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ORIGINAL ARTICLE

Quadratic estimators of covariance components in a multivariate mixed linear model

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Abstract It is known that the Henderson Method III (Biometrics 9:226–252, 1953) is of special interest for the mixed linear models because the estimators of the variance components are unaffected by the parameters of the fixed factor (or factors). This article deals with generalizations and minor extensions of the results obtained for the univariate linear models. A MANOVA mixed model is presented in a convenient form and the covariance components estimators are given on finite dimensional linear spaces. The results use both the usual parametric representations and the coordinate-free approach of Kruskal (Ann Math Statist 39:70–75, 1968) and Eaton (Ann Math Statist 41:528–538, 1970). The normal equations are generalized and it is given a necessary and sufficient condition for the existence of quadratic unbiased estimators for covariance components in the considered model.

Keywords Linear operator · Orthogonal projection · Quadratic form · Generalized least squares estimator · Estimable parametric function

1 Introduction

The purpose of this article is to extend the Henderson Method III (based on the fitting constants method) to multivariate mixed linear models in order to obtain quadratic unbiased estimators for covariance components.

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The study of variance components estimation in univariate linear models has been of interest to statisticians for the last six decades: Henderson (1953) proposed three methods for obtaining unbiased estimates of variance components; Zyskind (1967) gave necessary and sufficient conditions for ordinary least squares estimators (OLSE) to be best linear unbiased estimators (BLUE); Rao (1971a,b, 1976) developed minimum norm quadratic unbiased estimators (MINQUE) and minimum variance quadratic unbiased estimators (MIVQUE) for variance components; Hultquist and Atzinger (1972) obtained MIVQUE for parameters of the fixed effects and variance components. Complete surveys of MIVQUE, LSE, maximum likelihood estimators (MLE) and BLUE for parameters in linear models were presented by Kleffe (1977), Rao and Kleffe (1988) and Robinson (1991). Watson (1967) and Milliken (1971) treated algebraically the generalized least squares estimators (GLSE) of regression parameters. Olsen et al. (1976) obtained a minimal complete class of invariant quadratic unbiased estimators for two variance components. Klonecki and Zontek (1992) provided a method of constructing admissible biased non-negative estimators of variance components in unbalanced models.

The GLSE and MLE were obtained for parameters of some multivariate mixed linear models: Biorn (2004) provided that GLSE can be interpreted as a matrix weighted average of a group of GLSE where the weights are the inverse of their covariance matrices; Cossette and Luong (2003) used GLSE of covariance components for constructing Bayes estimators; Calvin and Dykstra (1991), and Bates and DebRoy (2004) used MLE or restricted MLE as iterative algorithms in which some steps were expressed as GLS problems. Beganu (1987a,b, 1992) obtained Gauss–Markov estimators of regression coefficients and covariance components for a multivariate mixed linear model in the balanced case.

The methods of estimation of covariance components in univariate linear models can also be employed in the multivariate corresponding models, but the implementation and computational techniques are very hard to use.

Therefore it is convenient that the multivariate mixed linear models be put into an appropriate form using a coordinate-free approach. Section 2 contains some definitions and notation required for this form.

In Sect. 3 submodels of the initial model are constructed and OLSE for parameters corresponding to submodels are derived. Section 4 deals with determining the estimating equations of the Henderson Method III in the multivariate case. The real finite dimensional inner product spaces and the linear operators are chosen according to considered model and some results obtained by Baksalary and Kala (1976) are used in Sect. 5. A generalization of some results developed by Seely (1970a,b) for some univariate fixed and mixed linear models is given in multivariate case and it is proved that necessary and sufficient conditions for estimability of parametric functions are the same. The covariance components estimators provided by this method are quadratic unbiased estimators which do not depend on the parameters of the fixed factors.

