第50卷第9期 中国科学技术大学学报 Vol. 50, No. 9
2020年9月 JOURNAL OF UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA Sep. 2020

文章编号:0253-2778(2020)09-1266-11

A Cholesky factor model in correlation modeling for discrete longitudinal data

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Abstract: A joint mean-correlation regression model framework was proposed for a family of generic discrete responses either balanced or unbalanced, and a Cholesky decomposition method was used for statistically meaningful reparameterization of correlation structures. To overcome computational intractability in maximizing the full likelihood function of the model, a computationally efficient Monte Carlo expectation maximization (MCEM) approach was proposed. Theoretical properties were also established for the resulting estimators. Simulation studies and a real data analysis show that the proposed approach yields highly efficient estimators for the parameters.

Key words: discrete longitudinal data; Cholesky decomposition; mean-correlation regression model; Monte Carlo expectation maximization

CLC number: O212.1 **Document code**: A doi:10.3969/j.issn.0253-2778.2020.09.006

2010 Mathematics Subject Classification: 62F12

Citation: LI Yezhen, ZHANG Weiping. A Cholesky factor model in correlation modeling for discrete longitudinal data[J]. Journal of University of Science and Technology of China, 2020, 50(9): 1266-1276.

李叶蓁,张伟平. 一种离散纵向数据相依结构建模的 Cholesky 因子模型[J]. 中国科学技术大学学报, 2020,50(9):1266-1276.

一种离散纵向数据相依结构建模的 Cholesky 因子模型

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摘要:对一类响应变量为离散型的平衡或非平衡纵向数据,提出了均值-相关系数联合回归模型框架,并且使用 Cholesky 分解方法对模型的相关结构进行参数化,使其具有良好的统计解释性. 为了解决似然推断中高维积分计算的难题,提出了一种高效的蒙特卡罗期望最大化(MCEM)算法,并证明了参数估计的渐近性质. 模拟实验和实际数据分析表明提出的方法是高度有效的.

关键词:离散纵向数据;Cholesky 分解;均值-相关系数回归模型;蒙特卡罗期望最大化算法

Received: 2020-03-30; **Revised**: 2020-06-18

Foundation item: Supported by the NSFC of China (11671374, 71771203, 71631006).

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0 Introduction

Longitudinal data, with repeated measurements collected from the same subject, are frequently encountered. Various models and methods for dealing with longitudinal data analysis are proposed in literature; see, among others, Refs. [1-2] for overviews of the methods in this area. It is well recognized that properly accounting for the correlation between these repeated measurements is important, not only for correct statistical inference, but also for efficiency in estimation. Recently, regression analysis of the covariance structure has attracted increasing attention. See Refs. [3-7] for related discussion. For discrete longitudinal data, however, there is no unified framework for the joint distribution of discrete longitudinal variables. Hence, modeling the within subject correlations/covariances are essentially case by case; see, for example, the Markov chain approach[8] for binary data, and other marginal approaches[9-10] for Poisson, multinomial, and other types of variables. The GEE approaches[11] and their variations have also been employed for studying discrete longitudinal data. For modeling a generic class of discrete and mixed types of variables in longitudinal data, Song et al.[12] proposed a Gaussian copula based approach to integrate separate one-dimensional generalized linear models into a joint regression analysis of continuous, discrete, and mixed correlated outcomes. Most recently, Tang et al.[13] proposed to model the discrete longitudinal responses with the Gaussian copula whose correlation matrix is modeled with the regression approach by using the hyperspherical parametrization[7].

We propose a copula-based joint mean-correlation modeling approach for discrete longitudinal data. The correlation structures for a family of generic discrete responses are decomposed by a moving average Cholesky decomposition. Unlike the hyperspherical parametrization in Ref. [13], the moving average Cholesky decomposition has a more direct interpretation of the statistical meaning and is particularly appealing because of the natural ordering of the variable in longitudinal data. Since the likelihood inference is computationally intractable in general, we develop a type of Monte Carlo expectation maximization (MCEM) based method for estimation.

The article is organized as follows. Section 1 introduces the joint mean-correlation model and the moving average Cholesky decomposition for correlation matrix. Section 2 provides the estimation procedure for our model. Section 3 presents extensive numerical simulations and a real data analysis. Conclusions are found in Section 4.

1 Models

1.1 Gaussian copula for discrete data

We denote by $\boldsymbol{y}_i=(y_{i1},\cdots,y_{im_i})^{\mathrm{T}}$ the m_i longitudinal measurements from the ith subject ($i=1,\cdots,n$), where the discrete response y_{ij} of interests is observed at time t_{ij}. Let $\boldsymbol{t}_i=(t_{i1},\cdots,t_{im_i})^{\mathrm{T}}$ and $\boldsymbol{x}_{ij}\in\mathbb{R}^p$ be the explanatory variable associated with the jth measurement of subject i. Here $\boldsymbol{t}_i$ and m_i can be subject specific so that the model is capable of handling unbalanced longitudinal data sets observed at irregularly spaced time points.

With multiple subjects, we denote the observations as $\{y_{ij},\boldsymbol{x}_{ij},t_{ij}\}$ ($i=1,\cdots,n$; $j=1,\cdots,m_i$). For categorical responses, we assume that y_{ij} follows an exponential family distribution so that the generalized linear models (GLMs) can be used for the discrete responses marginally[14]. That is, the probability mass function of y_{ij} takes the form $f(y)=c(y;\varphi)\exp\{[y\theta-\psi(\theta)]/\varphi\}$ with the canonical parameter θ and scale parameter φ.

