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► **To cite this version:**

Hanna Bacave, Pierre-Olivier Cheptou, Nikolaos Limnios, Nathalie Peyrard. Non-parametric Observation Driven HMM. 2024. hal-04053732v2

**HAL Id: hal-04053732**

**<https://hal.inrae.fr/hal-04053732v2>**

Preprint submitted on 17 Oct 2024

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## Non-parametric Observation Driven Hidden Markov Model

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### ARTICLE HISTORY

Compiled October 17, 2024

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## ABSTRACT

Hidden Markov models (HMM) are used in different fields to study the dynamics of a process that cannot be directly observed. However, in some cases, the structure of dependencies of a HMM is too simple to describe the dynamics of the hidden process. In particular, in some applications in finance and in ecology, the transition probabilities of the hidden Markov chain can also depend on the current observation. In this work, we are interested in extending the classical HMM to this situation. We refer to the extended model as the Observation Driven Hidden Markov Model (OD-HMM). We present a complete study of the general non-parametric OD-HMM with discrete and finite state spaces. We study its identifiability and the consistency of the maximum likelihood estimators. We derive the associated forward-backward equations for the E-step of the EM algorithm. The quality of the procedure is tested on simulated datasets. We illustrate the use of the model on an application on the study of annual plant dynamics. This work establishes theoretical and practical foundations for this framework that could be further extended to the parametric context in order to simplify estimation, and to hidden semi-Markov models for more realism.

## KEYWORDS

Non homogeneous HMM, identifiability, consistency, EM algorithm

## 1. Introduction

Hidden Markov Models (HMM, Cappé et al. 2005) are used in many different fields such as, e.g., medicine (Le Strat and Carrat 1999) to analyze epidemiological surveillance data, signal processing (Gales and Young 2008) for speech recognition, ecology (McClintock et al. 2020) to reconstruct hidden or partially observed ecological dynamics, bio-informatics (Yoon 2009) for the analysis of biological sequences, and finance (Engel and Hamilton 1990) to predict the regime of a monetary system thanks to the exchange rate. HMMs make it possible to study the dynamics of a process that cannot be directly observed. Indeed, in the above domains, the only observation available is an indirect information on the process of interest (e.g., symptoms of a disease), or another process driven by the hidden one (e.g., accelerometer data used to classify animal

behavior Leos-Barajas et al. 2017). In the field of HMM, results have been established on model identifiability (Allman et al. 2009; Cappé et al. 2005) and on the asymptotic properties of the Maximum Likelihood Estimator (MLE, Cappé et al. 2005). In practice, the MLE is computed using the Baum-Welch algorithm (Baum et al. 1970), a special case of the Expectation-Maximization algorithm for HMM (Dempster et al. 1977).

The HMM relies on two assumptions: the hidden process is modeled by a Markov chain, and the observations are independent, given the hidden chain. In some cases, this structure of dependencies is too simple to describe the dynamics of the hidden system. In particular, the next hidden state could depend not only on the current hidden state but also on the current observation, as we will see in some of the examples below. In this work we are interested in extending the classical HMM to this situation. We refer to the extended model as the Observation Driven Hidden Markov Model (OD-HMM) exemplified below. Theoretical results and inference algorithms for HMM do not directly apply to the OD-HMM, mainly because the transition probabilities are not constant across time in the OD-HMM and, instead, depend on the current observation. For this new dependency structure, it is necessary to study conditions for model identifiability and properties of the MLE. Furthermore, the forward-backward equations of the Baum-Welch algorithm must be adapted.

To highlight the usefulness of the OD-HMM, we present two applications where the hidden dynamics are driven by observations, one in ecology and one in finance. In ecology, the structure of the classical HMM is not always suitable to study the development of a partially observable species, in particular when the hidden and the observed processes represent two different life stages of the species, one dormant and one non-dormant. Let us consider the case of plants. In practice, we can only observe grown plants since the seeds in the soil are not attainable. The seeds remain in the soil for several years. This makes the use of a dynamical model with a hidden state, like a HMM, relevant. However, new seeds produced by the grown plants enter the soil each year. A classical HMM does not model this latter event. The OD-HMM is better suited.

The OD-HMM can also be used in finance as an extension of the Hamilton Markov-switching Model (Hamilton 1989), to study series of financial data that oscillate between two regimes. The characteristics of the observed financial data (e.g., mean, variance) depend on the hidden regime. In Engel and Hakkio (1996), the authors propose a study of the exchange rate of the European monetary system that can either be in a 'stable' or 'volatile' regime. The dependence structure of this model is similar to that of the OD-HMM since the exchange rate observed at time  $t - 1$  influences the regime it is in at time  $t$ .

An extension of HMM to the case where the current observation influences the transition of the hidden chain has already been considered in two contexts. First, in the two above-mentioned applied domains (Engel and Hakkio 1996; Pluntz et al. 2018a), specific OD-HMMs have been designed, in a parametric form, in order to estimate meaningful parameters for the application. Another set of works concerns the study of the properties of the MLE in models more general than OD-HMMs, but without providing a generic operational algorithm for model estimation (Ailliot and Pène 2015; Pouzo et al. 2022). Therefore, no complete tool kit exists at this time for a generic OD-HMM, providing model identifiability, theoretical properties of the MLE and an efficient implementation of the adaptation of the Baum-Welch algorithm to this model.

More precisely, the OD-HMM has been used in ecology to model the dynamics of annual plants (Pluntz et al. 2018a). In Pluntz et al. (2018a), the proposed model is a parametric model for the presence/absence of seeds as hidden states and the presence/absence of grown plants as observations. The main drivers of plants dynamics define the parameters. A simplification assumption considers a fixed probability of seed production equal to 1. Parameter estimation is performed by reformulating the model into the framework of classical HMM and applying the Baum-Welch algorithm. This article presents a parameterized OD-HMM dedicated to annual plant dynamics. Similarly, in Engel and Hakkio (1996), the model is specific to the financial application, with two hidden states.

From a theoretical point of view, a multitude of resources are available concerning the consistency of MLE for the classical HMM (Baum and Petrie 1966; Leroux 1992;

Gámiz et al. 2023), which we could have adapted to the OD-HMM case. However, other theoretical works on the properties of the MLE exist for more complex dependency structures between observations and hidden states than for the classical HMM (Ailliot and Pène 2015; Pouzo et al. 2022), and that include the OD-HMM as a particular case. In Ailliot and Pène (2015), the authors define the framework of non-homogeneous Markov-switching auto-regressive models and propose a study of the consistency of the MLE of this general model where the current observation and hidden state can depend on past observations on several time steps, as well as some applications in ecology. In this work, the state spaces can either be continuous or discrete but the results are given in the continuous case. The dependency structure of the OD-HMM is a particular case of the general framework of Ailliot and Pène (2015), even though it is not considered in their article. It is therefore possible to derive under which assumptions consistency of MLE for the OD-HMM is ensured, by traducing the generic results in Ailliot and Pène (2015) to the OD-HMM case. However, it remains to be done. In Pouzo et al. (2022), the author established sufficient conditions for the consistency and the local asymptotic normality of the MLE for a Markov regime switching model where transition probabilities can depend on covariates. Their results are established in the case where the observation state space is continuous and the hidden state space is discrete. Parameter estimation is only performed for a particular parametric version of the OD-HMM.

In conclusion, the works related to the OD-HMM dependency structure are either based on model parameters dedicated to a particular application (plant dynamics or finance), or on theoretical results for more general models or with continuous state space for the observed process. These latter ones can be used to derive consistency results for a general, non-parametric OD-HMM, but they do not provide an operational estimation algorithm. We can mention here the work of (Yujian 2005) where the OD-HMM was introduced as a HMM with states depending on observations. However, although the estimation procedure is described, there are no results on the asymptotic consistency of the MLE and the simulation study is very limited with no available code. The contribution of our work is a complete tool kit for the non-parametric OD-

HMM with finite state spaces that encompasses both its theoretical study (model identifiability and MLE consistency) and the design of an EM algorithm for MLE computation, with its implementation made available to the scientific community.

We begin in Section 2 by defining this model and studying its identifiability. Then, in Section 3, we study the consistency of the MLE, relying on the results of Ailliot and Pène (2015). We also provide the necessary modifications compared to the EM algorithm for HMM, in the Expectation step, and all detailed calculations to obtain the associated EM algorithm. In Section 4, we perform several simulation examples on simulated data in order to evaluate the quality of the EM estimators. Finally, in Section 5, we use a real data set to illustrate how the model can be exploited to estimate the mean duration of a seed bank in the soil.

## 2. The non-parametric OD-HMM

### 2.1. Model definition

Let us consider two sets of random variables, indexed by (discrete) time:  $Y_t$ , the observation at time  $t$ , with state space  $\Omega_Y = \{1, \dots, D\}$ , and  $Z_t$ , the hidden state at time  $t$ , with state space  $\Omega_Z = \{1, \dots, S\}$ . We study the evolution of the hidden and observed processes between the time  $t = 0$  and  $t = M$ , where  $1 \leq M < \infty$ . We denote the vector of all observations by  $Y_{0:M} = (Y_0, Y_1, Y_2, \dots, Y_M)$ . In the same way, the vector of all the hidden states, between  $t = 0$  and  $t = M$ , is denoted as  $Z_{0:M} = (Z_0, Z_1, \dots, Z_M)$ . In the most common version of a HMM, whose graphical representation is shown in Figure 1, left side,  $(Z_t)$  is a Markov chain and  $\mathbb{P}(Y_{0:M} = y_{0:M} \mid Z_{0:M} = z_{0:M}) = \prod_{t=0}^M \mathbb{P}(Y_t = y_t \mid Z_t = z_t)$ <sup>1</sup>.

We consider here an extension of the classical HMM, where the observation  $Y_{t-1}$  has an influence on the next hidden variable  $Z_t$ . This corresponds to the graphical representation of conditional independencies shown in Figure 1, right side.

**Definition 2.1** (OD-HMM). Let  $Y = (Y_t)_{t \in \mathbb{N}}$  be random variables mutually indepen-

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<sup>1</sup>By convention, we use uppercase letters,  $Z_t$  and  $Y_t$ , for random variables and lowercase letters,  $z_t$  and  $y_t$ , for realizations.



**Figure 1.** Graphical representation of conditional independencies in the chain  $(Z_t, Y_t)$  for an HMM (left) and for an OD-HMM (right).

dent conditionally to a sample path of the process  $Z = (Z_t)_{t \in \mathbb{N}}$ , such that  $Y_t$  depends only on  $Z_t$  and not all the path, i.e, for all  $y_{0:t} \in (\Omega_Y)^{t+1}$ , and all  $z_{0:t} \in (\Omega_Z)^{t+1}$ , the following relation holds true :

$$\mathbb{P}(Y_t = y_t \mid Z_{0:t} = z_{0:t}, Y_{0:t-1} = y_{0:t-1}) = \mathbb{P}(Y_t = y_t \mid Z_t = z_t).$$

The chain  $(Z_t, Y_t)_{t \in \mathbb{N}}$  is said to follow an Observation Driven HMM (OD-HMM) if, in addition, the process  $Z = (Z_t)_{t \in \mathbb{N}}$  satisfies the following property:

$$\mathbb{P}(Z_t = z_t \mid Z_{0:t-1} = z_{0:t-1}, Y_{0:t-1} = y_{0:t-1}) = \mathbb{P}(Z_t = z \mid Z_{t-1} = z_{t-1}, Y_{t-1} = y_{t-1}).$$

As a consequence, in a OD-HMM, the joint distribution of  $(Z_{0:M}, Y_{0:M})$  is fully determined by the following distributions. The initial probability is denoted  $\pi(z_0)$ , where:

$$\forall z_0 \in \Omega_Z, \pi(z_0) = \mathbb{P}(Z_0 = z_0).$$

The emission probability is denoted  $R(z_t, y_t)$ , where:

$$\forall z_t \in \Omega_Z, y_t \in \Omega_Y, R(z_t, y_t) = \mathbb{P}(Y_t = y_t \mid Z_t = z_t).$$

The transition probability is denoted  $P_{y_{t-1}}(z_{t-1}, z_t)$ , where:

$$\forall (z_t, z_{t-1}) \in \Omega_Z^2, y_{t-1} \in \Omega_Y, P_{y_{t-1}}(z_{t-1}, z_t) = \mathbb{P}(Z_t = z_t \mid Z_{t-1} = z_{t-1}, Y_{t-1} = y_{t-1}).$$



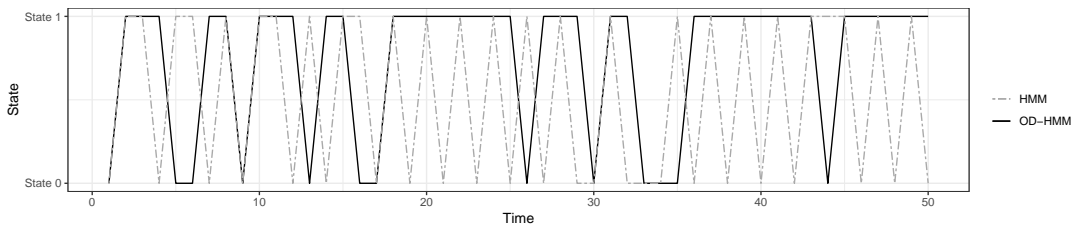
Note that due to the influence of observations on hidden states, the transition probability depends on the observation  $y_{t-1}$ . Therefore a specificity of this model is that there are as many transition matrices as observed states ( $D$ ), as opposed to the classical HMM. In this sense, the OD-HMM is non-homogeneous.

