



UNIVERSITÀ DI PISA



Sant'Anna
Scuola Universitaria Superiore Pisa



Consiglio Nazionale delle Ricerche

Book of Short Papers

SIS 2020



Società
Italiana di
Statistica

Editors: Alessio Pollice, Nicola Salvati and Francesco Schirripa Spagnolo

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PUBLISHED BY PEARSON

WWW.PEARSON.COM

ISBN 9788891910776

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Multivariate Mixed Hidden Markov Model for joint estimation of multiple quantiles

Modello Hidden Markov Multivariato ad effetti misti per la stima congiunta di quantili condizionati

Merlo Luca, Petrella Lea and Tzavidis Nikos

Abstract This paper develops a Mixed Hidden Markov Model for joint estimation of multiple quantiles in a multivariate linear regression for longitudinal data. This method accounts for association among multiple responses and study how the relationship between dependent and explanatory variables may vary across different quantile levels of the conditional distribution of the multivariate response variable. Unobserved heterogeneity sources and serial dependence are jointly modeled through the introduction of individual-specific, time-constant random coefficients and time-varying parameters that evolve over time with a Markovian structure, respectively. Estimation is carried out via a suitable EM algorithm without parametric assumptions on the random effects distribution. We assess the empirical behaviour of the proposed methodology through the analysis of the Millennium Cohort Study data.

Abstract Questo lavoro sviluppa un modello di Markov nascosto multivariato ad effetti misti per la stima congiunta di quantili marginali condizionati associati a variabili risposta multivariate, nell'ambito di una regressione lineare per dati longitudinali. La metodologia proposta consente di tenere conto dell'associazione esistente tra le variabili risposta e intende studiare come tale struttura di associazione varia quando si considerano diversi quantili della distribuzione condizionata della variabile risposta. Le fonti di eterogeneità non osservate, costanti e variabili nel tempo, vengono modellate congiuntamente introducendo effetti casuali costanti e coefficienti che variano nel tempo secondo una catena di Markov latente. La stima dei

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parametri è ottenuta tramite l'algoritmo EM senza formulare assunzioni parametriche sulla distribuzione degli effetti casuali. La validità del nostro approccio viene analizzata attraverso un'applicazione empirica con i dati del Millennium Cohort Study.

Key words: Longitudinal data, Mixed Hidden Markov Model, Multivariate Asymmetric Laplace Distribution, Quantile Regression, Random Effects Model

1 Introduction

Ever since quantile regression was first introduced in the seminal work of [6], it has attracted researchers' and practitioners' attention. It provides a way to model the conditional quantiles of a response variable with respect to a set of covariates in order to have a more complete picture of the entire conditional distribution compared to the classical mean regression. In a univariate quantile regression analysis, the likelihood based inferential approach to estimate the parameters relies on the introduction of the Asymmetric Laplace (AL) distribution: the maximization of the likelihood associated with the AL density is equivalent (in terms of parameter estimates) to the minimization of the quantile loss function of [6]. When multivariate response variables are concerned, the existing literature on quantile regression is less extensive due to the fact that there is not a unique definition of quantile for a multivariate random variable because there is no "natural" ordering in a p -dimensional space, for $p > 1$. Hence, the concept of multivariate quantile is still a debatable issue (see [7] and the references therein for relevant studies). Recently, [12] generalized the AL distribution inferential approach of the univariate case to a multivariate framework by using the Multivariate Asymmetric Laplace (MAL) distribution defined in [8]. By using the MAL distribution as likelihood based inferential tool, the authors sidestep the problem of defining a multivariate quantile, and meanwhile they implement a joint estimation of the marginal conditional quantiles of a multivariate response variable, taking into account for possible correlation among marginals.

When dealing with longitudinal data, because measurements recorded on the same individuals are likely correlated, the potential association between dependent observations should be taken into account in order to provide correct inferences. In such cases, random effect models have been proposed to accommodate for time-constant, within-subject correlation and between subject heterogeneity (see [10, 5]). However, when the assumption of time-constant random coefficients does not hold, adopting such model specification may lead to biased parameter estimates (see [3]). To account for serial heterogeneity, [4] suggested the use of Hidden Markov Models (HMM). The key assumption is the conditional independence of the response variables given a latent process that follows a Markov chain on a finite number of states. In this context, the application of HMMs is well justified by their versatility and mathematical tractability (see [11]).

