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TWO SPECIAL VARIANCE STRUCTURES IN THE GROWTH CURVE MODEL

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ABSTRACT. The properties of estimators of variance components, mainly their behaviour when normality assumption is violated, are studied in the growth curve model with special variance structures. The results of simulations are presented.

1. Introduction

The growth curve model was introduced by Potthoff and Roy [1], and during many years it has proved to be a very useful tool for different applications. It combines ANOVA and regression analysis in a special way, which does not have direct analogue in one-dimensional models. Its basic form is:

$$Y = XBZ + e,$$
$$\mathrm{E}(e) = 0, \quad \mathrm{var}\big(\mathrm{vec}(e)\big) = \Sigma \otimes I,$$

where $Y_{n\times p}$ is a matrix of n independent p-dimensional observations, $X_{n\times m}$ and $Z_{r\times p}$ are known design matrices (X is the ANOVA design matrix and Z is the matrix of regression design points) and $e_{n\times p}$ is the error matrix. $B_{m\times r}$ and $\Sigma_{p\times p}$ are unknown matrices of the first (regression coefficients) and the second (describing the dependence of the columns of Y) order parameters, respectively. The vec operator vectorizes a matrix by stacking its columns and the sign $\otimes$ denotes Kronecker product.

Standard least squares estimator of B — if B is estimable — is

$$\hat{B} = (X'X)^{-}X'Y\Sigma^{-1}Z'(Z\Sigma^{-1}Z')^{-}.$$

However, this estimator is a function of Σ, which is rarely known in practical applications, and therefore it has to be estimated. There is no problem estimating

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Σ when it is completely unknown. Under normality, its uniformly minimum variance unbiased invariant estimator (UMVUIE) is

$$\hat{\Sigma} = \frac{1}{n - r(X)} Y' M_X Y, \tag{1}$$

where $M_X = I - X(X'X)^- X'$ (for details see [3]). Problems arise in situations when the structure is partially known. It is because partial knowledge adds constraints to the estimation (optimization) process. In this case Σ can be expressed in the form

$$\Sigma = \sum_i \theta_i V_i \,,$$

where $\theta_i, i = 1, \dots, k < n(n+1)/2$ are unknown constants (variance components), and V_i are known matrices. The whole vector $\boldsymbol{\theta} = (\theta_1, \dots, \theta_k) \in \mathcal{F} = \{\boldsymbol{\theta}; \sum_i \theta_i V_i \geq 0\}$. Estimation of variance components in this general model was intensively studied in the past. However, special questions arise when different types of parametrization are used. Some applications came up with the following structures of the variance matrix:

(1) the uniform correlation structure (sometimes also called compound symmetry structure)

$$\Sigma = \sigma^2 \big((1-\rho) I + \rho \mathbf{1}\mathbf{1}' \big),$$

(2) the autoregressive correlation structure (also called serial correlation structure)

$$\Sigma = \sigma^2 \begin{pmatrix} 1 & \rho & \dots & \rho^{p-1} \\ \rho & 1 & \dots & \rho^{p-2} \\ \vdots & \vdots & \ddots & \vdots \\ \rho^{p-1} & \rho^{p-2} & \dots & 1 \end{pmatrix}.$$

Žežula [4] introduced simple estimators of both unknown parameters (σ^2 and ρ) based on (1), in both variance structures. In uniform variance structure model, explicit formulas are available:

$$\hat{\sigma}^2_S = \frac{\mathrm{Tr}(\hat{\Sigma})}{p} \,,$$

$$\hat{\rho}_S = \frac{1}{p-1} \left(\frac{\mathbf{1}'\hat{\Sigma}\mathbf{1}}{\mathrm{Tr}(\hat{\Sigma})} - 1 \right).$$

It has been shown that under normality these estimators are numerically very close to the UMVUEs, and supersede MLEs (measured by MSE). In autoregressive correlation structure model, estimator of σ^2 is the same as before, while estimator of ρ is the solutions of the following equation:

$$\hat{\sigma}^2 = \frac{\mathrm{Tr}(\hat{\Sigma})}{p}\,,$$
$$\hat{\rho}(p-1) + \hat{\rho}^2(p-2) + \cdots + \hat{\rho}^{\,p-1} = \frac{p}{2}\left(\frac{\mathbf{1}'\hat{\Sigma}\mathbf{1}}{\mathrm{Tr}(\hat{\Sigma})} - 1\right).$$

Only little is known about properties of these estimators. Wu [2] derives MLE of σ^2 only for the case when ρ is known. However, all these estimators are based on unbiased estimating equations (for details see [4]).

