreciable reduction, the potential users still face disheartening prospect of having to invert an m ×m matrix when m is too large.

The purpose of this thesis is to provide more efficient algorithm than any other algorithm related to W-matrix for the MINQUE procedure. We give here a new approach based on Lee and Kim(1988) as an extension of Kaplan's work(1983).

2. The Estimator of MINQUE

The basic model we shall use in the mixed model analysis of variance is the one given by Hartley and Rao(1967). It can be written as

$$y = X\alpha + Z_1 b_1 + Z_2 b_2 + \cdots + Z_c b_c + e \tag{2.1}$$

where

y is a vector of N observations;

α is a vector of k unknown constants, the fixed effects of the model;

X is an N × k incidence matrix of full column rank, corresponding to α;

Z_i is an N × m_i design matrix associated with the i-th random factor;

b_i is a vector of m_i variables, $i = 1,2,\cdots,c$;

e is an N × 1 vector of independent variables from $N(0, \sigma_0^2)$.

Suppose we wish to find the MINQUE of

$$L = p_0\sigma_0^2 + p_1\sigma_1^2 + \cdots + p_c\sigma_c^2, \tag{2.2}$$

the following procedure may be utilized (Kshirsagar 1983).
Step 1. Find $H_i = Z_i Z_i'$ $(i=0,1,\cdots,c)$ $Z_0 = I_N$.
Step 2. Find $H = \sum_{i=0}^{c} H_i$, $R = H^{-1} - H^{-1}X(X'H^{-1}X)^{-1}X'H^{-1}$.
Step 3. Find $s_{ij} = tr(RH_iRH_j)$, for all $i,j = 0,1,\cdots c$. Find $S = (s_{ij})$.
Step 4. Find $q_i = y'RH_iRy, i = 0,1\cdots,c$, and set $\underline{q}$ = vector of the q_i's.
Step 5. Find the solution of the equations $S\underline{\gamma} = \underline{q}$,

$$\text{where } \underline{\gamma}' = [\hat{\sigma}_0^2, \hat{\sigma}_1^2, \cdots, \hat{\sigma}_c^2] .$$

These are the MINQUEs of the individual variance components $\sigma_0^2, \sigma_1^2, \cdots, \sigma_c^2$.
Step 6. Replace σ_i^2 by its MINQUE $\hat{\sigma}_i^2$ in the linear function (2.2) to be estimated to get the MINQUE of L.

We shall now present a new procedure for the computation of MINQUE . From the main result by Lee and Kim(1988), we know that only necessary informations in forming W-matrix are knowing balanced matrices X_0, Z_0(i.e. there were one and only one observation in each cell), $\bar{y}$ which is the vector of cell means, e'e which is the error sum of squares, and diagonal matrix D containing the number of observations in each cell. The essence of this paper is using this result. Therefore the calculation related to the $N \times N$ inverse matrix H^{-1} will be treated as the calculation of the $n \times n$ matrix, where n is the number of nonempty cells. Obviously, n is smaller than m for crossed design with all interaction terms present, for nested designs, and for designs with many empty cells. But there exist designs, for example, which are additive or include only low-order interaction factors and that have few empty cells, whose m is much smaller than n. In this case, with assistance of matrix identity, the method can be transformed as the scheme of inverting $m \times m$ matrix, still using the balanced structure of matrix and vector. Thus, the present method reduces the computational requirements of MINQUE to a manageable level for many cases.

3. The MINQUE Procedure

When we copmare the unbalanced design matrices X and Z, where $Z = [Z_1 | Z_2 | \cdots | Z_c]$ to the balanced matrices X_0 and Z_0, respectively, then the matrices X and Z can be written as a product $X = TX_0$ and $Z = TZ_0$, where T is a replications matrix (See Kaplan (1983) or Lee and Kim(1988)). Also the matrix of cell frequencies D can be obtained as $D = T'T$. For example, in a two-way additive random effects model

$$y_{ijk} = \mu + \alpha_i + \beta_j + e_{ijk}$$

$$i=1,\cdots,I;\quad j=1,\cdots,J;\quad k=1,2,\cdots,n_i$$

with $I=2$, $J=2$, $n_{11}=n_{21}=2$, $n_{12}=3$, $n_{22}=1$, and the observations listed in the usual order $y'=(y_{111}, y_{112}, y_{121}, y_{122}, y_{123}, \cdots, y_{221})$, we would have

$$Z_1=\begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \qquad Z_2=\begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$Z_{01}=\begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \qquad Z_{02}=\begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$T=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad D=\begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

For the purpose of deriving necessary submatrices in MINQUE procedure, the following lemmas are needed (see Lee and Kim(1988) for the detailed derivations for these lemmas).