2 The multivariate mixed linear model

Consider the multivariate mixed linear model

$$Y = X\beta_0 + \sum_{h=1}^{k} Z_h\beta_h + e, \tag{1}$$

where Y is a matrix of N observations on the response variables which are row vectors of dimension p, X and Z_h are known $N\times m$, $N\times n_h$ matrices respectively, β_0 is an $m \times p$ matrix of unknown parameters, β_h an $n_h \times p$ matrix of random variables, $h = 1,2,\dots,k$, and e is an $N \times p$ matrix of unobservable random errors. It is assumed that the rows of β_h and e in (1) are independent and identically normal distributed random vectors with zero means and corresponding non-negative covariance matrices $\Sigma_h, h = 1,\dots,k$ and $\Sigma_e = \Sigma_{k+1}$.

The parameter space of this model is

$$\Omega = \left\{\theta = (\beta_0', \Sigma_1,\dots,\Sigma_{k+1})', \beta_0 \in \mathcal{L}_{p,m}, \Sigma_h \in \mathcal{S}_p, h = 1,\dots,k+1\right\},$$

where $\mathcal{L}_{p,m}$ is the set of $m\times p$ real matrices while $\mathcal{S}_p$ is the set of $p\times p$ symmetric non-negative matrices.

Then the random matrix Y in (1) has the expected value

$$E(Y \mid \theta) = X\beta_0 \tag{2}$$

and the covariance matrix

$$\text{cov}\ (\text{vec}\, Y' \mid \theta) = \sum_{h=1}^{k}(Z_h Z_h') \otimes \Sigma_h + I \otimes \Sigma_e \tag{3}$$

for θ arbitrary in Ω (vec Y' is an Np column vector obtained by rearranging the transposed rows of Y one below the other). I denotes the identity $N \times N$ matrix and "$\otimes$" stands for the Kronecker matrix product defined as usual: if A and B are elements from $\mathcal{L}_{p_1,p_2}$ and $\mathcal{L}_{q_1,q_2}$, respectively, then $A \otimes B = (a_{ij}B)$ is an element in $\mathcal{L}_{p_1q_1,p_2q_2}$.

Let $\mathcal{A} \subset \mathcal{L}_{p,N}$ be a finite dimensional linear space endowed with the inner product $\langle A,B\rangle = \text{tr}(AB')$ for all $A,B \in \mathcal{A}$. (The same trace inner product will be used for all linear spaces $\mathcal{L}_{p_1,p_2}$.)

Using the linear operators (2) and (3) it can be written that

$$E(\langle A,Y\rangle \mid \theta) = \langle A, E(Y \mid \theta)\rangle = \langle A, X\beta_0\rangle \tag{4}$$

$$\text{cov}(\langle A,Y\rangle, \langle B,Y\rangle \mid \theta) = \text{tr}(A\Sigma B') = \langle A, B\Sigma\rangle \tag{5}$$

for all $\theta \in \Omega$ and $A,B \in \mathcal{A}$, where Σ is the common covariance matrix of the rows of Y.

Hence $X\beta_0$ and Σ are the unique operators on $\mathcal{A}$ and on $\mathcal{S}_p$, respectively, that satisfy (4) and (5) for all $A, B, \in \mathcal{A}$ and $\theta \in \Omega$.

Concerning linear operator notions we use the following terms: let $(\mathcal{L}, \langle\cdot,\cdot\rangle)$ be a finite dimensional inner product space and let T be a linear operator from $\mathcal{L}$ to $\mathcal{A}$. The range of T is denoted by $R(T)$ and the null space of T by $N(T)$. The adjoint of T is the linear operator T^* from $\mathcal{A}$ into $\mathcal{L}$ which takes an element $A \in \mathcal{A}$ into the unique element T^*A in $\mathcal{L}$ having the property $\langle T^*A, B\rangle = \langle A, TB\rangle$ for all $B \in \mathcal{L}$. The rank of T is denoted by $r(T)$. The same notations are used for matrices except a prime for the transpose of a matrix.

