Computational Algorithm for the MINQUE and its Dispersion Matrix

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Abstract

The development of Minimum Norm Quadratic Unbiased Estimation (MINQUE) has introduced a unified approach for the estimation of variance components in general linear models. The computational problem has been studied by Liu and Senturia(1977) and Goodnight (1978, setting a-priori values to 0). This paper further simplifies the computation and gives efficient and compact computational algorithm for the MINQUE and dispersion matrix in general linear random model. Keywords: Δ-matrix, computational algorithm, variance components, MINQUE, linear random model, dispersion matrix, a-priori weights.

1. Introduction and Problem Formulation.

The traditional analysis of variance method and its modifications for the estimation of variance components have their origin from ad-hoc procedures and have few optimum properties if the design is unbalanced. Recently many papers have been devoted to the computational problems of maximum likelihood estimator (MLE) and restricted MLE (REMLE) of the variance components for general linear model (see Harville, 1977 for example), however relatively few for MINQUE. MINQUE is powerfull in that the method is a unified approach and the estimates are relatively insensitive to the a-priori values. Several modifications have been suggested (see P.S.S.R. Rao, 1975 for example), and some of them were derived because of computational complexities. This problem was considerably alleviated by the work of Liu and Senturia (1977). Consider the following general linear random model;

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$$Y = 1\mu + X^*_1\alpha_1 + \cdots + X^*_k\alpha_k + \epsilon \tag{1.1}$$

where Y is a $(n+1)$ vector of responses, 1 is a $(n+1)$ vector of 1's, μ is overall mean, X_i^* is given $(n+1)\times m_i$ matrix, α_i is m_i-vector of uncorrelated random variable with mean 0 and variance σ_i^2, ϵ is a vector of error component with mean 0 and variance σ^2, and finally all the components are uncorrelated.

Let C donote a $n\times(n+1)$ complete set of orthogonal contrast such that $C\,1=0$, $CC'=I_n$ Then $C'C=I-J/(n+1)$ where $J=1.1'$. Multiplying C to both sides cf (1.1) yields

$$Z = CY = X(\alpha_{-1} : \alpha_{-2} : \cdots : \alpha_{-k}) + C\epsilon \tag{1.2}$$

where $X_{n\times m} = C(X_1^* : \cdots X_k^*) = CX^*$, $m = \sum_1^k m_i$

Expectation and variance of the model (1.2), then is

$$E(Z) = 0$$

$$V(X) = \sigma_\cdot^2(I + \sum^k \rho_i V_i) = \sigma_\cdot^2 H \tag{1.3}$$

where $V_i = CX_iX_i'C'$, and $\rho_i = \sigma_i^2/\sigma_\cdot^2$

It can be shown that (Rao, 1971) MINQUE of the model (1.1) is equivalent to that of the model (1.2) and is obtained by solving the following systems of linear equations with respect to

$$\sigma' = (\sigma_1^2, \sigma_2^2, \cdots, \sigma_k^2, \sigma_\cdot^2),$$

$$S\sigma = u,$$

where S is $(k+1)$ dimensional symmetric matrix with its (i, j) th elements as

$\operatorname{tr}(RV_iRV_j)$, and n dimensional symmetric matrix

$$R = (I + r_1V_1 + \cdots + r_kV_k)^{-1},$$

and $k+1$ vector

$u = Z'RV_iRZ$ with $V_{k+1} = I$

and finally r_i is the a-priori weight of ρ_i

It will be assumed throughout that MINQUE is estimable or S is invertible. Also R is assumed to be determined uniquely.

2. Computational Algorithm of MINQUE

Let D_t denote a $m\times m$ diagonal matrix such as

$$D_t = \begin{bmatrix} t_1I_{m_1} & & \\ & t_iI_{m_i} & \\ & & t_kI_{m_k} \end{bmatrix} \tag{2.1}$$

for any choice of k-vector $t=(t_1, t_2, \cdots\cdots, t_k)$, Further i or j subscripted to D, let it be the diagonal matrix with i th or j th subdiagonal elements equal to 1 and all other elements equal to 0.

With the above convention, we have

$$V_i=XD_iX'$$
$$H=I+XD_\rho X' \quad (2.2)$$
$$R=(I+XD_rX')^{-1},$$

where ρ and r are k-vectors with their elements ρ_i and r_i respectively. From Rao (1973, p. 33), the following holds.

$$R=I-X(D_r^{-1}+X'X)^{-1}\ X' \quad (2.4)$$

For conveniency, let P be $m\times m$ matrix $(D_r^{-1}+X'X)^{-1}$ and let P_{ij} be $m_i\times m_j$ submatrix of P such that

$$P=\{P_{ij}\},\ i,j=1,2,\cdots,k.$$

Then $R=I-XPX'$ (2.5)

Hereafter $\sum_i^k$ will be used instead of $\sum_{i=1}^{k}$

Lemma 1

i) $X'XP=I_m-D_r^{-1}\ P$

ii) $\mathrm{tr}(R)=n-m-\sum_i^k\ \mathrm{tr}(P_{ii})/r_i$

iii) $X'RX=X'XPD_r^{-1}=D_r^{-1}PX'X=D_r^{-1}-D_r^{-1}\ PD_r^{-1}$

iv) $R(I+XD_tX')=I+XP\Delta_tX'$, where $\Delta_t=(D_t-D_r)D_r^{-1}$ for any t appropriately defined and $\mathrm{tr}(A)$ denotes the trace of a square matrix A.

