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Efficiency of the MLE in a multivariate parallel profile model with random effects

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ABSTRACT. In this paper we consider a multivariate parallel profile model with polynomial growth curves. The covariance structure based on a random effects model is assumed. The maximum likelihood estimators (MLE's) are obtained under the random effects covariance structure. The efficiency of the MLE is discussed.

1. Introduction

Suppose that m response variables $x_1, \dots, x_m$ have been measured at p different occasions on each of N individuals, and each individual belongs to one of k groups or treatments. Let $\boldsymbol{x}_j^{(g)}$ be an mp-vector of measurements on the j-th individual in the g-th group arranged as

$$\boldsymbol{x}_j^{(g)} = (x_{11j}^{(g)}, \dots, x_{1mj}^{(g)}, \dots\dots, x_{p1j}^{(g)}, \dots, x_{pmj}^{(g)})',$$

and assume that $\boldsymbol{x}_j^{(g)}$'s are independently distributed as $N_{mp}(\mu^{(g)}, \Omega)$, where Ω is an unknown $mp \times mp$ positive definite matrix, $j = 1, \dots, N_g$, $g = 1, \dots, k$. Further, we assume that mean profiles of k groups are parallel polynomial growth curves, i.e.,

$$\mu^{(g)} = (\mathbf{1}_p \otimes I_m)\xi^{(g)} + (B' \otimes I_m)\xi_2, \qquad g = 1, \dots, k, \tag{1.1}$$

where $\mathbf{1}_p$ is a p-vector of ones, $(\mathbf{1}_p \otimes I_m)$ defines the Kronecker product of $\mathbf{1}_p$ and the $m \times m$ identity matrix,

$$B = \begin{bmatrix} \mathbf{1}_p' \\ B_2 \end{bmatrix} = \begin{bmatrix} 1 & \cdots\cdots & 1 \\ t_1 & \cdots\cdots & t_p \\ \vdots & & \vdots \\ t_1^{q-1} & \cdots\cdots & t_p^{q-1} \end{bmatrix} \tag{1.2}$$

is a $q \times p$ within-individuals design matrix of rank q $(\leq p)$, $\xi^{(g)} : m \times 1$ and

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$\xi_2 : mq \times 1$ are vectors of unknown parameters. Yokoyama [7] considered a multivariate parallel profile model with

$$\mu^{(g)} = (\mathbf{1}_p \otimes I_m)\xi^{(g)} + \mu, \qquad g = 1, \dots, k.$$

Therefore, the model (1.1) means that μ has a linear structure. Without loss of generality, we may assume that $\xi^{(k)} = \mathbf{0}$. In the following we shall do this. Let

$$X = [\boldsymbol{x}_1^{(1)}, \dots, \boldsymbol{x}_{N_1}^{(1)}, \dots\dots, \boldsymbol{x}_1^{(k)}, \dots, \boldsymbol{x}_{N_k}^{(k)}]', \qquad N = N_1 + \dots + N_k.$$

Then the model of X can be written as

$$X \sim N_{N \times mp}(A_1 \Xi_1 (\mathbf{1}_p' \otimes I_m) + \mathbf{1}_N \xi_2' (B \otimes I_m), \Omega \otimes I_N), \tag{1.3}$$

where

$$A_1 = \begin{bmatrix} \mathbf{1}_{N_1} & & 0 \\ & \ddots & \\ 0 & & \mathbf{1}_{N_{k-1}} \\ & \cdots & \\ & 0 & \end{bmatrix}$$

is an $N \times (k-1)$ between-individuals design matrix of rank $k-1$ $(\leq N - p - 1)$, $\Xi_1 = [\xi^{(1)}, \dots, \xi^{(k-1)}]'$ is an unknown $(k-1) \times m$ parameter matrix. The model (1.3) may be called the multivariate parallel growth curve model. The model (1.3) with $B = I_p$ is a special case of mixed MANOVA-GMANOVA models considered by Chinchilli and Elswick [2], Kshirsagar and Smith [4, p. 85], etc. The mean structure of (1.3) can be written as