The purpose of this article is to extend the work of [12] by introducing a Mixed Hidden Markov Model (MHMM) to the longitudinal data setting to account for the correlation between responses. The MHMM (see [2]) encompasses Generalized Linear Mixed Models and HMMs as it accommodates time-constant and time-varying sources of random variation. Time-constant unobserved heterogeneity is described via individual-specific random coefficients while temporal effects are captured through state-specific effects that evolve over time depending on a hidden Markov chain. In order to prevent inconsistent parameter estimates due to misspecification of the random effects distribution, we adopt the Non-Parametric Maximum Likelihood (NPML) approach of [9] in which it is left unspecified and approximated by a discrete finite mixture distribution. Model parameters are estimated through maximum likelihood by using the Expectation-Maximization (EM) algorithm while standard error estimates rely on bootstrap resampling. From a computational perspective, we provide an efficient version of the EM algorithm with M-step updates in closed form for all model parameters.

2 Methodology

Let $\mathbf{Y}_{it} = (Y_{it}^{(1)}, \dots, Y_{it}^{(p)})$ be a continuous p -variate response variable vector and $\mathbf{X}_{it} = (X_{it}^{(1)}, \dots, X_{it}^{(k)})$ be a k -dimensional vector of explanatory variables for every subject $i = 1, \dots, N$ and time occasion $t = 1, \dots, T_i$. Given p quantile indexes $\boldsymbol{\tau} = (\tau_1, \dots, \tau_p)$, with $\tau_j \in (0, 1)$, $j = 1, \dots, p$, let $S_{it}(\boldsymbol{\tau})$, $i = 1, \dots, N$, $t = 1, \dots, T_i$ be a homogeneous, first-order, hidden Markov chain defined over a discrete states space $\mathcal{S} = \{1, \dots, M\}$ with initial and transition probabilities denoted by $\mathbf{q} = (q_1, \dots, q_M)$ and $\mathbf{Q} = \{q_{jk}\}$ over $\mathcal{S} \times \mathcal{S}$, respectively. Finally, let $\mathbf{b}_i(\boldsymbol{\tau})$ be a time-constant, subject-specific, random effects matrix having distribution $f_{\mathbf{b}}(\cdot | \boldsymbol{\tau})$ which, as they are meant to capture different unobserved characteristics, is independent of the hidden Markov chain, $S_{it}(\boldsymbol{\tau})$, and where $\mathbb{E}(\mathbf{b}_i(\boldsymbol{\tau})) = \mathbf{0}$ is used for parameter identifiability. We assume that the τ_j -th quantile of each of the j -th components of \mathbf{Y}_{it} can be modeled as a function of some explanatory variables. Let $\boldsymbol{\beta}(\boldsymbol{\tau}) = (\beta_1(\boldsymbol{\tau}), \dots, \beta_p(\boldsymbol{\tau}))$ be the $k \times p$ matrix of unknown regression coefficients. Then, the multivariate Mixed Hidden Markov Model (MHMM) is defined as follows:

$$\mathbf{Y}_{it} = \mathbf{X}_{it}\boldsymbol{\beta}(\boldsymbol{\tau}) + \mathbf{Z}_{it}\mathbf{b}_i(\boldsymbol{\tau}) + \mathbf{W}_{it}\boldsymbol{\alpha}_{s_{it}}(\boldsymbol{\tau}) + \boldsymbol{\varepsilon}_{s_{it}}(\boldsymbol{\tau}), \quad (1)$$

where \mathbf{Z}_{it} is a subset of \mathbf{X}_{it} , \mathbf{W}_{it} is a further subset of \mathbf{X}_{it} whose effects are assumed to vary over time, $\boldsymbol{\varepsilon}_{s_{it}}(\boldsymbol{\tau})$ denotes a p -dimensional vector of error terms with univariate component-wise quantiles (at fixed levels τ_1, \dots, τ_p , respectively) equal to zero and where the coefficients matrix $\boldsymbol{\alpha}_{s_{it}}(\boldsymbol{\tau})$ evolves over time according to the hidden Markov chain, $S_{it}(\boldsymbol{\tau})$, and takes one of the values in the set $\{\boldsymbol{\alpha}_1(\boldsymbol{\tau}), \dots, \boldsymbol{\alpha}_M(\boldsymbol{\tau})\}$.