Lemma 1. $T'H^{-1}T=(I+DZ_0Z_0')^{-1}D.$ (3.1)

Lemma 2. $XH^{-1}X=X_0MX_0$, where $M=(I+DZ_0Z_0')^{-1}D.$ (3.2)

Lemma 3. $Z'H^{-1}y = Z_0'M\bar{y}$. (3.3)

Lemma 4. $y'H^{-1}y = \bar{y}'M\bar{y} + e'e$. (3.4)

The following definitions of matrices are introduced for the simplicity of computation in MINQUE procedure.

$$B = (I+DZ_0Z_0')^{-1},\ C = B',\ M = BD,$$
$$J = (X_0'MX_0)^{-1},\ P = X_0JX_0'M,\ A = I-P,\ K = MA, \quad (3.5)$$
$$L = (CA)^2,\ V = A'BK,\ F = DL.$$

Define now the following matrix operators:

$$S1(A,B) = A'KB, \quad S2(A,B) = A'VB,$$
$$Q1(A,B) = S1(A,B), \quad Q2(A,B) = A'FB + e'e. \quad (3.6)$$

Now we can obtain the MINQUE estimators by use of above notations.

Result 1. The component s_{ij} for all $i,j = 1,2,\cdots,c$ is given by $s_{ij} = tr\{S1(Z_{0i}, Z_{0j})S1(Z_{0i}, Z_{0i})\}$ and s_{i0} for $i = 1,2,\cdots$ c is given by $s_{i0} = tr\{S2(Z_{0i}, Z_{0i})\}$. Also s_{00} is given by $s_{00} = tr(L) + N - n$.

Result 2. The element q_i for $i = 1,2,\cdots,c$ is given by $q_i = Q1(\bar{y},Z_{0i})Q1(Z_{0i},\bar{y})$ and q_0 is given by $q_0 = Q2(\bar{y},\bar{y})$.

The detailed explanation for these derivations is given in the Appendix. If we obtain the matrix S and the vector q, then we have only to solve the linear system $S\underline{\gamma} = \underline{q}$.

4. Conclusions

It has been shown that MINQUE algorithm developed herein needs the inversion of an $n \times n$ matrix, y, and e'e. Clearly, when n is small with respect to m, for example, the designs that are crossed designs with all interaction terms present, this algorithm will yield a considerable reduction in computational cost and effort. Conversely, if m is smaller than n, for instance, the design that are additive, Liu and Senturia's method seems to be superior to our procedure. In this point, Kaplan(1983) could not give a valid explanation. However, as shown by Lee Kim(1988), an $n \times n$ martix can be converted as a expression contained an $m \times m$ matrix. For example. the matrix B becomes $B=(I+DZ_0Z_0')^{-1}=I-DZ_0(I+Z_0'DZ_0)^{-1}Z_0'$ by help of well-known matrix identity: $(I+ST)^{-1} = I-S(I+TS)^{-1}T$. We see that $(I+DZ_0Z'_0)^{-1}$ is an $n \times n$ matrix and $(I+Z'_0DZ_0)^{-1}$ is an $m \times m$ matrix. Therefore, we also provide the advantage of using $\bar{y}$ and $e'e$ still using the inversion of an $m \times m$ matrix.

ACKNOWLEDGEMENTS

The authors wish to thank the referees for their helpful suggestions.

Appoendix

A. Derivation of Result 1

(1) The matrix S whose ij–th elements are

$$s_{ij} = \mathrm{tr}\{S1(Z_{0i},Z_{0j})S1(Z_{0j},Z_{0i})\} \text{ for all } i,j = 1,2,\cdots,c.$$

Proof. Note that

$$\begin{aligned} T'RT &= T'(H^{-1}-H^{-1}X(X'H^{-1}X)^{-1}X'H^{-1})T \\ &= M(I-X_0(X'_0MX_0)^{-1}X'_0M) \\ &= K. \end{aligned}$$

Then
$$\begin{aligned} s_{ij} &= \mathrm{tr}(RH_iRH_j) \\ &= \mathrm{tr}(Z'_iRZ_jZ'_jRZ_i) \\ &= \mathrm{tr}(Z'_{0i}T'RTZ_{0j}Z'_{0j}T'RTZ_{0i}) \\ &= \mathrm{tr}(Z'_{0i}KZ_{0j}Z'_{0j}KZ_{0i}) \\ &= \mathrm{tr}\{S1(Z_{0i},Z_{0j})S1(Z_{0j},Z_{0i})\}. \quad \blacksquare \end{aligned}$$

(2) The matrix S whose $i0$-th elements are

$$s_{i0} = \mathrm{tr}\{S2(Z_{0i},Z_{0i})\} \quad \text{for } i = 1,2,\cdots,c.$$

Proof. Observing that

$$\begin{aligned} T'H^{-1} &= T'(I-TZ_0Z'_0(I+DZ_0Z'_0)^{-1}T') \\ &= (I-DZ_0Z'_0(I+DZ_0Z'_0)^{-1})T' \\ &= (I+DZ_0Z'_0)^{-1}T' \end{aligned}$$

and

$$\begin{aligned} T'R &= T'(H^{-1} - H^{-1}TX_0(X_0'MX_0)^{-1}X_0'T'H^{-1}) \\ &= (I - MX_0(X_0'MX_0)^{-1}X_0')T'H^{-1} \\ &= A'BT'. \end{aligned}$$