$$E(X) = [A_1 \quad \mathbf{1}_N] \begin{bmatrix} \Xi_{11} & 0 \\ \xi_{21}' & \xi_{22}' \end{bmatrix} (B \otimes I_m), \tag{1.4}$$

where $\Xi_1 = \Xi_{11}$ and $\xi_2' = [\xi_{21}' \quad \xi_{22}']$. We note that the model (1.3) is the multivariate growth curve model (Reinsel [5]) with a linear restriction on mean parameters.

Chinchilli and Carter [1] discussed the LR test for a patterned covariance structure

$$\Omega = (\mathbf{1}_p \otimes I_m)\Sigma_\lambda(\mathbf{1}_p' \otimes I_m) + (W \otimes I_m)\Sigma_\tau(W' \otimes I_m) + I_p \otimes \Sigma_e,$$

in a multivariate GMANOVA model, where W is a known $p \times (p-1)$ matrix of rank $p-1$ such that $\mathbf{1}_p' W = \mathbf{0}$, Σ_τ is an arbitrary $m(p-1) \times m(p-1)$ positive semi-definite matrix, Σ_λ and Σ_e are arbitrary $m \times m$ positive semi-definite and positive definite matrices, respectively. We are now interested in a multivariate random effects covariance structure

$$\Omega = (\mathbf{1}_p \otimes I_m)\Sigma_\lambda(\mathbf{1}_p' \otimes I_m) + I_p \otimes \Sigma_e. \tag{1.5}$$

The covariance structure (1.5) is based on the following model:

$$\boldsymbol{x}_j^{(g)} = (\mathbf{1}_p \otimes I_m)(\xi^{(g)} + \lambda_j^{(g)}) + (B' \otimes I_m)\xi_2 + \boldsymbol{e}_j^{(g)}, \tag{1.6}$$

where $\lambda_j^{(g)}$'s and $\boldsymbol{e}_j^{(g)}$'s are independently distributed as $N_m(\mathbf{0}, \Sigma_\lambda)$ and $N_{mp}(\mathbf{0}, I_p \otimes \Sigma_e)$, respectively. From (1.6), we have

$$\mathrm{Var}(\boldsymbol{x}_j^{(g)}) = \Omega = (\mathbf{1}_p \otimes I_m)\Sigma_\lambda(\mathbf{1}_p' \otimes I_m) + I_p \otimes \Sigma_e.$$

Therefore, the model of X with random effects can be written as

$$\begin{aligned} X \sim N_{N\times mp}(&A_1\Xi_1(\mathbf{1}_p' \otimes I_m) + \mathbf{1}_N\xi_2'(B \otimes I_m), \\ &((\mathbf{1}_p \otimes I_m)\Sigma_\lambda(\mathbf{1}_p' \otimes I_m) + I_p \otimes \Sigma_e) \otimes I_N). \end{aligned} \tag{1.7}$$

Fujikoshi and Satoh [3] obtained the MLE's in the growth curve model with two different within-individuals design matrices when the covariance matrix has no structures, i.e., is any unknown positive definite. In this paper we consider the problems of estimating unknown mean parameters Ξ_1 and ξ_2 when Ω has the structure (1.5). By making this stronger assumption about Ω, we can expect to have more efficient estimators. In §2 we obtain the MLE's of Ξ_1 and ξ_2 in the model (1.7), using a canonical form of (1.7). In §3 it is shown how much gains can be obtained for the maximum likelihood estimation of Ξ_1 by assuming a multivariate random effects covariance structure.

