PRELIMINARY REPORT

Growth Curve Models with Linear Structure for Location and Variance Parameters

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SUMMARY

Growth curve models for the analysis of longitudinal data often involve many parameters, which may be the cause of loss of efficiency in the inference or poor interpretation of the results of analysis. This paper proposes to introduce a family of linear structures into the fixed location parameters and the variance-covariance parameters in growth curve models. This leads to the models with fewer unknown parameters, resulting in increased efficiency and easier interpretation in analysis. A noniterative algorithm is also provided for estimating unknown parameters in the model.

Key words: Growth curve; Random effect; Repeated measurements; Unbalanced data; Noniterative estimation procedure; Parallel profile; GMANOVA

1. Introduction

Growth curve models were implied by Wishart(1938) and formulated specifically by Potthoff and Roy (1964) for analyzing longitudinal data. Similar models were proposed by Rao(1965) and Khatri(1966). Grizzle and Allen(1969) proposed a unified formula for growth curve models. Laird and Ware(1982) generalized them to the analysis of unbalanced growth curve data, and proposed a method for estimating unknown parameters based on E-M algorithm. Vonesh and Carter(1987) proposed alternative efficient method of inference using a noniterative algorithm. Fujikoshi (1994) gave a review of recent developments on random effects models for balanced and unbalanced data. In many situations of growth curve analysis, more than one groups with respect to the sort of treatments are dealt with. Hirotsu(1991, 1993) remarked that the treatment effect may be not homogeneous over the subjects, in such a case the covariance of 'between-individual' effects should vary over groups, where the use of heteroscedastic model is needed.

A natural extension of the model proposed by Vonesh and Carter(1987) may be given by

$$\mathbf{y}_i = X_i \Phi \mathbf{d}_i + X_i \Psi \mathbf{z}_i + X_i \mathbf{b}_i + \mathbf{e}_i, \quad i = 1, \dots, N, \quad (1.1)$$

for N distinct individuals, where $\mathbf{y}_i = (y_{i1}, \dots, y_{ir_i})'$ is an $r_i \times 1$ vector of repeated measurements on the i th individual, X_i is an $r_i \times q$ matrix of known explanatory variables with $\text{rank} X_i = q \leq r_i$, $\mathbf{d}_i = (d_{i1}, \dots, d_{ig})'$ is a $g \times 1$ vector of group indicator variables for the i th individual, $\mathbf{z}_i$ is an $h \times 1$ vector of fixed baseline covariables; Φ and Ψ are $q \times g$ and $q \times h$ matrices of fixed regression coefficients, respectively; $\mathbf{e}_i$ is an $r_i \times 1$ vector of within-individual random error, $\mathbf{b}_i$ is a $q \times 1$ vector of between-individual random variation. It is further assumed that $\mathbf{b}_i$ and $\mathbf{e}_i$ have the multivariate normal distributions with $E(\mathbf{b}_i) = \mathbf{0}$, $E(\mathbf{e}_i) = \mathbf{0}$,

$$\text{Cov}(\mathbf{b}_i, \mathbf{b}_{i'}) = \delta_{ii'} \sum_{m=1}^g d_{im} \Delta_m, \quad (1.2)$$

$$\text{Cov}(\mathbf{e}_i, \mathbf{e}_{i'}) = \delta_{ii'} \sum_{m=1}^g d_{im} \sigma_m^2 I_{r_i}, \quad (1.3)$$

$$\text{Cov}(\mathbf{b}_i, \mathbf{e}_{i'}) = O_{q \times r_{i'}}, \quad i, i' = 1, \dots, N,$$

where δ_{ij} denotes Kronecker delta, and I_{r_i} is the $r_i \times r_i$ identity matrix.

Then Model (1.1) can be expressed alternatively as

$$\mathbf{y}_i = X_i \Lambda \mathbf{a}_i + X_i \mathbf{b}_i + \mathbf{e}_i, \quad i = 1, \dots, N, \quad (1.4)$$

where $\mathbf{a}_i = (\mathbf{d}_i', \mathbf{z}_i')'$ is the $(g+h) \times 1$ vector of between-individual covariates for the i th individual; $\Lambda = [\Phi; \Psi]$ is the $q \times (g+h)$ matrix of fixed regression coefficients. Vonesh and Carter's model can be given in Model (1.4) when $\Delta_1 = \dots = \Delta_g$ and $\sigma_1^2 = \dots = \sigma_g^2$.