For parsimoniously modeling the mean of y_{ij}, $\mu_{ij}=E(y_{ij})$, the traditional strategy of GLM is applied to incorporate the available explanatory variable $\boldsymbol{x}_{ij}$:

$$g(\mu_{ij})=\boldsymbol{x}_{ij}^{\mathrm{T}}\boldsymbol{\beta} \tag{1}$$

with the known transformation $g(\cdot)$ and unknown model parameter $\boldsymbol{\beta}$.

To fill the gap between the marginal distributions and the joint distributions, we consider the copula model. A function $C(u_1,\cdots,u_d)$ is called a copula function if it is a distribution function with each of its margins uniformly distributed on [0, 1]. That is,

$$C(\boldsymbol{u})=P(U_1\leqslant u_1,\cdots,U_d\leqslant u_d),$$

where each U_j ($j=1,\cdots,d$) is uniformly distributed on [0,1] and $\boldsymbol{u}=(u_1,\cdots,u_d)$. The Sklar's theorem ensures the existence of such multivariate function. In the context of longitudinal data, the joint distribution function of $\boldsymbol{y}_i$ and a copula $C(u_{i1},\cdots,u_{im_i})$ are connected via

$$\begin{aligned}F_{m_i}(\boldsymbol{y}_i)=P(Y_{i1}\leqslant y_{i1},\cdots,Y_{im_i}\leqslant y_{im_i})=\\P(F_{i1}(Y_{i1})\leqslant F_{i1}(y_{i1}),\cdots,\\F_{im_i}(Y_{im_i})\leqslant F_{im_i}(y_{im_i}))=\\F(F_{i1}^{-1}(u_{i1}),\cdots,F_{im_i}^{-1}(u_{im_i}))=\\C(u_{i1},\cdots,u_{im_i})\end{aligned}\tag{2}$$

where $u_{ij}=F_{ij}(y_{ij})$, $j=1,\cdots,m_i$ and $F_{ij}(\cdot)$ is the marginal cumulative distribution function of y_{ij}. In this paper, we use the Gaussian copula as it has the additional advantage of allowing a flexible parametric dependence structure. Then the joint distribution of $\boldsymbol{y}_i$ in (2) is

$$F_{m_i}(\boldsymbol{y}_i)=\Phi_{m_i}(z_{i1},\cdots,z_{im_i};\boldsymbol{R}_i)=\Phi_{m_i}(\boldsymbol{z}_i;\boldsymbol{R}_i)\tag{3}$$

where $\Phi_{m_i}(\cdots;\boldsymbol{R}_i)$ is the probability distribution function (PDF) of the m_i dimensional normal distribution with zero mean and correlation matrix $\boldsymbol{R}_i$, and $z_{ij}=\Phi^{-1}\{F_{ij}(y_{ij})\}$ for $j=1,\cdots,m_i$, with $\Phi(\cdot)$ being the PDF of the univariate standard normal distribution.

It should also be noticed that the entries of $\boldsymbol{R}_i$ are not directly the coefficients of correlation between the discrete observations, but they determine the dependence of the longitudinal observations via Eq. (3). Song[15] discussed the connection between the correlation coefficients in $\boldsymbol{R}_i$ and those of the observed variables explicitly.

1.2 Moving average Cholesky decomposition

Modeling correlation (and covariance) matrices can be challenging due to the positive-definiteness constraint. This problem can be removed by infusing regression-based ideas into Cholesky decomposition[16].

The standard Cholesky decomposition of an $m_i\times m_i$ positive definite covariance matrix is of the following form:

$$\boldsymbol{\Sigma}_i=\boldsymbol{C}_i\boldsymbol{C}_i^{\mathrm{T}}\tag{4}$$

where $\boldsymbol{C}_i=(c_{ijk})$ is a lower triangular matrix with positive diagonal elements and its entries are difficult to interpret. Pre-multiplying $\boldsymbol{C}_i$ by the inverse of $\boldsymbol{D}_i=\mathrm{diag}(c_{i11},c_{i22},\ldots,c_{im_im_i})$ leads to an alternative Cholesky decomposition (ACD)[17], and keeps $\boldsymbol{D}_i$ outside, and we have

$$\boldsymbol{\Sigma}_i=\boldsymbol{D}_i(\boldsymbol{D}_i^{-1}\boldsymbol{C}_i)(\boldsymbol{C}_i^{\mathrm{T}}\boldsymbol{D}_i^{-1})\boldsymbol{D}_i=\boldsymbol{D}_i\widetilde{\boldsymbol{L}}_i\widetilde{\boldsymbol{L}}_i^{\mathrm{T}}\boldsymbol{D}_i\tag{5}$$

where $\widetilde{\boldsymbol{L}}_i=\boldsymbol{D}_i^{-1}\boldsymbol{C}_i$ is obtained from a slightly different standardised $\boldsymbol{C}_i$, dividing each row by its corresponding diagonal entry.

For statistical interpretation of the below-diagonal entries of $\widetilde{\boldsymbol{L}}_i$, it is clear that $\boldsymbol{D}_i^{-1}(\boldsymbol{z}_i-\bar{\boldsymbol{z}}_i)$ has $\widetilde{\boldsymbol{L}}_i\widetilde{\boldsymbol{L}}_i^{\mathrm{T}}$ as the standard Cholesky decomposition of its covariance matrix and

$$\boldsymbol{\varepsilon}_i=(\boldsymbol{D}_i\widetilde{\boldsymbol{L}}_i)^{-1}(\boldsymbol{z}_i-\bar{\boldsymbol{z}}_i),$$

its vector of innovations, has $\mathrm{Cov}(\varepsilon_i)=\boldsymbol{I}_{m_i}$. Denote $\widetilde{\boldsymbol{L}}_i=(L_{ijk})$ and $\boldsymbol{D}_i=(\sigma_{ij})$, we obtain variable-order, moving average representation for the standardized $\dfrac{(z_{ij}-\bar{z}_{ij})}{\sigma_{ij}}$ as

$$\frac{(z_{ij}-\bar{z}_{ij})}{\sigma_{ij}}=\varepsilon_{ij}+\sum_{k=1}^{j-1}L_{ijk}\varepsilon_{ik}\tag{6}$$