2. The MLE's

First we reduce the model (1.7) to a canonical form. Let $H = [H_1 \quad N^{-1/2}\mathbf{1}_N \quad H_3]$ be an orthogonal matrix of order N such that

$$\begin{aligned}[] [A_1 \quad \mathbf{1}_N] &= [H_1 \quad N^{-1/2}\mathbf{1}_N]\begin{bmatrix} L_{11} & \mathbf{0} \\ l_{21}' & N^{1/2} \end{bmatrix} \\ &= H_{(2)}L, \end{aligned}$$

where $H_1 : N \times (k-1)$, and $L_{11} : (k-1) \times (k-1)$ is a lower triangular matrix. Similarly, let $Q = [p^{-1/2}\mathbf{1}_p \quad Q_2' \quad Q_3']'$ be an orthogonal matrix of order p such that

$$\begin{aligned} \begin{bmatrix} \mathbf{1}_p' \otimes I_m \\ B_2 \otimes I_m \end{bmatrix} &= \begin{bmatrix} p^{1/2}I_m & 0 \\ R_{21} & R_{22} \end{bmatrix}\begin{bmatrix} p^{-1/2}\mathbf{1}_p' \otimes I_m \\ Q_2 \otimes I_m \end{bmatrix} \\ &= RQ_{(2)}, \end{aligned}$$

where $Q_2 : (q-1) \times p$, and $R_{22} : m(q-1) \times m(q-1)$ is a lower triangular matrix. Then the mean structure of (1.7) can be written as

(2.1) $$A_1 \Xi_1 (\mathbf{1}_p' \otimes I_m) + \mathbf{1}_N \xi_2'(B \otimes I_m) = p^{-1/2} H_1 \Theta_1 (\mathbf{1}_p' \otimes I_m) + N^{-1/2} \mathbf{1}_N \theta_2' Q_{(2)},$$

where

$$\Theta_1 = p^{1/2} L_{11} \Xi_1, \qquad \theta_2' = N^{1/2} \xi_2' R + \boldsymbol{l}_{21}' [\Xi_1 \quad 0] R.$$

Here we note that (Ξ_1, ξ_2) is an invertible function of (Θ_1, θ_2). In fact, Ξ_1 and ξ_2 can be expressed in terms of Θ_1 and θ_2 as

(2.2) $$\Xi_1 = p^{-1/2} L_{11}^{-1} \Theta_1, \qquad \xi_2' = N^{-1/2} \theta_2' R^{-1} - N^{-1/2} \boldsymbol{l}_{21}' [p^{-1/2} L_{11}^{-1} \Theta_1 \quad 0].$$

Using the above transformation, we can write a canonical form of (1.7) as

(2.3) $$Y = H' X (Q' \otimes I_m) = \begin{bmatrix} Y_{11} & Y_{12} & Y_{13} \\ \boldsymbol{y}_{21}' & \boldsymbol{y}_{22}' & \boldsymbol{y}_{23}' \\ Y_{31} & Y_{32} & Y_{33} \end{bmatrix} \sim N_{N \times mp}(E(Y), \Psi \otimes I_N),$$

where the mean $E(Y)$ and the covariance matrix Ψ are given by

(2.4) $$E(Y) = \begin{bmatrix} \Theta_{11} & 0 & 0 \\ \theta_{21}' & \theta_{22}' & \mathbf{0}' \\ 0 & 0 & 0 \end{bmatrix}, \qquad \begin{bmatrix} \Theta_{11} & 0 \\ \theta_{21}' & \theta_{22}' \end{bmatrix} = L \begin{bmatrix} \Xi_{11} & 0 \\ \xi_{21}' & \xi_{22}' \end{bmatrix} R,$$

$\Theta_1 = \Theta_{11}$, $\theta_2' = [\theta_{21}' \quad \theta_{22}']$, $\Theta_{11} : (k-1) \times m$, $\theta_{21} : m \times 1$, $\theta_{22} : m(q-1) \times 1$,

(2.5) $$\Psi = (Q \otimes I_m) \Omega (Q' \otimes I_m) = \begin{bmatrix} p\Sigma_\lambda + \Sigma_e & 0 \\ 0 & I_{p-1} \otimes \Sigma_e \end{bmatrix},$$

$$p\Sigma_\lambda + \Sigma_e : m \times m, \qquad I_{p-1} \otimes \Sigma_e : m(p-1) \times m(p-1).$$

