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SELECTED MODELS AND METHODS OF PARAMETER ESTIMATION IN GROWTH CURVES WITH CONCOMITANT VARIABLES

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Summary

This paper presents some growth curve models with concomitant variables. One of them is a new one. These models differ with regard to the values of concomitant variables that can be varied for all experimental units or all time points or for both of them simultaneously. Moreover, suitable methods of parameter estimation and some connections between them are displayed.

Key words and phrases: growth curve methods, concomitant variables, linear mathematical models, parameter estimation methods.

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1. Introduction

The growth curve method is used for the analysis of data, which are obtained when the studied feature is measured on *n* units in *p*-time points. This method can be used to describe the change of course of the feature using polynomial regression in the fixed time interval. It is used to estimate polynomial coefficients and elements of covariance matrix and to verify hypotheses about equality of suitable coefficients for different groups in considered curves. This method was presented by Potthoff and Roy (1964).

In statistical literature one can find numerous works and books that contain solutions of particular problems connected with growth curves. They include among others: different patterns of covariance matrices with the consequence of this in parameters estimation (Lee, 1988), estimation of variance and covariance components in random models (Žežula, 1993), or extension of growth curve model by taking into consideration more parameters matrices of *B* than in Potthoff-Roy's model. Those last models are named the sum of profiles or extended growth curves. The broad theory for the sum of profiles model under the nested subspace condition was given by von Rosen in numerous papers (for example: von Rosen, 1989) and summed up in the book written by Kollo and von Rosen (2005). The theory presented in that book and papers comprise profiles corresponding to different degree of polynomial for the successive group of units.

In this paper we are interested in growth curves estimators when other variables beyond the time have influence on changing studied variable values in time. The values of these additional variables can be measured too, and these values can change in successive time points. These additional variables are called concomitant variables. In such models we have two groups of parameters. They are polynomial and regression coefficients. The number of concomitant variables in the model is denoted by *s*.

A few different types of dependence between the studied feature and concomitant variables can be considered in those models. A few cases can be distinguished when:

a) The concomitant variables values are different and fixed for individual units, but each of this values determine the studied feature value in successive points of time. It can be for example a body mass of animal before a fat.

b) The concomitant variables values are changed in time, but are the same for all experimental units. They can be e.g. meteorological elements on the field in horticular experiments. These values characterize climatic conditions in time points and flow in the studied plant feature.

c) The values of concomitant variables are different for both of them simultaneously i.e. for all units and all points of time. The example of this situation can be the following: for the plants that are grown on various plots and for which the change of their features are studied in time, the contents of mineral components in soil for all plots in the same time points can be measured too.

So additional aspects ought to be taken into consideration during the modelling of change of value of the feature under influence of concomitant variables. The following example illustrates this situation when the dynamics of plant fruit-bearing is considered in the time domain than must determined if:

- reaction on the influence of concomitant value is the same for all plants,
- different group of plants can react to this influence in various way,
- values of concomitant variables are the same or different for all units in separate time points.

2. Models and suitable estimation methods

2.1. Potthoff-Roy's method

The first model to be presented is Potthoff and Roy's (1964) one that does not contain concomitant variables. It is a multivariable model presented in the following form

$$\mathrm{Y} = \mathrm{ABT} + \mathrm{E}\,, \tag{2.1}$$

where *Y* is $n \times p$-matrix of observations of feature on *n* experimental units in p time points, *A* is $n \times a$-known matrix which divides experimental units on *a* group, *B* - is $a \times q$-matrix of unknown coefficients in searched polynomial growth curves of $q-1$ degree, *T* is $q \times p$- matrix that include the successive powers of time points from 0 to *q*-1 (it is Vandermon's matrix) that defines internal structure of observations and *E* is a $n \times p$ - matrix of random errors. If all units are homogeneous then $A = J_n$, where J_n is a vector of *n* ones, but if observations are subject to two way classification then matrix *A* is a non full rank. To continue our considerations in this paper, matrix *A* is taken as in a one way classification without the column of ones.