All above mentioned estimators were derived under normality assumption, i.e.,

$$\mathrm{vec}(Y) \sim N\big(\mathrm{vec}(XBZ), \Sigma \otimes I\big)\,.$$

The estimator of σ^2 is unbiased in both structures, while the estimator of ρ is biased. The most common criterion for comparison of biased estimators is the mean square error (MSE), which turns into variance for unbiased ones.

Our main question was, how these estimators behave when the data are non-normal, and compare it with the normal case. In particular, we were interested in the following questions:

- How the bias of the estimators changes under different distributions?
- What happens with the MSE of the estimators?

To put it other way, we wanted to study the robustness of estimators of σ^2 and ρ with respect to the violation of normality assumption.

Second problem is connected with MSE. MSE of $\hat{\sigma}^2$ and $\hat{\rho}$ in the model with uniform correlation structure can be expressed also by means of the true values of parameters (see [4]):

$$\begin{aligned}\mathrm{MSE}_*\ \hat{\sigma}^2 &= \frac{2\sigma^4}{n-r(X)} \cdot \frac{1+(p-1)\rho^2}{p}, \\ \mathrm{MSE}_*\ \hat{\rho} &= \frac{2}{n-r(X)} \cdot \frac{(1-\rho)^2\big(1+(p-1)\rho\big)^2}{p(p-1)} + o\left(n^{-1}\right).\end{aligned} \tag{2}$$

Therefore, one possible way of estimating MSE is by substitution of estimated values into these relations. We can call them naive MSE estimators. We were interested, whether such estimators are good ones, i.e., whether they are close to their true values.

Third problem concerns $\hat{\rho}$. This estimator is biased, and its distribution is difficult to tackle. R. A. Fisher developed a transformation of sample correlation coefficient, so-called Z-transformation, which has asymptotically normal distribution (thus allowing easy testing of the coefficient). The well-known formula for the transformation is:

$$Z = \frac{1}{2} \ln \left(\frac{1+\hat{\rho}_n}{1-\hat{\rho}_n} \right),$$

where $\hat{\rho_n}$ is the standard normal-theory estimator of ρ. We were interested in how this transformation of $\hat{\rho}$ behaves under different base distributions.

2. Simulations

Model describing quadratic growth in two groups was used for simulations, with altogether 27 observations. This is quite a typical sample size in many biological applications, and our aim wasn't to study the effect of different sample sizes. The dimensions used were as follows: $n = 27$ (11 observations in the first group, and 16 in the second one), $p = 4$, $m = 2$, $r = 3$. The chosen value of matrix B used in our simulations, as well as those of X and Z and sample size, was based on data from [1]. Values of σ^2 and ρ were also chosen. Then, error term was added to known product XBZ. As base distributions for this were used: normal $N(0{,}1)$, $N(5{,}1)$, $N(0{,}16)$, $N(0{,}625)$, mixture of normal and exponential $0.3N(0{,}1)+0.7Exp(1)$, beta $B(2{,}2)$, $B(1/2{,}1/2)$, $B(3/4{,}5/4)$, Laplace $La(1)$. At first, independent errors from a base distribution were generated. Then, mean value of the distribution was subtracted (with the exception of $N(5{,}1)$), and finally, linear transformation was done in order to get required correlation structure in all rows.

In all cases the value of σ^2 coincided with the variance of the base distribution used. The considered values of parameter ρ were:

(i) in model with uniform correlation structure: -0.3, -0.1, 0.1, 0.5, 0.75, 0.96 (here ρ must belong to $\langle -1/(p-1); 1\rangle$, see [4]);

(ii) in model with autoregressive correlation structure: -0.75, -0.5, -0.1, 0.1, 0.5, 0.75, 0.96 (here ρ can belong to the whole interval $\langle -1; 1\rangle$).

In each case 5000 models were generated and parameter estimates were computed.

