A note on the application of the Oakes’ identity to obtain the observed information matrix of hidden Markov models

Francesco Bartolucci, Alessio Farcomeni and Fulvia Pennoni

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Abstract

We derive the observed information matrix of hidden Markov models by the application of the Oakes (1999)’s identity. The method only requires the first derivative of the forward-backward recursions of Baum and Welch (1970), instead of the second derivative of the forward recursion, which is required within the approach of Lystig and Hughes (2002). The method is illustrated by an example based on the analysis of a longitudinal dataset which is well known in sociology.

Keywords: Expectation-Maximization algorithm, Local identifiability, Latent Markov model, Longitudinal data, Standard Errors

1 Introduction

Hidden Markov (HM) models have been developed early in the literature on stochastic processes as extensions for measurement errors of the standard Markov chain model; for one of the oldest relevant contributions about these models, see Baum and Petrie (1966).
HM models have received much attention in the time-series analysis literature, due to their wide applicability and easy interpretation (for an up-to-date review see Zucchini and MacDonald, 2009). These models are also finding an increasing popularity for the analysis of longitudinal data (see Bartolucci et al., 2010).

The main tool for maximum likelihood (ML) estimation of the parameters of an HM model is the Expectation-Maximization (EM) algorithm, which is based on certain forward-backward recursions. This algorithm and these recursions were developed by Baum and colleagues in a series of papers specifically for HM models (Baum and Petrie, 1966; Baum and Egon, 1967; Baum et al., 1970). Then, the EM algorithm was put in a more general context in the widely cited paper of Dempster et al. (1977).

A drawback of the afore mentioned algorithm is that it does not provide, as a by-result, the standard errors for the parameter estimates. This is because it uses neither the observed nor the expected information matrix, which are suitable transformations of the second derivative matrix of the model log-likelihood. From the inverse of these matrices, we obtain standard errors for the parameter estimates. Then, from the output of the EM algorithm, we have not an obvious method for assessing the precision of these maximum likelihood estimates. The information matrix is also important to check the local identifiability of the model through its rank; see McHugh (1956) and Goodman (1974) among others.

Computing the information matrix (observed or expected) of a latent variable model, as an HM model, is considered a difficult task. Several methods have been proposed to overcome this difficulty; for a review see Lystig and Hughes (2002) and McLachlan and Krishnan (2008). One of the more interesting solutions was proposed by Louis (1982). This solution is based on the missing information principle as defined by Orchard and Woodbury (1972). According to this principle, the observed information matrix can be expressed as the difference between two matrices corresponding to the complete information, which we would be able to compute if we knew the latent states, and the missing
information due to the unobserved variables. However, this correction term is difficult in general to compute; see Oakes (1999) for further comments and Turner et al. (1998) for related techniques.

Oakes (1999) presented an alternative approach, with respect to that of Louis (1982), to compute the observed information matrix of a latent variable model. In particular, he derived an explicit formula for the second derivative matrix of the model log-likelihood which involves the first derivative of the conditional expectation of the score of the complete data log-likelihood, given observed data.

Specifically for HM models, Lystig and Hughes (2002) proposed a method for exactly computing the observed information matrix based on the second derivative of the forward recursion of Baum et al. (1970) which is used to compute the model log-likelihood; for a similar method see Bartolucci (2006). The method of Lystig and Hughes (2002) has become rather popular in the HM literature. Among the methods related to the EM algorithm, we also mention that proposed by Bartolucci and Farcomeni (2009) which is very simple to implement and requires a small extra code over that required for the ML estimation. However, since it is based on the numerical derivative of the score, the obtained information matrix may be considered an approximation of the true one. Also note that, in order to obtain standard errors for the parameter estimates, we can alternatively use a parametric bootstrap method (Efron and Tibshirani, 1993), as described in Zucchini and MacDonald (2009). Even if the standard errors obtained in this way may be more reliable with respect to those based on the information matrix, the method may be computationally costly and, in any case, does not allow us to check for local identifiability in an obvious way.

In this paper, we show how to apply the Oakes (1999) identity to obtain the observed information matrix of an HM model. As we will show, the proposed method only requires the first derivative of the forward-backward recursions of Baum et al. (1970), whereas the method of Lystig and Hughes (2002) requires the second derivative of the forward
recursion. On the other hand, the proposed method is superior to that of Bartolucci and Farcomeni (2009) since it allows us to exactly compute the observed information matrix. To the best of our knowledge, an implementation of the Oakes (1999)'s identity for HM models, as the one we propose here, is not available in the literature.

The proposed approach is illustrated through an application based on a well-known longitudinal dataset. For the specific HM model used in this application, we make available some R functions\(^1\) to compute the information matrix and then obtaining the standard errors for the parameter estimates.

In the following, we first briefly review the EM algorithm and the Oakes (1999)'s identity in their general versions. In Section 3 we propose an implementation of this identity for HM models on the basis of a suitable reparametrization. Then, in Section 4 we describe the application of the proposed method in connection with the analysis of the dataset mentioned above.