The model is non-parametric in the sense that there is no restriction of the values of the transition and the emission matrices (this can sometimes also be referred to as a fully parametric model). Even though the model is non-parametric, for the sake of simplicity, we will refer to these distributions as the model parameters. Since they are all probabilities with a constraint to add up to one, the set of parameters is  $\theta = \left( (P_y(z', z), y \in \Omega_Y, z' \in \Omega_Z, z \in \Omega_Z \setminus \{S\}), (R(z, y), z \in \Omega_Z, y \in \Omega_Y \setminus \{D\}) \right)$ . It takes values in  $\Theta = [0, 1]^{|\Omega_Z|(|\Omega_Z|-1)|\Omega_Y| + (|\Omega_Y|-1)|\Omega_Z|}$ . We do not include the initial distribution  $\pi$  because we will not consider its MLE estimation.

To illustrate the difference in the behavior of the HMM and the OD-HMM, we plot two simulated hidden chains in Figure 2. The first one, in solid line, is simulated according to an OD-HMM with two possible states for the observation and for the hidden chain. The two transition matrices and the emission matrix are as follows:

$$P_0 = \begin{pmatrix} 0.2 & 0.8 \\ 0.8 & 0.2 \end{pmatrix}, P_1 = \begin{pmatrix} 0.8 & 0.2 \\ 0.2 & 0.8 \end{pmatrix}, R = \begin{pmatrix} 0.8 & 0.2 \\ 0.2 & 0.8 \end{pmatrix}.$$

The second one, in dashed line, is simulated with a HMM, ignoring that the transition can depend on the observation, and with a transition matrix equal to the first transition matrix of the OD-HMM. The emission matrix is the same as above.



**Figure 2.** Realization of hidden chains simulated from an OD-HMM and from a HMM. The first one (solid line) is simulated according to an OD-HMM with two possible states for the observation and, therefore, two transition matrices. The second one (dashed line) is simulated with a HMM with a transition matrix equal to the first transition matrix of the OD-HMM. The emission matrix is the same for the two simulations.

The simulations demonstrate the difference between the two models in terms of sojourn time in a given state. Specifically, the OD-HMM simulation shows longer sojourn time in state 1.

Note that, as in a classical HMM, the hidden chain of a OD-HMM is Markovian.

**Proposition 2.2** (Markovianity of the hidden chain in a OD-HMM). *If  $(Z_t, Y_t)_{t \in \mathbb{N}}$  follows an OD-HMM model, then the hidden chain  $(Z_t)_{t \in \mathbb{N}}$  is Markovian. The associated transition probability is equal to  $\sum_{y_{t-1} \in \Omega_Y} \mathbb{P}(Z_t = z_t | Y_{t-1} = y_{t-1}, Z_{t-1} = z_{t-1}) \mathbb{P}(Y_{t-1} = y_{t-1} | Z_{t-1} = z_{t-1})$ .*

See Appendix A for the demonstration.

## 2.2. Generic identifiability

As explained in Allman et al. (2009), the requirement of identifiability may be too strict when considering statistical parameter estimation. Indeed, for some models, only a subset of parameters of measure zero may not be identifiable and in practice estimation will perform well. We therefore consider generic identifiability and we provide sufficient conditions to ensure the generic identifiability of the parameters of the OD-HMM, by an application of the results in Allman et al. (2009). We first recall the definition of generic identifiability.

**Definition 2.3** (Generic identifiability). Let  $\mathcal{F}(\Theta) = \{\mathbb{P}_\theta, \theta \in \Theta\}$  be a family of probability distributions parameterized by  $\theta$ . We say that the model's parameters  $\theta$  are generically identifiable if the elements of  $\Theta$  that do not satisfy  $\mathbb{P}_\theta = \mathbb{P}_{\theta'} \implies \theta = \theta'$  are of measure zero in the parameter space.

This means that any observed dataset has a probability of one of being drawn from a distribution with identifiable parameters. In Allman et al. (2009), the authors established the following proposition on generic identifiability for HMM.

**Proposition A** (Generic identifiability for HMM (Allman et al. 2009)<sup>2</sup>). *The param-*

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<sup>2</sup>Propositions from the literature are numbered by capital letters, while propositions corresponding to new

eters of a HMM with  $r$  hidden states and  $k$  observable states are generically identifiable from the marginal distribution of  $2L + 1$  consecutive variables provided that  $L$  satisfies:

$$\binom{L + k - 1}{k - 1} \geq r.$$

In order to establish sufficient conditions for the generic identifiability of the OD-HMM parameters  $\theta$ , we first reformulate the model  $\mathcal{M}_\theta^{ODHMM}$  into an equivalent HMM,  $\mathcal{M}_\theta^{HMM}$ , with the dimension of the state space of the hidden variable being  $r = |\Omega_Z| \times |\Omega_Y|$  and an observed state space of dimension  $k = |\Omega_Y|$ , and whose transition and emission probabilities are functions of  $\theta$ . Using Proposition A, we establish sufficient conditions for the generic identifiability of the parameters of  $\mathcal{M}_\theta^{HMM}$ . We then establish that if  $\theta \neq \theta'$ , then  $\mathcal{M}_\theta^{HMM}$  and  $\mathcal{M}_{\theta'}^{HMM}$  are not the same model. Therefore the condition for generic identifiability also holds for the original OD-HMM model,  $\mathcal{M}_\theta^{ODHMM}$ .

Let us first present the reformulation of a OD-HMM model  $(Z_t, Y_t)$  as a HMM. The hidden variable is  $H_t = (Z_t, Y_t) \in \Omega_Z \times \Omega_Y$  and the observed variable is a copy of  $Y_t$ , i.e.,  $O_t = Y_t \in \Omega_Y$ . The couple  $(H_t, O_t)$  satisfies the definition of a HMM since  $H_t$  is a Markov chain, and conditionally to  $(H_t)$ , the  $O_t$ s are mutually independent and each  $O_t$  depends only on  $H_t$ . We now express  $P^{\text{HMM}}$ , the transition matrix, and  $R^{\text{HMM}}$ , the emission matrix of  $\mathcal{M}_\theta^{HMM}$ , using the parameters of  $\mathcal{M}_\theta^{ODHMM}$  :

$$P_\theta^{\text{HMM}}(h_{t-1}, h_t) = R(z_t, y_t)P_{y_{t-1}}(z_{t-1}, z_t), \quad R_\theta^{\text{HMM}}(h_t, o_t) = \mathbf{1}_{(y_t=o_t)}.$$

Then, using Proposition A, we know that the parameters of  $\mathcal{M}_\theta^{HMM}$  (i.e., the elements of the transition matrix  $P_\theta^{\text{HMM}}$  and the emission matrix  $R_\theta^{\text{HMM}}$ ) are generically

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results are numbered by Arabic numbers.

identifiable when the observed chain is longer than  $2L + 1$ , where  $L$  satisfies:

$$\binom{L + |\Omega_Y| - 1}{|\Omega_Y| - 1} \geq |\Omega_Z| |\Omega_Y|.$$

It is easy to show (see Appendix B) that two different parameters  $\theta$  and  $\theta'$  of an OD-HMM that lead to the same transition matrix  $P^{\text{HMM}}$ , and the same emission matrix  $R^{\text{HMM}}$ , are equal ( $\theta = \theta'$ ). Therefore, generic identifiability also holds for  $\mathcal{M}_\theta^{\text{ODHMM}}$ .

**Proposition 2.4** (Generic identifiability for OD-HMM). *The parameters of an OD-HMM with  $|\Omega_Z|$  hidden states and  $|\Omega_Y|$  observable states are generically identifiable from the marginal distribution of  $2L + 1$  consecutive variables, provided that  $L$  satisfies:*

$$\binom{L + |\Omega_Y| - 1}{|\Omega_Y| - 1} \geq |\Omega_Z| |\Omega_Y|.$$

**Example 2.5.** For  $|\Omega_Z| = 2$  and  $|\Omega_Y| = 2$ , the parameters  $\theta$  are identifiable as soon as the chain has more than  $2L + 1 = 7$  observations. Indeed,

$$\binom{L + 2 - 1}{2 - 1} \geq 2 \times 2 \quad \Leftrightarrow \quad L \geq 3.$$

**Example 2.6.** For  $|\Omega_Z| = 7$  and  $|\Omega_Y| = 3$ , the parameters  $\theta$  are identifiable as soon as the chain has more than  $2L + 1 = 11$  observations. Indeed,

$$\binom{L + 3 - 1}{3 - 1} \geq 7 \times 3 \quad \Leftrightarrow \quad L \geq 5.$$

The condition on the minimal length of the observation sequence is easily satisfied. Furthermore, it is easy to see that when the cardinal of  $\Omega_Z$  increases (while  $|\Omega_Y|$  remains constant), the minimal value of  $L$  satisfying the condition also increases. On the contrary, when  $|\Omega_Y|$  increases (while  $|\Omega_Z|$  remains constant), this value decreases.

### 3. Maximum likelihood estimation

We are interested in the calculation of the Maximum Likelihood Estimator (MLE), denoted  $\hat{\theta}_{M,z_0}$  (or, for the sake of simplicity,  $\hat{\theta}$ ), defined by the following formula:

$$\hat{\theta} = \arg \max_{\theta} L(\theta; y_{0:M}; z_0),$$

where  $L(\theta; y_{0:M}; z_0) = \mathbb{P}_{\theta}(Y_{0:M} = y_{0:M} \mid Z_0 = z_0)$  is the likelihood.

#### 3.1. Consistency

We work on a probability space  $(\Omega_Z \times \Omega_Y, \mathcal{P}(\Omega_Z \times \Omega_Y), \mathbb{P}_{\theta}, \theta \in \Theta)$  together with the counting measure  $\mu$ .

As shown in Ailliot and Pène (2015, Theorem 2), we can obtain the consistency of the MLE of a more general model, referred to as the Non-Homogeneous Markov-Switching Auto-Regressive model (NHMS-AR model), in which the state spaces can be either continuous or discrete, but the results are given in the continuous case. The NHMS-AR model is based on the following two assumptions:

- The distribution of  $Z_t$ , conditionally to  $\{Z_{t'} = z_{t'}\}_{t' < t}$  and  $\{Y_{t'} = y_{t'}\}_{t' < t}$ , only depends on  $y_{t-s:t-1}$  and  $z_{t-1}$ , where  $s \in \{1, \dots, t\}$ .
- The distribution of  $Y_t$ , conditionally to  $\{Z_{t'} = z_{t'}\}_{t' < t}$  and  $\{Y_{t'} = y_{t'}\}_{t' < t}$ , only depends on  $y_{t-s:t-1}$  and  $z_t$ .

The OD-HMM is a particular case of the NHMS-AR model, where  $s = 1$  and where  $y_t$  does not depend on  $y_{t-1}$ . Moreover, the chain  $(Z_t)$  is non-homogeneous with respect to time because  $P_y$  depends on  $y \in \Omega_Y$ .