To address the second problem in uniform correlation model, the MSE estimate was computed by two methods. First, it was computed by substitution of parameter estimates into formula (2). Second, using the knowledge of the true parameter value, it was computed by the standard formula

$$\mathrm{MSE} = \frac{1}{m} \sum_{i=1}^{m} (u_i - w)^2,$$

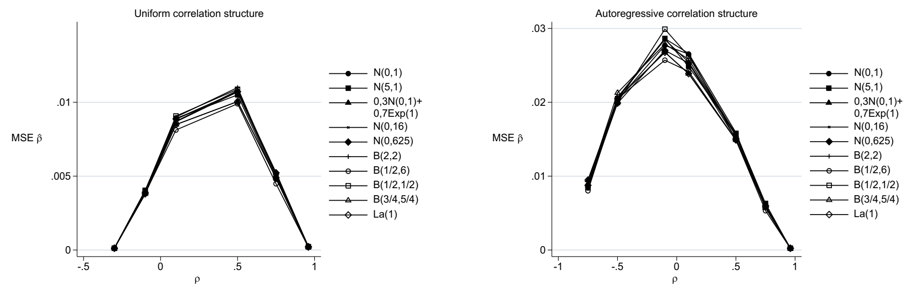

FIGURE 1. Influence of the change of true value of parameter ρ to MSE of its estimator.

where m (=5000) is the number of observations, u_i are the estimates computed, and w is true value of relevant parameter.

3. Results

The arithmetic mean of estimates of both parameters was not influenced by the change of distribution. This statistic was close to the true values of parameters for all chosen distributions and all chosen values of parameters. It means that all used distributions gave results comparable to $N(0,1)$, and no substantial bias appeared. Realize that the departures from normality were of different types: high skewness, heavy tails, short tails, U-shaped density. In this sense all proposed estimators are robust.

However, MSE was influenced by the change of distribution in both considered models. This claim concerns primarily the MSE of $\hat{\sigma}^2$; MSE $\hat{\rho}$ varied little with the change of distribution.

MSE of $\hat{\sigma}^2$ depended on the true value of σ^2 — relative error increased with the parameter value.

MSE was also influenced by the change of the true value of ρ:

- estimator $\hat{\sigma}^2$: MSE was smaller for true values of parameter ρ close to zero (Figure 2),
- estimator $\hat{\rho}$: MSE was smaller for true values of parameter ρ close to its upper and lower bound (Figure 1).

The dependence on the true value of ρ is opposite for the two parameter estimators — when one has the smallest MSE, the second has the biggest MSE.

Figure 2 shows quite big differences in MSE of $\hat{\sigma}^2$ between different base distributions:

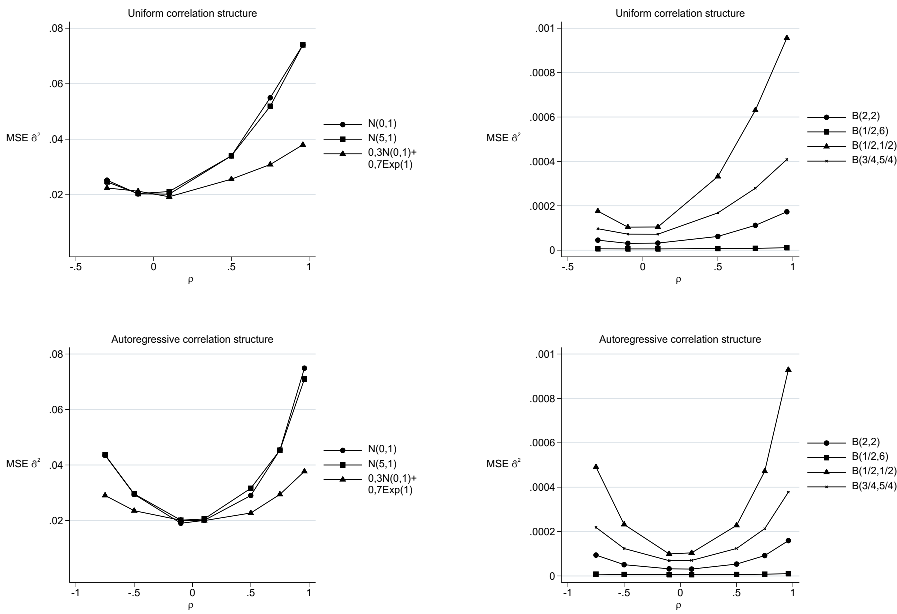

FIGURE 2. Influence of the change of true value of parameter ρ to MSE of estimator of parameter σ^2.