3 The OLSE corresponding to submodels

In the sequel we consider that all the factors of the model (1) are fixed. The submodel i of the initial model (1) has a design matrix $U_i = (X, Z_1, \ldots, Z_i) \in \mathcal{L}_{(m+\sum_{h=1}^{i} n_h),N}$ and the corresponding parameter space

$$\Omega_i = \left\{\theta_i = (\beta_0', \beta_1', \ldots, \beta_i')' : \beta_0 \in \mathcal{L}_{p,m}, \beta_h \in \mathcal{L}_{p,n_h}, h = 1, \ldots, i\right\} \tag{6}$$

for $i = 1, 2, \ldots, k$. The random matrix Y in the submodel i has expectation

$$E(Y \mid \theta_i) = X\beta_0 + \sum_{h=1}^{i} Z_h\beta_h = U_i\theta_i \tag{7}$$

and covariance matrix

$$\mathrm{cov}(\mathrm{vec}\, Y' \mid \theta_i) = I \otimes \Sigma_e \tag{8}$$

for all $\theta_i \in \Omega_i, i = 1, \ldots, k$.

If we denote $U_0 = X \in \mathcal{L}_{N,m}$ and $\Omega_0 = \left\{\theta_0 = \beta_0 : \beta_0 \in \mathcal{L}_{p,m}\right\}$ then we can form $k + 1$ submodels of the model (1) all of them being considered linear models with fixed effects.

The normal equations $U_i'U_i\theta_i = U_i'Y$ are solved to obtain OLSE

$$\hat{\theta}_i = (U_i'U_i)^- U_i'Y \tag{9}$$

of θ_i, corresponding to the i submodel under assumptions (6), (7) and (8), $i = 0, 1, \ldots, k$. $(U_i'U_i)^-$ is a generalized inverse of $U_i'U_i$ when U_i is not of full column rank. Therefore $\hat{\theta}_i$ exists, satisfies the normal equations and $\langle\lambda_i, \hat{\theta}_i\rangle$ is a BLUE for parameter function $\langle\lambda_i, \theta_i\rangle$ if $\lambda_i \in R(U_i')$ (Seely and Zyskind 1971).

Then there exists $A \in \mathcal{A}$ such that $\langle\lambda_i, \hat{\theta}_i\rangle = \langle U_i^*A, \hat{\theta}_i\rangle = \langle A, U_i\hat{\theta}_i\rangle =$ $= \langle A, P_iY\rangle$, where the linear operator

$$P_i = U_i(U_i'U_i)^-\, U_i' \tag{10}$$

from $\mathcal{A}$ into $\mathcal{A}$ is the orthogonal projection onto $R(U_i)$, i.e. P_i is symmetric, idempotent and uniquely determined operator regardless of the choice of $(U_i'U_i)^-$. Hence, by (10) and (7), $E(\langle\lambda_i, \hat{\theta}_i\rangle \mid \theta_i) = \langle A, P_i U_i \theta_i\rangle = \langle A, U_i\theta_i\rangle = \langle\lambda_i, \theta_i\rangle$ and covariance matrix of $\hat{\theta}_i$ is minimum in the class of all linear unbiased estimators of $\langle\lambda_i, \theta_i\rangle$, $(\mathrm{cov}\,(\mathrm{vec}\widetilde{\theta}_i{}' \mid \theta_i) - \mathrm{cov}\,(\mathrm{vec}\hat{\theta}_i{}' \mid \theta_i)$ is non-negative definite for all $\widetilde{\theta}_i$ verifying $E(\langle\lambda_i, \widetilde{\theta}_i\rangle \mid \theta_i) = \langle\lambda_i, \theta_i\rangle)i = 0, 1, \ldots, k$.