Therefore, to take advantage of the results from Ailliot and Pène (2015) in the case of the OD-HMM, we consider the transition matrix of the couple  $(Z_t, Y_t)$  denoted  $\tilde{P}_{\theta}$

and defined by:

$$\forall (i, a), (j, b) \in \Omega_Z \times \Omega_Y, \quad \tilde{P}_\theta(i, a; j, b) = P_a(i, j; \theta)R(j, b; \theta).$$

Thus, the coupled Markov chain  $(Z_t, Y_t)_{t \in \mathbb{N}}$  is homogeneous, with the transition operator  $\tilde{P}_\theta$ , and the stationary distribution  $\tilde{\pi}_\theta$  of  $(Z_t, Y_t)$ . Moreover, the probability and the expectation, corresponding to the stationary distribution  $\tilde{\pi}_\theta$ , are denoted, respectively, as  $\bar{\mathbb{P}}_\theta$  and  $\bar{\mathbb{E}}_\theta$ , and are, respectively,  $\bar{\mathbb{P}}_\theta(\cdot) = \mathbb{P}_{\theta, \tilde{\pi}_\theta}(\cdot)$ , and  $\bar{\mathbb{E}}_\theta(\cdot) = \mathbb{E}_{\theta, \tilde{\pi}_\theta}(\cdot)$ . Finally, the marginal distribution of the stationary distribution  $\bar{\mathbb{P}}_\theta$  of  $(Y)$ , is referred to as  $\bar{\mathbb{P}}_\theta^Y$ .

The direct transposition of Theorem 2 with its assumptions, from Ailliot and Pène (2015), to the case of the OD-HMM, with our notations, takes the form of the following Proposition B with its related assumptions (we will check if they are always satisfied or not for the OD-HMM in a second step):

- (A1)  $\Theta$  is a compact space;
- (A2) The chain  $(Z_t, Y_t)_{t \in \mathbb{N}}$  is ergodic with an invariant probability for each  $\theta \in \Theta$  denoted  $\tilde{\pi}_\theta$ ;
- (A3) The elements of  $\bar{\mathbb{P}}_\theta$  are absolutely continuous with respect to  $\mathbb{P}_\theta$  for all  $\theta \in \Theta$ ;
- (A4) The elements of  $P_y$  and  $R$  are continuous in  $\theta$ , for any  $y$  in  $\Omega_Y$ .

Under the above assumptions, Theorem 2 from Ailliot and Pène (2015) leads to the following proposition:

**Proposition B** (Consistency of the NHMS-AR model MLE (Ailliot and Pène 2015), in the particular case of the OD-HMM MLE). *Let  $\theta^*$  be the true value of the parameter  $\theta$ . Under the model assumptions (A1) - (A4) and the following ones:*

- (1)  $0 < P_{y,-} := \min_{\theta, z_0, y_0, z_1} P_{y_0}(z_0, z_1; \theta) \leq P_{y,+} := \max_{\theta, z_0, y_0, z_1} P_{y_0}(z_0, z_1; \theta) < \infty$ ;
- (2)  $B_- = \bar{\mathbb{E}}_{\theta^*} [\ln(\min_{\theta} \sum_{z_0 \in \Omega_Z} R(z_0, Y_0; \theta))] < \infty$ ;
- (3)  $B_+ = \bar{\mathbb{E}}_{\theta^*} [\ln(\max_{\theta} \sum_{z_0 \in \Omega_Z} R(z_0, Y_0; \theta))] < \infty$ ;
- (4)  $\forall \theta \in \Theta, \sum_{z \in \Omega_Z} R(z, Y_0) < \infty, \mathbb{P}_{\theta^*}$ -a.s.;

(5)  $\forall \theta \in \Theta$ , for  $\mu$ -a.e., and for any probability  $\alpha$  on  $\Omega_Z \times \Omega_Y$ ,  $\lim_{k \rightarrow \infty} \|\alpha \tilde{P}^k - \tilde{\pi}_\theta\|_1 = 0$ , where the  $\|\cdot\|_1$  can be either the  $L^1$  norm or the total variation norm, which differ by a multiplicative constant  $1/2$ .

Then, for any  $z_0 \in \Omega_Z$ , the limit values of the MLE  $\hat{\theta}_{M,z_0}$ , as  $M \rightarrow \infty$ , are contained in the space  $\{\theta \in \Theta; \bar{\mathbb{P}}_\theta^Y = \bar{\mathbb{P}}_{\theta^*}^Y\}$   $\mathbb{P}_{\theta^*}$ -a.s..

We now focus on the assumptions (A1) to (A4) and (1) to (5) and we check if they are always satisfied by a OD-HMM, in order to propose a version of the above proposition fully adapted to the OD-HMM. First we introduce the following proposition, an intermediate result about the ergodicity of the chain  $(Z_t, Y_t)$ .

**Proposition 3.1.** *If the Markov chain  $(Z_t)_{t \in \mathbb{N}}$  is ergodic, then the Markov chain  $(Z_t, Y_t)_{t \in \mathbb{N}}$  is ergodic too and its stationary distribution is referred to as  $\tilde{\pi}_\theta$ .*

**Proof.** From ergodicity of  $(Z_t)$ , for any  $i, j \in \Omega_Z$  there exists a finite sequence of states (a path with positive probabilities)  $i \rightarrow i_1 \rightarrow i_2 \rightarrow \dots \rightarrow i_k \rightarrow j$ . As  $\sum_{y \in \Omega_Y} R(i, y) = 1$ , there exists at least  $a_i \in \Omega_Y$  such that  $R(i, a_i) > 0$ , then the path  $(i, a_i) \rightarrow (i_1, a_{i_1}) \rightarrow \dots \rightarrow (i_k, a_{i_k}) \rightarrow (j, a_j)$  exists. So, the Markov chain  $(Z_t, Y_t)$  is irreducible.

Now to prove the aperiodicity of the chain  $(Z_t, Y_t)$ , we have, since  $(Z_t)$  is ergodic, that there exists a state, say  $i_0 \in \Omega_Z$ , such that two different closed paths exist, i.e.,  $i_0 \rightarrow i_1 \rightarrow \dots \rightarrow i_k \rightarrow i_0$  and  $i_0 \rightarrow i'_1 \rightarrow \dots \rightarrow i'_m \rightarrow i_0$  such that  $GCD\{k+1, m+1\} = 1$ . We also have  $(i_0, a_{i_0}) \rightarrow (i_1, a_{i_1}) \rightarrow \dots \rightarrow (i_k, a_{i_k}) \rightarrow (i_0, a_{i_0})$  and  $(i_0, a_{i_0}) \rightarrow (i'_1, a'_{i_1}) \rightarrow \dots \rightarrow (i'_m, a'_{i_m}) \rightarrow (i_0, a_{i_0})$  for which we also have the same lengths  $k+1$  and  $m+1$ , so the Markov chain  $(Z_t, Y_t)$  is aperiodic and, finally, since it is finite, it will be ergodic.  $\square$

**Remark 1.** In the case where all the elements of the transition matrices  $P_y$  are strictly positive, the Markov chain  $(Z_t)$  is ergodic. Consequently, the assumption of Proposition 3.1 is satisfied, and, consequently, the Markov chain  $(Z, Y)$  is ergodic.

**Remark 2.** Moreover, for a HMM, if the elements of the transition matrix  $P$  are not necessary strictly positive, but, the Markov chain  $(Z_t)$  is assumed to be ergodic, then

there exists an integer  $n_0 \geq 1$  such that :

$$\forall n \geq n_0, \forall i, j \in \Omega_Z, P^n(i, j) > 0.$$

**Remark 3.** In the case of the OD-HMM, since we have a finite number of transition matrices  $P_y, y \in \Omega_Y$ , there exists an integer  $n_0 \geq 1$  such that :

$$\forall n \geq n_0, \forall i, j \in \Omega_Z, \forall y \in \Omega_Y, P_y^n(i, j) > 0.$$

Using the intermediate Proposition 3.1 and the model assumptions, we will now examine if the assumptions leading to Proposition B are satisfied for the OD-HMM.

We first consider the model assumptions (A1) to (A4). Assumption (A1) is obviously satisfied by a OD-HMM. To satisfy assumption (A2), we assume that the Markov chain  $(Z_t)$  is ergodic, and on the basis of Proposition 3.1, the chain  $(Z, Y)$  is ergodic as well. Assumption (A3) is satisfied since the state spaces  $\Omega_Z$  and  $\Omega_Y$  are discrete. Assumption (A4) is satisfied in the discrete and non-parametric case, which is the case studied here. Each element of the  $P_y$  and  $R$  matrices is continuous with respect to  $\theta$ . Thus, to satisfy assumptions (A1) to (A4), we just have to assume that the Markov chain  $(Z_t)$  is ergodic.

Let us now consider assumptions (1) to (5) in Proposition B. Assumption (1) is satisfied when all the elements of the transition matrices  $P_y$  are positive or, at least, asymptotically for a value  $n \geq n_0$ , as explained in Remark 1 and Remark 3. Besides, since the transition matrices are stochastic,  $\max_{\theta, z_0, y_0, z_1} P_{y_0}(z_0, z_1; \theta) \leq 1$ . Assumptions (2), (3) and (4) are satisfied since any column of the emission matrix  $R$  includes at least one non-zero element. Indeed, if a column of the emission matrix  $R$  were equal to zero, it could be removed. Therefore, the quantity  $\sum_{z_0 \in \Omega_Z} R(z_0, Y_0; \theta)$  is strictly positive and finite. Assumption (5) is satisfied because the chain  $(Z_t, Y_t)_{t \in \mathbb{N}}$  is ergodic according to Proposition 3.1. Moreover, the convergence is exponentially fast.

We finally obtain the following proposition concerning the consistency of the MLE of the OD-HMM. This proposition holds under the model assumption that  $(Z_t)$  is



ergodic.

**Proposition 3.2** (Consistency of the OD-HMM MLE). *Let  $\theta^*$  be the true value of the parameters. For all  $z_0 \in \Omega_Z$ , the limit values of the MLE  $\hat{\theta}_{M,z_0}$ , as  $M \rightarrow \infty$ , are contained in the space  $\{\theta \in \Theta; \bar{\mathbb{P}}_\theta^Y = \bar{\mathbb{P}}_{\theta^*}^Y\}$   $\mathbb{P}_{\theta^*}$ -a.s..*

Note that in the parametric case (still with discrete and finite state spaces), it will be necessary to study assumption (A4) in order to obtain conditions to ensure the consistency of the OD-HMM MLE estimator.

### 3.2. EM algorithm

We now present how to compute the MLE of  $\theta$  using the Expectation-Maximization algorithm (EM, Dempster et al. 1977). To take the influence of the previous observation  $Y_{t-1}$  on the current hidden state  $Z_t$  into account, as shown in Figure 1, right side, we propose an adaptation of the EM for HMM (Cappé et al. 2005).

We consider the situation where we have  $C$  realizations  $(Y_{c,t})$  of  $C$  independent identically distributed OD-HMM  $(Z_{c,t}, Y_{c,t})$ , where  $c \in \{1, \dots, C\}$  with  $1 \leq C < \infty$  and  $t \in \{0, \dots, M\}$  with  $1 \leq M < \infty$ . In the following, we denote the tuple of the hidden states at time  $t$  for chain 1 to chain  $C$  by  $Z_{1:C,t} = (Z_{1,t}, Z_{2,t}, \dots, Z_{C,t})$ . In the same way, we denote by  $Y_{1:C,t} = (Y_{1,t}, Y_{2,t}, \dots, Y_{C,t})$  the tuple of the observations at time  $t$  for the  $C$  chains. Moreover, we denote  $\pi(z_{c,0}; \theta)$ ,  $P_{y_{c,t-1}}(z_{c,t-1}, z_{c,t}; \theta)$  and  $R(z_{c,t}, y_{c,t}; \theta)$  the probabilities defining the OD-HMM with parameter  $\theta$ .

With these notations, the complete likelihood  $L_{comp}(\theta; z_{1:C,0:M}, y_{1:C,0:M})$ , denoted  $L_{comp}$ , is equal to (see Appendix C):

$$\begin{aligned} L_{comp} &= \mathbb{P}(Z_{1:C,0:M} = z_{1:C,0:M}, Y_{1:C,0:M} = y_{1:C,0:M} | \theta) \\ &= \prod_{c=1}^C \left[ \pi(z_{c,0}; \theta) R(z_{c,0}, y_{c,0}; \theta) \prod_{t=1}^M P_{y_{c,t-1}}(z_{c,t-1}, z_{c,t}; \theta) R(z_{c,t}, y_{c,t}; \theta) \right]. \end{aligned}$$

The EM algorithm is an iterative algorithm that relies on the expectation of  $L_{comp}$

and that converges to a local maximum of the likelihood  $\mathbb{P}(Y_{1:C,0:M} = y_{1:C,0:M}|\theta)$ . At each iteration, it computes:

$$\begin{aligned}\theta(m+1) &= \arg \max_{\theta} \mathbb{E} \left[ \ln L_{comp}(\theta; Z_{1:C,0:M}, Y_{1:C,0:M}) | Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right], \\ &= \arg \max_{\theta} Q(\theta|\theta^{(m)})\end{aligned}\quad (1)$$

where  $\theta^{(m)}$  is the parameter estimator at iteration  $m$  of EM.