This model is considered under assumption that rows of matrix *Y* are uncorrelated, but columns are correlated with common covariance matrix $\underset{pp}{\Sigma}$. Additionally, a matrix of observations is a multivariate normally distributed. This assumption can be presented as

$$Y \sim N_{np}(ABT, \underset{pp}{\Sigma} \otimes I_n)$$

where I_n is a unit matrix of n dimension.

Estimators of parameters in this model that are coefficients in polynomials in matrix B and covariance matrix Σ obtained by maximum likelihood method (Kshirsagar, 1988) are given in following form:

$$\hat{B} = (A'A)^{-1} A'Y\hat{\Sigma}^{-1}T'(T\hat{\Sigma}^{-1}T')^{-1} \tag{2.2}$$

and

$$\hat{\Sigma} = \frac{1}{n} Y'[I_n - A(A'A)^{-1} A']Y\,. \tag{2.3}$$

2.2 Growth curves with fixed value of concomitant variables

In many situations, when the course of changes of the feature is related to feature values before the study for each unit or additionally to values of other features, then model is the following

$$Y = ABT + \underset{ns}{X}\,\underset{sp}{\Gamma} + E\,, \tag{2.4}$$

where the matrices Y, A, B, T are the same as in model (2.1) and X is $n \times s$ -matrix of values of s concomitant variables for each of n units and Γ is $s \times p$ -matrix of unknown regression coefficients in p time points. Suitable estimators of B and Γ obtained by generalized least squares method were given in the paper by Wesołowska-Janczarek (1996). If the covariance matrix was known there were following:

$$\hat{\boldsymbol{\gamma}} = R[\Sigma^{-1} \otimes X' - \Sigma^{-1}T'(T\Sigma^{-1}T')^{-1}T\Sigma^{-1} \otimes X'A(A'A)^{-1}A']\mathbf{y}$$

where $\underset{ps,ps}{R} = [\Sigma^{-1} \otimes X'X - \Sigma^{-1}T'(T\Sigma^{-1}T')^{-1}T\Sigma^{-1} \otimes X'A(A'A)^{-1}A'X]^{-1}$ (2.5)

and $\hat{\beta} = \{[(T\Sigma^{-1}T')^{-1}T\Sigma^{-1} \otimes (A'A)^{-1}A']\mathbf{y} - (T\Sigma^{-1}T')^{-1}T\Sigma^{-1} \otimes (A'A)^{-1}A'X\}\hat{\boldsymbol{\gamma}}$

where $\boldsymbol{\gamma} = vec(\Gamma)$, $\boldsymbol{\beta} = vec(B)$ and $\mathbf{y} = vec(Y)$ and operator $vec()$ sets columns of the matrix one under another.

If Σ is unknown then it can be replaced by

$$\hat{\Sigma} = \frac{1}{n} Y'[I_n - A(A'A)^{-1} A']Y .$$

2.3. Growth curve with concomitant variables changing in time and the same values for all units

In same experiments there are additional factors that can be influenced in the studied feature and these changing values can be measured in considered time points. This income ought to be taken into consideration and it can be considered in two ways. The first is when concomitant variables value are the same for all units in successive time points and the second is when these values are different for each of the units and for all time points. Now we consider the first of this ways.

A suitable model and parameter estimation were presented in the paper by Wesołowska-Janczarek and Fus (1996). This model is the following

$$Y = ABT + J_n \boldsymbol{\gamma}' X + E , \tag{2.6}$$

where the matrices *Y*, *A*, *B*, *T* and *E* are the same in model (2.1), *X* is $s \times p$ - matrix of values of these *s* variables in successive time points, $\boldsymbol{\gamma}$ is a vector of *s* regression coefficients at concomitant variables and J_n is the vector of *n* ones.