It is known (Rao 1973) the result:

Lemma 1 *Let P_i be the linear operator* (10). *Then P_i is an orthogonal projection on $R(U_i)$, if and only if P_i is an orthogonal projection on $R(X) + \sum_{h=1}^{i} R(Z_h), i = 1, \ldots, k$.*

Using the definition and the properties of an orthogonal projection (see Halmos 1957) onto a vectorial space endowed with an inner product and Lemma 1 we can find the following results:

Lemma 2 *Let P_i be the linear operator* (10). *Then P_i is an orthogonal projection on $R(U_i)$, if and only if it is an orthogonal projection on $R(XX') + \sum_{h=1}^{i} R(Z_h Z_h'), i = 1, \ldots, k$.*

Corollary 1 *P_i given by* (10) *is an orthogonal projection on $R(X) + \sum_{h=1}^{i} R(Z_h)$ iff it is an orthogonal projection on $R(XX') + \sum_{h=1}^{i} R(Z_h Z_h'), i = 1, \ldots, k$.*

Lemma 3 *If P_i is an orthogonal projection on $R(U_i)$, then $R(XX')$, $R(Z_h Z_h') \subset N(P_k - P_i)$, $h = 1, \ldots, i$; $i = 0, 1, \ldots, k-1$.*

Proof It follows from Lemma 1 and Corollary 1 that P_i and P_k are orthogonal projections on $R(XX') + \sum_{h=1}^{i} R(Z_h Z_h')$ and, on $R(XX') + \sum_{h=1}^{k} R(Z_h Z_h')$, respectively, where $i = 1, \ldots, k-1$.

If $Z_h Z_h' A_h$ is arbitrary in $R(Z_h Z_h')$ with $A_h \in \mathcal{A}$ we have $(P_k - P_i) Z_h Z_h' A_h = 0$ for $h = 1, \ldots, i$ and $i = 1, \ldots, k-1$. A similar result is obtained for $(P_k - P_i) XX'A = 0$ for all $A \in \mathcal{A}$ and $i = 0, 1, \ldots, k-1$.

4 The generalized fitting constants method

Henderson's three methods for estimating variance components in some univariate linear models were generalized to obtain unbiased estimators for covariance components in some multivariate linear regression models.

Using a matrix formulation Searle (1971) showed that Henderson Method III can be the preferred estimation procedure for the mixed linear models but it has three major shortcomings:

- There are no necessary and sufficient conditions for the existence of variance and covariance estimators,
- There are too many equations and
- The provided estimators can be negative definite quadratic forms.

The purpose of this section is to show that the first two shortcomings can be removed for the multivariate mixed linear model (1). Thus under assumptions expressed by (2) and (3) of the initial model let $Y'P_iY$ be generalized quadratic forms corresponding to the symmetric matrix P_i given by (10), $i = 0, 1, \ldots, k$. Their expected values can be derived under normality assumption by using the results obtained by Magnus and Neudecker (1979) and Neudecker (1990) as

$$E(Y'P_iY \mid \theta) = \beta_0'X'P_iX\beta_0 + \sum_{h=1}^{k} \mathrm{tr}(P_iZ_hZ_h') \cdot \Sigma_h + \mathrm{tr}P_i \cdot \Sigma_e$$

for $\theta \in \Omega$ and $i = 0, 1, \ldots, k$. Then the expected values

$$E[Y'(P_k - P_i)Y \mid \theta] = \beta_0'X'(P_k - P_i)X\beta_0 + \sum_{h=1}^{k} \mathrm{tr}[(P_k - P_i)Z_hZ_h'] \cdot \Sigma_h \\ + \mathrm{tr}(P_k - P_i) \cdot \Sigma_e,$$

become

$$E[Y'(P_k - P_i)Y \mid \theta] = \sum_{h=i+1}^{k} \mathrm{tr}[(P_k - P_i)Z_hZ_h'] \cdot \Sigma_h + [r(U_k) - r(U_i)] \cdot \Sigma_e \tag{11}$$

since, using Lemma 3, we have that $(P_k - P_i)X\beta_0 = 0$ for all $\beta_0 \in \mathcal{L}_{p,m}$ and $\mathrm{tr}[(P_k - P_i)Z_hZ_h'] = \langle (P_k - P_i)Z_h, Z_h \rangle = 0$ for $h = 1, \ldots, i$ and $i = 0, 1, \ldots, k-1$. As P_k is aan orthogonal projection on $R(U_k)$, the mean of the difference of the quadratic forms $Y'Y$ and $Y'P_kY$ under the initial conditions, i.e. $\theta \in \Omega$, is

$$E[Y'(I - P_k)Y \mid \theta] = [N - r(U_k)] \cdot \Sigma_e \tag{12}$$

The Henderson Method III consists in equating each difference of two quadratic forms to its expected value which is calculated under the assumptions of the initial model.