The intermediate quantity  $Q(\theta|\theta^{(m)})$  can be broken down into three terms, one depending on the initial distribution, another depending on the transition matrix, and the last one depending on the emission distribution (see Appendix C).

$$\begin{aligned}Q(\theta|\theta^{(m)}) &= \mathbb{E} \left[ \ln \mathbb{P}(Y_{1:C,0:M}, Z_{1:C,0:M}|\theta) | Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right] \\ &= \sum_{c=1}^C \sum_{z_0 \in \Omega_Z} \ln(\pi(z_0; \theta)) \times \mathbb{P}(Z_{c,0} = z_0 | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \\ &+ \sum_{c=1}^C \sum_{t=1}^M \sum_{(z,z') \in \Omega_Z^2} \ln(P_{y_{c,t-1}}(z, z'; \theta)) \\ &\times \mathbb{P}(Z_{c,t-1} = z, Z_{c,t} = z' | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \\ &+ \sum_{c=1}^C \sum_{t=0}^M \sum_{z' \in \Omega_Z} \ln(R(z', y_{c,t}; \theta)) \times \mathbb{P}(Z_{c,t} = z' | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}).\end{aligned}$$

A detailed derivation of all the formulas for the E step and the M step are available in Appendix C. Only the main elements are presented here.

### 3.2.1. E step

At iteration  $m$ , the E step consists in computing the marginal probabilities of interest that appear in the expression of  $Q(\theta|\theta^{(m)})$ . They are:

- $\forall 0 \leq t \leq M, \forall c \in \{1, \dots, C\}, \forall z_t \in \Omega_Z,$

$$\rho_{c,t}^{(m)}(z_t) = \mathbb{P}(Z_{c,t} = z_t | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)});$$

- $\forall 1 \leq t \leq M, \forall c \in \{1, \dots, C\}, \forall (z_{t-1}, z_t) \in \Omega_Z^2,$

$$\xi_{c,t}^{(m)}(z_{t-1}, z_t) = \mathbb{P}(Z_{c,t-1} = z_{t-1}, Z_{c,t} = z_t | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}).$$

To obtain  $\rho_{c,t}^{(m)}(z_t)$  and  $\xi_{c,t}^{(m)}(z_{t-1}, z_t)$ , we introduce the following variables:

- $\alpha_{c,t}^{(m)}(z_t)$ , such that,  $\forall 0 \leq t \leq M, \forall c \in \{1, \dots, C\}, \forall z_t \in \Omega_Z,$

$$\alpha_{c,t}^{(m)}(z_t) = \mathbb{P}(Y_{c,0:t} = y_{c,0:t}, Z_{c,t} = z_t | \theta^{(m)});$$

- $\beta_{c,t}^{(m)}(z_t)$ , such that,  $\forall 0 \leq t < M, \forall c \in \{1, \dots, C\}, \forall z_t \in \Omega_Z,$

$$\beta_{c,t}^{(m)}(z_t) = \mathbb{P}(Y_{c,t+1:M} = y_{c,t+1:M} | Z_{c,t} = z_t, Y_{c,t} = y_{c,t}, \theta^{(m)}).$$

The E step works by using the Forward-Backward algorithm. The only specificity in the Forward-Backward algorithm for the OD-HMM compared to that of the HMM is in the expression of  $\beta_{c,t}^{(m)}(z_t)$ , in the Backward algorithm because it is taken conditionally to the current observations  $y_{c,t}$ . It is computed by using the following recurrence formula :

$$\forall 0 \leq t < M, \forall c \in \{1, \dots, C\}, \forall z_t \in \Omega_Z,$$

$$\beta_{c,t}^{(m)}(z_t) = \sum_{z_{t+1} \in \Omega_Z} R^{(m)}(z_{t+1}, y_{c,t+1}) \beta_{c,t+1}^{(m)}(z_{t+1}) P_{y_{c,t}}^{(m)}(z_t, z_{t+1}),$$

where  $\beta_{c,M}^{(m)}(z_M) = 1$ .

The quantities  $\alpha_{c,t}^{(m)}(z_t)$  and  $\beta_{c,t}^{(m)}(z_t)$  are used to compute  $\rho_{c,t}^{(m)}(z_t)$  and  $\xi_{c,t}^{(m)}(z_{t-1}, z_t)$ , as in the classical EM for HMM.

### 3.2.2. $M$ step

In the  $M$  step we resolve the maximization problem (1) to obtain the expression of updated parameters. We express these parameters in terms of  $\rho_{c,t}^{(m)}(z_t)$  and  $\xi_{c,t}^{(m)}(z_{t-1}, z_t)$  as follows:

- $\forall y \in \Omega_Y, \forall z_t \in \Omega_Z, \forall z_{t-1} \in \Omega_Z,$

$$P_y^{(m+1)}(z_{t-1}, z_t) = \frac{\sum_{c=1}^C \sum_{t=1}^M \xi_{c,t}^{(m)}(z_{t-1}, z_t) \mathbb{1}_{(y_{c,t-1}=y)}}{\sum_{c=1}^C \sum_{t=1}^M \sum_{z'_t \in \Omega_Z} \xi_{c,t}^{(m)}(z_{t-1}, z'_t) \mathbb{1}_{(y_{c,t-1}=y)}};$$

- $\forall z_t \in \Omega_Z, \forall y \in \Omega_Y,$

$$R^{(m+1)}(z_t, y) = \frac{\sum_{c=1}^C \sum_{t=0}^M \rho_{c,t}^{(m)}(z_t) \mathbb{1}_{(y_{c,t}=y)}}{\sum_{c=1}^C \sum_{t=0}^M \rho_{c,t}^{(m)}(z_t)}.$$

### 3.2.3. Initialization and stopping criterion

Since the result of EM can be sensible to the initialization, we simulate  $N_{init}$  sets of initial parameter values using a uniform probability distribution  $\mathcal{U}[0, 1]$  for each element of  $\theta$ , and normalizing them to obtain probabilities. We then run the EM algorithm for each of them.

The algorithm is stopped when the first of the two criteria is met: either a number  $N_{iter}$  of iterations is reached or the algorithm has converged. To check for convergence, at each iteration  $m$ , we compute a distance between the estimator at iteration  $m$  and the one at iteration  $m + 1$ . Since the set of parameters  $\theta$  is composed of matrices ( $P$  and  $R$ ), and the rows of these matrices all add up to one, we consider the following distance between the  $i$ -th row of  $\theta^{(m)}$ , denoted  $\theta_i^{(m)}$ , and  $\theta_i^{(m+1)}$  :

$$dist(\theta_i^{(m)}, \theta_i^{(m+1)}) = \sqrt{\sum_{k=1}^K (\theta_{i,k}^{(m)} - \theta_{i,k}^{(m+1)})^2},$$

	True parameters
<b>Example 1</b>	$P_0^* = \begin{pmatrix} 0.2 & 0.8 \\ 0.8 & 0.2 \end{pmatrix}, P_1^* = \begin{pmatrix} 0.8 & 0.2 \\ 0.2 & 0.8 \end{pmatrix}, R^* = \begin{pmatrix} 0.8 & 0.2 \\ 0.2 & 0.8 \end{pmatrix}$
<b>Example 2</b>	$P_0^* = \begin{pmatrix} 0.6 & 0.4 \\ 0.4 & 0.6 \end{pmatrix}, P_1^* = \begin{pmatrix} 0.4 & 0.6 \\ 0.6 & 0.4 \end{pmatrix}, R^* = \begin{pmatrix} 0.2 & 0.8 \\ 0.8 & 0.2 \end{pmatrix}$
<b>Example 3</b>	$P_0^* = \begin{pmatrix} 0.2 & 0.8 \\ 0.8 & 0.2 \end{pmatrix}, P_1^* = \begin{pmatrix} 0.8 & 0.2 \\ 0.2 & 0.8 \end{pmatrix}, R^* = \begin{pmatrix} 0.4 & 0.6 \\ 0.6 & 0.4 \end{pmatrix}$

**Table 1.** True transition and emission matrices for the three simulation examples.

where  $K$  is the length of  $\theta_i^{(m)}$  and  $\theta_{i,k}^{(m)}$  is the  $k$ -th element of row  $\theta_i^{(m)}$  ( $K = |\Omega_Z|$  or  $K = |\Omega_Y|$ ). When the average distance over all rows of all matrices of  $\theta$  is smaller than a given threshold  $\epsilon$ , we consider that the algorithm has converged.

When the  $N_{init}$  algorithms have converged or stopped, we keep the best estimator, i.e., the one that is associated with the larger likelihood  $\mathbb{P}(Y_{1:C,0:M} = y_{1:C,0:M}|\theta)$ . The likelihood is easily computed using the  $\alpha$ s and  $\beta$ s.

#### 4. Validation of the estimation procedure on simulated data

In order to validate the estimation procedure, we realize three simulation examples on datasets simulated from the OD-HMM with different values of true parameters, whose transition and emission matrices are provided in Table 1, corresponding to problems of increasing difficulty. In the first simulation example, the transition and emission matrices are very contrasted. In the second simulation example, the elements of the transition matrices are chosen close to  $1/2$ . In the last simulation example, the rows of the emission matrix are similar, so the observations provide little information on the hidden process. Note that according to Proposition 2.4, the OD-HMM of the three simulation examples are generically identifiable as soon as the chain has more than seven observations.

For the sake of comparison, we also provide estimators for the three examples based on a HMM model.

We first describe the protocol common to all the simulation examples and we then present and discuss the results.

#### 4.1. Protocol

For a given simulation example, associated with the true parameters  $\theta^*$  (presented in Table 1) and a given  $C$ , we set the initial distribution to  $\pi = (1, 0)$  and we simulated  $C$  chains  $(Z_{c,t})$  and  $(Y_{c,t})$  of length  $M = 500$ . We then ran the EM algorithm for OD-HMM and the EM for HMM to obtain the parameter estimators,  $\hat{\theta}^{\text{OD-HMM}}$  and  $\hat{\theta}^{\text{HMM}}$ , respectively, from the  $C$  observed chains. There are six parameters to estimate. We ran the EM with  $N_{init} = 10$ ,  $N_{iter} = 750$ , and  $\epsilon = 0.001$ . To quantify the difference between  $\theta^*$  and  $\hat{\theta}$ , we used the following distance between the  $i$ -th row of  $\theta^*$ , and  $\hat{\theta}$ :

$$\text{dist}(\theta_i^*, \hat{\theta}_i) = \frac{1}{K} \sum_{k=1}^K \frac{|\theta_{i,k}^* - \hat{\theta}_{i,k}|}{\theta_{i,k}^*},$$