Under the assumptions $Y \sim N_{np}(ABT + J_n \boldsymbol{\gamma}' X ; \Sigma \otimes I_n)$ and $\Sigma > 0$ estimators of parameters in this model obtained by the maximum likelihood method were given in following form:

$$\begin{aligned}
n\hat{\Sigma} &= (Y - A\hat{B}T - \mathbf{1}_n \hat{\boldsymbol{\gamma}}' X)'(Y - A\hat{B}T - \mathbf{1}_n \hat{\boldsymbol{\gamma}}' X) \\
\hat{B}_{\hat{\Sigma}} &= (A'A)^{-} A'(Y - \mathbf{1}_n \hat{\boldsymbol{\gamma}}' X)\hat{\Sigma}^{-1} T'(T\hat{\Sigma}^{-1} T')^{-1} \\
\hat{\boldsymbol{\gamma}}_{\hat{\Sigma}} &= [\mathbf{1}'_n Y - \mathbf{1}'_n A(A'A)^{-} A'Y\hat{\Sigma}^{-1} T'(T\hat{\Sigma}^{-1} T')^{-1} T]\hat{\Sigma}^{-1} X' R_{\hat{\Sigma}} \\
R_{\hat{\Sigma}} &= [nX\hat{\Sigma}^{-1} X' - \mathbf{1}'_n A(A'A)^{-} A'\mathbf{1}_n X\hat{\Sigma}^{-1} T'(T\hat{\Sigma}^{-1} T')^{-1} T\hat{\Sigma}^{-1} X']^{-1}.
\end{aligned} \tag{2.7}$$

The values of these estimators can be calculated by the iterative method where in the first step the following form of a matrix will be taken $\hat{\Sigma} = Y'[I_n - A(A'A)^{-1}A]Y$.

This model can be changed if the reaction of each of *a* groups units on influence the same values of concomitant variables can be various. Then model (2.6) can be written in the following (Wesołowska-Janczarek, 1996)

$$Y = ABT + A\Gamma X + E = A[B \vdots \Gamma]\begin{bmatrix} T \\ \cdots \\ X \end{bmatrix} + E = AB^*T^* + E\,, \tag{2.8}$$

where Γ is a $a \times s$ - matrix where the elements are unknown regression coefficients between the studied feature *y* and concomitant variables for each of *a* group. Estimators B^* i Σ can be obtained from (2.2) and (2.3) if *B* and *T* will be replaced by B^* i T^*.

2.4. Growth curve with changing in time concomitant variables and when their values are different for all units in all time points

Now the values of studied feature depended on *s* concomitant variables for each of *n* units as previously but their values are different for each of *n* units and for each of *p* time points. Experimental data are composed of matrix *Y* of the studied feature values taken on *n* units in *p* time points and *p* $n \times s$ - matrices X_i $(i = 1,..., p)$ of values of *s* concomitant variables in *i* time point for each of *n* units. Here there are two cases, too. The first is when changes of values of concomitant variables in each of *i*-time point are random and independent from time and the other if concomitant variables values are changed in time too.

A) First case

In the first case the concomitant variables values cannot be marked in the model, together with growth curve, but this changeability cannot be omitted. It can be done by proper estimation of covariance matrix. Suitable method of estimation growth curves with elimination of concomitant variables changeability was proposed in the paper by Wesołowska-Janczarek (2007). It is a two-stage method. In the first step regression coefficients are estimated $\boldsymbol{\gamma}'_i = [\gamma_{i1}, \gamma_{i2},..., \gamma_{is}]$ for each $i = 1,..., p$ time points using linear regression relation between *i*-column of matrix $Y = [\mathbf{y}_1, \mathbf{y}_2,..., \mathbf{y}_p]$ and $\boldsymbol{\gamma}_i$ using $n \times s$ - matrix X_i. Then

$$\mathbf{y}_i = X_i \boldsymbol{\gamma}_i + \boldsymbol{\varepsilon}_i \quad \text{dla} \quad i = 1,..., p . \tag{2.9}$$

From here estimator of $\boldsymbol{\gamma}_i$ obtained by the least square method is

$$\boldsymbol{\gamma}_i = (X_i' X_i)^{-1} X_i' y_i \quad \text{for} \quad i = 1,..., p \tag{2.10}$$

and n estimator of covariance matrix for observations matrix Y can be obtained using n-dimension vectors of residuals

$$\mathbf{u}_i = \mathbf{y}_i - \hat{X}_i \hat{\boldsymbol{\gamma}}_i \qquad \text{for } i = 1,.., p . \tag{2.11}$$

Then these vectors can be put together into a matrix $\underset{np}{U} = [\mathbf{u}_1, \mathbf{u}_2,....,\mathbf{u}_p]$, and an estimator of covariance matrix $\boldsymbol{\Sigma}$ that must be used into Potthoff-Roy method in (2.2) to estimate curves is the following

$$S = U'[I_n - A(A'A)^{-1} A]U \tag{2.12}$$

or $\hat{\boldsymbol{\Sigma}} = S$.