If we make no special assumption about the structures of the regression coefficient matrix Λ and of the variance-covariance matrices Δ_m , $m = 1, \dots, g$, Model (1.4) may involve quite large number of parameters relative to N in many practical cases, which may be the cause of loss of efficiency in the inference or poor aspects of the results of analysis. In this paper we introduce a family of linear structures into parameters of the matrices Λ and Δ_m in Model (1.4), which would lead to increase in efficiency of the inference and easier interpretation in the analysis of growth curve data.

2. Linear structures for parameters

In order to obtain accurate estimates of parameters and clear aspects of the structure of the regression model, it may be effective to assume that some parameters are known (it is often

assumed to be zero) rather than unknown or that some parameters share a common value. Several researchers have considered the estimation of Λ under the linear condition $C_1\Lambda C_2 = O$ where C_1 and C_2 are some known matrices, but no simple approach has been offered (e.g. Anderson and Olkin, 1985; von Rosen, 1989, 1991). In this section, we propose an alternative procedure for reducing the number of distinct parameters by introducing a family of linear structures into the location and variance-covariance parameters in Model (1.4).

2.1. LINEAR STRUCTURE FOR LOCATION PARAMETERS

Let $\Phi = (\phi_1, \dots, \phi_g)$ and $\Psi = (\psi_1, \dots, \psi_h)$. Then we assume that Φ and Ψ have linear structures as follows.

$$\begin{aligned}\phi_u &= B_u \gamma + \mathbf{f}_u, & u = 1, \dots, g, \\ \psi_v &= C_v \nu, & v = 1, \dots, h,\end{aligned}$$

where B_u and C_v are prespecified known matrices. $\mathbf{f}_u$ is a vector of prespecified known elements, γ and ν are vectors of unknown parameters to be estimated with

$$\begin{aligned}\text{rank}(B_u) &= \dim(\gamma) = \ell_b, & u = 1, \dots, g, \\ \text{rank}(C_v) &= \dim(\nu) = \ell_c, & v = 1, \dots, h.\end{aligned}$$

Denoting $B = (B'_1, \dots, B'_g)'$, $F = (\mathbf{f}_1, \dots, \mathbf{f}_g, \mathbf{0}_1, \dots, \mathbf{0}_h)$ and $C = (C'_1, \dots, C'_h)'$, we have

$$\Lambda = \text{Mat}_q \left[\begin{pmatrix} B & O \\ O & C \end{pmatrix} \begin{pmatrix} \gamma \\ \nu \end{pmatrix} \right] + F = \text{Mat}_q(G\lambda) + F, \quad (2.1)$$

where $G = \begin{pmatrix} B & O \\ O & C \end{pmatrix}$ is the $[q(g+h)] \times \ell$ matrix with prespecified known elements and $\lambda = (\gamma', \nu')'$ is the $\ell (= \ell_b + \ell_c)$ vector of unknown parameters; $\text{Mat}_q()$ denotes the function from an $qn \times 1$ vector to the $q \times n$ matrix that is defined by

$$\text{Mat}_q(\mathbf{z}) = (\mathbf{z}_1, \dots, \mathbf{z}_n),$$

where $\mathbf{z} = (\mathbf{z}'_1, \dots, \mathbf{z}'_n)'$ with $q \times 1$ vectors $\mathbf{z}_j, j = 1, \dots, n$. Then it yields that Model (1.4) can be generalized as

$$\begin{aligned}y_i &= X_i[\text{Mat}_q(G\lambda) + F]\mathbf{a}_i + X_i\mathbf{b}_i + \mathbf{e}_i, \\ &= \mathbf{c}_i + Z_i\lambda + X_i\mathbf{b}_i + \mathbf{e}_i, \quad i = 1, \dots, N,\end{aligned}$$

where $\mathbf{c}_i = X_i F \mathbf{a}_i$, and $Z_i = X_i (\mathbf{a}_i' \otimes I_q) G$, $i = 1, \dots, N$. Since $\mathbf{c}_i$ is known, we can assume $F = O$ (and therefore $\mathbf{c}_i = \mathbf{0}$) without loss of generality. So, it can be clear that the resulted growth curve model is included to the mixed effect model proposed by Laird, Lange and Stram (1987) as a special case.