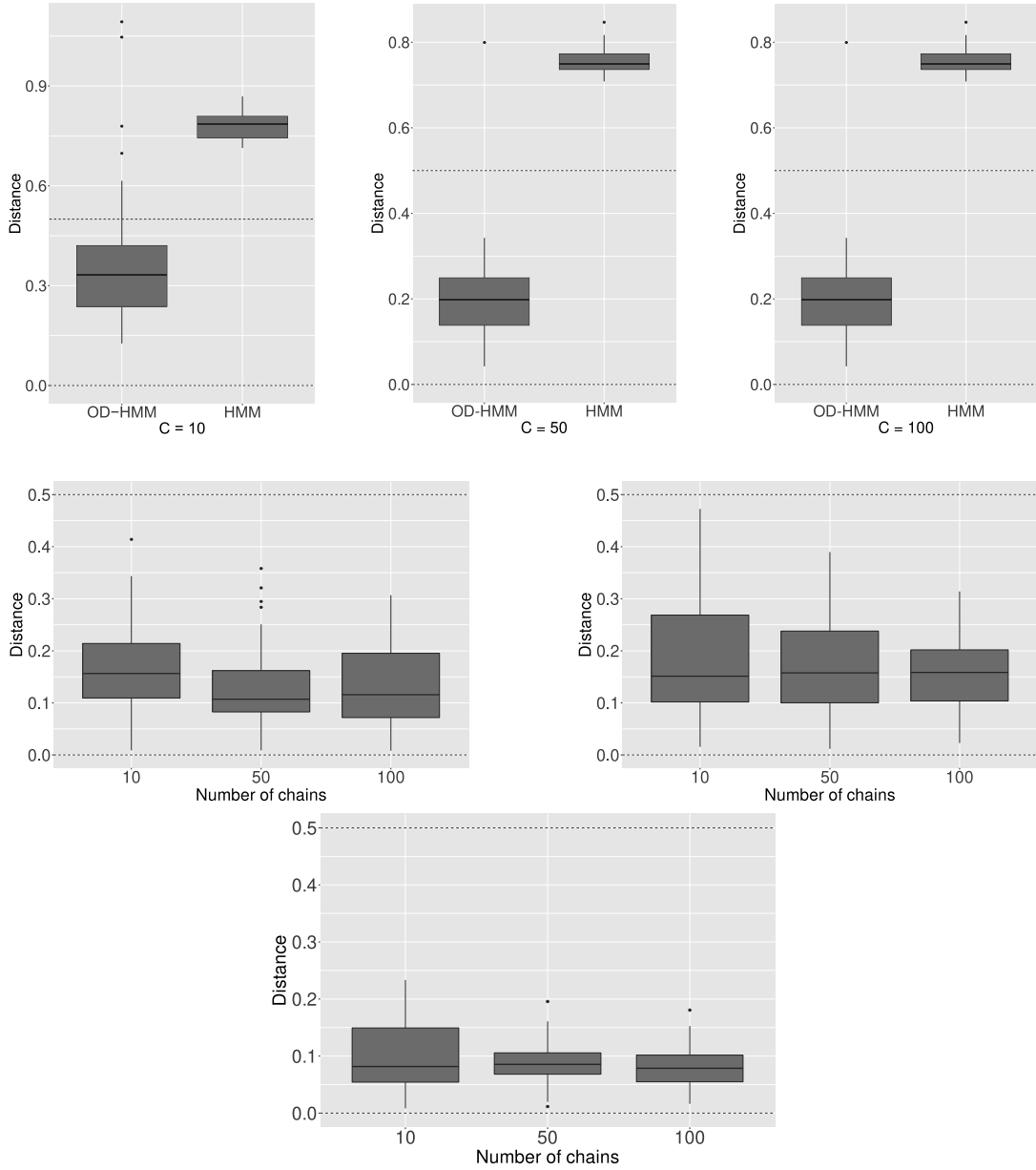
where  $K$  is the length of  $\theta_i$  and  $\theta_{i,k}$  is the  $k$ -th element of the  $\theta$   $i$ -th row ( $K = |\Omega_Z|$  or  $K = |\Omega_Y|$ ). We also computed a global distance, defined as the mean of all distances over each row of the model parameters. Note that in the case of an estimation based on an HMM model, in order to compare the transition matrix estimated by EM for HMM, denoted as  $\hat{P}^{\text{HMM}}$ , with the two true transition matrices  $P_0^*$  and  $P_1^*$ , we calculate the distance between  $\hat{P}^{\text{HMM}}$  and  $P_0^*$ , and then between  $\hat{P}^{\text{HMM}}$  and  $P_1^*$ .

In order to capture the variability in the EM estimators, we repeated this protocol 50 times. Finally, we reproduce the whole procedure for increasing numbers of chains:  $C = 10, 50, 100$ .

#### 4.2. Results

##### 4.2.1. First simulation example

First, we compare the results of EM for OD-HMM and those obtained using EM for HMM on data simulated from the parameters of simulation example 1 (given in Table 1). In Figure 3, we display the boxplots of the average errors, over all parameters for the two methods.



**Figure 3.** Simulation example 1: The top line of the figure displays boxplots of the distance between  $\hat{\theta}^{\text{OD-HMM}}$  and  $\theta^*$  (left boxplot of each figure on the top line) and  $\hat{\theta}^{\text{HMM}}$  and  $\theta^*$  (right boxplot of each figure on the top line) for increasing values of the number of chains ( $C = 10, 50$  and  $100$ ). The second line displays the boxplot of the distance between  $\hat{P}_0$  and  $P_0^*$  (on the middle line at left),  $\hat{P}_1$  and  $P_1^*$  (on the middle line at right) and, the bottom line shows the boxplot between the estimated emission matrix and the true one for increasing values of the number of chains ( $C = 10, 50$  and  $100$ ).

Regardless of the number of chains, the EM algorithm for OD-HMM provides higher quality estimators. This was expected since the data are generated from an OD-HMM with true parameters, matrices  $P_0^*, P_1^*$ , that are significantly different from each other.

We now take a more detailed look at the quality of the estimators provided by the EM for OD-HMM. First, looking at the top line of Figure 3, we observe that the average distance between the estimated parameters  $\hat{\theta}$  and the true parameters  $\theta^*$  is decreasing between  $C = 10$  and  $C = 50$  and remain constant between  $C = 50$  and  $C = 100$ . Regardless of the number of chains, the mean value, over the repetitions, of this average distance is lower than 0.160 (i.e., a 16% error) which is of very good quality. The convergence rate is 100%.

If we now specifically consider the transition matrices (see Figure 3, on the middle line), we observe that the quality of the estimator is quite poor for  $C = 10$  chains. Indeed, the median distance between  $\hat{P}_0$  and  $P_0^*$  is slightly above 0.15, and, in the worst case, the distance can exceed 0.4. However, the estimation results for  $C = 50$  and  $C = 100$  chains are more satisfactory. The median distance between  $\hat{P}_0$  and  $P_0^*$  is less than 0.15. Moreover, the estimators do not exceed 33% error (except for the two highest extreme values with  $C = 50$ ). The median distance between  $\hat{P}_1$  and  $P_1^*$  is also around 0.15 for all values of  $C$ . We can observe that for  $C = 10$  and  $C = 50$ , the quality of the estimator of  $P_1$  is not as good as that of the estimator of  $P_0$ . In particular, the results are more variable and the ninth deciles are higher for  $P_1$  than for  $P_0$ . On average, the distance between  $\hat{P}_0$  and  $P_0^*$  is 0.163 for  $C = 10$  and 0.135 for  $C = 50$  and  $C = 100$ . The one between  $\hat{P}_1$  and  $P_1^*$  is 0.20 for  $C = 10$ , and then decreases to 0.165 for  $C = 50$  and 0.155 for  $C = 100$ .

The estimator of the emission matrix is of very good quality (see Figure 3, on the bottom line) even if the results for  $C = 100$  have slightly larger variations than those of  $C = 50$ . The median value is lower than 0.1 and the distance does not exceed 0.3.

To conclude, in the case where the matrices are contrasted, i.e., the matrices  $P_0$  and  $P_1$  are distant from the matrix composed of 1/2 and the rows of  $R$  are very different from each other, the estimation by the EM algorithm for OD-HMM is satisfactory.



#### 4.2.2. *Second simulation example*

In this example, the transition matrices (given in Table 1) are close. When comparing the estimators from the EM for OD-HMM and for HMM, we observe that there is no clear domination of one model on the other, it varies with  $C$  as shown in the top line of Figure 4. The reason is maybe that in this example, the influence of the observations on the transition matrices is not strong. Therefore, the OD-HMM is close to a classical HMM.

Let us focus now on the estimator from EM for OD-HMM. Compared to the simulation example 1, the transition matrices are close to the matrix composed of  $1/2$ . Therefore, in theory, estimating the transition matrices should be more difficult, and this is the case. However, the average distance between the estimated and the true parameters remains lower than 0.22 and decreases with  $C$ ; it is, on average, 0.212 for  $C = 10$  chains, 0.164 for  $C = 50$  chains and 0.160 for  $C = 100$  chains, with more variability for  $C = 50$  chains than for  $C = 100$ .

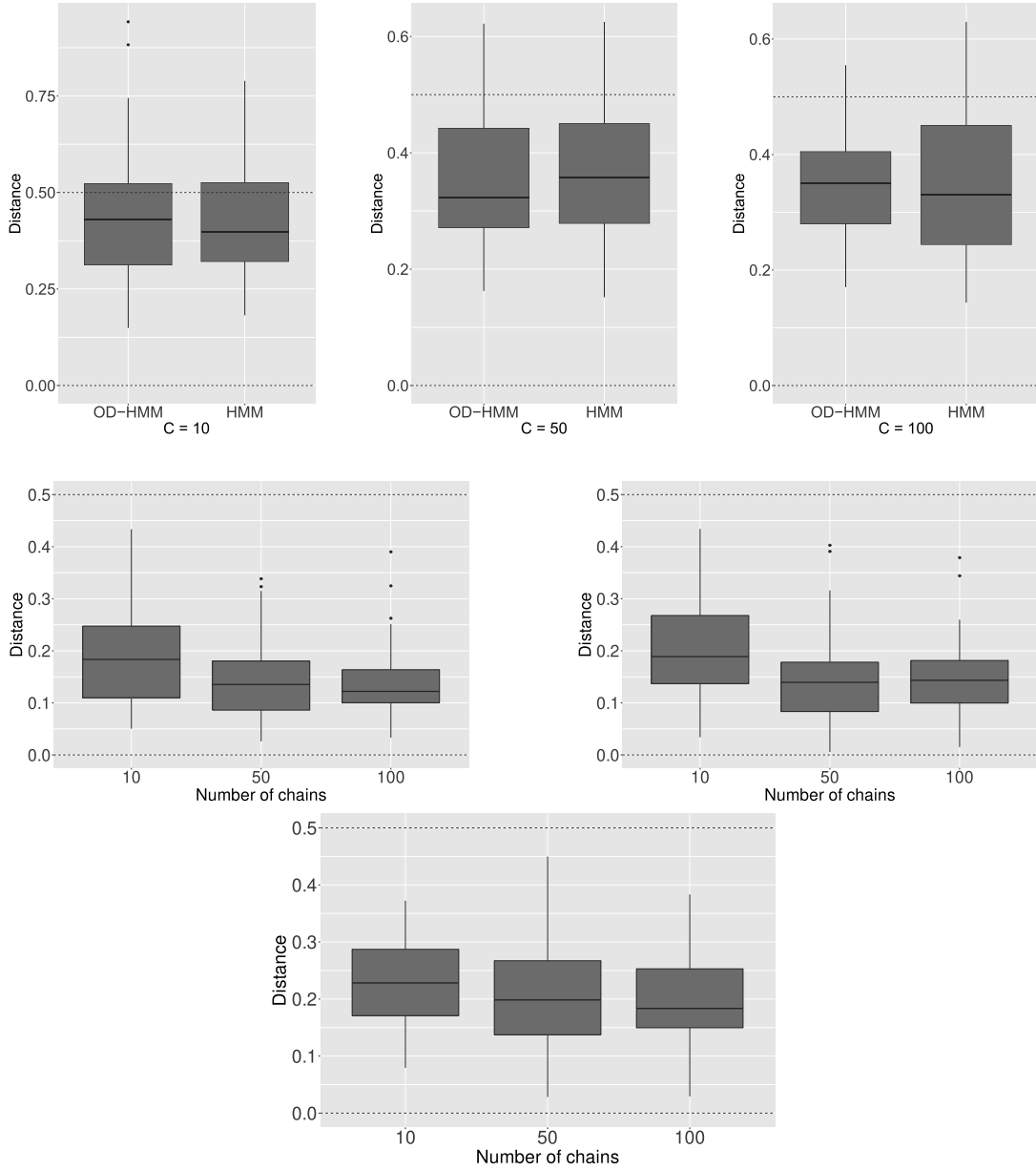
The distances for the transition matrices and for the emission matrices are displayed separately on middle and bottom lines of Figure 4. There is no more systematic decrease of the distance with  $C$ .

We can see that the distance between  $\hat{P}_0$  and  $P_0^*$  remains low, while the distance between  $\hat{P}_1$  and  $P_1^*$  has increased compared to simulation example 1. The distances between the estimated and the true emission matrices are also greater than the distances in the simulation example 1. Indeed, the median distance for  $C = 10$  is 0.23 and decreases to 0.18 for  $C = 100$  chains.

#### 4.2.3. *Third simulation example*

In the third simulation example, the two transition matrices are the same as in the first example; they are not close. The conclusion of the comparison between the results of EM for OD-HMM and EM for HMM is qualitatively the same, but quantitatively the difference between the quality of the two estimators is closer (see Figure 5).