It is worth noticing that if values of concomitant variables are the same for all units in individual time points i.e.

$$\underset{ns}{X_i} = J_n \otimes [x_{1i}, x_{2i},..., x_{si}] \quad i = 1,..., p \tag{2.13}$$

then in (2.12) there is

$$U'[I - A(A'A)^{-1} A']U = Y'[I - A(A'A)^{-1} A']Y \tag{2.14}$$

(see Wesołowska-Janczarek and Kolczyńska, 2008) and estimators obtained by two-step methods are the same as gained by Patthoff-Roy's method.

B) Second case

In the case when concomitant variables values are changing in time, the dependence between feature of y and concomitant variables ought to be taken into consideration in the model.

A proposal for the model is the following

$$\mathbf{y} = (T' \otimes A)vec(B) + D\boldsymbol{\gamma} + e \tag{2.15}$$

where $\mathbf{y} = vec(Y)$, $\boldsymbol{\gamma} = [\gamma' , \gamma'_2 ,..., \gamma'_p]'$, $\boldsymbol{\beta} = vec(B)$, $\otimes$ is a Kronecker product of two matrices and D is $np \times ps$ - matrix of the form:

$$\underset{np,sp}{D} = \begin{bmatrix} X_1 & 0 & \dots & 0 \\ 0 & X_2 & \dots & 0 \\ \hline 0 & 0 & \cdots & X_p \end{bmatrix} = diag(X_1, X_2,..., X_p), \tag{2.16}$$

and matrices of X_i are the same as in formula (2.9).

This linear model (2.15) can be written as:

$$\mathbf{y} = [(T' \otimes A) \vdots D] \begin{bmatrix} \boldsymbol{\beta} \\ \boldsymbol{\gamma} \end{bmatrix} + e \tag{2.17}$$

B1) $\Sigma_Y = \sigma^2 I_{np}$

If the feature in time points is uncorrelated, then $\Sigma_Y = \sigma^2 (I_n \otimes I_p)$ then using least square method estimators of vector of parameters can be obtained in the form:

$$\begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix} = \begin{bmatrix} TT' \otimes A'A & (T \otimes A')D \\ \hline D'(T' \otimes A) & D'D \end{bmatrix}^{-1} \begin{bmatrix} T \otimes A' \\ D' \end{bmatrix} \mathbf{y}. \tag{2.18}$$

If moreover $X_1 = X_2 = ... = X_p = X$,then $D = I_p \otimes X$ and

$$\begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix} = \begin{bmatrix} TT' \otimes A'A & T \otimes A'X \\ \hline T' \otimes X'A) & I \otimes X'X \end{bmatrix}^{-1} \begin{bmatrix} T \otimes A' \\ I \otimes X' \end{bmatrix} \mathbf{y}. \tag{2.19}$$

If additionally condition $A'X = 0$ be fulfilled then

$$\hat{\boldsymbol{\beta}} = [(TT')^{-1} \otimes (A'A)^{-1}](T \otimes A')\mathbf{y} = [(TT')^{-1}T \otimes (A'A)^{-1}A]'\mathbf{y}$$

and (2.20)

$$\hat{\boldsymbol{\gamma}} = (I \otimes (X'X)^{-1})(I \otimes X)\mathbf{y} = [I \otimes (X'X)^{-1}X']\mathbf{y}$$

and then these formulas can be written as:

$$\hat{B} = (A'A)^{-1}A'YT'(TT')^{-1}$$

and (2.21)

$$\hat{\Gamma} = (X'X)^{-1}X'Y \quad \text{where} \quad \hat{\Gamma} = [\hat{\boldsymbol{\gamma}}_1, \hat{\boldsymbol{\gamma}}_2, ..., \hat{\boldsymbol{\gamma}}_p]$$

and it is means that the estimator of coefficients in growth curves is the same as given by (2.2) with $\hat{\Sigma} = \sigma^2 I_{np}$.

