A comparisons of some criteria for states selection of the latent Markov model for longitudinal data

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Outline

Introduction

- Background:

  Latent Markov (LM) models (Wiggins, 1973; Bartolucci et al., 2012) are successfully applied in the analysis of longitudinal data: they allow to take into account several aspects, such as serial dependence between observations, measurement errors, unobservable heterogeneity

  LM models assume that one or more occasion-specific response variables depends only on a discrete latent variable characterized by a given number of latent states which in turn depends on the latent variables corresponding to the previous occasions according to a first-order Markov chain

  LM models are characterized by several parameters: the initial probabilities to belong to a given latent state, the transition probabilities from a latent state to another one, the conditional response probabilities given the discrete latent variable

- Problem: a crucial point with LM models is represented by the selection of the number of latent states

- Aim: we compare the behavior of several model selection criteria to choose the number of latent states

  Special attention is devoted to classification-based criteria that take explicitly into account the partition of observations in different latent states, through a specific measurement of the quality of classification, denoted as entropy

Multivariate basic LM model: notation

- $\boldsymbol{Y}^{(t)} = (Y_1^{(t)}, \ldots, Y_r^{(t)})$: vector of discrete categorical response variables Y_j ($j = 1, \ldots, r$) observed at time t ($t = 1, \ldots, T$), having c_j categories
- $\boldsymbol{Y} = (\boldsymbol{Y}^{(1)}, \ldots, \boldsymbol{Y}^{(T)})$: vector of observed responses made of the union of vectors $\boldsymbol{Y}^{(t)}$; usually, it is referred to repeated measurements of the same variables Y_j ($j = 1, \ldots, r$) on the same individuals at different time points
- $U^{(t)}$: latent state at time t with state space $\{1, \ldots, k\}$
- $\boldsymbol{U} = (U^{(1)}, \ldots, U^{(T)})$: vector describing the latent process

Multivariate basic LM model: main assumptions

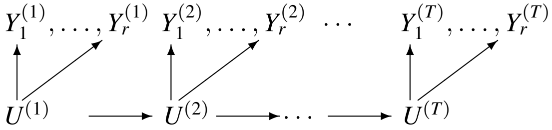
- vectors $\boldsymbol{Y}^{(t)}$ $(t = 1, \ldots, T)$ are conditionally independent given the latent process $\boldsymbol{U}$ and the response variables in each $\boldsymbol{Y}^{(t)}$ are conditionally independent given $U^{(t)}$ (local independence), i.e.,

  each occasion-specific observed variable $Y_j^{(t)}$ is independent of $Y_j^{(t-1)}, \ldots, Y_j^{(1)}$ and of each $Y_h^{(t)}$, for all $h \neq j = 1, \ldots, r$, given $U^{(t)}$

- latent process $\boldsymbol{U}$ follows a first-order Markov chain with k latent states, i.e.,

  each latent variable $U^{(t)}$ is independent of $U^{(t-2)}, \ldots, U^{(1)}$, given $U^{(t-1)}$

LM:



Multivariate basic LM model: parameters

- $k\sum_{j=1}^r (c_j-1)$ conditional response probabilities

  $\phi_{jy|u}^{(t)} = p(Y_j^{(t)} = y|U^{(t)} = u) \quad j = 1,\dots,r;\ t = 1,\dots,T;\ u = 1,\dots,k;\ y = 0,\dots,c_j-1$

  $\phi_{\boldsymbol{y}|u}^{(t)} = \prod_{j=1}^r \phi_{jy|u}^{(t)} = p(Y_1^{(t)} = y_1,\dots,Y_r^{(t)} = y_r|U^{(t)} = u)$

- $(k-1)$ initial probabilities

  $\pi_u = p(U^{(1)} = u) \quad u = 1,\dots,k$

- $(T-1)k(k-1)$ transition probabilities

  $\pi_{u|v}^{(t|t-1)} = p(U^{(t)} = u|U^{(t-1)} = v) \quad t = 2,\dots,T;\ u,v = 1,\dots,k$