If we now look at the quality of the OD-HMM estimator, this simulation example is the most difficult: since the rows of the emission matrix are similar, it is more difficult



**Figure 4.** Simulation example 2: The top line of the figure displays boxplots of the distance between  $\hat{\theta}^{\text{OD-HMM}}$  and  $\theta^*$  (left boxplot of each figure on the top line) and  $\hat{\theta}^{\text{HMM}}$  and  $\theta^*$  (right boxplot of each figure on the top line) for increasing values of the number of chains ( $C = 10, 50$  and  $100$ ). The second line displays the boxplot of the distance between  $\hat{P}_0$  and  $P_0^*$  (on the middle line at left),  $\hat{P}_1$  and  $P_1^*$  (on the middle line at right) and, the bottom line shows the boxplot between the estimated emission matrix and the true one for increasing values of the number of chains ( $C = 10, 50$  and  $100$ ).

than for simulation examples 1 and 2 to know which hidden state has generated the observation. One consequence is that we encountered a problem of label switching, i.e., the roles of the two hidden states in the matrices were switched during the estimation procedure. We considered that label switching occurs when the average distance

between the rows of  $\theta^*$  and of  $\hat{\theta}$  is smaller when we permute the hidden state than when we do not. We observed 50% of label switching for  $C = 10$ , 36% for  $C = 50$ , and 32% for  $C = 100$ . The distances we discuss now are obtained after correction of label switching when present.

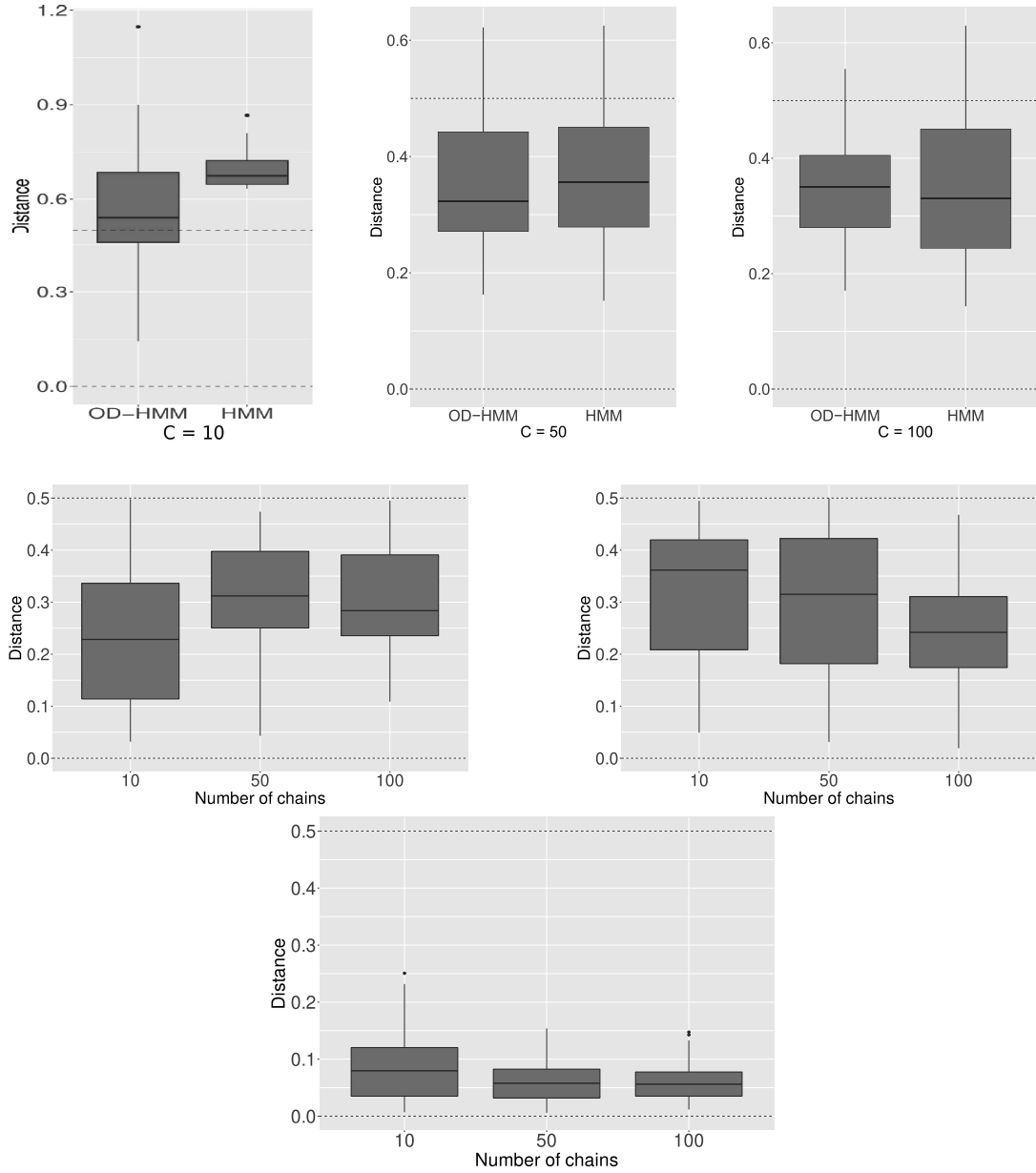
We observed that the quality of the estimator is really less good than in the two first simulation examples. Indeed, the average distance between the estimated parameters and the true ones decreases from 0.31 to 0.25 when  $C$  increases, which is larger than before. The poor estimator quality for  $C = 10$  can be explained by the fact that 28% of the EM did not converge. For the other values of  $C$ , the convergence rate is 100%.

If we look at the transition matrices (Figure 5, middle line) and the emission matrix (Figure 5, bottom line) separately, we observe that the quality of the estimator of the former is strongly degraded, while the estimator of the latter is of a quality similar to that of the the first simulation example.

## 5. Applications to plant dynamics on real data

In this section, we present the use of the OD-HMM for analyzing annual plant dynamics. As mentioned in the introduction, a recent model for plant dynamics is from the family of OD-HMMs but with a specific parameterization of the transition matrices (Pluntz et al. 2018a). We do not pretend that the non-parametric OD-HMM will lead to better estimators of plant dynamics than these models. In this section, we illustrate, on data from the dataset used in Pluntz et al. (2018a), the advantage of taking into account the fact that the current hidden state depends on the previous observation, compared to an HMM approach. We show how a key statistic of the dynamics - the average duration of the seed stock persistence - can be better estimated.

The dataset utilized in this study comes from the Biovigilance research project. This project was conducted between the years 2002 and 2009 and aimed to monitor the abundance of weed species in French agroecosystems. A total of 38 weed species in 325 fields were monitored over a four-year period (Fried 2010). In practice we used the dataset after conversion into records of presence or absence, as in Pluntz et al. (2018b).



**Figure 5.** Simulation example 3: The top line of the figure displays boxplots of the distance between  $\hat{\theta}^{\text{OD-HMM}}$  and  $\theta^*$  (left boxplot of each figure on the top line) and  $\hat{\theta}^{\text{HMM}}$  and  $\theta^*$  (right boxplot of each figure on the top line) for increasing values of the number of chains ( $C = 10, 50$  and  $100$ ). The second line displays the: boxplot of the distance between  $\hat{P}_0$  and  $P_0^*$  (on the middle line at left),  $\hat{P}_1$  and  $P_1^*$  (on the middle line at right) and, the bottom line shows the boxplot between the estimated emission matrix and the true one for increasing values of the number of chains ( $C = 10, 50$  and  $100$ ).

So for a given weed species, the available observations are  $(y_0, \dots, y_3)$  with  $y_t \in \{0, 1\}$ , and the hidden chain  $(z_0, \dots, z_3)$  corresponds to the presence or absence of seeds in the seed bank. To illustrate the data, we present in Table 2 (column Data) the repartition of the observed trajectories among the 16 possible trajectories for four species (which

will be studied below): *Lactuca serriola*, *Matricaria chamomilla*, *Sonchus oleraceus*, *Taraxacum officinale*.

Trajectory	<i>Lactuca serriola</i>			<i>Matricaria chamomilla</i>		
	Data	HMM	OD-HMM	Data	HMM	OD-HMM
(0, 0, 0, 0)	153	122	124	128	84	92
(0, 0, 0, 1)	7	8	7	10	9	8
(0, 0, 1, 0)	1	9	5	6	10	9
(0, 0, 1, 1)	4	3	3	2	3	5
(0, 1, 0, 0)	5	4	8	5	12	11
(0, 1, 0, 1)	0	4	1	1	8	6
(0, 1, 1, 0)	0	5	7	3	6	4
(0, 1, 1, 1)	4	1	0	3	5	4
(1, 0, 0, 0)	3	15	13	6	7	17
(1, 0, 0, 1)	0	3	0	0	8	4
(1, 0, 1, 0)	0	0	0	1	5	4
(1, 0, 1, 1)	0	1	0	0	2	1
(1, 1, 0, 0)	0	1	8	7	6	5
(1, 1, 0, 1)	0	1	0	0	4	3
(1, 1, 1, 0)	0	0	1	3	5	3
(1, 1, 1, 1)	0	0	0	2	3	1

Trajectory	<i>Sonchus oleraceus</i>			<i>Taraxacum officinale</i>		
	Data	HMM	OD-HMM	Data	HMM	OD-HMM
(0, 0, 0, 0)	112	91	92	138	82	87
(0, 0, 0, 1)	12	14	14	12	5	4
(0, 0, 1, 0)	12	3	9	5	12	8
(0, 0, 1, 1)	4	6	8	4	6	9
(0, 1, 0, 0)	15	10	7	13	83	9
(0, 1, 0, 1)	5	7	3	2	2	4
(0, 1, 1, 0)	3	7	5	2	8	8
(0, 1, 1, 1)	1	5	5	0	5	3
(1, 0, 0, 0)	7	7	13	1	13	9
(1, 0, 0, 1)	0	5	2	0	3	4
(1, 0, 1, 0)	0	5	5	0	11	4
(1, 0, 1, 1)	1	7	3	0	7	5
(1, 1, 0, 0)	3	7	4	0	4	7
(1, 1, 0, 1)	2	5	0	0	3	7
(1, 1, 1, 0)	0	1	1	0	6	5
(1, 1, 1, 1)	0	1	0	0	7	4

**Table 2.** Repartition of the length 4 trajectories among the 16 possible ones, in the data, in the HMM simulations and in the OD-HMM simulations, for the four weed species studied.

For a given weed species, we estimated  $\hat{P}_0$ ,  $\hat{P}_1$  and  $\hat{R}$ , with the EM algorithm for OD-HMM. We then simulated the trajectories of 100 chains of length 500 using these estimators from which we estimated the average time of continuous presence of seeds in the soil (average duration of seed stock persistence). For the sake of comparison,

we performed the same estimation using EM for HMM instead. We ran this procedure for the four species mentioned above and classified as non-dormant in the literature and also according to the estimators obtained in Pluntz et al. 2018a. Consequently, the seed stock persistence must be low for these species.

Species	Model	Min.	1st Quant.	Median	Mean	3rd Quant.	Max.
<i>Lactuca serriola</i>	OD-HMM	1	1	3	3.854	5	39
	HMM	1	7	19	25.94	37	162
<i>Matricaria chamo.</i>	OD-HMM	1	1	2	2.066	3	15
	HMM	1	3	6	7.654	10	46
<i>Sonchus oleraceus</i>	OD-HMM	1	2	4	5.616	8	46
	HMM	1	5	10	14.85	21	129
<i>Taraxacum offic.</i>	OD-HMM	1	4	8	11.14	15	75
	HMM	1	17	43	60.47	81	373

**Table 3.** Comparison of the average duration of seeds stock persistence estimated by EM for HMM, and by EM for OD-HMM for four weed species. These species are classified as non dormant species based on biological knowledge and also according to the estimators obtained in Pluntz et al. 2018a. Data are from the Biovigilance dataset.

Results are presented in Table 3. The estimator of the average duration of seed stock persistence based on the OD-HMM is clearly in better agreement with what is expected from biological knowledge. On the contrary, the estimated duration with the EM for HMM is excessively high. This may be due to the fact that in the HMM model, the probability to remain in state one in the hidden chain must be high to compensate for the arrival of new seeds by standing flora, which is not taken into account. We can see from Table 2 that when simulating the same number of trajectories of length 4 than in the data, the repartition among the 16 possible ones is quite similar between the data, the HMM simulations and the OD-HMM simulations. However, for the HMM model this is only possible with an unrealistic estimation of the dynamics of the hidden chain.