2 Preliminaries

We give in this section the necessary background about the EM algorithm and the Oakes (1999)'s identity in general; then we recall some important features about HM models.

2.1 EM algorithm and observed information matrix

The EM algorithm (Dempster et al., 1977) is an iterative algorithm for finding the ML estimator of models with missing variables and has a special role in the literature on latent variable models.

With reference to an observed sample, let \(\ell(\theta)\) denote the log-likelihood of the latent variable model of interest, where \(\theta\) is the vector of parameters. As it is well known, the EM algorithm is based on the complete data log-likelihood, denoted as \(\ell^*(\theta)\), which is the

\(^1\)through a website to be indicated later
log-likelihood that we could compute if we knew the value of the latent variables for each every sample unit. In particular, to maximize \( \ell(\theta) \), the algorithm alternates the following steps until convergence:

- **E-step**: compute the conditional expected value of the complete data log-likelihood given the current estimate of \( \theta \), denoted by \( \hat{\theta} \), and the observed data. This expected value is denoted by \( Q(\theta|\hat{\theta}) \);

- **M-step**: maximize \( Q(\theta|\hat{\theta}) \) with respect to \( \theta \).

We now consider the score and the observed information matrix corresponding to the model log-likelihood \( \ell(\theta) \). These are defined, respectively, as

\[
 s(\theta) = \frac{\partial \ell(\theta)}{\partial \theta} \quad \text{and} \quad J(\theta) = -\frac{\partial^2 \ell(\theta)}{\partial \theta \partial \theta'}.
\]

It may be simply proved that

\[
 s(\theta) = \frac{\partial Q(\theta|\hat{\theta})}{\partial \theta} \bigg|_{\hat{\theta} = \theta}.
\]

Consequently, the Oakes (1999)’s identity states that:

\[
 J(\theta) = -\left\{ \frac{\partial^2 Q(\theta|\hat{\theta})}{\partial \theta \partial \theta'} \bigg|_{\hat{\theta} = \theta} + \frac{\partial^2 Q(\theta|\hat{\theta})}{\partial \theta' \partial \theta'} \bigg|_{\hat{\theta} = \theta} \right\}.
\] (1)

This identity then involves two components. The first component is the second derivative of the conditional expected value of the complete-data log-likelihood given the observed data. This component is simple to obtain from the EM algorithm. The second component involved in (1) is the first derivative of the score for the same expected log-likelihood with respect to the current value of the parameters.

### 2.2 Hidden Markov models

Consider now a sequence of \( T \) response variables \( Y^{(1)}, \ldots, Y^{(T)} \), which are collected in the vector \( Y \). These response variables may be continuous or categorical and we may even
observe a vector of multivariate outcomes at each $t$. In the following, we briefly review the assumptions of an HM model for these data and then how to apply the EM algorithm for ML estimation of the resulting model.

2.2.1 Assumptions

An HM model relies on the following basic assumptions:

- the response variables $Y^{(1)}, \ldots, Y^{(T)}$ are conditionally independent given a sequence of unobserved variables $U^{(1)}, \ldots, U^{(T)}$ giving rise to a latent process vector denoted by $U$;

- every response variable $Y^{(t)}$, $t = 1, \ldots, T$, depends on the latent process $U$ only through $U^{(t)}$;

- the latent process $U$ follows a Markov chain with $k$ states labelled from 1 to $k$.

We consider in particular HM models in which:

- the conditional distribution of $Y^{(t)}$ given $U^{(t)}$ is time-homogenous;

- the latent Markov chain is of first-order and time-homogeneous.

Parameters of the model are then the initial probabilities of the latent process, denoted $\lambda_u = f_{U^{(1)}}(u)$ with $u = 1, \ldots, k$ and the transition probabilities $\pi_{u|\bar{u}} = f_{U^{(t)}|U^{(t-1)}}(u|\bar{u})$ with $t = 2, \ldots, T$ and $\bar{u}, u = 1, \ldots, k$. The initial probabilities are collected in the $k$-dimensional column vector $\lambda$ and the transition probabilities are collected in the $k \times k$ matrix $\Pi$, with each row denoted $\pi'_{\bar{u}}$, where $\pi_{\bar{u}} = (\pi_{1|\bar{u}}, \ldots, \pi_{k|\bar{u}})'$.

In the above expressions, $f_{U^{(t)}}(u)$ denotes the probability mass function of the distribution of $U^{(t)}$, whereas $f_{U^{(t)}|U^{(t-1)}}(u|\bar{u})$ denotes the probability mass function of $U^{(t)}$ given $U^{(t-1)}$. A similar convention will be used to denote density functions.

Furthermore, when the response variables are categorical with a reduced number of categories (labelled from 1 to $c$), we introduce the additional notation $\phi_{y|u} = f_{Y^{(t)}|U^{(t)}}(y|u)$
with \( u = 1, \ldots, k \) and \( y = 0, \ldots, c - 1 \). The probabilities are collected in the \( c \times k \) matrix \( \Phi \) which is made of the column vectors \( \phi_u \), with \( \phi = (\phi_1|u, \ldots, \phi_{c|u})' \).