- $\#\text{par} = k\sum_{j=1}^r (c_j-1) + (k-1) + (T-1)k(k-1)$

Multivariate basic LM model: probability distributions

- $p(\boldsymbol{U} = \boldsymbol{u}) = \pi_u \prod_{t=2}^T \pi_{u|v}^{(t|t-1)} = \pi_u \cdot \pi_{u_2|u}^{(2|1)} \dots \pi_{u_T|u_{T-1}}^{(T|T-1)}$
- $p(\boldsymbol{Y} = \boldsymbol{y}|\boldsymbol{U} = \boldsymbol{u}) = \prod_{t=1}^T \phi_{\boldsymbol{y}|u}^{(t)} = \phi_{\boldsymbol{y}|u}^{(1)} \cdot \phi_{\boldsymbol{y}|u}^{(2)} \dots \phi_{\boldsymbol{y}|u}^{(T)}$
- manifest distribution of $\boldsymbol{Y}$

$$p(\boldsymbol{Y} = \boldsymbol{y}) = \sum_{\boldsymbol{u}} p(\boldsymbol{Y} = \boldsymbol{y}, \boldsymbol{U} = \boldsymbol{u}) = \sum_{\boldsymbol{u}} p(\boldsymbol{U} = \boldsymbol{u}) \cdot p(\boldsymbol{Y} = \boldsymbol{y}|\boldsymbol{U} = \boldsymbol{u})$$
$$= \sum_{u} \pi_u \phi_{\boldsymbol{y}|u}^{(1)} \cdot \sum_{u_2} \pi_{u_2|u}^{(2|1)} \phi_{\boldsymbol{y}|u}^{(2)} \dots \sum_{u_T} \pi_{u_T|u_{T-1}}^{(T|T-1)} \phi_{\boldsymbol{y}|u}^{(T)}$$
$$= \sum_{u} \sum_{u_2} \dots \sum_{u_T} \pi_u \prod_{t=2}^{T} \pi_{u|v}^{(t|t-1)} \prod_{t=1}^{T} \phi_{\boldsymbol{y}|u}^{(t)}$$

Note that computing $p(\boldsymbol{Y} = \boldsymbol{y})$ involves all the possible k^T configurations of vector $\boldsymbol{u}$

Multivariate basic LM model: maximum likelihood (ML) estimation

- Log-likelihood of the model

$$\ell(\boldsymbol{\theta}) = \sum_{\boldsymbol{y}} n_{(\boldsymbol{y})} \log[p(\boldsymbol{Y} = \boldsymbol{y})]$$

  - $\boldsymbol{\theta}$: vector of all model parameters (π_u, $\pi_{u|v}^{(t|t-1)}$, $\phi_{jy|u}^{(t)}$)
  - $n_{(\boldsymbol{y})}$: frequency of the response configuration $\boldsymbol{y}$ in the sample

- $\ell(\boldsymbol{\theta})$ may be maximized with respect to $\boldsymbol{\theta}$ by an *Expectation-Maximization (EM) algorithm* (Dempster *et al.*, 1977)

EM algorithm

Complete data log-likelihood of the model

$$\ell^*(\boldsymbol{\theta}) = \sum_{j=1}^{r}\sum_{t=1}^{T}\sum_{u=1}^{k}\sum_{y=0}^{c-1} a_{juy}^{(t)} \log \phi_{jy|u}^{(t)} + \\ + \sum_{u=1}^{k} b_u^{(1)} \log \pi_u + \sum_{t=2}^{T}\sum_{v=1}^{k}\sum_{u=1}^{k} b_{vu}^{(t)} \log \pi_{u|v}^{(t|t-1)}$$

- $a_{juy}^{(t)}$: frequency of subjects responding by y for the j-th response variable and belonging to latent state u, at time t
- $b_u^{(1)}$: frequency of subjects in latent state u at time 1
- $b_{vu}^{(t)}$: frequency of subjects which move from latent state v to u at time t

EM algorithm

- The algorithm *alternates two steps* until convergence in $\ell(\boldsymbol{\theta})$:

  E: compute the expected values of frequencies $a_{juy}^{(t)}$, $b_u^{(1)}$, and $b_{vu}^{(t)}$, given the observed data and the current value of $\boldsymbol{\theta}$, so as to obtain the expected value of $\ell^*(\boldsymbol{\theta})$

  M: update $\boldsymbol{\theta}$ by maximizing the expected value of $\ell^*(\boldsymbol{\theta})$ obtained above; explicit solutions for $\boldsymbol{\theta}$ estimations are available

- The E-step is performed by means of certain recursions which may be easily implemented through matrix notation (Bartolucci, 2006)

Forward and backward recursions

To efficiently compute the probability $p(\boldsymbol{Y} = \boldsymbol{y})$ and the posterior probabilities $f_{u|\boldsymbol{y}}^{(t)}$ and $f_{u|v,\boldsymbol{y}}^{(t|t-1)}$ we can use forward and backward recursions for obtaining the following intermediate quantities

- Forward recursions

$$q_{u,\boldsymbol{y}}^{(t)} = p(U^{(t)} = u, \boldsymbol{Y}^{(1)}, \ldots, \boldsymbol{Y}^{(t)}) = \sum_{v=1}^{k} q_{v,\boldsymbol{y}}^{(t-1)} \pi_{u|v}^{(t|t-1)} \phi_{\boldsymbol{y}|u}^{(t)} \quad u = 1, \ldots, k$$

starting with $q_{u,\boldsymbol{y}}^{(1)} = \pi_u \phi_{\boldsymbol{y}|u}^{(1)}$

- Backward recursions

$$\bar{q}_{v,\boldsymbol{y}}^{(t)} = p(\boldsymbol{Y}^{(t+1)}, \ldots, \boldsymbol{Y}^{(T)} | U^{(t)} = v) = \sum_{u=1}^{k} \bar{q}_{u,\boldsymbol{y}}^{(t+1)} \pi_{u|v}^{(t+1|t)} \phi_{\boldsymbol{y}|u}^{(t+1)} \quad v = 1, \ldots, k$$

starting with $\bar{q}_{v,\boldsymbol{y}}^{(T)} = 1$

Model selection criteria

- A crucial point with LM models concerns the selection of k, the number of latent states
- We may rely on the literature about finite mixture models and hidden Markov models
- The most well-known criteria are
  - Akaike's Information Criterion (AIC - Akaike, 1973)

$$\mathrm{AIC} = -2\ell(\boldsymbol{\theta}) + 2 \cdot \#\mathrm{par}$$

    or its variants:
  - Consistent AIC (CAIC)

$$\mathrm{CAIC} = -2\ell(\boldsymbol{\theta}) + \#\mathrm{par} \cdot (\log(n) + 1)$$

  - AIC3

$$\mathrm{AIC3} = -2\ell(\boldsymbol{\theta}) + 3 \cdot \#\mathrm{par}$$

  - Bayesian Information Criterion (BIC - Schwarz, 1978)

$$\mathrm{BIC} = -2\ell(\boldsymbol{\theta}) + \#\mathrm{par} \cdot \log(n)$$

Classification-based criteria

Some criteria are developed in the context of the classification likelihood approach, based on the relation

$$\ell^*(\boldsymbol{\theta}) = \ell(\boldsymbol{\theta}) - \text{EN}$$

where EN is the entropy and it denotes a penalization term which measures the quality of the partition and it is defined as (Hernando et al., 2005)

$$\begin{aligned}\text{EN} &= -\sum_{u_1}\ldots\sum_{u_T} f_{u_1,\ldots u_T|\boldsymbol{y}} \log(f_{u_1,\ldots u_T|\boldsymbol{y}}) = \\ &= -\sum_{u_1}\ldots\sum_{u_T} f^{(1)}_{u_1|\boldsymbol{y}} \cdot f^{(2|1)}_{u_2|u_1,\boldsymbol{y}} \cdot \ldots \cdot f^{(t|t-1)}_{u_t|u_{t-1},\boldsymbol{y}} \cdot \ldots \cdot f^{(T|T-1)}_{u_T|u_{T-1},\boldsymbol{y}} \cdot \\ &\cdot [\log(f^{(1)}_{u_1|\boldsymbol{y}}) + \log(f^{(2|1)}_{u_2|u_1,\boldsymbol{y}}) + \ldots + \log(f^{(t|t-1)}_{u_t|u_{t-1},\boldsymbol{y}}) + \ldots + \log(f^{(T|T-1)}_{u_T|u_{T-1},\boldsymbol{y}})]\end{aligned}$$