Our objective is to provide joint estimation of the p marginal conditional quantiles of \mathbf{Y}_{it} taking into account for potential correlation among the dependent variables. Conditional on the hidden state occupied at time t , $S_{it}(\boldsymbol{\tau})$, and on the

individual-specific random coefficients, $\mathbf{b}_i(\tau)$, observations from the same individual are independent and the following equality holds:

$$f_{\mathbf{Y}|S,\mathbf{b}}(\mathbf{y}_{it} | \mathbf{y}_{i1:t-1}, s_{i1:t}, \mathbf{b}_i, \tau) = f_{\mathbf{Y}|S,\mathbf{b}}(\mathbf{y}_{it} | s_{it}, \mathbf{b}_i, \tau), \quad (2)$$

where $\mathbf{y}_{i1:t-1}$ represents the history of the responses for the i -th subject up to time $t-1$ and $s_{i1:t}$ is the individual sequence of states up to time t .

In order to derive maximum likelihood estimates for the regression model in (1), we consider the Multivariate Asymmetric Laplace (MAL) distribution, $\mathcal{M}\mathcal{A}\mathcal{L} \sim (\boldsymbol{\mu}_{it}, \mathbf{D}\tilde{\boldsymbol{\xi}}, \mathbf{D}\Sigma\mathbf{D})$ (see [8]), whose conditional density function is given by:

$$f_{\mathbf{Y}|S,\mathbf{b}}(\mathbf{y}_{it} | s_{it}, \mathbf{b}_i, \tau) = \frac{2 \exp\left\{(\mathbf{y}_{it} - \boldsymbol{\mu}_{it})' \mathbf{D}^{-1} \Sigma^{-1} \tilde{\boldsymbol{\xi}}\right\}}{(2\pi)^{p/2} |\mathbf{D}\Sigma\mathbf{D}|^{1/2}} \left(\frac{\tilde{m}_{it}}{2 + \tilde{d}}\right)^{\nu/2} K_{\nu}\left(\sqrt{(2 + \tilde{d})\tilde{m}_{it}}\right), \quad (3)$$

where the location parameter $\boldsymbol{\mu}_{it}$ is defined by the linear model $\boldsymbol{\mu}_{it} = \boldsymbol{\mu}(s_{it}, \mathbf{b}_i, \tau) = \mathbf{X}_{it}\boldsymbol{\beta}(\tau) + \mathbf{Z}_{it}\mathbf{b}_i(\tau) + \mathbf{W}_{it}\boldsymbol{\alpha}_{s_{it}}(\tau)$, $\mathbf{D}\tilde{\boldsymbol{\xi}} \in \mathbb{R}^p$ is the scale (or skew) parameter with $\mathbf{D} = \text{diag}[d_1, \dots, d_p]$, $d_j > 0$ and $\tilde{\boldsymbol{\xi}} = [\tilde{\xi}_1, \tilde{\xi}_2, \dots, \tilde{\xi}_p]'$ having generic element $\tilde{\xi}_j = \frac{1-2\tau_j}{\tau_j(1-\tau_j)}$, $j = 1, \dots, p$. $\tilde{\boldsymbol{\Sigma}}$ is a $p \times p$ positive definite matrix such that $\Sigma = \Lambda\Psi\Lambda$, with Ψ being a correlation matrix and $\Lambda = \text{diag}[\sigma_1, \dots, \sigma_p]$, with $\sigma_j^2 = \frac{2}{\tau_j(1-\tau_j)}$, $j = 1, \dots, p$. Moreover, $\tilde{m}_{it} = (\mathbf{y}_{it} - \boldsymbol{\mu}_{it})' (\mathbf{D}\Sigma\mathbf{D})^{-1} (\mathbf{y}_{it} - \boldsymbol{\mu}_{it})$, $\tilde{d} = \tilde{\boldsymbol{\xi}}' \Sigma \tilde{\boldsymbol{\xi}}$, and $K_{\nu}(\cdot)$ denotes the modified Bessel function of the third kind with index parameter $\nu = (2-p)/2$. The constraints imposed on $\tilde{\boldsymbol{\xi}}$ and Λ represent necessary conditions for model identifiability for any fixed quantile level τ_1, \dots, τ_p and guarantee that $\mu_{it}^{(j)}$ is the τ_j -th conditional quantile function of $Y_{it}^{(j)}$ given $S_{it}(\tau)$ and \mathbf{b}_i , for $j = 1, \dots, p$.

It is worth noting that our methodology reduces to the (multivariate) linear quantile Hidden Markov Model of [4] when $\mathbf{W}_{it} = \mathbf{1}$ and $\mathbf{b}_i(\tau) = \mathbf{0}$ for all $i = 1, \dots, N$ and $t = 1, \dots, T_i$; whereas it reduces to the (multivariate) linear quantile Mixed Model of [10] when there is only one state of the hidden Markov chain, i.e. $M = 1$.