### 2.3 Application of the EM algorithm

It is well known that the above model may be estimated by an EM algorithm formulated as in Baum et al. (1970); see also Bartolucci et al. (2010) and Zucchini and MacDonald (2009).

Suppose that we observe \( n \geq 1 \) independent realizations of \( Y \), denoted by \( y_1, \ldots, y_n \), with every \( y_i \) having elements \( y_i(t), t = 1, \ldots, T \). Note that, in the case of time-series data, we can only observe a single realization of \( Y \) and then \( n = 1 \); in this case, \( T \) is typically large. On the other hand, in the case of longitudinal data, \( n \) is often large as compared to \( T \). Our results apply invariably and the model log-likelihood may be expressed as

\[
\ell(\eta) = \sum_i \log f_Y(y_i) = \sum_y n_y \log f_Y(y),
\]

where \( \eta \) is a vector containing all the parameters in \( \Phi, \pi, \) and \( \Pi \), \( f_Y(y) \) is the probability mass function of \( Y \) seen as a function of \( \eta \). This function can be computed by a forward recursion which is described in Appendix 1. Moreover, \( n_y \) is frequency of the response configuration \( y = (y^{(1)}, \ldots, y^{(T)})' \) and the sum \( \sum_y \) is extended to all response configurations observed at least once.

We now specialize the EM algorithm for the case of categorical outcomes mentioned at the end of the previous section. Let \( a_{uy}^{(t)} \), with \( t = 1, \ldots, T, \ u = 1, \ldots, k, \ y = 0, \ldots, c - 1 \), denote the frequency of \( U^{(t)} = u \) and \( Y^{(t)} = y \), let \( b_u^{(t)} \), with \( t = 1, \ldots, T, \ u = 1, \ldots, k \), denote the frequency of \( U^{(t)} = u \), and let \( c_{\bar{u}uu}^{(t)} \), with \( t = 2, \ldots, T, \ \bar{u}, u = 1, \ldots, k \), denote the joint frequency of the latent states \( U^{(t-1)} = \bar{u} \) and \( U^{(t)} = u \). Every E-step of the EM algorithm consists of computing the conditional expected value of these frequencies given
the observed data and the current value of the parameter vector denoted by $\hat{\eta}$, that is

$$\hat{a}_{uy}^{(t)} = \sum_i f_{U(u)}(u|y_i) I(y_i^{(t)} = y) = \sum_y n_y f_{U(u)}(u|y) I(y^{(t)} = y),$$

$$\hat{b}_u^{(1)} = \sum_i f_{U(u)}(u|y_i) = \sum_y n_y f_{U(u)}(u|y),$$

$$\hat{c}_{uu}^{(t)} = \sum_i f_{U(u-1),U(u)}(y|y_i) = \sum_y n_y f_{U(u-1),U(u)}(u|y),$$

where $1(\cdot)$ is the indicator function equal to 1 if its argument is true. These expected values involve posterior probabilities that may be computed by recursions illustrated in Appendix 1.

Then, the M-step consists of maximizing the conditional expected value, given the observed data and $\hat{\eta}$, of the complete data log-likelihood, which may be decomposed as

$$Q(\eta|\eta) = Q_1(\Phi|\eta) + Q_2(\pi|\eta) + Q_3(\Pi|\eta),$$

with

$$Q_1(\Phi|\eta) = \sum_y \sum_t \sum_u \hat{a}_{uy}^{(t)} \log \phi_{y|u},$$

$$Q_2(\pi|\eta) = \sum_u \hat{b}_u^{(1)} \log \lambda_u,$$

$$Q_3(\Pi|\eta) = \sum_{t>1} \sum_{\bar{u}} \sum_u \hat{c}_{uu}^{(t)} \log \pi_{u|\bar{u}}.$$

Explicit expressions are available to maximize separately each of these expressions. In fact, at every M-step $\phi_{y|u}$ is set proportional to $\sum_t \hat{a}_{uy}^{(t)}$, $\lambda_u$ to $\hat{b}_u^{(1)}$, and $\pi_{u|\bar{u}}$ to $\sum_{t>1} \hat{c}_{uu}^{(t)}$; see Bartolucci et al. (2010) for a more detailed description.