Thus a linear system in the covariance components $\Sigma_1, \ldots, \Sigma_k$ and Σ_e is obtained in the form

$$\begin{cases} \displaystyle\sum_{h=i+1}^{k} \mathrm{tr}(Q_{i+1}Z_hZ_h') \cdot \Sigma_h + [r(U_k) - r(U_i)] \cdot \Sigma_e = Y'Q_{i+1}Y, \quad i = 0, 1, \ldots, k-1 \\ [N - r(U_k)] \cdot \Sigma_e = Y'Q_{k+1}Y \end{cases} \tag{13}$$

where

$$Q_{i+1} = P_k - P_i, \quad Q_{k+1} = I - P_k \tag{14}$$

are the matrices of the quadratic forms (11) and (12).

Hence the estimating system (13) obtained in Henderson Method III for linear model (1) has $k+1$ equations and $\Sigma_1, \ldots, \Sigma_k, \Sigma_e = \Sigma_{k+1}$ unknown $p \times p$ symmetric non-negative matrices representing the components of the covariance matrix (3).

5 Consistency and estimability

In most references to the Henderson Method III it was assumed that the estimating equations are consistent so that no complications arise with regard to estimability. In the sequel it will be shown that even if $\Sigma_1, \ldots, \Sigma_{k+1}$ are estimable it does not follow that the Eqs. (13) are consistent.

Denote by

$$\Omega_{k+1} = \left\{\Sigma_\theta = (\Sigma_1, \ldots, \Sigma_{k+1})', \Sigma_h \in \mathcal{S}_p, h = 1, \ldots, k+1\right\}$$

the set of parameters representing the covariance components in model (1). A linear parametric function $\big((\lambda, \Sigma_\theta)\big) = \sum_{h=1}^{k+1} \lambda_h \Sigma_h$ with $\lambda = (\lambda_1, \ldots, \lambda_{k+1})' \in R^{k+1}$ is said to be estimable if there exists a linear function of $Y'Y$ whose expectation is equal to $\big((\lambda, \Sigma_\theta)\big)$ for all $\Sigma_\theta \in \Omega_{k+1}$.

Let H and W be linear operators from R^{k+1} to $\mathcal{L}_{N,N}$ such that

$$H\rho = \sum_{h=1}^{k+1} (Z_h Z_h') \rho_h = \sum_{h=1}^{k+1} V_h \rho_h, \quad W\rho = \sum_{h=1}^{k+1} Q_h \rho_h$$

for $\rho \in R^{k+1}$, where $V_{k+1} = I$ and Q_h are given by (14), $h = 1, \ldots, k+1$. Then the adjoint operator W^* of W from $\mathcal{L}_{N,N}$ to R_p^{k+1} is defined by

$$W^* A = (\langle Q_1, A\rangle, \ldots, \langle Q_{k+1}, A\rangle)'$$

for arbitrary $A \in \mathcal{L}_{N,N}$. Hence form of $W^* H\rho$ will be

$$W^* H\rho = \left(\sum_{h=1}^{k+1} \langle Q_1, V_h\rangle \rho_h, \ldots, \sum_{h=1}^{k+1} \langle Q_{k+1}, V_h\rangle \rho_h\right)' \tag{15}$$

for $\rho \in R^{k+1}$.