In the case of a continuous parametric distribution for the random effects, the likelihood for the model in (1)-(3) involves the integration over the distribution of the random effects, $f_{\mathbf{b}}(\cdot | \tau)$. Such integral cannot be solved analytically and maximum likelihood parameter estimates can be obtained through numerical integration techniques. In addition parametric assumptions on the distribution of the random coefficients can be too restrictive and misspecification of the mixing distribution can lead to biased parameter estimates. For these reasons, we may rely on the Non-parametric Maximum Likelihood (NPML) estimation theory of [9]: $f_{\mathbf{b}}(\cdot | \tau)$ is left unspecified and we approximate it by using a discrete distribution on $G < N$ locations, $\mathbf{b}_g(\tau)$, with associated probabilities defined by $\pi_g(\tau) = \Pr(\mathbf{b}_i(\tau) = \mathbf{b}_g(\tau))$, $i = 1, \dots, N$ and $g = 1, \dots, G$. That is, $\mathbf{b}_i(\tau) \sim \sum_{g=1}^G \pi_g(\tau) \delta_{\mathbf{b}_g}(\tau)$ where δ_{θ} is a one-point distribution putting a unit mass at θ . In this case, if we suppress the index τ to simplify the notation, the observed data likelihood of the model has the form:

Multivariate Mixed Hidden Markov Model for joint estimation of multiple quantiles

$$L(\Phi_\tau) = \prod_{i=1}^N \prod_{g=1}^G \sum_{\mathcal{S}^{T_i}} \left\{ \left[\prod_{t=1}^{T_i} f_{\mathbf{Y}|S, \mathbf{b}}(\mathbf{y}_{it} | s_{it}, \mathbf{b}_g) \right] q_{s_{i1}} \prod_{t=2}^{T_i} q_{s_{it-1}s_{it}} \right\} \pi_g, \quad (4)$$

where $\Phi_\tau = (\beta, \mathbf{D}, \Psi, \mathbf{b}_1, \dots, \mathbf{b}_G, \pi_1, \dots, \pi_G, \alpha_1, \dots, \alpha_M, \mathbf{q}, \mathbf{Q})$ denotes the vector of model parameters and $f_{\mathbf{Y}|S, \mathbf{b}}(\mathbf{y}_{it} | s_{it}, \mathbf{b}_g)$ represents the response distribution of unit i of being in the hidden state s_{it} at time t and of belonging to the g -th component of the finite mixture, which is assumed to have a MAL density in (3) with location parameter given by $\mu_{it} = \mu(s_{it}, \mathbf{b}_g, \tau) = \mathbf{X}_{it}\beta(\tau) + \mathbf{Z}_{it}\mathbf{b}_g(\tau) + \mathbf{W}_{it}\alpha_{s_{it}}(\tau)$.

2.1 Estimation

Given the representation in (4), let us denote by w_{ig} the indicator variable that is equal to 1 if the i -th unit belongs to the g -th component of the finite mixture, and 0 otherwise. Similarly let u_{itj} be equal to 1 if unit i is in state j at time t and 0 otherwise; let v_{itjk} be equal to 1 if unit i is in state j at time $t-1$ and in state k at time t , and 0 otherwise. Finally, we denote by z_{itjg} the indicator of the i -th individual being in state j at time t and coming from the g -th component of the mixture. The log-likelihood for the complete data has the following form:

$$\ell_c(\Phi_\tau) = \sum_{i=1}^N \left\{ \sum_{g=1}^G w_{ig} \log \pi_g + \sum_{j=1}^M u_{i1j} \log q_j + \sum_{t=2}^{T_i} \sum_{j=1}^M \sum_{k=1}^M v_{itjk} \log q_{jk} + \sum_{t=1}^{T_i} \sum_{j=1}^M \sum_{g=1}^G z_{itjg} \log f_{\mathbf{Y}|S, \mathbf{b}}(\mathbf{y}_{it} | S_{it} = j, \mathbf{b}_g) \right\}. \quad (5)$$

In the E-step of the algorithm, the presence of the unobserved indicator variables $w_{ig}, u_{itj}, v_{itjk}$ and z_{itjg} is handled by taking their conditional expectation given the observed data and the current parameter estimates. Calculation of such quantities may be addressed via an adaptation of the forward and backward variables; see [14]. Subsequently, the M-step solutions are updated by maximizing the conditional expectation of (5) given the observed data and the current parameter estimates with respect to Φ_τ and solving the M-step equations. We derive closed form update expressions of the model parameters, based on the mixture representation of the MAL distribution. Finally, the E- and M-steps are alternated until convergence. To avoid convergence to local maxima, for each value of the pair (G, M) , we initialize model parameters using a multi-start strategy.