## 6. Conclusion

Even though the OD-HMM framework was already encountered in the literature, its use up until now has been limited to specific cases dedicated to certain applications. With this work we exhibit the theoretical guaranties and an estimation algorithm

in the non-parametric case, which should facilitate sharing and use by the scientific community.

Concerning the theoretical aspect, we studied the consistency of the MLE of the OD-HMM by transposing the work of Ailliot and Pène (2015) to the case of the OD-HMM. The next step would be to prove the asymptotic normality of the MLE of the OD-HMM, either by extending the work of Bickel et al. (1998) and Gámiz et al. (2023) proposed for a classical HMM, or by adapting the work of Pouzo et al. (2022) proposed for more complex structures including the case of the OD-HMM. Extending the notion of reliability of a system modeled by an HMM (Durand and Gaudoin 2016; Gámiz et al. 2023) to the OD-HMM case may be an interesting perspective.

On the practical side, we derived the EM algorithm for OD-HMM to estimate the parameters of the model. By performing three experiments, we found that when the values of the true parameters  $P^*$  and  $R^*$ , or just  $R^*$  are contrasted, the estimation procedure provides good results. However, it is not recommended to use the EM algorithm for OD-HMM when the true emission matrix  $R^*$  is not contrasted. These experiments were conducted on observation trajectories of a maximum length of 500 to avoid the appearance of possible numerical problems. Moreover, we carried out the experiments for  $C$  varying from 10 to 100 chains, in order to be able to run more simulation examples in a faster way, although running the algorithm on a larger number of chains would certainly improve the quality of the estimator. In the same way, although the EM algorithm for OD-HMM presented here is built for any size of discrete and finite state spaces, we only tested the  $2 \times 2$  case to perform multiple experiments and to be able to detect the possible appearance of label switching, as in the third proposed experiment. To work with more complex systems (more trajectories and states) it would be wise to consider a parametric model, as underlined in Bazzi et al. (2022) : "*A key challenge is to specify an appropriate and parsimonious function that links the lagged dependent variables to future transition probabilities*".

Since this work was motivated by the need of more realism in the modeling of applications, we envisage extending the OD-HMM to the case where the hidden chain is

a semi-Markov chain (Barbu and Limnios 2008; Abdullah and Hoek 2022; Yu 2016). The sojourn time distribution will then be generalized to any probability distribution and not only to a geometric one as in a HMM. The challenge will then be to adapt the framework of Hidden Semi-Markov Models (HSMM) to the case of OD-HSMM by modeling the impact of observations on sojourn time distribution. Results on identifiability of HSMM and properties of the MLE (Barbu and Limnios 2008) will also have to be adapted, as well as the EM algorithm for HSMM to the OD-HSMM (Bulla 2006; Barbu and Limnios 2008; Yu 2016).

### **Code and data availability**

The algorithm is implemented in R. All the R codes used for the numerical experiments are available in two GitLab repositories. The functions corresponding to the EM algorithm for OD-HMM (for any size of the state spaces) are contained in an R package, available at the following link : <https://forgemia.inra.fr/hanna.bacave/odhmm>. The functions used to run the experiments in Section 4 and Section 5 can be found in the following repository: [https://forgemia.inra.fr/hanna.bacave/article\\_odhmm](https://forgemia.inra.fr/hanna.bacave/article_odhmm). For Section 5, the data used is available at the following link : <https://hal.science/hal-01801122>.

### **Acknowledgments**

The authors would like to thank Elise Maigne (MIAT-INRAE) for her advice on good practices for code reproducibility and for her support in the process of building the GitLab repository and the package.

### **Funding details**

This work was supported by the French National Research Agency (ANR) under Grant ANR-21-CE40-005 (project HSMM-INCA).



## **Disclosure statement**

The authors report that there are no competing interests to declare.

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## Appendix A. Demonstration of Markovianity of the hidden chain in an OD-HMM

**Proposition A.1** (Markovianity of the hidden chain in an OD-HMM). *If  $(Z_t, Y_t)_{t \in \mathbb{N}}$  follows an OD-HMM model, then the hidden chain  $(Z_t)_{t \in \mathbb{N}}$  is Markovian. The associated transition probability is equal to  $\sum_{y_{t-1} \in \Omega_Y} \mathbb{P}(Z_t = z_t | Y_{t-1} = y_{t-1}, Z_{t-1} = z_{t-1}) \mathbb{P}(Y_{t-1} = y_{t-1} | Z_{t-1} = z_{t-1})$ .*

Indeed, we have:

$$\begin{aligned}
 \mathbb{P}(Z_t = z_t | Z_{0:t-1} = z_{0:t-1}) &= \sum_{y_{t-1} \in \Omega_Y} \mathbb{P}(Z_t = z_t, Y_{t-1} = y_{t-1} | Z_{0:t-1} = z_{0:t-1}) \\
 &= \sum_{y_{t-1} \in \Omega_Y} \mathbb{P}(Z_t = z_t | Y_{t-1} = y_{t-1}, Z_{t-1} = z_{t-1}) \times \\
 &\quad \mathbb{P}(Y_{t-1} = y_{t-1} | Z_{0:t-1} = z_{0:t-1}) \\
 &= \sum_{y_{t-1} \in \Omega_Y} \mathbb{P}(Z_t = z_t | Y_{t-1} = y_{t-1}, Z_{t-1} = z_{t-1}) \times \\
 &\quad \mathbb{P}(Y_{t-1} = y_{t-1} | Z_{t-1} = z_{t-1}) \\
 &= \sum_{y_{t-1} \in \Omega_Y} \mathbb{P}(Z_t = z_t, Y_{t-1} = y_{t-1} | Z_{t-1} = z_{t-1}) \\
 &= \mathbb{P}(Z_t = z_t | Z_{t-1} = z_{t-1})
 \end{aligned}$$

## Appendix B. Generic identifiability

Let us consider two ODHMMs, the first one with parameter  $\theta$  and the second with parameter  $\theta'$ . The transition matrix and emission matrix are  $P_y$  and  $R$ , and  $P'_y$  and  $R'$  respectively. We assume that their reformulations as a HMM lead to the same model, i.e.  $\mathcal{M}_\theta^{HMM} = \mathcal{M}_{\theta'}^{HMM}$  and we show that this implies that  $\theta = \theta'$ .

If the two transition matrices  $P_\theta^{\text{HMM}}$  and  $P_{\theta'}^{\text{HMM}}$  are identical, we have:

$$\left\{ \begin{array}{l} P_\theta^{\text{HMM}}((0, 0), (0, 0)) = P_{\theta'}^{\text{HMM}}((0, 0), (0, 0)) \\ P_\theta^{\text{HMM}}((0, 0), (0, 1)) = P_{\theta'}^{\text{HMM}}((0, 0), (0, 1)) \\ \dots \\ P_\theta^{\text{HMM}}((0, 0), (0, D)) = P_{\theta'}^{\text{HMM}}((0, 0), (0, D)) \end{array} \right.$$

Using the definition of  $P_\theta^{\text{HMM}}$  in terms of the original OD-HMM, we obtain:

$$\left\{ \begin{array}{l} P_0(0, 0)R(0, 0) = P'_0(0, 0)R'(0, 0) \\ P_0(0, 0)R(0, 1) = P'_0(0, 0)R'(0, 1) \\ \dots \\ P_0(0, 0)R(0, D) = P'_0(0, 0)R'(0, D) \end{array} \right.$$

Adding all the lines leads to:

$$P_0(0, 0) \left[ \sum_{d=0}^D R(0, d) \right] = P'_0(0, 0) \left[ \sum_{d=0}^D R'(0, d) \right].$$

Since  $\sum_{d=0}^D R(0, d) = 1$  and  $\sum_{d=0}^D R'(0, d) = 1$  we obtain  $P_0(0, 0) = P'_0(0, 0)$ . If we replace  $P'_0(0, 0)$  by  $P_0(0, 0)$  in the above system we also obtain that  $\forall d \in \{0, \dots, D\}$ ,  $R(0, d) = R'(0, d)$ .

We can perform the same calculations with all possible values for  $(z_{t-1}, y_{t-1}, z_t)$

and we will obtain that  $P_{y_{t-1}}(z_{t-1}, z_t) = P'_{y_{t-1}}(z_{t-1}, z_t)$  and that  $\forall y_t \in \{0, \dots, D\}$ ,  $R(z_t, y_t) = R'(z_t, y_t)$ . This establishes that if  $\mathcal{M}_\theta^{HMM} = \mathcal{M}_{\theta'}^{HMM}$ , then  $\mathcal{M}_\theta^{ODHMM} = \mathcal{M}_{\theta'}^{ODHMM}$ .

## Appendix C. Calculations of EM algorithm

Note that another EM solution to estimate the non parametric OD-HMM could be to use the classical EM for HMM to estimate the non-parametric HMM in which the hidden state is the pair  $(Z_t, Y_t)$ , i.e. the  $\mathcal{M}_\theta^{HMM}$  model defined in Section 2.2. It would require a second step after estimation to recover the transition and the emission matrices of the OD-HMM from the estimated transition and emission matrices of the  $\mathcal{M}_\theta^{HMM}$  model. Furthermore, the number of parameters in the  $\mathcal{M}_\theta^{HMM}$  is  $|\Omega_Z| \times |\Omega_Y| \times (|\Omega_Z| \times |\Omega_Y| - 1)$ , which is larger than in the original OD-HMM  $(|\Omega_Z| \times (|\Omega_Z| - 1) \times |\Omega_Y| + |\Omega_Z| \times (|\Omega_Y| - 1))$ .

### C.1. Complete likelihood expression

We recall the definition of the complete likelihood that we will denote  $L_{comp}$ .

$$L_{comp} = L(\theta; z_{1:C,0:M}, y_{1:C,0:M}) = \mathbb{P}(Y_{1:C,0:M} = y_{1:C,0:M}, Z_{1:C,0:M} = z_{1:C,0:M} | \theta).$$

Since the  $C$  chains are i.i.d we have:



$$\begin{aligned}
L_{comp} &= L(\theta; z_{1:C,0:M}, y_{1:C,0:M}) \\
&= \prod_{c=1}^C \mathbb{P}(Z_{c,0:M} = z_{c,0:M}, Y_{c,0:M} = y_{c,0:M} | \theta) \\
&= \prod_{c=1}^C \mathbb{P}(Z_{c,M} = z_{c,M}, Y_{c,M} = y_{c,M} | Z_{c,0:M-1} = z_{c,0:M-1}, Y_{c,0:M-1} = y_{c,0:M-1}, \theta) \\
&\quad \times \mathbb{P}(Z_{c,0:M-1} = z_{c,0:M-1}, Y_{c,0:M-1} = y_{c,0:M-1} | \theta) \\
&= \dots \\
&= \prod_{c=1}^C \prod_{t=1}^M \mathbb{P}(Z_{c,t} = z_{c,t}, Y_{c,t} = y_{c,t} | Z_{c,t-1} = z_{c,t-1}, Y_{c,t-1} = y_{c,t-1}, \theta) \\
&\quad \times \mathbb{P}(Z_{c,0} = z_{c,0}, Y_{c,0} = y_{c,0} | \theta) \\
&= \prod_{c=1}^C \prod_{t=1}^M \mathbb{P}(Y_{c,t} = y_{c,t} | Z_{c,t} = z_{c,t}, \theta) \mathbb{P}(Z_{c,t} = z_{c,t} | Z_{c,t-1} = z_{c,t-1}, Y_{c,t-1} = y_{c,t-1}, \theta) \\
&\quad \times \mathbb{P}(Y_{c,0} = y_{c,0} | Z_{c,0} = z_{c,0}, \theta) \mathbb{P}(Z_{c,0} = z_{c,0}, \theta)
\end{aligned}$$

Finally,

$$L(y_{1:C,0:M}, z_{1:C,0:M} | \theta) = \prod_{c=1}^C \left[ \pi(z_{c,0}) R(z_{c,0}, y_{c,0}) \prod_{c,t=1}^M P_{y_{c,t-1}}(z_{c,t-1}, z_{c,t}) R(z_{c,t}, y_{c,t}) \right].$$