The family of structures represented by (2.1) contains the non-specified structure as a special case: that is, setting $G = I_{q(g+h)}$ and $\boldsymbol{\lambda} = \text{vec}(\Lambda)$, we have the identity $\Lambda = \text{Mat}_q(I_{q(g+h)} \text{vec}(\Lambda))$. Furthermore, we see that many useful structures can be expressed in Formula (2.1), some of which are illustrated as below.

Example 1 Parallel profile structure that is specified by $\Phi = (\boldsymbol{\mu}', \mathbf{1}_g \otimes \boldsymbol{\beta}')'$, $\boldsymbol{\mu} = (\mu_1, \dots, \mu_g)'$ (see, Srivatrava, 1987; Yokoyama and Fujikoshi, 1993; Yokoyama, 1993), can be expressed as $\Phi = \text{Mat}_q(B\boldsymbol{\gamma})$ where $\boldsymbol{\gamma} = (\boldsymbol{\mu}, \boldsymbol{\beta})'$ and $B = \sum_{u=1}^g \boldsymbol{\delta}_u^{(g)} \otimes B_u$ with

$$B_u = \begin{pmatrix} \boldsymbol{\delta}_u^{(g)'} & \mathbf{0}_{q-1}' \\ O_{(q-1) \times g} & I_{q-1} \end{pmatrix}, \quad u = 1, \dots, g.$$

Example 2 Structure for the model in which all between-individual covariables have no-interaction effect with “time” variable that is specified by $\Psi = (\boldsymbol{\alpha}, O_{h \times (q-1)})'$ can be expressed as $\Psi = \text{Mat}_q(C\boldsymbol{\alpha})$, where $C = \sum_{v=1}^h \boldsymbol{\delta}_v^{(h)} \otimes C_v$ with

$$C_v = \begin{pmatrix} \boldsymbol{\delta}_v^{(h)'} \\ O_{(q-1) \times h} \end{pmatrix}, \quad v = 1, \dots, h.$$

2.2. LINEAR STRUCTURE FOR VARIANCE PARAMETERS

In a similar argument to previous subsection, we also introduce a family of linear structures into the variance parameters. Let σ_m^2 be the parameter defined by (1.3) and Δ_m be the matrix defined by (1.2). Then we assume that they have linear structures as below,

$$\sigma_m^2 = \mathbf{h}_m' \boldsymbol{\tau},$$

$$\Delta_m = \text{Mat}_q(R_m \boldsymbol{\xi}) + V_m, \quad m = 1, \dots, g.$$

where $\mathbf{h}_m$ is a $k_e \times 1$ known vector, $\boldsymbol{\tau}$ is a $k_e \times 1$ vector of parameters, R_m is a $q^2 \times k_b$ known matrix of $\text{rank } R_m = k_b \leq q^2$, $\boldsymbol{\xi}$ is a $k_b \times 1$ vector of parameters, and V_m is a $q \times q$ known matrix.

Example 3 Uniform within-individual error model can be derived from

$$\mathbf{h}_m = \mathbf{h}_1, \quad m = 2, \dots, g.$$

Example 4 Uniform between-individual variation model can be derived from

$$R_m = R_1, \quad \text{and} \quad V_m = V_1, \quad m = 2, \dots, g.$$

Example 5 Null between-individual variation model can be derived from

$$k_b = 0, \quad \text{and} \quad V_m = O_{q \times q}, \quad m = 1, \dots, g.$$

3. Inference on λ

3.1. KNOWN VARIANCE

Let $\theta = (\tau', \xi')'$ denote the vector consisting of the $k = k_e + k_b$ distinct parameters. When θ is known, if we let $\mathbf{u}_i = (X_i' X_i)^{-1} X_i' \mathbf{y}_i$, $i = 1, \dots, N$, then the best linear unbiased estimator of λ is given by the generalized least squares estimator (c.f. Vonesh and Carter(1987), Laired, Lange and Stram(1987)),