Then we can prove, for any $1\leqslant j,k\leqslant m_i$, the correlation coefficient between z_{is} and z_{it} is given by

$$R_{ijk}=\mathrm{corr}(z_{ij},z_{ik})=\frac{\sum_{s=1}^{j\wedge k}L_{ijs}L_{iks}}{\sqrt{\sum_{s=1}^{j}L_{ijs}^2\sum_{s=1}^{k}L_{iks}^2}}\tag{7}$$

This property is a great motivation for modeling a correlation matrix.

In our approach, we parameterize the moving average parameters $\{L_{ijk}\}_{j>k}$ to overcome the over-parametrization problem. We propose to model these unconstrained parameters collectively via a regression model

$$L_{ijk}=\boldsymbol{w}'_{ijk}\gamma \tag{8}$$

where $\boldsymbol{w}_{ijk}\in\mathbb{R}^q$ is the explanatory variable and γ is the $q\times 1$ unknown parameters, we need to examine the covariates of the ith subject at the corresponding observations. We follow the convention of longitudinal data analysis by taking $\boldsymbol{w}_{ijk}$ as some function of the time lag $|t_{ij}-t_{ik}|$ between observations, which effectively ensures the correlation to be stationary. Other time-dependent covariates may also be meaningfully exploited. Thus our regression approach for the correlations can incorporate a broad class of covariates available for explaining the covariations between longitudinal measurements.

2 Estimation

We use the GLM for the responses marginally characterized by marginal parameters $\boldsymbol{\eta}=(\boldsymbol{\beta},\varphi)$, the copula model 3 for the joint distribution, and the Cholesky model for the correlation $\boldsymbol{R}_i$ with the parameters γ in (8). By combining all unknown parameters in this modeling framework, we write collectively the parameter vector of interest as $\boldsymbol{\theta}=(\boldsymbol{\beta},\varphi,\boldsymbol{\gamma})$. Then we are ready to develop the maximum likelihood estimators with the discrete longitudinal responses:

$$L(\theta)=\prod_{i=1}^{n}P(Y_{i1}=y_{i1},\cdots,Y_{im_i}=y_{im_i})=\prod_{i=1}^{n}P(y_{i1}-1<Y_{i1}\leqslant y_{i1},\cdots,y_{im_i}-1<Y_{im_i}\leqslant y_{im_i})=\prod_{i=1}^{n}\int\cdots\int_{z_i^-<\boldsymbol{u}\leqslant z_i}\phi_{m_i}(\boldsymbol{u};\boldsymbol{R}_i)\mathrm{d}\boldsymbol{u} \tag{9}$$

where $z_i=(z_{i1},\cdots,z_{im_i})^{\mathrm{T}}$ and $\boldsymbol{z}_i^-=(z_{i1}^-,\cdots,z_{im_i}^-)^{\mathrm{T}}$ with

$$z_{ij}=\Phi^{-1}\{F_{ij}(y_{ij})\},\ z_{ij}^-=\Phi^{-1}\{F_{ij}(y_{ij}-1)\},$$

and $z_{ij}^-=-\infty$ when y_{ij} takes the smallest possible value on its support.

However, evaluating the likelihood (9) involves the probability distribution functions of the m_i-dimensional normal distribution, whose analytical form is not available and numerical approximation is required. The computational cost of numerical approximation is high and may not scale easily to even a moderate number of repeat measurements. In fact, directly calculating the distribution function of each subject i specified by (2) requires 2^{m_i} summations of lower dimensional distribution functions as in the approach of Ref. [12], and the computational cost grows exponentially with m_i.

Inspired by Ref. [18], we implement a type of Monte Carlo expectation maximization (MCEM) algorithm[19] to estimate this integral. The expectation maximization (EM) algorithm[20] is a method to maximize the likelihood function in the presence of missing data $\boldsymbol{z}$. This is done iteratively. In the E-step one calculates the Q function, viz.

$$Q(\boldsymbol{\gamma},\hat{\boldsymbol{\gamma}}^{(m)})=\int_{\boldsymbol{z}}f(\boldsymbol{z}\mid\boldsymbol{y};\hat{\boldsymbol{\gamma}}^{(m)})\ln f(\boldsymbol{z};\boldsymbol{\gamma})\mathrm{d}\boldsymbol{z} \tag{10}$$

which is the expectation of the log likelihood with respect to the conditional predictive distribution $f(\boldsymbol{z}\mid\boldsymbol{y};\boldsymbol{R}(\hat{\boldsymbol{\gamma}}^{(m)}))$, under the current value of the model parameters $\hat{\boldsymbol{\gamma}}^{(m)}$ at the mth iteration. The Q function is then maximized in the M-step to find the new value of the model parameters, viz.

$$\hat{\boldsymbol{\gamma}}^{(m+1)}=\underset{\boldsymbol{\gamma}}{\arg\max}\,Q(\boldsymbol{\gamma},\hat{\boldsymbol{\gamma}}^{(m)}) \tag{11}$$

These steps are repeated iteratively until convergence. When the Q function is not available in closed form, a Monte Carlo estimate of the required expectation can be used instead. This is the MCEM algorithm. The Q function is replaced by

$$Q(\boldsymbol{\gamma},\hat{\boldsymbol{\gamma}}^{(m)})=\frac{1}{K}\sum_{k=1}^{K}\ln f(\boldsymbol{z}_k;\boldsymbol{R}(\hat{\boldsymbol{\gamma}}^{(m)})) \tag{12}$$

in the E-step, where $\boldsymbol{z}_1,\cdots,\boldsymbol{z}_K$ are drawn from $f(\boldsymbol{z}\mid\boldsymbol{y};\hat{\boldsymbol{\gamma}}^{(m)})$.