Proof

i) $X'XP=(-D_r^{-1}+D_r^{-1}+X'X)P=I_m-D_r^{-1}P$ from the definition of P.

ii) $\mathrm{tr}(R)=\mathrm{tr}(I_n-XPX')=n-\mathrm{tr}(X'XP)=n-m+\sum_i^kP_{ii}/r_i$

iii) $X'RX=X'(I-XPX')=X'X-X'XPX'X=X'X(I-PX'X)=X'XPD_r^{-1}$ from i).

iv) $R(I+XD_tX')=I-XPX'+RXD_tX'$

$RX=(I-XPX')X=X-XPX'X=XPD_r^{-1}$ from i)

Hence $RXD_tX'-XPX'=XPD_r^{-1}D_tX'-XPX'=XPD_r^{-1}(D_t-D_r)X=XP\Delta_tX'$ and the result follows.

Using the above lemma, we have the the following expressions for the elements of S-matrix and u-vector.

$$s_{ij}=\mathrm{tr}(RV_iRV_j),\ \text{for } i,j=1,2,\cdots,\ k$$

$$=\mathrm{tr}[D_i(I-PD_r^{-1})D_j(I-PD_r^{-1})]/r_ir_j \text{ from iii)}$$
$$=\mathrm{tr}[D_{ij}-PD_r^{-1}D_{ji}-PD_r^{-1}D_{ij}+D_iPD_r^{-1}D_jPD_r^{-1}]/r_ir_j$$

where $D_{ij}=D_iD_j=\begin{cases}\phi, & \text{if } i\neq j\\ I_{mi}, & \text{if } i=j\end{cases}$

Letting $||A||$ denote the sums of square for all the elements of matrix A, the following results can be oftained for $i,j=1.2.\cdots k$.

$$s_{ij}=\begin{cases}||P_{ij}||\ r_ir_j, & \text{if } i\neq j\\ [m_i-\frac{2}{r_i}\mathrm{tr}(P_{ii})+\frac{1}{r_i^2}||P_{ii}||]/r_i^2, & \text{if } i=j\end{cases} \tag{2.8}$$

$$s_{i,k+1}=\mathrm{tr}(RV_iR), \text{ for } i=1,2,\cdots, k$$
$$=\mathrm{tr}\ RV_iR(R^{-1}-\textstyle\sum_j^k r_jV_j)$$
$$=\mathrm{tr}(RV_i)-\textstyle\sum_j^k r_js_{ij}$$
$$=\mathrm{tr}(D_iX'RXD_i)-\textstyle\sum_j^k r_js_{ij}$$
$$=m_i/r_i-\mathrm{tr}(P_{ii})/r_i^2-\textstyle\sum_i^k r_js_{ij} \text{ from iii)} \tag{2.9}$$

$$s_{k+1,k+1}=\mathrm{tr}(RR)$$
$$=\mathrm{tr}[R(R^{-1}-\textstyle\sum_j^k r_jV_j)R]$$
$$=\mathrm{tr}(R)-\textstyle\sum_j^k r_jS_{j,k+1}$$
$$=n-m-\textstyle\sum_j^k\mathrm{tr}(P_{jj})/r_j-\sum_j^k r_jS_{i,k+1} \tag{2.10}$$

$$u_i=Z'RV_iRZ, \text{ for } i=1,2,\cdots, k$$
$$=Z'RXD_iX'RZ$$
$$=Z'XPD_iPX'Z/r_i^2, \text{ from iii)} \tag{2.11}$$

$$u_{k+1}=Z'RRZ$$
$$=Z'R(R^{-1}-\textstyle\sum_j^k r_jV_j)RZ$$
$$=Z'RZ-\textstyle\sum_j^k r_ju_j$$
$$=Z'Z-Z'XPX'Z-\textstyle\sum_j^k r_ju_j \tag{2.12}$$

Finally $Z'Z$, $Z'X$, $X'X$ can be obtained from the mean adjusted sums of square matrix usually calculated for normal equation.