3 Application

To investigate the behaviour of the proposed methodology, we analyse the data from the Millennium Cohort Study (MCS) which has been studied by [1] and [13] in the context of M-quantile regression with time-constant random-effects. The MCS is a longitudinal survey which aims at better addressing the effects of social disadvan-

tage on children’s outcomes in the UK. The two outcomes of interest, emotional problems and behavioural problems, measured by the SDQ internalizing score and by the SDQ externalizing score, respectively, were collected at ages 3, 5 and 7 years. A description of the included demographic and socio-economic covariates can be found in [13]. We used the proposed model with constant random intercepts and time-varying random slopes specified for age. A summary of the results when $\tau = (0.25, 0.25)$, $\tau = (0.50, 0.50)$ and $\tau = (0.75, 0.75)$ is reported in Table 1. The estimated regression coefficients are consistent with those obtained by [13]. In particular, we selected a number of mixture components equal to $G = (3, 5, 5)$ at quantile levels 0.25, 0.50 and 0.75 respectively, and we identified a decreasing number of hidden states $M = (5, 4, 3)$ as the analyzed quantile level increases.

τ -th quantile	(0.25, 0.25) [G = 3, M = 5]		(0.50, 0.50) [G = 5, M = 4]		(0.75, 0.75) [G = 5, M = 3]	
	SDQ _{Int}	SDQ _{Ext}	SDQ _{Int}	SDQ _{Ext}	SDQ _{Int}	SDQ _{Ext}
Intercept	0.864 (0.126)	1.846 (0.178)	1.267 (0.215)	3.925 (0.251)	3.790 (0.288)	4.275 (0.412)
Age year scal	1.379 (0.010)	-0.804 (0.016)	1.234 (0.009)	-0.634 (0.011)	-0.583 (0.021)	-0.244 (0.031)
Age2 year scal	0.045 (0.005)	0.193 (0.009)	0.077 (0.011)	0.208 (0.013)	0.104 (0.018)	0.287 (0.024)
ALE 11	0.022 (0.008)	0.036 (0.016)	0.086 (0.018)	0.113 (0.019)	0.116 (0.039)	0.205 (0.055)
SED 4	0.070 (0.023)	0.105 (0.045)	0.175 (0.038)	0.221 (0.030)	0.201 (0.051)	0.398 (0.076)
Kessm	0.090 (0.009)	0.143 (0.012)	0.167 (0.009)	0.189 (0.012)	0.208 (0.018)	0.299 (0.025)
Degree	-0.350 (0.109)	-0.894 (0.149)	-0.526 (0.114)	-1.482 (0.171)	-0.703 (0.160)	-1.267 (0.232)
GCSE	-0.217 (0.110)	-0.582 (0.150)	-0.352 (0.113)	-0.430 (0.166)	-0.413 (0.149)	-0.427 (0.213)
White	-0.090 (0.061)	-0.143 (0.097)	-0.075 (0.149)	0.059 (0.160)	-0.216 (0.203)	0.320 (0.303)
Male	-0.062 (0.016)	0.793 (0.030)	0.027 (0.037)	0.950 (0.045)	0.082 (0.080)	0.944 (0.119)
IMDScore	-0.022 (0.005)	-0.036 (0.009)	-0.025 (0.008)	-0.027 (0.010)	-0.027 (0.020)	-0.045 (0.029)
Eng eth stratum	-0.043 (0.159)	-0.168 (0.174)	0.122 (0.193)	0.144 (0.220)	0.174 (0.241)	-0.025 (0.374)
Eng dis stratum	-0.003 (0.031)	0.003 (0.072)	0.085 (0.047)	0.106 (0.050)	0.156 (0.111)	0.337 (0.175)

Table 1 Point estimates with non-parametric bootstrap standard errors in parentheses ($B = 1000$ re-samples) for different quantile levels. Parameter estimates are displayed in boldface when significant at the standard 5% level. The number of mixture components G and hidden states M are selected according to the BIC criteria.

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