with

$$f_{u|\boldsymbol{y}}^{(t)} = \frac{q_{u,\boldsymbol{y}}^{(t)} \cdot \bar{q}_{u,\boldsymbol{y}}^{(t)}}{p(\boldsymbol{Y} = \boldsymbol{y})}$$

$$f_{u|v,\boldsymbol{y}}^{(t|t-1)} = \frac{f_{v,u|\boldsymbol{y}}^{(t-1,t)}}{f_{v|\boldsymbol{y}}^{(t-1)}} = \frac{q_{v,\boldsymbol{y}}^{(t-1)} \pi_{u|v}^{(t|t-1)} \phi_{\boldsymbol{y}^{(t)}|u} \bar{q}_{u,\boldsymbol{y}}^{(t)}}{p(\boldsymbol{Y} = \boldsymbol{y})} \cdot \frac{p(\boldsymbol{Y} = \boldsymbol{y})}{q_{v,\boldsymbol{y}}^{(t-1)} \bar{q}_{v,\boldsymbol{y}}^{(t-1)}} =$$

$$= \pi_{u|v}^{(t|t-1)} \phi_{\boldsymbol{y}^{(t)}|u} \cdot \frac{\bar{q}_{u,\boldsymbol{y}}^{(t)}}{\bar{q}_{v,\boldsymbol{y}}^{(t-1)}}$$

We may also formulate an approximation for EN, under the assumption that $u^{(t)}$ are independent given $\boldsymbol{Y}$:

- $\mathrm{EN}_1 = -\sum_{u_1}\dots\sum_{u_T} f_{u|\mathbf{y}}^{(t)} \log(f_{u|\mathbf{y}}^{(t)})$
- or a possible variant of EN_1 given by $\mathrm{EN}_2 = -\sum_{u_1}\dots\sum_{u_T} f_{u|\mathbf{y}}^{(t)} \log(f_{u|\mathbf{y}}^{(t)})/T$
- Example: T=3

$$
\begin{aligned}
\mathrm{EN} &= -\sum_u\sum_v\sum_z f_{u,v,z|\mathbf{y}} \log(f_{u,v,z|\mathbf{y}}) = \\
&= f_{z|v,\mathbf{y}}^{(3|2)} \cdot f_{v|u,\mathbf{y}}^{(2|1)} \cdot f_{u|\mathbf{y}}^{(1)} \cdot \\
&\cdot [\log(f_{z|v,\mathbf{y}}^{(3|2)}) + \log(f_{v|u,\mathbf{y}}^{(2|1)}) + \log(f_{u|\mathbf{y}}^{(1)})] \\
\mathrm{EN}_1 &= -[f_{u|\mathbf{y}}^{(1)} \cdot \log(f_{u|\mathbf{y}}^{(1)}) + f_{v|\mathbf{y}}^{(2)} \cdot \log(f_{v|\mathbf{y}}^{(2)}) + f_{z|\mathbf{y}}^{(3)} \cdot \log(f_{z|\mathbf{y}}^{(3)})] \\
\mathrm{EN}_2 &= \frac{1}{3}\mathrm{EN}_1
\end{aligned}
$$

Some classification-based criteria are (McLachlan and Peel, Chap. 6)