Then

$$\begin{aligned} s_{i0} &= tr(RH_iRH_0) \\ &= tr(RZ_iZ_i'R) \\ &= tr(Z_{0i}'T'RRTZ_{0i}) \\ &= tr(Z_{0i}'A'BDB'A\ Z_{0i}) \\ &= tr(Z_{0i}'A'BMA\ Z_{0i}) \text{ using } M = DB' \\ &= tr(Z_{0i}'A'BKZ_{0i}) \\ &= tr(Z_{0i}'VZ_{0i}) \\ &= tr\{S2(Z_{0i}, Z_{0i})\}. \quad \blacksquare \end{aligned}$$

(3) The 00-th element of S is

$$s_{00} = tr(L) + N - n.$$

Proof. Use the fact that

$$\begin{aligned} R &= H^{-1} - H^{-1}TX_0JX_0'T'H^{-1} \\ &= I - T(Z_0Z_0' + B'X_0JX_0')BT'. \end{aligned}$$

Then, $s_{00} = tr(RR) = tr(L) + N - n$ from the definition of L. $\blacksquare$

B. Derivation of Result 2

(4) The elements of q_i for $i = 1, 2, \cdots, c$ are given by

$$q_i = Q1(y, Z_{0i})Q1(Z_{0i}\bar{y}).$$

Proof.

$$\begin{aligned} y'RZ_i &= y'(H^{-1} - H^{-1}TX_0JX_0'T'H^{-1})TZ_{0i} \\ &= y'H^{-1}T(I - X_0JX_0'M)Z_{0i} \\ &= y'TB'AZ_{0i} \\ &= \bar{y}'DB'AZ_{0i} \\ &= \bar{y}'KZ_{0i}. \end{aligned}$$

Then (4) is established. ■

(5) The element q_0 is $q_0 = Q_2(\bar{y},\bar{y})$.

Proof. For the simplicity of notation,

let $E = Z_0Z_0' + B'X_0JX_0'$.

Then
$$\begin{aligned} q_0 &= y'RRy \\ &= y'(I-TEBT')^2y \\ &= y'(I-2TEBT')y + y'(TEBDEBT')y \\ &= \bar{y}'D\bar{y} + e'e - 2\bar{y}'DEBD\bar{y} + \bar{y}'D(EBD)^2\bar{y} \\ &= \bar{y}'D(I-EBD)^2\bar{y} + e'e \\ &= Q2(\bar{y},\bar{y}). \end{aligned}$$
■

References

(1) Corbeil, R. R., and Searle, S. R.(1976). Restricted maximum likelihood(REML) estimation of variance components in the mixed model, *Technometrics*, Vol. 18,31-38.

(2) Giesbrecht, F. G.(1983). An efficient procedure for computing MINQUE of variance components and generalized least squares estimates of fixed effects, *Communications in Statistics—Theory and Methods.*, Vol. 12(18), 2169—2177.

(3) Hartley, H.O., and Rao, J.N.K(1967). Maximum likelihood estimation for the mixed analysis of variance model, *Biometrika,* Vol. 54,93-108.

(4) Harville, D. A.(1977). Maximum likelihood approaches to variance component estimation and to realted problems,
Journal of the American Statistical Association, Vol. 72, 320-340.

(5) Hemmerle, W.J., and Hartley, H.O.(1973). Computing maximum likelihood estimates for the mixed A.O.V. model using the *W* transformation, *Technometrics,* Vol. 15, 81 9-831.

(6) Kaplan, J.S.(1983). A method for calculating MINQUE estimators of variance components, *Journal of the American Statistical Association,* Vol. 78, 476-477.

(7) Kennedy, W.J., and Gentle, J.E.(1980). *Statistical Computing,* Marcel Dekker, Inc.

(8) Kshirsagar, A.M.(1983). *A Course in Linear Models,* New York, Marcel Dekker, Inc.

(9) Lee, J.T., and Kim, B.C.(1988). A new approach for the W-matrix, *Journal of Statistical Computation and Simulation* Vol. 29, 241-254.

(10) Liu, Lon-Mu, and Senturia, Jerome.(1977). Computation of MINQUE variance component estimators, *Journal of the American Statistical Association,* Vol. 72, 867-8 68.

(11) Searle, S.R.(1979). Notes on variance component estimation : A detailed account of maximum likelihood and kindred methodology. Report Number BU-673M, Biometric Unit. Ithaca, New York : Cornell University Press.

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

(13) Rao, C.R., and Kleffe, J.(1980). Estimation of variance components. *Handbook of Statistics,* Vol.1, North Holland, 1-40.

(14) Wansbeek, T.(1980). A regression interpreation of the computation of MINQUE variance component estimates, *Journal of the American Statistical Association,* Vol. 75, 375-376.