Summarizing the above, MINQUE computation of the model (1.1) proceeds as in the following.

i) Compute $m+1$ dimensional mean adjusted sums of square matrix

$$\begin{bmatrix}Z'Z & Z'X\\ \text{Symm} & X'X\end{bmatrix}$$

ii) Determine the a-priori values, r, and compute $m\times m$ matrix

$$P=(D_r^{-1}+X'X)^{-1}$$

iii) Follow (2.8) through (2.12) to obtain S and u

iv) Obtain MINQUE by solving $S\sigma=u$.

It can easily be observed from above that once mean adjusted sums of square matrix in step (i) and the inversion of a $m\times m$ symmetric matrix is obtained, S matrix and u-vector needs number of multiplications proportional to m^2.

3. Dispersion matrix of MINQUE

For derivation of dispersion matrix of MINQUE, normality is assumed, and since MINQUE is unbiased regardless of the a-priori values, variance of the estimator is mean square error.

Rewrite $S\sigma=u$ of (1.4) as

$$\sigma=S^{-1}u=Z'A_iZ \tag{3.1}$$

where $A_i=\sum_j^{k+1}s^{ij}RV_jR$

$$=s^{i,k+1}R(I+XD_{si}X')R, \text{ for } i=1,2,\cdots,k \tag{3.2}$$

and s_i subscripted to D-matrix is k vector with j th element $s^{ij}/s^{i,k+1}$ and s^{ij} is (i,j) th element of S^{-1}

Using the result of Searle (1971, p.55), variance of the statistic in (3.1) becomes

$$V(\sigma)=2\sigma^4\mathrm{tr}(A_iHA_jH), \text{ for } i,j=1,2,\cdots k+1$$

Now tr (A_iHA_jH)

$$=(s^{i,k+1}s^{j,k+1})\mathrm{tr}[R(I+XD_{sj}X')RHR(I+XD_pX')RH] \tag{3.3}$$

The quantity inside the trace is equal to

$$(I+XP\Delta_{si}X')\ (I+P\Delta_pX')\ (I+XP\Delta_{si}X')\ (I+XP\Delta_pX')$$

using iv) of lemma 1. Applying the property that the trace is invariant under the cyclic permutation of the operand matrices, the following lemma holds.

Lemma 2

The (i,j) th element of the dispersion matrix of MINQUE for the model (1.1) is

$$2\sigma^4s^{i,k+1}s^{j,k+1}[n-m+\mathrm{tr}(T_iT_pT_jT_p)]$$

where T_i and T_p are $m\times m$ matrices such as

$$T_p=I+X'XP\Delta_p=I+(I-D_r^{-1}P)\Delta_p \text{ and}$$

$$T_i=I+X'XP\Delta s_i=I+(I-D_r^{-1}P)\Delta s_i,$$

for $i,j=1,2,\cdots k+1$

4. Conclusions

It has been shown that MINQUE algorithm developed herein needs number of multiplications proportional to the square of total number of levels once the mean adjusted sums of suquares for the response and design matrix and the inversion of $m \times m$ symmetric matrix is obtained. As the studies by Hess (1979), Huh and Webster (1981) suggests, MINQUE could yield sensitive estimates if the weights of the a-priori values are under-estimated. Hence the suggestions of the a-priori values equal to 1 (Rao, 1972), or equal to 0 (Goodnight, 1978) could yield bad estimates. The properties of the MINQUE could be further investigated utilizing the algorithm on the dispersion matrix developed.

REFERENCES

(1) Goodnight, J.H. (1978). Computing MIVQUEO estimates of variance components. SAS Technical Report, SAS Institute Inc., Cary, NC.

(2) Harville, D.A. (1977). Maximum likelihood approaches to variance component estimation and to related problems (invited paper). *Journal of the American Statistical Association,* 77.

(3) Hess, J.L. (1979). Sensitivity of MINQUE with respect to a priori weights. *Biometrics.* 35, 645-649.

(4) Huh, M.Y. and Webster, J.T. (1981). Sensitivty of MINQUE in the two-way classification. submitted for publication to *Technometrics.*

(5) Liu, L.M. and Senturia, Jerome (1977). Computation of MINQUE variance component estimates. *Journal of the American Statistical Association,* 72, 867-868

(6) Rao, C.R. (1971). Estimation of variance and covariance components-MINQUE theory. *Journal of Multivariate Analysis,* 1, 257-275.

(7) Rao, C.R. (1972). Estimation of variance and covariance components in linear modelr. *Journal of the American Statistical Association,* 67, 112-115.

(8) Rao, C.R. (1973). *Linear Statistical Inference and its Applicatinns,* John Wiley and Sons 33.

(9) Rao, P.S.S.R. (1975). Theory of MINQUE-Review. Discussion paper no. 118. Indian Statistical Institue, New Delhi.

(10) Searle, S.R.(1971). *Linear Models,* John Wiley and Sons, 55.