- Classification Likelihood information Criterion (CLC)

$$\mathrm{CLC} = -2\ell(\boldsymbol{\theta}) + 2 \cdot \mathrm{EN}$$

- Approximated Integrated Classification Likelihood criterion (ICL-BIC)

$$\mathrm{ICL} - \mathrm{BIC} = \mathrm{BIC} + 2 \cdot \mathrm{EN}$$

- Normalized Entropy Criterion (NEC)

$$\mathrm{NEC} = \frac{\mathrm{EN}}{\ell(\boldsymbol{\theta}) - \ell_1(\boldsymbol{\theta})} \quad k \geq 2$$

  where $\ell_1(\boldsymbol{\theta})$ is the maximum log-likelihood in case of $k = 1$, and $\mathrm{NEC} = 1$ if $k = 1$

- Approximated NECs:

$$\mathrm{NEC}_1 = \frac{\mathrm{EN}_1}{\ell(\boldsymbol{\theta}) - \ell_1(\boldsymbol{\theta})} \quad k \geq 2$$

$$\mathrm{NEC}_2 = \frac{\mathrm{EN}_2}{\ell(\boldsymbol{\theta}) - \ell_1(\boldsymbol{\theta})} \quad k \geq 2$$

Monte Carlo simulation study

- We compare
  - AIC, CAIC, AIC3, BIC
  - CLC, ICL-BIC, NEC, NEC_1, NEC_2
- 100 samples with a given size n and coming from a multivariate LM model, characterized by r binary $(y = 0, 1)$ response variables observed in T time occasions, k latent states, and given values of initial probabilities π_u, transition probabilities $\pi_{u|v}^{(t|t-1)}$, conditional response probabilities $\phi_{jy|u}^{(t)}$
- $n = 250, 500, 1000$
- $r = 1, 3, 5$
- $T = 5, 10$
- $k = 2, 3$
- all analyses are implemented in R software

Main results

Scenery 1

- $n = 250$, $T = 5$, $k = 2$
- $\phi^{(t)}_{j0|u=1} = 0.8 = \phi^{(t)}_{j1|u=2}$, $\quad \phi^{(t)}_{j0|u=2} = 0.2 = \phi^{(t)}_{j1|u=1}$
- $\pi_1 = 0.5 = \pi_2$
- $\pi^{(t|t-1)}_{1|1} = 0.7 = \pi^{(t|t-1)}_{2|2}$, $\quad \pi^{(t|t-1)}_{1|2} = 0.3 = \pi^{(t|t-1)}_{2|1}$ (time homogenous assumption)
- $r = 1, 3, 5$

Main results

Scenery 1: Relative frequencies of k chosen on the basis of several criteria

k	BIC	AIC	AIC3	CAIC	NEC	NEC_1	NEC_2	CLC	ICL-BIC
$r = 1$									
1	**0.52**	0.00	0.10	**0.63**	**1.00**	**1.00**	**0.99**	**1.00**	**1.00**
2	**0.48**	0.98	0.90	0.37	0.00	0.00	0.01	0.00	0.00
3	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$r = 3$									
1	0.00	0.00	0.00	0.00	**0.88**	**0.92**	0.00	**0.88**	**0.95**
2	1.00	0.83	0.98	1.00	0.10	0.07	0.96	0.10	0.04
3	0.00	0.16	0.02	0.00	0.01	0.01	0.04	0.01	0.01
4	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.01	0.00
$r = 5$									
1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	1.00	0.77	1.00	1.00	1.00	1.00	1.00	1.00	1.00
3	0.00	0.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	0.00	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Main results

Scenery 2

- $n = 250$, $T = 5$, $k = 2$
- $\phi^{(t)}_{j0|u=1} = 0.7 = \phi^{(t)}_{j1|u=2}, \quad \phi^{(t)}_{j0|u=2} = 0.3 = \phi^{(t)}_{j1|u=1}$
- $\pi_1 = 0.5 = \pi_2$
- $\pi^{(t|t-1)}_{1|1} = 0.9 = \pi^{(t|t-1)}_{2|2}, \quad \pi^{(t|t-1)}_{1|2} = 0.1 = \pi^{(t|t-1)}_{2|1}$ (time homogenous assumption)
- $r = 1, 3, 5$