The Dunn-Smyth residuals[21] are a useful diagnostic tool for generalized linear modeling, which are used here as a device for numerical approximation of the integrand in Eq. (9). Let u_{ij} be independent draws from a standard uniform random variable U(0,1). We first define $u_{ij} = F_{ij}(y_{ij}) + u_{ij} f_{ij}(y_{ij})$, which are uniformly distributed on the (0,1) interval, if y_{ij} has the marginal distribution function F_{ij}. A Dunn-Smyth residual is then defined by $\zeta_{ij} = \Phi^{-1}(u_{ij})$. The distribution of these residuals, conditional on the data and marginal distributions, is a truncated multivariate normal with an identity covariance matrix. We can write the distribution of the vector of Dunn-Smyth residuals as

$$g(\boldsymbol{\zeta}_i) = \frac{\prod_{j=1}^{d} \phi(\zeta_{ij})}{\prod_{j=1}^{d} f_{ij}(y_{ij})} \tag{13}$$

This distribution has positive probability only in the region of integration of the likelihood defined in Eq. (9), making it a candidate for importance sampling to estimate this integral.

Theorem 2.1 The likelihood of the discrete Gaussian copula can be approximated by importance sampling with K sets of Dunn-Smyth residuals

$$L(\boldsymbol{\beta}, \varphi, \boldsymbol{\theta} \mid \boldsymbol{y}_1, \cdots, \boldsymbol{y}_n) = \prod_{i=1}^{n} \int_{z_i^- < z \leqslant z_i} \phi_{d_i}(\boldsymbol{z}; \boldsymbol{R}_i(\boldsymbol{\gamma})) \mathrm{d}z \simeq \prod_{i=1}^{n} \prod_{j=1}^{d_i} f_{ij}(y_{ij}) \prod_{i=1}^{n} \sum_{k=1}^{K} \frac{\phi_{d_i}(\zeta_i^k; \boldsymbol{R}_i(\boldsymbol{\gamma}))}{\prod_{j=1}^{d_i} \phi(\zeta_{ij}^k)},$$

where f_{ij} is the marginal density of variable j and observation i, and ζ_i are Dunn-Smyth residuals distributed by g.

Proof We can approximate the likelihood by importance sampling with K sets of Dunn-Smyth residuals

$$L_i(\boldsymbol{\beta}, \varphi, \boldsymbol{\gamma} \mid \boldsymbol{y}_i) = \int_{z_i^- < z \leqslant z_i} \phi_{d_i}(\boldsymbol{z}; \boldsymbol{R}_i(\boldsymbol{\gamma})) \mathrm{d}z = \int_{z_i^- < z \leqslant z_i} \phi_{d_i}(\boldsymbol{z}; \boldsymbol{R}_i(\boldsymbol{\gamma})) \frac{\prod_{j=1}^{d_i} f_{ij}(y_{ij})}{\prod_{j=1}^{d_i} \phi(z_{ij})} g(\boldsymbol{z}) \mathrm{d}z = \prod_{j=1}^{d_i} f_{ij}(y_{ij}) \int_{z_i^- < z \leqslant z_i} \frac{\phi_{d_i}(\boldsymbol{z}; \boldsymbol{R}_i(\boldsymbol{\gamma}))}{\prod_{j=1}^{d_i} \phi(z_{ij})} g(\boldsymbol{z}) \mathrm{d}z \tag{14}$$

which can be approximated using K samples from g, viz.

$$L_i(\boldsymbol{\beta}, \varphi, \boldsymbol{\gamma} \mid \boldsymbol{y}_i) \simeq \prod_{j=1}^{di} f_{ij}(y_{ij}) \sum_{k=1}^{K} \frac{\phi_{d_i}(\zeta_i^k; \boldsymbol{R}_i(\boldsymbol{\gamma}))}{\prod_{j=1}^{d_i} \phi(\zeta_{ij}^k)} \tag{15}$$

The parameters $(\boldsymbol{\beta}, \varphi, \boldsymbol{\gamma})$ are estimated via the algorithm in two steps. First, the marginal parameters $(\boldsymbol{\beta}, \varphi)$ are estimated by assuming independence, as with independence estimating equations. Second, these estimates $(\hat{\boldsymbol{\beta}}, \hat{\varphi})$ are plugged into the likelihood $L(\boldsymbol{\beta}, \varphi, \boldsymbol{\gamma} \mid \boldsymbol{y}_1, \cdots, \boldsymbol{y}_n)$, defined in Eq. (14). The resulting plug-in likelihood $L(\boldsymbol{\gamma} \mid \hat{\boldsymbol{\beta}}, \hat{\varphi}, \boldsymbol{y}_1, \cdots, \boldsymbol{y}_n)$ is maximized for correlation parameters $\boldsymbol{\gamma}$. Such algorithms have good asymptotic properties, including asymptotic efficiency relative to maximum likelihood[22].

We note that the observations $\boldsymbol{y}_i \sim f(\boldsymbol{y}, \eta, \boldsymbol{\gamma})$ for $i \in \{1, \cdots, n\}$. To establish the theoretical properties, we assume the following regularity conditions hold.