What concerns the second problem in uniform correlation model, Figure 3 shows the ratio MSE $\hat{\rho}/\text{MSE}_* \hat{\rho}$ for different base distributions. We can see that this ratio is close to 1 for all chosen distributions and all true values of ρ. As a result, naive MSE estimator of $\hat{\rho}$ is usable.

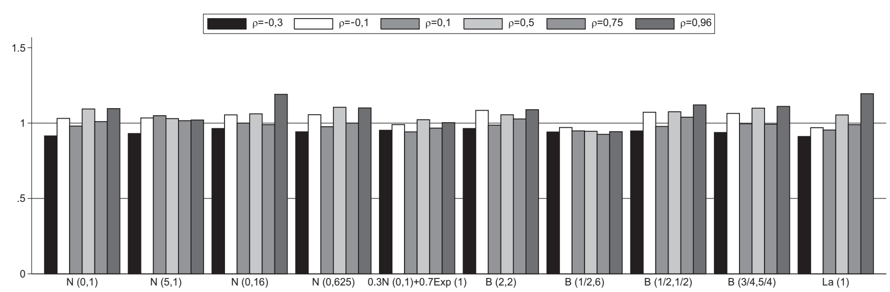

FIGURE 3. The ratio $\text{MSE}\hat{\rho}/\text{MSE}_*\hat{\rho}$.

For the estimator $\hat{\sigma}^2$ MSE of both types is comparable only for normal distribution. Figure 4 shows that for other distributions the ratio $\mathrm{MSE}\,\hat{\sigma}^2/\mathrm{MSE}_*\,\hat{\sigma}^2$ is markedly different from 1. We can conclude, that estimator of σ^2 is much more sensitive to the change of distribution than that of ρ.

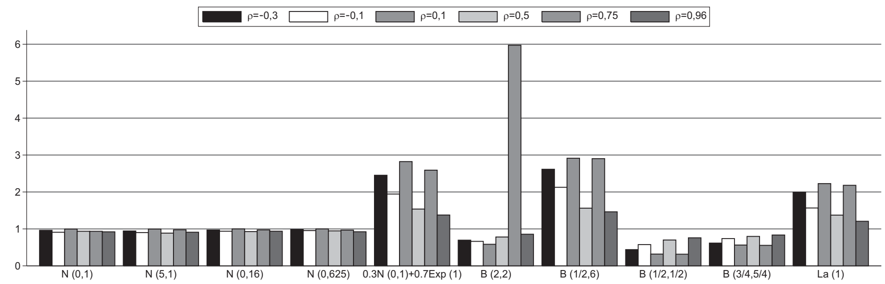

FIGURE 4. The ratio $\mathrm{MSE}\hat{\sigma}^2/\mathrm{MSE}_*\hat{\sigma}^2$.

The third problem concerned the Z-transformation of $\hat{\rho}$. The main question of interest was whether this transformation can bring approximate normality. It is to be stressed, that used estimators of ρ arise in a quite different way than Pearsonian sample correlation coefficient, and in the uniform model even the lower bound is different. However, the Z-transformation has variance stabilization property in the normal case, and therefore it was interesting to investigate its behaviour in this case (this question was proposed to one of the authors by Sir D. Cox). When the transformation was applied, three tests of normality of the empirical distribution were carried out by: Shapiro—Wilk, Shapiro—Francia and Jarque—Bera. These tests indicate that Z-transformation is not very useful for considered estimators of ρ. In the model with uniform correlation structure the hypothesis of normality was rejected mostly when the true value of parameter ρ was close to its constraints. The situation was opposite for the second correlation structure — the hypothesis was rejected mostly when the true value of parameter ρ was close to zero.

4. Summary

The distributional change does not seem to have substantial influence on bias of unknown parameters in both considered models. Bias does not also depend on true value of parameters. On the other hand, MSE of estimators seems to be sensitive to the type of distribution, and to the true value of parameters. In particular, MSE of estimator $\hat{\rho}$ was sensitive only to the change of true value of ρ. On the other hand, MSE of estimator $\hat{\sigma}^2$ was strongly influenced by distributional changes, and by true values of both σ^2 and ρ.

The naive MSE estimator of $\hat{\rho}$ in the uniform correlation model is usable, but we cannot recommend using the naive MSE estimator of $\hat{\sigma}^2$ when the error distribution is not normal.

Z-transformation of the estimators of ρ, also is not recommended in the investigated models.

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