It is easy to notice from (14) and Lemma 3 that $\langle Q_{i+1}, V_h\rangle = \langle (P_k - P_i) Z_h, Z_h\rangle = 0$ for $h = 1, \ldots, i; i = 0, 1, \ldots, k-1$ and $\langle Q_{k+1}, V_h\rangle = \langle (I - P_k) Z_h, Z_h\rangle = 0$ for $h = 1, \ldots, k$. Then the coefficients of Σ_h in the estimating

Eqs. (13) are the same as the coefficients corresponding to ρ_h in (15), $h = 1,\ldots,k+1$.

Writing the entries (i,j) of Σ_h, the second terms of the Eqs. (13) become $Y_i' Q_h Y_j, h = 1,\ldots,k+1$, where Y_i is the i column of the random matrix Y. Then it is obtained a vector of quadratic forms

$$W^*(Y_jY_i') = (\langle Q_1, Y_jY_i'\rangle,\ldots,\langle Q_{k+1}, Y_jY_i'\rangle)'$$

for all $i,j = 1,\ldots,p$. Therefore, if Σ_θ verifies Eqs. (13) then $\Sigma_\theta(i,j) = (\Sigma_1(i,j),\ldots,\Sigma_{k+1}(i,j))'$ will verify the equations

$$W^*H\Sigma_\theta(i,j) = W^*(Y_jY_i') \tag{16}$$

for $i,j = 1,\ldots,p$.

It follows that the conditions regarding consistency and estimability for the multivariate mixed linear model without interactions (1) are similar to conditions for the corresponding univariate model (Seely 1970b).

Theorem 1 *The estimating Eqs.* (13) *are consistent if*

$$R(W'H) = R(W'). \tag{17}$$

Proof The relation $R(W) \cap N(H^*) = \{0\}$ is equivalent to (17). Let $A \in R(W) \cap N(H^*)$. Then there exists $\delta(i,j) \in R^{k+1}$ such that $H^*W\delta(i,j) = 0$. By adding the $k+1$ equations of (16) and denoting $\sum_{h=1}^{k+1} V_h = V$, we have $\sum_{h=1}^{k+1}\langle V, Q_h\rangle\delta_h(i,j) = \langle V, W\delta(i,j)\rangle = 0$, that is $W\delta(i,j) = 0$. Then the Eqs. (16) and (13) and consistent.

A necessary and sufficient condition for parametric functions to be estimable found by Seely (1970b) can be developed for model (1) as follows:

Theorem 2 *Let W be a linear operator such that*

$$R(W) + N(H^*) = R(XX')^\perp \tag{18}$$

The parametric function $((\lambda, \Sigma_\theta))$ is estimable if and only if there exists $\rho \in R^{k+1}$ such that $H^*W\rho = \lambda$.

Corollary 2 *If ρ and λ verify the equation $H^*W\rho = \lambda$, then $\sum_{h=1}^{k+1}\rho_h Y'Q_h Y$ is a quadratic unbiased estimator of the parametric function $((\lambda, \Sigma_\theta))$.*

Proof For i and j fixed in $\{1, 2, \ldots, p\}$ the corresponding element of the estimator has expectation

$$E\left[\sum_{h=1}^{k+1} \rho_h(i,j) Y_i' Q_h Y_j\right] = \sum_{h=1}^{k+1} \rho_h(i,j) E(W' Y_j Y_i')$$
$$= (\rho(i,j), W^* H \Sigma_\theta(i,j)) = (\lambda(i,j), \Sigma_\theta(i,j))$$

where (.,.) is the usual inner product in R^{k+1}.

Corollary 3 *If the linear operator W satisfies the relations (17) and (18) and if $\hat{\Sigma}_\theta$ is the solution of (13), then $((\lambda, \hat{\Sigma}_\theta))$ is a quadratic unbiased estimator of $((\lambda, \Sigma_\theta))$ for $\lambda \in R(H'W)$.*

Proof From Theorem 1 it follows that Eqs. (13) have a unique solution $\hat{\Sigma}_\theta$. If $\lambda \in R(H'W)$, then there exists a ρ such that $\lambda = H^* W \rho$, which means that $((\lambda, \Sigma_\theta))$ is estimable by Theorem 2. Then Corollary 2 can be used.

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