Condition C1 The parameter space Θ contains an open set of which the true parameter $\boldsymbol{\theta}_0$ is an interior point.

Condition C2 There exists an open subset of $\boldsymbol{\omega} \in \Omega$ containing $\boldsymbol{\eta}_0$ and an integrable function $M_r(\boldsymbol{y})$, such that for every $\boldsymbol{\eta} \in \omega$ and $\boldsymbol{y} \in \boldsymbol{y}$,

$$|\partial^3 \ln f(\boldsymbol{y}, \boldsymbol{\eta}, \boldsymbol{\gamma}) / \partial^3 \eta_r| \leqslant M_r(\boldsymbol{y})$$

for $r \in \{1, \cdots, \dim(\boldsymbol{\eta})\}$, where $E_{\boldsymbol{\eta}_0}\{M_r(\boldsymbol{y})\} < \infty$.

Condition C3 For $r \in \{1, \cdots, \dim(\boldsymbol{\eta})\}$ there are bounded functions $V_r(\boldsymbol{y})$ such that in the neighborhood of $\boldsymbol{\eta}_0$ for any fixed γ,

$$\{\partial \ln f(\boldsymbol{y}, \boldsymbol{\eta}, \boldsymbol{\gamma}) / \partial \eta_r\}^2 \leqslant V_r(\boldsymbol{y})$$

with $E_{\boldsymbol{\eta}_0}\{V_r(\boldsymbol{y})\} < \infty$.

Theorem 2.2 Under the conditions C1～C3, the estimators $(\hat{\boldsymbol{\beta}}, \hat{\varphi}, \hat{\boldsymbol{\gamma}})$ are consistent and asymptotically normally distributed.

The technical proof is given in Appendix.

3 Numerical studies

3.1 Simulations

In this section, we conduct simulation studies to investigate the finite performances of the proposed method. In each of the studies, we generated 500 data sets and took sample sizes $n=50$, 100 and 200, and the Monte Carlo sample size $K=200$. We also compared our method to the GEE method[23] and the generalized linear mixed-effects models(GLMM)[24] for estimating the parameters in the mean model and the dispersion. In GEE method, we assume unstructured correlations, and in GLMM, we consider time as random effects. All simulations were conducted in R.

Study 3.1 In this study we consider that the marginal distributions F_{ij} ($j=1,\ldots,m_i$) for n subjects as the negative binomial distribution $y_{ij}\sim \text{NegBin}(\delta,\mu_{ij})$ with mean μ_{ij} and variance $\mu_{ij}+\mu_{ij}^2/\varphi$, where $\varphi>0$ is the over-dispersion parameter and the numbers of repeated measurements m_i for each subject satisfies $m_i-1\sim \text{Binomial}(5, 0.8)$. The mean was then parameterized as $\mu_{ij}=\exp(x_{ij}^{\mathrm{T}}\beta)$ to allow dependence on explanatory variables, and the variance exceeds its mean (i. e. over-dispersion). The explanatory variables x_{ij1} and x_{ij2} were bivariate normal with correlation 0.5. The parameters in the correlation matrix was set as $L_{ijk}=\gamma_0+w_{ijk1}\gamma_1+w_{ijk2}\gamma_2$ for the moving-average (MA) structure as in Eq. (6) with $\boldsymbol{w}_{ijk}=\{1,t_{ij}-t_{ik},(t_{ij}-t_{ik})^2\}^{\mathrm{T}}$ and the measurement times t_{ij}s were uniformly distributed. The true parameters were taken as $\boldsymbol{\beta}=(\beta_0,\beta_1,\beta_2)=(1,-0.3,0.5)$, $\delta=4$ and $\boldsymbol{\gamma}=(\gamma_0,\gamma_1,\gamma_2)=(0.5,-0.3,0.3)$.

Tab. 1 shows the accuracy of the estimated parameters in terms of their mean biases (MB) and standard deviations (SD) in three methods. For the GLMM method, the dispersion parameter is fixed, because the estimation of it is always unstable. We can see the biases and the standard deviations decrease as the sample size increases, and all the biases are small especially when n is large. Compared to the GEE and GLMM estimates for the parameters in the mean model, our method have very competitive performances. In terms of dispersion parameter, the bias of our method is about one-half of the GEE, and of course GLMM. For the biases of other mean parameters, our method performs much better than GLMM, probably because we need to correctly model the random effect additionally in GLMM. And the SD of our method are slightly smaller than GLMM. Additionally, we can see that the biases are close but always smaller than GEE, and the SD of our method are much smaller than the SD of GEE. It shows that our method is more stable than GEE. All above show the advantage of proposed method.

Tab. 1 Simulation results for Study 3.1. Mean bias (MB) and standard deviation (SD) of mean parameters

	our method			GEE			GLMM		
	50	100	200	50	100	200	50	100	200
MB_{β_0}	0.010	0.000	0.001	0.007	0.002	0.001	0.116	0.112	0.115
SD_{β_0}	0.085	0.060	0.041	0.128	0.129	0.137	0.096	0.067	0.047
MB_{β_1}	0.002	0.003	0.002	0.002	0.001	0.005	0.005	0.005	0.000
SD_{β_1}	0.052	0.038	0.023	0.096	0.089	0.109	0.053	0.040	0.025
MB_{β_2}	0.000	0.002	0.002	0.003	0.009	0.003	0.005	0.006	0.002
SD_{β_2}	0.055	0.038	0.026	0.119	0.158	0.093	0.057	0.040	0.028
MB_{ψ}	0.767	0.359	0.166	1.464	0.913	0.381	—	—	—
SD_{ψ}	1.817	1.075	0.660	2.395	1.916	1.401	—	—	—
MB_{γ_0}	0.001	0.006	0.004	—	—	—	—	—	—
SD_{γ_0}	0.151	0.103	0.073	—	—	—	—	—	—
MB_{γ_1}	0.072	0.003	0.001	—	—	—	—	—	—
SD_{γ_1}	0.917	0.613	0.438	—	—	—	—	—	—
MB_{γ_2}	0.081	0.010	0.008	—	—	—	—	—	—
SD_{γ_2}	1.151	0.764	0.532	—	—	—	—	—	—