### 3 Observed information matrix for HM models

First of all, we consider a reparametrization of the model such that the new parameter vector, denoted by $\theta$, is variation independent and is contained in $\mathcal{R}^s$ for a suitable $s$. Then, we show how to implement the Oakes (1999)'s identity by exploiting this reparametrization.
3.1 Reparametrization of the model

The conditional response probabilities are reparametrized through \( c - 1 \) logits referred to the first category, that is

\[
\alpha_{y|u} = \log \frac{\phi_{y+1|u}}{\phi_{1|u}}, \quad u = 1, \ldots, k, \quad y = 1, \ldots, c - 1,
\]

which are included in the \((c-1)\)-dimensional column vectors \( \alpha_u \); moreover, by \( \alpha \) we denote the vector made of the subvectors \( \alpha_1, \ldots, \alpha_k \). It is worth noting that the choice of the baseline category is irrelevant for the inference and shall be guided only by interpretability reasons. The initial probabilities are transformed similarly by the logits

\[
\beta_u = \log \frac{\lambda_{u+1}}{\lambda_1}, \quad u = 1, \ldots, k - 1,
\]

which are collected in the \((k-1)\)-dimensional column vector \( \beta \). Finally, the transition probabilities are parametrized through logits referred to the diagonal element, that is

\[
\gamma_{\bar{u}u} = \log \frac{\pi_{u|\bar{u}}}{\pi_{\bar{u}|u}}, \quad \bar{u}, u = 1, \ldots, k, \quad u \neq \bar{u},
\]

which are collected in the \((k-1)\)-dimensional vectors \( \gamma_{\bar{u}} \) for \( u = 1, \ldots, k \); we also denote by \( \gamma \) the overall vectors made of the subvectors \( \gamma_1, \ldots, \gamma_k \).

It is convenient to express the above vectors of logits in matrix notation. In particular, we can easily show that \( \alpha \) may be obtained by stacking the vectors

\[
\alpha_u = A \log \phi_u, \quad u = 1, \ldots, k,
\]

where \( A = (-1_{c-1} \quad I_{c-1}) \), with \( 1_h \) denoting a column vector of \( h \) ones and \( I_h \) an identity matrix of the same dimension. The inverse transformation is

\[
\phi_u = [1'_k \exp(\tilde{A} \alpha_u)]^{-1} \exp(\tilde{A} \alpha_u), \quad \tilde{A} = \begin{pmatrix} 0'_{c-1} \\ I_{c-1} \end{pmatrix}, \quad (5)
\]

where \( 0_h \) is column vector of \( h \) zeros. Similarly, we have that

\[
\beta = B \log \lambda,
\]
with $B = (-1_{k-1} \ I_{k-1})$; the inverse transformation of the last expression is defined as in (5) on the basis of the matrix $B$ defined in a similar way as $A$. Finally, the vector $\delta$ is made of the subvectors $\delta_{\bar{u}}$, $\bar{u} = 1, \ldots, k$, with

$$\delta_{\bar{u}} = C_{\bar{u}} \log \pi_{\bar{u}},$$

where

$$C_{\bar{u}} = \begin{pmatrix} I_{\bar{u}-1} & -1_{\bar{u}-1} & O_{\bar{u}-1,k-\bar{u}} \\ O_{k-\bar{u},\bar{u}-1} & -1_{k-\bar{u}} & I_{k-\bar{u}} \end{pmatrix},$$

with $O_{hj}$ denoting an $h \times j$ matrix of zeros. The inverse transformation, to obtain $\pi_{\bar{u}}$ from $\delta_{\bar{u}}$, is as in (5), with $\tilde{A}$ substituted by

$$\tilde{C}_{\bar{u}} = \begin{pmatrix} I_{\bar{u}-1} & O_{\bar{u}-1,k-\bar{u}} \\ 0'_{\bar{u}-1} & 0'_{k-\bar{u}} \\ O_{k-\bar{u},\bar{u}-1} & I_{k-\bar{u}} \end{pmatrix}.$$

The new vector of parameters $\theta$ is obtained by stacking the single parameters vectors, that is $\theta = (\alpha', \beta', \gamma')'$. Obviously, provided that all probabilities $\pi_{y|\bar{u}}$, $\lambda_{\bar{u}}$, and $\pi_{u|\bar{u}}$ are strictly positive, $\theta \in \mathcal{R}^s$, with $s = (c-1)k + k - 1 + k(k-1)$, and is a one-to-one transformation of the original parameter vector $\eta$, which instead belongs to a more complex space.

### 3.2 Computing the observed information matrix

First of all, adopting the above reparametrization, the expected value of the complete data log-likelihood may be expressed as

$$Q(\theta|\bar{\theta}) = Q_1(\alpha|\bar{\theta}) + Q_2(\beta|\bar{\theta}) + Q_3(\gamma|\bar{\theta}),$$

where, using the matrix notation, we have

$$Q_1(\alpha|\bar{\theta}) = \sum_{\bar{u}} \hat{a}'_{\bar{u}} \log \phi_{\bar{u}},$$

$$Q_2(\beta|\bar{\theta}) = (\hat{b}^{(1)})' \log \lambda,$$

$$Q_3(\gamma|\bar{\theta}) = \sum_{\bar{u}} \hat{c}'_{\bar{u}} \log \pi_{\bar{u}},$$
with \( \hat{a}_u \) denoting a column vector with elements \( \sum_t \hat{a}_{uy}^{(t)} \), \( y = 0, \ldots, c - 1 \), \( \hat{b}^{(1)}_u \) denoting a column vector with elements \( \hat{b}_u^{(1)} \), \( u = 1, \ldots, k \), and \( \hat{c}_u \) denoting a vector with elements \( \sum_{t>1} c_u^{(t)} \), \( u = 1, \ldots, k \). Consequently, by applying standard rules about log-linear models, we have the following score vectors for the complete-data log-likelihood:

\[
\frac{\partial Q_1(\alpha|\theta)}{\partial \alpha} = \sum_u \tilde{A}'(\hat{a}_u - \hat{b}_u^{(1)} \phi_u),
\]

\[
\frac{\partial Q_2(\beta|\theta)}{\partial \beta} = \tilde{B}'(\hat{b}^{(1)} - n\lambda),
\]

\[
\frac{\partial Q_3(\gamma|\theta)}{\partial \gamma} = \sum_u \tilde{C}'_u(\hat{c}_u - \hat{b}_u^{(+)} \pi_u).
\]

where \( \Omega_{\phi_u} = \text{diag}(\phi_u) - \phi_u \phi_u' \), \( \Omega_{\lambda} \) and \( \Omega_{\pi_u} \) are defined in a similar way, and \( \hat{b}_u^{(+)} = \sum_{t>1} \hat{b}_u^{(t-1)} \). Similar, we have the second derivative matrices:

\[
\frac{\partial^2 Q_1(\alpha|\theta)}{\partial \alpha \partial \alpha'} = -\sum_u \hat{b}_u^{(1)} \tilde{A}' \Omega_{\phi_u} \tilde{A},
\]

\[
\frac{\partial^2 Q_2(\beta|\theta)}{\partial \beta \partial \beta'} = -n \tilde{B}' \Omega_{\lambda} \tilde{B},
\]

\[
\frac{\partial^2 Q_3(\gamma|\theta)}{\partial \gamma \partial \gamma'} = -\sum_u \hat{b}_u^{(+)} \tilde{C}'_u \Omega_{\pi_u} \tilde{C}_u.
\]

It is straightforward to see that the second derivative in (1) is a block-diagonal matrix, with blocks corresponding to above three derivatives, that is

\[
\frac{\partial^2 Q(\theta|\theta)}{\partial \theta \partial \theta'} = \text{diag} \left( \frac{\partial^2 Q_1(\alpha|\theta)}{\partial \alpha \partial \alpha'}, \frac{\partial^2 Q_2(\beta|\theta)}{\partial \beta \partial \beta'}, \frac{\partial^2 Q_3(\gamma|\theta)}{\partial \gamma \partial \gamma'} \right).
\]

Moreover, in order to compute the second component in (1) we need the first derivatives of the expected frequencies in (6), (7), and (8) with respect to \( \tilde{\theta} \). More precisely, we have

\[
\frac{\partial^2 Q(\theta|\theta)}{\partial \theta \partial \theta'} = \left( \frac{\partial^2 Q_1(\alpha|\theta)}{\partial \theta \partial \alpha'}, \frac{\partial^2 Q_2(\beta|\theta)}{\partial \theta \partial \beta'}, \frac{\partial^2 Q_3(\gamma|\theta)}{\partial \theta \partial \gamma'} \right),
\]

where

\[
\frac{\partial^2 Q_1(\alpha|\theta)}{\partial \theta \partial \alpha'} = \sum_u \left( \frac{\partial \hat{a}_u'}{\partial \theta} - \frac{\partial \hat{b}_u^{(t)}(t)}{\partial \theta} \phi_u' \right) \tilde{A},
\]

\[
\frac{\partial^2 Q_2(\beta|\theta)}{\partial \theta \partial \beta'} = \frac{\partial \hat{b}_u^{(1)}(1)}{\partial \theta} \tilde{B},
\]

\[
\frac{\partial Q_3(\gamma|\theta)}{\partial \gamma} = \sum_u \left( \frac{\partial \hat{c}_u'}{\partial \theta} - \frac{\partial \hat{b}_u^{(1)}(1)}{\partial \theta} \pi_u' \right) \tilde{C}_u.
\]
How to compute the first derivatives of the above expected values with respect to $\hat{\theta}$ is shown in Appendix 2.

Once the observed information at the ML estimate of $\theta$ has been obtained through (1) exploiting the above results, on the basis of this matrix we can obtain the standard errors and check identifiability in the usual way. In particular, the standard errors are obtained by computing the square root of the elements in the main diagonal of $J(\hat{\theta})^{-1}$. Then, local identifiability is checked through the rank of $J(\hat{\theta})$; nevertheless, that this matrix is of full rank is required in order to compute its inverse.