$$\hat{\lambda}(\theta) = \left[G' \left\{ \sum_{i=1}^N (\mathbf{a}_i \mathbf{a}_i') \otimes \Gamma_i^{-1}(\theta) \right\} G \right]^{-1} G' \sum_{i=1}^N \mathbf{a}_i \otimes \{ \Gamma_i^{-1}(\theta) \mathbf{u}_i \}, \quad (3.1)$$

where

$$\Gamma_i(\theta) = \sum_{m=1}^g d_{im} \left\{ \text{Mat}_q(R_m \xi) + V_m + (\mathbf{h}_m' \tau)(X_i' X_i)^{-1} \right\}.$$

The variance-covariance matrix of $\hat{\lambda}(\theta)$ is

$$\Omega(\theta) = \left[G' \left\{ \sum_{i=1}^N (\mathbf{a}_i \mathbf{a}_i') \otimes \Gamma_i^{-1}(\theta) \right\} G \right]^{-1}. \quad (3.2)$$

The formula of (3.1) and (3.2) reduce to the results due to Vonesh and Carter (1987) when $G = I_{q(g+h)}$, $k_b = q^2$, $k_e = 1$, $R_m = I_{q^2}$, $V_m = O_{q \times q}$ and $\mathbf{h}_m = 1$, $m = 1, \dots, g$.

3.2. UNKNOWN VARIANCE

When the covariance vector θ is unknown, we can estimate λ by substituting unbiased estimate of θ into (3.1). An unbiased estimate of θ is given by the method of Reinsel(1985) which is based on the individual error mean squares,

$$v_i^2 = \mathbf{y}_i' \left\{ I_{r_i} - X_i (X_i' X_i)^{-1} X_i' \right\} \mathbf{y}_i / (r_i - q),$$

and the “between-individual sample variance-covariance” matrices

$$Q_m = U_m' \{I_{N_m} - Z_m(Z_m'Z_m)^{-1}Z_m'\} U_m / (N_m - h - 1)$$

where $U_m = (\mathbf{u}_{i_1^{(m)}}, \dots, \mathbf{u}_{i_{N_m}^{(m)}})'$, and $Z_m = \begin{pmatrix} 1 & \cdots & 1 \\ \mathbf{z}_{i_1^{(m)}} & \cdots & \mathbf{z}_{i_{N_m}^{(m)}} \end{pmatrix}'$ with $J_m = \{i | \mathbf{d}_i = \boldsymbol{\delta}_m^{(g)}\} = \{i_1^{(m)}, \dots, i_{N_m}^{(m)}\}$. Let $H = (\mathbf{h}_1', \dots, \mathbf{h}_g')'$. Then an unbiased estimator of $\boldsymbol{\tau}$ is given by

$$\hat{\boldsymbol{\tau}} = (H'W_eH)^{-1}H'W_e\mathbf{s},$$

where $\mathbf{s} = (s_1^2, \dots, s_g^2)'$,

$$s_m^2 = \left[\sum_{i \in J_m} (r_i - q) \right]^{-1} \sum_{i \in J_m} (r_i - q) v_i^2, \quad m = 1, \dots, g,$$

and $W_e = \sum_{m=1}^g [\sum_{i \in J_m} (r_i - q)] \boldsymbol{\delta}_m^{(g)} \boldsymbol{\delta}_m^{(g)'}.$ The induced unbiased estimator of σ_m^2 is given by

$$\hat{\sigma}_m^2 = \mathbf{h}_m' \hat{\boldsymbol{\tau}}, \quad m = 1, \dots, g.$$