Study 3.2 The data sets were generated from the model

$$y_{ij} \sim \text{Bernoulli}(p_{ij}),$$
$$\text{logit}(p_{ij}) = \beta_0 + x_{ij1}\beta_1 + x_{ij2}\beta_2,$$
$$L_{ijk} = \gamma_0 + w_{ijk1}\gamma_1 + w_{ijk2}\gamma_2,$$
$$i = 1, \cdots, n;\ j = 1, \cdots, m_i,$$

where again the measurement times t_{ij}'s were uniform and $m_i - 1 \sim \text{Binomial}(5, 0.8)$. The covariate $\boldsymbol{x}_{ij} = (x_{ij1}, x_{ij2})^{\mathrm{T}}$ was generated from a standard bivariate normal distribution with zero correlation. We took the covariates for the correlations as $\boldsymbol{w}_{ijk} = \{1, t_{ij} - t_{ik}, (t_{ij} - t_{ik})^2\}^{\mathrm{T}}$. The parameters were set as $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2) = (1.0, -0.3, 0.5)$ and

$$\boldsymbol{\gamma} = (\gamma_0, \gamma_1, \gamma_2) = (0.5, -0.3, 0.3).$$

Tab. 2 shows that the results are qualitatively similar to those in Study 3.1. When $n = 50$ and 100, the mean biases of GEE are slightly smaller than our method, but the standard deviations are lager than our method. And when $n = 200$, our method has the best performance. Overall, our method performs promisingly and indicates the potential benefit for estimating the mean model incorporating the correlations in the longitudinal data by using a parsimonious correlation model.

Tab. 2 Simulation results for Study 3.2. Mean bias (MB) and standard deviation (SD) of mean parameters

	our method			GEE			GLMM		
	50	100	200	50	100	200	50	100	200
MB_{β_0}	0.027	0.026	0.017	0.051	0.031	0.018	0.141	0.044	0.015
SD_{β_0}	0.225	0.149	0.105	0.235	0.153	0.106	1.092	0.501	0.106
MB_{β_1}	0.018	0.012	0.004	0.011	0.008	0.008	0.020	0.012	0.006
SD_{β_1}	0.169	0.116	0.089	0.174	0.128	0.090	0.197	0.122	0.094
MB_{β_2}	0.018	0.016	0.001	0.011	0.010	0.004	0.025	0.017	0.003
SD_{β_2}	0.186	0.119	0.090	0.193	0.123	0.090	0.198	0.132	0.096
MB_{γ_0}	0.063	0.057	0.016	—	—	—	—	—	—
SD_{γ_0}	0.299	0.207	0.128	—	—	—	—	—	—
MB_{γ_1}	0.139	0.113	0.076	—	—	—	—	—	—
SD_{γ_1}	1.904	1.219	0.771	—	—	—	—	—	—
MB_{γ_2}	0.238	0.076	0.029	—	—	—	—	—	—
SD_{γ_2}	2.385	1.460	1.460	—	—	—	—	—	—

3.2 Online shopping data

E-commerce application has become one of the most commonly used Internet applications all over the world. Research on behavior of shopping users, especially its impact on purchasing, is of great significance to deeply understand user's online purchase behavior, discover high potential users, and promote consumption.

In this section, we consider an application of our methods using online shopping logs data accumulated by Tmall.com. We analyze a randomly selected sample of $n = 1\ 000$ visits to Tmall.com from May to October in 2015. The response variable is the number of times a user make purchases. Users on average made 4.23 visits with a standard deviation 1.92, resulting in a highly unbalanced repeated measurement data set. We also consider a set of covariates that could explain the variation in users' consumption behavior, including users' personal information and shopping logs. Tab. 3 describes these explanatory variables in detail. In the application, the nonlinear effect of age is assumed including age^2 among the covariates.

The model described in Section 1 is fitted on this dataset. To account for the over-dispersion, we used a parametric negative binomial regression model for the mean,

$$\text{action}_{ij} \sim \text{NegBin}(\varphi, \mu_{ij}),$$
$$\ln(\mu_{ij}) = \ln(\text{time}_{ij}) + \beta_0 + \beta_1 \text{click}_{ij} + \beta_2 \text{favor}_{ij} + \beta_3 \text{age}_i + \beta_4 \text{age}_i^2 + \beta_5 \text{gender}_i,$$

where φ is the over-dispersion parameter, time_{ij} is the month of time from the start day. The $\ln(\text{time}_{ij})$ is needed to account for different observation periods.