Note that the standard errors obtained as above are referred to the ML estimate of the parameter vector $\theta$. However, we can simply express the standard errors for the corresponding estimate of the initial parameter vector $\eta$ by the delta method. In particular, we first compute

$$
\left( \frac{\partial \theta'}{\partial \eta} \bigg|_{\eta=\hat{\eta}} \right) J(\hat{\theta})^{-1} \left( \frac{\partial \theta}{\partial \eta'} \bigg|_{\eta=\hat{\eta}} \right)
$$

to estimate the variance-covariance matrix of $\hat{\eta}$ and then we obtain the corresponding standard errors as the square root of the elements in the main diagonal of this matrix. In particular, the derivative matrix of $\theta$ with respect of $\eta$ may be simply constructed as a block diagonal matrix with blocks corresponding to the derivative of $\alpha_u$ with respect to every $\phi_u, u = 1, \ldots, k$, to the derivative of $\beta$ with respect to $\pi'$, and to the derivative of $\pi_u$ with respect to $\delta_u, \bar{u} = 1, \ldots, k$. For instance, we have

$$
\frac{\partial \alpha'_u}{\partial \phi} = \Omega_{\phi_u} \hat{A}
$$

and in similar way we can compute the other other blocks.

Finally, it is important to consider that the method described above may be simply adapted to more sophisticated HM models in which, for instance, the transition probabilities are time-heterogeneous, the distribution of the response variables given the latent state is assumed to belong to a certain parametric family, and/or covariates are included in the model; see Bartolucci et al. (2010). However, we prefer to focus on a specific, but
important, HM model in order to make the description of the proposed methods simpler to understand.

4 Example

In order to illustrate the proposed approach, we analyze a well-known dataset based on 5 annual waves of the National Youth Survey (Elliot et al., 1989). The dataset concerns 237 individuals who were aged 13 years in 1976. The use of marijuana was measured by an ordinal response variable for each wave, having the following three categories: “never in the past year” (coded as 1); “no more than once in a month in the past year” (coded as 2); “once a month in the past year” (coded as 3). Such data have been also used for empirical illustrations by Lang et al. (1999), Vermunt and Hagenaars (2004), and Bartolucci (2006).

With \( k = 2 \) we obtain the estimates of the conditional response probabilities displayed in Table 1. The table also reports the standard errors obtained with the proposed method and those obtained using the parametric bootstrap with a number of sample repetitions equal to 1000. Moreover, in Tables 2 and 3 we show the estimates of the initial probabilities and of the transition probabilities respectively, together with the corresponding standard errors.

| \( y \) | \( u = 1 \) | \( u = 2 \) | \( u = 1 \) | \( u = 2 \) | \( u = 1 \) | \( u = 2 \) |
|---|---|---|---|---|---|---|
| 1 | 0.9552 | 0.0791 | 0.0137 | 0.0338 | 0.0096 | 0.0315 |
| 2 | 0.0437 | 0.4623 | 0.0131 | 0.0339 | 0.0090 | 0.0338 |
| 3 | 0.0011 | 0.4586 | 0.0024 | 0.0398 | 0.0024 | 0.0358 |

Table 1: Estimates of the parameters \( \phi_{y|u} \) and corresponding standard errors obtained by the proposed method (s.e.) and a parametric bootstrap method based on 1,000 samples (boot.s.e.).
Table 2: Estimates of the parameters $\lambda_u$ and corresponding standard errors obtained by the proposed (s.e.) method and a parametric bootstrap method based on 1,000 samples (boot.s.e.).

| $u$ | est. | s.e. | boot.s.e. |
|-----|------|------|-----------|
| 1   | 0.9466 | 0.0178 | 0.0166 |
| 2   | 0.0534 | 0.0178 | 0.0166 |

Table 3: Estimates of the parameters $\pi_{u|\bar{u}}$ and corresponding standard errors obtained by the proposed method (s.e.) and a parametric bootstrap method based on 1,000 samples (boot.s.e.).

| $\bar{u}$ | $u = 1$ | $u = 2$ | $u = 1$ | $u = 2$ | $u = 1$ | $u = 2$ |
|-----------|---------|---------|---------|---------|---------|---------|
| 1         | 0.8774  | 0.1226  | 0.0157  | 0.0157  | 0.0140  | 0.0140  |
| 2         | 0.0319  | 0.9681  | 0.0316  | 0.0316  | 0.0268  | 0.0268  |

For this application, through the proposed recursion we easily obtain the standard errors for the parameter estimates. Moreover, as shown in Tables 1, 2, and 3, these standard errors are always very close to the corresponding parametric bootstrap standard errors. This confirms the validity of the proposed method to compute the observed information matrix.

We also estimated the HM model $k = 3$ classes, however the information matrix $J(\hat{\theta})$ is singular because one of the transition probabilities becomes equal to 0, so that we cannot state that this model is locally identifiable.
Appendix 1: Efficient implementation of recursions

Manifest distribution of the response variables

In order to efficiently compute the manifest probability \( f_Y(y) \), let \( q^{(t)}(y) \) denote the column vector with elements \( f_{U,Y,Y^{(t)}}(u,y^{(1)},\ldots,y^{(t)}) \), for \( u = 1, \ldots, k \). Then, we have

\[
q^{(t)}(y) = \begin{cases} 
\text{diag}(m_y^{(t)}), & t = 1, \\
\text{diag}(m_y^{(t)})(q^{(t-1)}(y))^\top, & t = 2, \ldots, T,
\end{cases}
\]

(12)

where \( m_y \) is a \( k \) dimensional column vector containing the probabilities \( \phi_{y|u}, u = 1, \ldots, k \). At the end of this recursions we obtain \( f_Y(y) \) as \( q^{(T)}(y)^\top 1 \), where \( 1 \) denotes a column vector of ones of suitable dimension. In implementing this recursion, attention must be payed to the case of large values of \( T \) because, as \( t \) increases, the probabilities in \( q^{(t)}(y) \) could become negligible; see Scott (2002) for remedial measures.