Main results

Scenery 2: Relative frequencies of k chosen on the basis of several criteria

k	BIC	AIC	AIC3	CAIC	NEC	NEC_1	NEC_2	CLC	ICL-BIC
$r = 1$									
1	0.35	0.01	0.02	**0.53**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**
2	0.65	0.98	0.97	**0.47**	0.00	0.00	0.00	0.00	0.00
3	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00
$r = 3$									
1	0.00	0.00	0.00	0.00	**1.00**	**1.00**	0.09	**1.00**	**1.00**
2	1.00	0.92	0.995	1.00	0.00	0.00	0.855	0.00	0.00
3	0.00	0.07	0.005	0.00	0.00	0.00	0.015	0.00	0.00
4	0.00	0.01	0.00	0.00	0.00	0.00	0.015	0.00	0.00
5	0.00	0.00	0.00	0.00	0.00	0.00	0.025	0.00	0.00
$r = 5$									
1	0.00	0.00	0.00	0.00	0.285	**0.77**	0.00	0.285	**0.55**
2	1.00	0.78	0.995	1.00	0.59	0.22	0.98	0.59	**0.445**
3	0.00	0.205	0.005	0.00	0.03	0.005	0.015	0.035	0.005
4	0.00	0.01	0.00	0.00	0.07	0.005	0.005	0.070	0.00
5	0.00	0.005	0.00	0.00	0.025	0.00	0.000	0.025	0.00

Main results

Scenery 3

- $n = 500$, $T = 5$, $k = 3$
- $\phi^{(t)}_{j0|u=1} = 0.9 = \phi^{(t)}_{j1|u=2}$, $\phi^{(t)}_{j0|u=2} = 0.1 = \phi^{(t)}_{j1|u=1}$, $\phi^{(t)}_{j0|u=3} = 0.4$, $\phi^{(t)}_{j1|u=3} = 0.6$
- $\pi_1 = \pi_2 = \pi_3 = 0.33$
- $\pi^{(t|t-1)}_{1|1} = \pi^{(t|t-1)}_{2|2} = \pi^{(t|t-1)}_{3|3} = 0.80$, $\pi^{(t|t-1)}_{2|1} = 0.15 = \pi^{(t|t-1)}_{2|3}$, $\pi^{(t|t-1)}_{3|1} = 0.05 = \pi^{(t|t-1)}_{1|3}$, $\pi^{(t|t-1)}_{1|2} = 0.10 = \pi^{(t|t-1)}_{3|2}$ (time homogenous assumption)
- $r = 1, 3, 5$

Main results

Scenery 3: Relative frequencies of k chosen on the basis of several criteria

k	BIC	AIC	AIC3	CAIC	NEC	NEC_1	NEC_2	CLC	ICL-BIC
$r=1$									
1	0.00	0.00	0.00	0.00	**1.00**	**1.00**	**0.92**	**1.00**	**1.00**
2	**1.00**	**0.98**	**0.99**	**1.00**	0.00	0.00	0.07	0.00	0.00
3	0.00	0.02	0.01	0.00	0.00	0.00	0.01	0.00	0.00
$r=3$									
1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	0.03	0.00	0.00	0.10	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**
3	0.97	0.81	1.00	0.90	0.00	0.00	0.00	0.00	0.00
4	0.00	0.19	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$r=5$									
1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	0.00	0.00	0.00	0.00	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**
3	1.00	0.78	0.99	1.00	0.00	0.00	0.00	0.00	0.00
4	0.00	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00
5	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Conclusions

- We compared several criteria for the selection of the number of latent states in the LM models
- We observed that:
  - AIC, BIC and their variants present a better general behavior with respect to the classification-based criteria
  - classification-based criteria tend to underestimate the true number of latent states, mainly for the univariate case
  - the behavior of classification-based criteria improves by increasing the number of observed response variables
  - by increasing the number k of latent states the performance of all considered criteria gets worse
- For further developments of our work, we would like to study in deep extended versions of entropy and classification-based criteria to improve the performance of the latent states selection process
- We will refer to the most recent developments in the context of hidden Markov models: see Durand and Guedon (2012) for a discussion about the tendency of entropy to overestimate the uncertainty and for a new proposal to decompose the global entropy in conditional entropies

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