Tab. 3　Variable descriptions

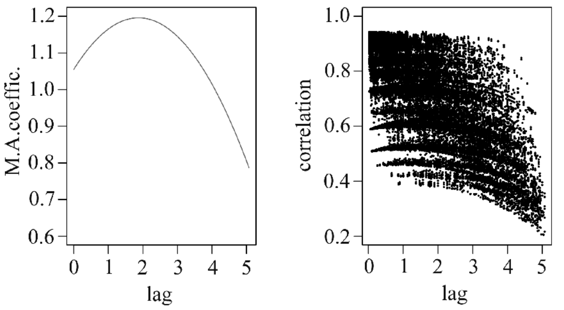
variable	description
action	number of times a user make purchases
age	1 for <18; 2 for [18,24]; 3 for [25,29] 4 for [30,34]; 5 for [35,39]; 6 for [40,49] 7 for ≥50
age²	square of age
gender	0 for female, 1 for male
merchant	number of merchants clicked
click	number of items clicked
favor	number of items added to favourite

Tab. 4 reports the estimates of the regression parameters. And also as a comparison, a GLMM approach with visit-time as random effect was implemented. From the results, we notice that all the explanatory variables are statistically significant. The variable click is a positively significant variable, indicating that users who click more will have more chance to make purchases, given other explanatory variables. The times users make purchases is negatively related to favor and gender. Since gender takes 1 for a man and 0 for a woman, it is obvious that a man tends to make less purchases. And the fact that favor is negatively correlated to purchase suggests users who add an item to favorites may be less likely to buy it at the same time. As for nonlinear relations, the quadratic effects of age is negatively significant, which means that middle-aged people will make more purchases. The over-dispersion parameter $\hat{\delta}=0.682$ is significant, suggesting that the counts are over-dispersed.

Tab. 4　Estimates of the parameters

	our method			GLMM		
	Est.	SE	p-value	Est.	SE	p-value
(intercept)	−3.693	0.514	<0.01	−3.688	0.482	<0.01
click	0.045	0.004	<0.01	0.034	0.004	<0.01
favor	−0.244	0.051	<0.01	−0.189	0.043	<0.01
age	1.133	0.219	<0.01	1.195	0.204	<0.01
age²	−0.098	0.023	<0.01	−0.109	0.021	<0.01
gender	−0.113	0.049	0.021	−0.120	0.047	0.01
φ	0.682	0.028	<0.01	0.832	−	−

For the parameters in the correlation, we obtained $\hat{\gamma}_0=1.055$, $\hat{\gamma}_1=0.142$, $\hat{\gamma}_2=-0.037$. We summarize the fitting with some plots. Fig. 1(a) shows the plots of the fitted M. A. coefficient versus the time lag, suggesting that a polynomial model for correlations is reasonable. The curved pattern between the correlation and time in Fig. 1(b) is interesting, which may be due to the fact that purchases made within a short period of time are more correlated to each other but such an effect becomes weaker in a relative longer term.



(a) plot of fitted M.A. coefficient versus time lag　(b) plot of fitted correlations versus time lag

Fig. 1　The online shopping data

4 Conclusion

With discrete longitudinal data, we propose a mean-correlation model based on moving average Cholesky decomposition. For this class of models, computing the full likelihood is often infeasible. Therefore, we propose a computationally efficient MCEM approach for model estimation. Our method can deal with any set of marginal distributions in Gaussian copula model, and is simple and flexible to implement. We assess the performance by a series of simulation studies which show that our approach has very competitive performances. Overall, the proposed framework is revealing some informative features from the statistical modeling for generic data with temporal dependence. It is benefits to discover interesting dependence properties of the covariance structures. Topics for future research include the feature selection for the mean-correlation model and the model diagnostic tools for assessing model adequacy.

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Appendix

Our method is a two-step estimation procedure, where we estimate $\boldsymbol{\beta}$ and φ from a marginal likelihood and then maximize the conditional likelihood given these estimates. By treating $\boldsymbol{\beta}$ and φ as nuisance parameters, we can get consistent estimators of parameters $\boldsymbol{\gamma}$.

Proof of Theorem 2.2

Let $\boldsymbol{\theta}_0=(\boldsymbol{\eta}_0, \boldsymbol{\gamma}_0)$ be the true parameters, and $\hat{\boldsymbol{\eta}}$ be the estimated coefficients where $\hat{\boldsymbol{\eta}}_j$ is found by maximizing the jth marginal likelihood,

$$\hat{\boldsymbol{\eta}}_j=\underset{\boldsymbol{\eta}_j}{\operatorname{argmax}} \ln L_j(\boldsymbol{y}_j, \boldsymbol{\eta}_j) \tag{A1}$$

Because maximizing Eq. (A1) is equivalent to using independence estimating equations in the GEE framework[23], which is consistent under Condition C1 and Condition C2, we now state a result, without proof, concerning the consistency of the marginal parameters.

Lemma A.1 Under some regular conditions C1~C3, $\hat{\boldsymbol{\eta}}\to\boldsymbol{\eta}_0$ in probability as $n\to\infty$.

Analogously to the proof of standard maximum likelihood estimation in Ref. [25], we define

$$\tau(\boldsymbol{\gamma})=\frac{1}{n}\ln\frac{L(\boldsymbol{y}; \hat{\boldsymbol{\eta}}, \boldsymbol{\gamma})}{L(\boldsymbol{y}; \hat{\boldsymbol{\eta}}, \boldsymbol{\gamma}_0)}=\frac{1}{n}\sum_{i=1}^{n}\ln\frac{f(\boldsymbol{y}_i; \hat{\boldsymbol{\eta}},\boldsymbol{\gamma})}{f(\boldsymbol{y}_i; \hat{\boldsymbol{\eta}},\boldsymbol{\gamma}_0)} \tag{A2}$$

However, we cannot use the law of large numbers directly to show this converges to its expectation under $\boldsymbol{\theta}_0$ as each summand of $\tau(\boldsymbol{\gamma})$ is a function of all the data, through $\hat{\boldsymbol{\eta}}$. Instead, we develop the following result.