In the multivariate case, the same recursion as in (12) may be used, with \( m_y \) substituted by the vector \( m_y \) with elements corresponding the conditional probability of the response vector \( y \) given every possible value of the corresponding latent state. For further details on this, and the following recursion, see Zucchini and MacDonald (2009) and Bartolucci et al. (2010).

Posterior distribution of the latent variables

Let \( \bar{q}^{(t)}(y) \) be the column vector with elements \( f_{Y^{(t+1)},\ldots,Y^{(T)}|U^{(t)}}(\bar{u},y^{(t+1)},\ldots,y^{(T)}) \), \( \bar{u} = 1, \ldots, k \). This vector may computed by the backward recursion

\[
\bar{q}^{(t)}(y) = \begin{cases} 
1, & t = T, \\
\Pi\text{diag}(m_y^{(t+1)})(\bar{q}^{(t+1)}(y))^\top, & t = T-1, \ldots, 1.
\end{cases}
\]

Then, the \( k \)-dimensional column vector \( f^{(t)}(y) \) with elements \( f_{U|Y}(u|y), u = 1, \ldots, k \), is obtained as

\[
f^{(t)}(y) = \frac{1}{f_Y(y)}\text{diag}[q^{(t)}(y)]q^{(t)}(y), \quad t = 1, \ldots, T.
\]

(13)
Moreover, the \( k \times k \) matrix \( F^{(t)}(\mathbf{y}) \), with elements \( f_{U(t-1),U(t)}(\bar{u},u|\mathbf{y}) \) arranged by letting \( \bar{u} \) run by row and \( u \) by column, is obtained as

\[
F^{(t)}(\mathbf{y}) = \frac{1}{f_{Y}(\mathbf{y})} \text{diag}[q^{(t-1)}(\mathbf{y})] \Pi \text{diag}[m_{y(t)}] \text{diag}[q^{(t)}(\mathbf{y})],
\]

for \( t = 2, \ldots, T \).

Appendix 2: derivative of the expected frequencies

The derivatives of the expected frequencies in (9), (10), and (11) may be obtained by substituting in (2), (3), and (4) every posterior probability with the corresponding derivative with respect to the parameters of interest. For instance, from (2) we have that the derivative matrix

\[
\frac{\partial \hat{a}'_{\bar{u}}}{\partial \hat{\theta}}
\]

has the following elements

\[
\frac{\partial \hat{a}'_{\bar{u}y}}{\partial \theta_j} = \sum_y n_y \frac{\partial f_{U(t)|Y}(u|\mathbf{y})}{\partial \theta_j} I(y^{(t)} = y),
\]

for \( y = 1, \ldots, c \), where \( \hat{\theta}_j \) is an arbitrary element of \( \hat{\theta} \).

In order to compute the derivative of \( f_{U(t)|Y}(u|\mathbf{y}) \), and also that of \( f_{U(t-1),U(t)}|Y \), with respect to every parameter \( \hat{\theta}_j \) we can proceed as in Lystig and Hughes (2002) and Bartolucci (2006). In particular, let

\[
q^{(t,j)}(\mathbf{y}) = \frac{\partial q^{(t)}(\mathbf{y})}{\partial \theta_j} \quad \text{and} \quad \bar{q}^{(t,j)}(\mathbf{y}) = \frac{\partial \bar{q}^{(t)}(\mathbf{y})}{\partial \theta_j},
\]

and let \( \phi_u^{(j)} \), \( \lambda^{(j)} \), and \( \Pi^{(j)} \) be defined in a similar way as the derivatives of \( \phi_u \), \( \lambda \), and \( \Pi \) with respect to \( \hat{\theta}_j \); in a similar way also define \( m_y^{(j)} \). Finally, the vectors in (15) may be obtained by the following recursions:

\[
q^{(t)}(\mathbf{y}) = \begin{cases} 
\text{diag}(m_{y(t)}^{(j)}) \lambda + \text{diag}(m_{y(t)}) \lambda^{(j)}, & t = 1, \\
\text{diag}(m_{y(t)}^{(j)}) \Pi' q^{(t-1)}(\mathbf{y}) + \text{diag}(m_{y(t)}) (\Pi^{(j)})' q^{(t-1)}(\mathbf{y}) + \text{diag}(m_{y(t)}) \Pi' (\bar{q}^{(t-1,j)}(\mathbf{y})) & t = 2, \ldots, T, 
\end{cases}
\]
and
\[ \hat{q}^{(t)}(y) = \begin{cases} 0 & t = T, \\
\Pi^{(j)} \text{diag}(m^{(t+1)}_{y^{(t+1)}}) \hat{q}^{(t+1)}(y) + \Pi \text{diag}(m^{(j)}_{y^{(t+1)}}) q^{(t+1)}(y) + \\
\Pi \text{diag}(m^{(t+1)}_{y^{(t+1)}}) \hat{q}^{(t+1,j)}(y), & t = T - 1, \ldots, 1. \end{cases} \]