From (2.3), it is easy to see that the MLE's of Θ_1 and θ_2 are given by

$$\hat{\Theta}_1 = Y_{11}, \qquad \hat{\theta}_2' = \boldsymbol{y}_{2(12)}',$$

where $\boldsymbol{y}_{2(12)}' = [\boldsymbol{y}_{21}' \quad \boldsymbol{y}_{22}']$. Hence the MLE's of Ξ_1 and ξ_2 are given by

(2.6) $$\hat{\Xi}_1 = p^{-1/2} L_{11}^{-1} Y_{11}, \quad \hat{\xi}_2' = N^{-1/2} \boldsymbol{y}_{2(12)}' R^{-1} - N^{-1/2} \boldsymbol{l}_{21}' [p^{-1/2} L_{11}^{-1} Y_{11} \quad 0].$$

Now we express the MLE's given in (2.6) in terms of the original observations. Let

(2.7) $$\tilde{A}_1 = \left(I_N - \frac{1}{N} \mathbf{1}_N \mathbf{1}_N' \right) A_1, \qquad \tilde{B}_2 = B_2 \left(I_p - \frac{1}{p} \mathbf{1}_p \mathbf{1}_p' \right).$$

Then, from the definitions of L and R it is seen that

$$H_1 = \tilde{A}_1 L_{11}^{-1}, \qquad \boldsymbol{l}'_{21} = \frac{1}{\sqrt{N}} \mathbf{1}'_N A_1,$$

$$Q_2 \otimes I_m = R_{22}^{-1}(\tilde{B}_2 \otimes I_m), \qquad R_{21} = \frac{1}{\sqrt{p}}(B_2 \mathbf{1}_p \otimes I_m).$$

Using these results, we have the following theorem.

THEOREM 2.1. *The MLE's of* Ξ_1 *and* ξ_2 *in the multivariate parallel profile model* (1.7) *are given as follows:*

$$\hat{\Xi}_1 = \frac{1}{p}(\tilde{A}'_1\tilde{A}_1)^{-1}\tilde{A}'_1 X(\mathbf{1}_p \otimes I_m),$$

$$\hat{\xi}'_{21} = \frac{1}{p}\left[\bar{\boldsymbol{x}}'\{(I_p - \tilde{B}'_2(\tilde{B}_2\tilde{B}'_2)^{-1}B_2) \otimes I_m\} - \frac{1}{N}\mathbf{1}'_N A_1(\tilde{A}'_1\tilde{A}_1)^{-1}\tilde{A}'_1 X\right](\mathbf{1}_p \otimes I_m),$$

$$\hat{\xi}'_{22} = \bar{\boldsymbol{x}}'\{(\tilde{B}'_2(\tilde{B}_2\tilde{B}'_2)^{-1}) \otimes I_m\},$$

where $\tilde{A}_1$ *and* $\tilde{B}_2$ *are given by* (2.7), *and* $\bar{\boldsymbol{x}}$ *is the sample mean vector of observations of all the groups.*

We note that the MLE's of unknown variance parameters Σ_λ and Σ_e in the model (1.7) are complicated and impractical. The MLE's of Σ_λ and Σ_e in the model (1.7) are the same ones as in the model of Yokoyama [7], in which μ has no structures. For a detailed discussion of the MLE's of these parameters, see Yokoyama [7].