Lemma A.2 Let $l_n(\boldsymbol{\theta})=l_n(\boldsymbol{\eta},\boldsymbol{\gamma})=\ln L(\boldsymbol{y};\boldsymbol{\eta},\boldsymbol{\gamma})=\sum_{i=1}^{n}\ln f(\boldsymbol{y}_i; \boldsymbol{\eta},\boldsymbol{\gamma})$, we have $l_n(\hat{\boldsymbol{\eta}}, \boldsymbol{\gamma})/n\to E_{\boldsymbol{\theta}_0}\ln f(\boldsymbol{y},\boldsymbol{\eta}_0,\boldsymbol{\gamma})$ in probability as $n\to\infty$.

Proof Under Conditions C1 ~ C3 one has that, for any fixed $\boldsymbol{\gamma}$, the Taylor expansion of the standardized likelihood around $\boldsymbol{\eta}_0$ is

$$\frac{1}{n}l_n(\hat{\boldsymbol{\eta}}, \boldsymbol{\gamma})=\frac{1}{n}l_n(\boldsymbol{\eta}_0, \boldsymbol{\gamma})+\frac{1}{n}(\hat{\boldsymbol{\eta}}-\boldsymbol{\eta}_0)^{\mathrm{T}}\frac{\partial}{\partial\boldsymbol{\eta}}l_n(\boldsymbol{\eta}, \boldsymbol{\gamma})\big|_{\tilde{\boldsymbol{\eta}}} \tag{A3}$$

where $\tilde{\boldsymbol{\eta}}$ is between $\hat{\boldsymbol{\eta}}$ and $\boldsymbol{\eta}_0$. By the Cauchy-Schwarz inequality, the last term is

$$\left\|\frac{1}{n}(\hat{\boldsymbol{\eta}}-\boldsymbol{\eta}_0)^{\mathrm{T}}\frac{\partial}{\partial\boldsymbol{\eta}}l_n(\boldsymbol{\eta}, \boldsymbol{\gamma})\big|_{\tilde{\boldsymbol{\eta}}}\right\|\leqslant\frac{1}{n}\|\hat{\boldsymbol{\eta}}-\boldsymbol{\eta}_0\|\times\left\|\frac{\partial}{\partial\boldsymbol{\eta}}l_n(\boldsymbol{\eta}, \boldsymbol{\gamma})\big|_{\tilde{\boldsymbol{\eta}}}\right\| \tag{A4}$$

By Lemma A.1, we know $\|\hat{\boldsymbol{\eta}}-\boldsymbol{\eta}_0\|=o_p(1)$. We then look at the square of the last term, viz.

$$\left\|\frac{\partial}{\partial\boldsymbol{\eta}}l_n(\boldsymbol{\eta}, \boldsymbol{\gamma})\big|_{\tilde{\boldsymbol{\eta}}}\right\|^2=\sum_{r=1}^{\dim(\boldsymbol{\eta})}\left\{\sum_{i=1}^{n}\frac{\partial}{\partial\boldsymbol{\eta}_r}\ln f(\boldsymbol{y}_i,\boldsymbol{\eta},\boldsymbol{\gamma})\big|_{\tilde{\boldsymbol{\eta}}}\right\}^2=O_p(n^2) \tag{A5}$$

which follows from the regularity conditions. Hence

$$\left\|\frac{\partial}{\partial\boldsymbol{\eta}}l_n(\boldsymbol{\eta}, \boldsymbol{\gamma})\big|_{\tilde{\boldsymbol{\eta}}}\right\|=O_p(n) \tag{A6}$$

So the remainder term in Eq. (A3) is given by

$$\left\|\frac{1}{n}(\hat{\boldsymbol{\eta}}-\boldsymbol{\eta}_0)^{\mathrm{T}}\frac{\partial}{\partial\boldsymbol{\eta}}l_n(\boldsymbol{\eta},\boldsymbol{\gamma})\big|_{\tilde{\boldsymbol{\eta}}}\right\|\leqslant\frac{1}{n}o_p(1)O_p(n)=o_p(1) \tag{A7}$$

This in turn implies

$$\frac{1}{n}l_n(\hat{\boldsymbol{\eta}}, \boldsymbol{\gamma})=\frac{1}{n}l_n(\boldsymbol{\eta}_0,\boldsymbol{\gamma})+o_p(1) \tag{A8}$$

Therefore for any $\boldsymbol{\gamma}$, $l_n(\hat{\boldsymbol{\eta}}, \boldsymbol{\gamma})/n\to E_{\boldsymbol{\theta}_0}\ln f(\boldsymbol{y},\boldsymbol{\eta}_0,\boldsymbol{\gamma})$ in probability. The proof is completed.

Now we can return to the standard proof, it can be easily shown that

$$\tau(\boldsymbol{\gamma})=\frac{1}{n}\sum_{i=1}^{n}\ln\frac{f(\boldsymbol{y}_i;\ \hat{\boldsymbol{\eta}},\boldsymbol{\gamma})}{f(\boldsymbol{y}_i;\ \hat{\boldsymbol{\eta}},\boldsymbol{\gamma}_0)}\to E_{\boldsymbol{\theta}_0}\{\ln\frac{f(\boldsymbol{y},\boldsymbol{\eta}_0,\boldsymbol{\gamma})}{f(\boldsymbol{y},\boldsymbol{\eta}_0,\boldsymbol{\gamma}_0)}\}=-K(\boldsymbol{\theta}_0,\ \boldsymbol{\theta})<0 \tag{A9}$$

unless $f(\boldsymbol{y},\boldsymbol{\theta})=f(\boldsymbol{y};\ \boldsymbol{\theta}_0)$, and $\hat{\boldsymbol{\theta}}\to\boldsymbol{\theta}_0$ in probability and hence $\hat{\boldsymbol{\gamma}}\to\boldsymbol{\gamma}_0$ in probability. Then through the standard process, we can easily obtain the asymptotic normality.

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