Finally, the first derivative of \( f_Y(y) \) with respect to \( \theta_j \) is obtained as \( f_Y^{(j)}(y) = (q^{(T,j)})'1 \). In a similar way, considering (13) and (14), we obtain the vector \( f^{(t,j)}(y) \) and \( F^{(t,j)}(y) \), having elements corresponding to the derivatives of \( f_{U(t)|Y}(u|y) \) and \( f_{U(t-1),U(t)|Y} \) with respect to every parameter \( \hat{\theta}_j \).

References

Bartolucci, F. (2006). Likelihood inference for a class of latent Markov models under linear hypotheses on the transition probabilities. *Journal of the Royal Statistical Society, series B*, 68:155–178.

Bartolucci, F. and Farcomeni, A. (2009). A multivariate extension of the dynamic logit model for longitudinal data based on a latent Markov heterogeneity structure. *Journal of the American Statistical Association*, 104:816–831.

Bartolucci, F., Farcomeni, A., and Pennoni, F. (2010). An overview of latent Markov models for longitudinal categorical data. *arXiv:1003.2804*.

Baum, L. and Egon, J. (1967). An inequality with applications to statistical estimation for probabilistic functions of a Markov process and to a model for ecology. *Bull. Amer. Meteorol. Soc.*, 73:360–363.

Baum, L. and Petrie, T. (1966). Statistical inference for probabilistic functions of finite state Markov chains. *Annals of Mathematical Statististics*, 37:1554–1563.

Baum, L., Petrie, T., Soules, G., and Weiss, N. (1970). A maximization technique occu-
ring in the statistical analysis of probabilistic functions of Markov chains. *Annals of Mathematical Statistics*, 41:164–171.

Dempster, A. P., Laird, N. M., and Rubin, D. B. (1977). Maximum likelihood from incomplete data via the EM algorithm (with discussion). *Journal of the Royal Statistical Society, Series B*, 39:1–38.

Efron, B. and Tibshirani, R. (1993). *An Introduction to the Bootstrap*. Chapman & Hall, New York.

Elliot, D. S., Huizinga, D., and Menard, S. (1989). *Multiple Problem Youth: Delinquency, Substance Use, and Mental Health Problems*. Springer-Verlag, New York.

Goodman, L. A. (1974). Exploratory latent structure analysis using both identifiable and unidentifiable models. *Biometrika*, 61:215–231.

Lang, J. B., McDonald, J. W., and Smith, P. W. F. (1999). Association modeling of multivariate categorical responses: a maximum likelihood approach. *Journal of the American Statistical Association*, 94:1161–71.

Louis, T. (1982). Finding the observed information matrix when using the EM algorithm. *Journal of the Royal Statistical Society, Series B*, 44:226–233.

Lystig, T. C. and Hughes, J. (2002). Exact computation of the observed information matrix for hidden Markov models. *Journal of Computational and Graphical Statistics*, 11:678–689.

McHugh, R. B. (1956). Efficient estimation and local identification in latent class analysis. *Psychometrika*, 21:331–347.

McLachlan, G. J. and Krishnan, T. (2008). *The EM Algorithm and Extensions: Second Edition*. Wiley, New Jersey.
Oakes, D. (1999). Direct calculation of the information matrix via the EM algorithm. 
*Journal of the Royal Statistical Society, Series B*, 61:479–482.

Orchard, T. and Woodbury, M. (1972). A missing information principle: theory and applications. In Le Cam L.M., N. J. and L., S. E., editors, *Proc. Sixth Berkeley Symp. on Math. Statist. and Prob.*, volume 1, pages 697–715, Berkeley. University of California Press.

Scott, S. L. (2002). Bayesian methods for hidden Markov models: Recursive computing in the 21st century. *Journal of the American Statistical Association*, 97:337–351.

Turner, T. R., Cameron, M. A., and Thomson, P. J. (1998). Hidden Markov chains in generalized linear models. *The Canadian Journal of Statistics / La Revue Canadienne de Statistique*, 26:107–125.

Vermunt, J. and Hagenaars, J. (2004). Ordinal longitudinal data analysis. In R.C. Hauspie, N. C. and Molinari, L., editors, *Methods in Human Growth Research*. Cambridge University Press.

Zucchini, W. and MacDonald, I. L. (2009). *Hidden Markov Models for time series: an introduction using R*. Springer-Verlag, New York.