3. Efficiency of $\hat{\Xi}_1$

In this section we consider the efficiency of the MLE for Ξ_1 in the case when the covariance structure (1.5) is assumed. Let S_w be the matrix of the sums of squares and products due to the within variation, i.e.,

$$S_w = X'H_3H'_3X = \sum_{g=1}^{k}\sum_{j=1}^{N_g}(\boldsymbol{x}_j^{(g)} - \bar{\boldsymbol{x}}^{(g)})(\boldsymbol{x}_j^{(g)} - \bar{\boldsymbol{x}}^{(g)})',$$

where $\bar{\boldsymbol{x}}^{(g)}$ is the sample mean vector of observations of the g-th group. When no special assumptions about Ω are made, the MLE of Ξ_1 is given by

(3.1) $$\tilde{\Xi}_1 = (\tilde{A}'_1\tilde{A}_1)^{-1}\tilde{A}'_1 X S_w^{-1}(\mathbf{1}_p \otimes I_m)\{(\mathbf{1}'_p \otimes I_m)S_w^{-1}(\mathbf{1}_p \otimes I_m)\}^{-1}$$

(see, e.g., Srivastava [6]). The estimators $\hat{\Xi}_1$ and $\tilde{\Xi}_1$ have the following properties.

Theorem 3.1. *In the multivariate parallel profile model* (1.7) *it holds that both the estimators* $\hat{\Xi}_1$ *and* $\tilde{\Xi}_1$ *are unbiased, and*

$$\mathrm{Var}(\mathrm{vec}(\hat{\Xi}_1)) = \frac{1}{p}(p\Sigma_\lambda + \Sigma_e) \otimes (\tilde{A}_1'\tilde{A}_1)^{-1},$$

$$\mathrm{Var}(\mathrm{vec}(\tilde{\Xi}_1)) = \frac{1}{p}\left\{1 + \frac{m(p-1)}{N-k-m(p-1)-1}\right\}(p\Sigma_\lambda + \Sigma_e) \otimes (\tilde{A}_1'\tilde{A}_1)^{-1},$$

where $\tilde{A}_1$ *is given by* (2.7).

Proof. From (2.2), (2.6) and $\tilde{A}_1'\tilde{A}_1 = L_{11}'L_{11}$, we obtain the result on $\hat{\Xi}_1$. It can be shown that for any positive definite covariance matrix Ω,

$$E(\tilde{\Xi}_1) = \Xi_1$$

and

$$\mathrm{Var}(\mathrm{vec}(\tilde{\Xi}_1)) = \left\{1 + \frac{m(p-1)}{N-k-m(p-1)-1}\right\}\{(\mathbf{1}_p' \otimes I_m)\Omega^{-1}(\mathbf{1}_p \otimes I_m)\}^{-1} \otimes (\tilde{A}_1'\tilde{A}_1)^{-1}$$

(see, e.g., Fujikoshi and Satoh [3], Yokoyama [7]). Under the assumption that

$$\Omega = (\mathbf{1}_p \otimes I_m)\Sigma_\lambda(\mathbf{1}_p' \otimes I_m) + I_p \otimes \Sigma_e,$$

it holds that

$$\{(\mathbf{1}_p' \otimes I_m)\Omega^{-1}(\mathbf{1}_p \otimes I_m)\}^{-1} = \frac{1}{p}(p\Sigma_\lambda + \Sigma_e),$$

which proves the desired result on $\tilde{\Xi}_1$.

From Theorem 3.1, we obtain

$$\mathrm{Var}(\mathrm{vec}(\tilde{\Xi}_1)) - \mathrm{Var}(\mathrm{vec}(\hat{\Xi}_1)) = \frac{m(p-1)}{p\{N-k-m(p-1)-1\}}(p\Sigma_\lambda + \Sigma_e) \otimes (\tilde{A}_1'\tilde{A}_1)^{-1} > 0, \quad (3.2)$$

which implies that $\hat{\Xi}_1$ is more efficient than $\tilde{\Xi}_1$ in the model (1.7). This shows that we can get a more efficient estimator for Ξ_1 by assuming a multivariate random effects covariance structure. Especially, when p is large relative to N, we can obtain greater gains. It is not simple and is left as a future problem how much gains can be obtained for the maximum likelihood estimation of ξ_2 by assuming the covariance structure (1.5).

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