B2) $\hat{\Sigma}_y = \underset{pp}{\Sigma} \otimes I_n$

If the known covariance matrix in (2.17) is different from $\sigma^2 I_{np}$ then to estimate matrices of parameters the generalized least squares method can be used. Then the normal equations are as follows:

$$\begin{bmatrix} T \otimes A' \\ D' \end{bmatrix} (\Sigma \otimes I_n)^{-1} [T' \otimes A \vdots D] \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix} = \begin{bmatrix} T \otimes A' \\ D' \end{bmatrix} (\Sigma \otimes I_n)^{-1} \mathbf{y}$$

and the estimator of vector of parameters is

$$\begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix} = \begin{bmatrix} T\Sigma^{-1}T' \otimes A'A & (T\Sigma^{-1} \otimes A')D \\ D'(\Sigma^{-1} \otimes I_n) & D'(\Sigma^{-1} \otimes I_n)D \end{bmatrix}^{-1} \begin{bmatrix} T\Sigma^{-1} \otimes A' \\ D'(\Sigma^{-1} \otimes I_n) \end{bmatrix} \mathbf{y}. \quad (2.22)$$

These estimators can be written in the form:

$$\hat{\boldsymbol{\gamma}} = R^* \{D'(\Sigma^{-1} \otimes I_n) - (\Sigma^{-1}T'(T\Sigma^{-1}T')^{-1}T\Sigma^{-1} \otimes A(A'A)^{-1}A')\}\mathbf{y}$$

where (2.23)

$$R^* = \{D'(\Sigma^{-1} \otimes I_n)D - D'[\Sigma^{-1}T'(T\Sigma^{-1}T')^{-1}T\Sigma^{-1} \otimes A(A'A)^{-1}A']D\}^{-1}$$

and $\hat{\boldsymbol{\beta}} = \{[(T\Sigma^{-1}T')]^{-1}T\Sigma^{-1} \otimes (A'A)^{-1}A'] \cdot$

$$[I - DR^{*}D'[\Sigma^{-1}T'(T\Sigma^{-1}T')^{-1}T\Sigma^{-1} \otimes A(A'A)^{-1}] - DR^{*}D'(\Sigma^{-1} \otimes I_n)]\}\mathbf{y}.$$

If additionally $X_1 = X_2 = ...X_p = X$, then $D = I_p \otimes X$ and the estimators of $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ are the same as in (2.5) for model (2.4). Moreover, if the covariance matrix Σ is not known, then as the estimator can be taken a matrix $S = \frac{1}{n}Y'[I_n - A(A'A)^{-1}A']Y$.

3. Concluding remarks

The growth curve with concomitant variables is the method to which problems of polynomial regression with multiple regression are connected.

The review of known models and proper estimation methods is supplemented by a new model for growth curve with concomitant variables, whose values are different for all units and for all time points simultaneously. This model (2.17) and the proper parameter estimation method was considered under assumptions $\Sigma_y = \sigma^2 I_{np}$ and $\Sigma_y = \Sigma \otimes I_n$.

A choice of the proper model and suitable estimation method ought to be compiliant with the problem character and data that are the disposal of the experimenter.

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WYBRANE MODELE I METODY ESTYMACJI PARAMETRÓW W KRZYWYCH WZROSTU ZE ZMIENNYMI TOWARZYSZĄCYMI

Streszczenie

Dla problemu krzywych wzrostu ze zmiennymi towarzyszącymi dokonano przeglądu różnych modeli uwzględniając trzy przypadki zróżnicowanych wartości zmiennych towarzyszących dla: różnych jednostek, dla różnych punktów czasowych oraz jednocześnie dla obu z nich. Podano odpowiednie metody estymacji parametrów i związki zachodzące między nimi. Model i estymacja parametrów dla najbardziej ogólnego trzeciego z wymienionych przypadków są nową propozycją zawartą w tej pracy.

Słowa kluczowe: krzywe wzrostu, zmienne towarzyszące, liniowe modele matematyczne, estymacja parametrów.

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