In terms of $\boldsymbol{\xi}$, let $R = (R_1', \dots, R_g')'$ and

$$D_m(\hat{\boldsymbol{\tau}}) = Q_m - \mathbf{h}_m' \hat{\boldsymbol{\tau}} \sum_{i \in J_m} c_i (X_i' X_i)^{-1}, \quad m = 1, \dots, g,$$

where $c_i = [1 - (\mathbf{1}, \mathbf{z}_i')(Z_m'Z_m)^{-1}(\mathbf{1}, \mathbf{z}_i)'] / (N_m - h - 1)$, $i \in J_m$, $m = 1, \dots, g$. Then the weighted least square estimator $\hat{\boldsymbol{\xi}}$ of $\boldsymbol{\xi}$ is given by

$$\hat{\boldsymbol{\xi}} = (R'W_bR)^{-1}R'W_b \sum_{m=1}^g \boldsymbol{\delta}_m^{(g)} \otimes \text{vec}(D_m(\hat{\boldsymbol{\tau}}) - V_m),$$

which is unbiased, where $W_b = \sum_{m=1}^g (N_m - h - 1) (\boldsymbol{\delta}_m^{(g)} \boldsymbol{\delta}_m^{(g)'} \otimes I_{q^2})$. The induced estimator of Δ_m may be given by

$$\tilde{\Delta}_m(\hat{\boldsymbol{\xi}}) = \text{Mat}_q(R_m \hat{\boldsymbol{\xi}}) + V_m, \quad m = 1, \dots, g. \quad (3.3)$$

One disadvantage of (3.3) is that $\tilde{\Delta}_m(\hat{\boldsymbol{\xi}})$ could fail to be positive semidefinite. In such a case we modify $\tilde{\Delta}_m(\hat{\boldsymbol{\xi}})$ to construct an estimate of Δ_m that is at least positive semidefinite. Suppose that $\tilde{\boldsymbol{\eta}}_m = (\tilde{\eta}_{1m}, \dots, \tilde{\eta}_{qm})'$ is the vector of eigen-values of $\tilde{\Delta}_m(\hat{\boldsymbol{\xi}})$, and that $\tilde{\Delta}_m(\hat{\boldsymbol{\xi}})$ can be expressed as $\tilde{\Delta}_m(\hat{\boldsymbol{\xi}}) = T_m \text{diag}(\tilde{\boldsymbol{\eta}}_m) T_m'$, where T_m is an orthogonal matrix. Then $\tilde{\Delta}_m(\hat{\boldsymbol{\xi}})$ in (3.3) will be non-positive semidefinite if $\min \{\tilde{\eta}_{jm} | j = 1, \dots, q\} < 0$. To guarantee positive semidefinite estimate of Δ_m , we consider the modified estimator

$$\hat{\Delta}_m(\hat{\boldsymbol{\xi}}) = \begin{cases} \tilde{\Delta}_m(\hat{\boldsymbol{\xi}}), & \text{if } \min \{\tilde{\eta}_{jm} | j = 1, \dots, q\} \geq 0, \\ T_m \text{diag}(\hat{\boldsymbol{\eta}}_m) T_m', & \text{if } \min \{\tilde{\eta}_{jm} | j = 1, \dots, q\} < 0, \end{cases}$$

where $\hat{\eta}_m = (\hat{\eta}_{1m}, \dots, \hat{\eta}_{qm})'$, $\hat{\eta}_{jm} = (|\tilde{\eta}_{jm}| + \tilde{\eta}_{jm})/2$, $j = 1, \dots, q$.

If we now denote by $\hat{\theta} = (\hat{\tau}', \hat{\xi}')'$ the vector estimate of $\theta = (\tau', \xi')'$, then an estimated generalized least squares estimate of λ is

$$\hat{\lambda}(\hat{\theta}) = \left[G' \left\{ \sum_{i=1}^N (\mathbf{a}_i \mathbf{a}_i') \otimes \Gamma_i^{-1}(\hat{\theta}) \right\} G \right]^{-1} G' \sum_{i=1}^N \mathbf{a}_i \otimes \{ \Gamma_i^{-1}(\hat{\theta}) \mathbf{u}_i \}, \quad (3.4)$$

where

$$\Gamma_i(\hat{\theta}) = \sum_{m=1}^g d_{im} \{ \hat{\Delta}_m(\hat{\xi}) + (\mathbf{h}_m' \hat{\tau})(X_i' X_i)^{-1} \}.$$

Its estimated variance-covariance matrix is obtained from (3.2) as follows,

$$\hat{\Omega}(\hat{\theta}) = \left[G' \left\{ \sum_{i=1}^N (\mathbf{a}_i \mathbf{a}_i') \otimes \Gamma_i^{-1}(\hat{\theta}) \right\} G \right]^{-1}$$

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