## C.2. Intermediate quantity calculation expression

We recall the definition of the intermediate quantity, where  $\theta^{(m)}$  is the value of the parameters at iteration  $m$ .

$$Q(\theta | \theta^{(m)}) = \mathbb{E} \left[ \ln(\mathbb{P}(Y_{1:C,0:M}, Z_{1:C,0:M} | \theta) | Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)}) \right].$$

We replace the complete likelihood by its expression and we take its logarithm. We denote  $X = \ln(\mathbb{P}(Y_{1:C,0:M} = y_{1:C,0:M}, Z_{1:C,0:M} = z_{1:C,0:M} | \theta))$  and we obtain:

$$\begin{aligned}
X &= \ln(\mathbb{P}(Y_{1:C,0:M} = y_{1:C,0:M}, Z_{1:C,0:M} = z_{1:C,0:M} | \theta)) \\
&= \ln \left\{ \prod_{c=1}^C \left[ \pi(z_{c,0}) R(z_{c,0}, y_{c,0}) \prod_{t=1}^M P_{y_{c,t-1}}(z_{c,t-1}, z_{c,t}) R(z_{c,t}, y_{c,t}) \right] \right\} \\
&= \sum_{c=1}^C \ln[\pi(z_{c,0})] + \ln \left[ \prod_{t=0}^M R(z_{c,t}, y_{c,t}) \right] + \ln \left[ \prod_{t=1}^M P_{y_{c,t-1}}(z_{c,t-1}, z_{c,t}) \right] \\
&= \sum_{c=1}^C \ln[\pi(z_{c,0})] + \sum_{t=0}^M \ln[R(z_{c,t}, y_{c,t})] + \sum_{t=1}^M \ln[P_{y_{c,t-1}}(z_{c,t-1}, z_{c,t})]
\end{aligned}$$

Let us denote  $Q = Q(\theta | \theta^{(m)})$ , we can break down  $Q$  as follows:

$$\begin{aligned}
Q &= Q(\theta | \theta^{(m)}) \\
&= \mathbb{E} \left\{ \sum_{c=1}^C \left[ \ln \pi(Z_{c,0}) + \sum_{t=0}^M \ln R(Z_{c,t}, Y_{c,t}) \right. \right. \\
&\quad \left. \left. + \sum_{t=1}^M \ln P_{Y_{c,t-1}}(Z_{c,t-1}, Z_{c,t}) \right] \mid Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right\} \\
&= \sum_{c=1}^C \left\{ \mathbb{E} \left[ \ln \pi(Z_{c,0}) \mid Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right] \right. \\
&\quad \left. + \mathbb{E} \left[ \sum_{t=0}^M \ln R(Z_{c,t}, Y_{c,t}) \mid Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right] \right. \\
&\quad \left. + \mathbb{E} \left[ \sum_{t=1}^M \ln P_{Y_{c,t-1}}(Z_{c,t-1}, Z_{c,t}) \mid Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right] \right\} \\
&= \sum_{c=1}^C \left\{ \mathbb{E} \left[ \ln \pi(Z_{c,0}) \mid Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right] \right. \\
&\quad \left. + \sum_{t=0}^M \mathbb{E} \left[ \ln R(Z_{c,t}, Y_{c,t}) \mid Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right] \right. \\
&\quad \left. + \sum_{t=1}^M \mathbb{E} \left[ \ln P_{Y_{c,t-1}}(Z_{c,t-1}, Z_{c,t}) \mid Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right] \right\}
\end{aligned}$$

where

$$\begin{aligned} \mathbb{E} \left[ \ln \pi(Z_{c,0}) \mid Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right] &= \sum_{z_{c,0} \in \Omega_Z} \ln \pi(z_{c,0}) \\ &\times \mathbb{P}(Z_{c,0} = z_{c,0} \mid Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}), \end{aligned}$$

and:

$$\begin{aligned} \mathbb{E} \left[ \ln R(Z_{c,t}, Y_{c,t}) \mid Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right] &= \sum_{z_{c,t} \in \Omega_Z} \ln R(z_{c,t}, y_{c,t}) \\ &\times \mathbb{P}(Z_{c,t} = z_{c,t} \mid Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \end{aligned}$$

In the same way, we have:

$$A = \mathbb{E} \left[ \ln P_{Y_{c,t-1}}(Z_{c,t-1}, Z_{c,t}) \mid Y_{1:C,0:M} = y_{1:C,0:M}, \theta^{(m)} \right]$$

where :

$$\begin{aligned} A &= \sum_{(z_{c,t}, z_{c,t-1}) \in \Omega_Z^2} \ln P_{y_{c,t-1}}(z_{c,t-1}, z_{c,t}) \\ &\times \mathbb{P}(Z_{c,t} = z_{c,t}, Z_{c,t-1} = z_{c,t-1} \mid Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \end{aligned}$$

We finally obtain:

$$\begin{aligned} Q(\theta \mid \theta^{(m)}) &= \sum_{c=1}^C \sum_{z_{c,0} \in \Omega_Z} \ln \pi(z_{c,0}) \mathbb{P}(Z_{c,0} = z_{c,0} \mid Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \\ &+ \sum_{c=1}^C \sum_{t=1}^M \sum_{(z_{c,t}, z_{c,t-1}) \in \Omega_Z^2} \ln P_{y_{c,t-1}}(z_{c,t-1}, z_{c,t}) \\ &\times \mathbb{P}(Z_{c,t-1} = z_{c,t-1}, Z_{c,t} = z_{c,t} \mid Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \\ &+ \sum_{c=1}^C \sum_{t=0}^M \sum_{z_{c,t} \in \Omega_Z} \ln R(z_{c,t}, y_{c,t}) \mathbb{P}(Z_{c,t} = z_{c,t} \mid Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \end{aligned}$$

### C.3. E Step calculations

During the E Step, we want to calculate the marginal probabilities of interest appeared in the expression of  $Q(\theta|\theta^{(m)})$ . We denote:

- $\rho_{c,t}^{(m)}(z_t) = \mathbb{P}(Z_{c,t} = z_t | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)})$ ,
- $\xi_{c,t}^{(m)}(z_{t-1}, z_t) = \mathbb{P}(Z_{c,t-1} = z_{t-1}, Z_{c,t} = z_t | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)})$ .

To obtain  $\rho_{c,t}^{(m)}(z_t)$  and  $\xi_{c,t}^{(m)}(z_{t-1}, z_t)$ , we introduce the following variables:

- $\alpha_{c,t}^{(m)}(z_t)$ , such as  $\alpha_{c,t}(z_t) = \mathbb{P}(Y_{c,0:t} = y_{c,0:t}, Z_{c,t} = z_t | \theta^{(m)})$  ;
- $\beta_{c,t}^{(m)}(z_t)$ , such as  $\beta_{c,t}(z_t) = \mathbb{P}(Y_{c,t+1:M} = y_{c,t+1:M} | Z_{c,t} = z_t, Y_{c,t} = y_{c,t}, \theta^{(m)})$ .

#### C.3.1. Forward algorithm for computing the $\alpha$ s

We begin by expressing  $\alpha_0(z_{c,0})$  :

$$\begin{aligned} \alpha_{c,0}^{(m)}(z_{c,0}) &= \mathbb{P}(Y_{c,0} = y_{c,0}, Z_{c,0} = z_{c,0} | \theta^{(m)}) \\ &= \mathbb{P}(Y_{c,0} = y_{c,0} | Z_{c,0} = z_{c,0}, \theta^{(m)}) \mathbb{P}(Z_{c,0} = z_{c,0} | \theta^{(m)}) \\ &= R(z_{c,0}, y_{c,0})^{(m)} \pi(z_{c,0})^{(m)} \end{aligned}$$

Now, given that  $\forall 1 \leq t \leq M$ , we have:

$$\begin{aligned}
\alpha_{c,t}^{(m)}(z) &= \mathbb{P}(Y_{c,0:t} = y_{c,0:t}, Z_{c,t} = z | \theta^{(m)}) \\
&= \mathbb{P}(Y_{c,0:t} = y_{c,0:t} | Z_{c,t} = z, \theta^{(m)}) \mathbb{P}(Z_{c,t} = z | \theta^{(m)}) \\
&= \mathbb{P}(Y_{c,t} = y_{c,t} | Z_{c,t} = z, \theta^{(m)}) \mathbb{P}(Y_{c,0:t-1} = y_{c,0:t-1} | Z_{c,t} = z, \theta^{(m)}) \mathbb{P}(Z_{c,t} = z | \theta^{(m)}) \\
&= \mathbb{P}(Y_{c,t} = y_{c,t} | Z_{c,t} = z \theta^{(m)}) \mathbb{P}(Y_{c,0:t-1} = y_{c,0:t-1}, Z_{c,t} = z | \theta^{(m)}) \\
&= R^{(m)}(z, y_{c,t}) \times \sum_{z_{c,t-1} \in \Omega_Z} \mathbb{P}(Y_{c,0:t-1} = y_{c,0:t-1}, Z_{c,t} = z, Z_{c,t-1} = z_{c,t-1} | \theta^{(m)}) \\
&= R^{(m)}(z, y_{c,t}) \sum_{z_{c,t-1} \in \Omega_Z} \mathbb{P}(Z_{c,t} = z | Y_{c,0:t-1} = y_{c,0:t-1}, Z_{c,t-1} = z_{c,t-1}, \theta^{(m)}) \\
&\quad \times \mathbb{P}(Y_{c,0:t-1} = y_{c,0:t-1}, Z_{c,t-1} = z_{c,t-1} | \theta^{(m)}) \\
&= R^{(m)}(z, y_{c,t}) \times \sum_{z_{c,t-1} \in \Omega_Z} \mathbb{P}(Z_{c,t} = z | Y_{c,t-1} = y_{c,t-1}, Z_{c,t-1} = z_{c,t-1}, \theta^{(m)}) \\
&\quad \times \alpha_{c,t-1}^{(m)}(z_{c,t-1}) \\
&= R^{(m)}(z, y_{c,t}) \times \sum_{z_{c,t-1} \in \Omega_Z} P_{y_{c,t-1}}^{(m)}(z_{c,t-1}, z) \times \alpha_{c,t-1}^{(m)}(z_{c,t-1}).
\end{aligned}$$

We therefore obtain the forward recursive expression:

$$\forall 1 \leq t \leq M, \alpha_{c,t}^{(m)}(z) = R^{(m)}(z, y_{c,t}) \sum_{z_{c,t-1} \in \Omega_Z} \alpha_{c,t-1}^{(m)}(z_{c,t-1}) P_{y_{c,t-1}}^{(m)}(z_{c,t-1}, z).$$

### C.3.2. Backward algorithm for computing the $\beta$ s

We start by initializing  $\beta_M^{(m)}(z)$ . By convention we set  $\beta_M^{(m)}(z) = 1$ .

Now, given that  $\forall 1 \leq t \leq M - 1$ , we have:

$$\begin{aligned}
\beta_{c,t}^{(m)}(z) &= \mathbb{P}(Y_{c,t+1:M} = y_{c,t+1:M} | Z_{c,t} = z, Y_{c,t} = y_{c,t}, \theta^{(m)}) \\
&= \sum_{z_{c,t+1} \in \Omega_Z} \mathbb{P}(Y_{c,t+1:M} = y_{c,t+1:M}, Z_{c,t+1} = z_{c,t+1} | Z_{c,t} = z, Y_{c,t} = y_{c,t}, \theta^{(m)}) \\
&= \sum_{z_{c,t+1} \in \Omega_Z} \mathbb{P}(Y_{c,t+2:M} = y_{c,t+2:M} | Y_{c,t+1} = y_{c,t+1}, Z_{c,t+1} = z_{c,t+1}, \theta^{(m)}) \\
&\quad \times \mathbb{P}(Y_{c,t+1} = y_{c,t+1}, Z_{c,t+1} = z_{c,t+1} | Y_{c,t} = y_{c,t}, Z_{c,t} = z, \theta^{(m)}) \\
&= \sum_{z_{c,t+1} \in \Omega_Z} \beta_{c,t+1}^{(m)}(z_{c,t+1}) \mathbb{P}(Z_{c,t+1} = z_{c,t+1} | Y_{c,t} = y_{c,t}, Z_{c,t} = z, \theta^{(m)}) \\
&\quad \times \mathbb{P}(Y_{c,t+1} = y_{c,t+1} | Z_{c,t+1} = z_{c,t+1}, \theta^{(m)}) \\
&= \sum_{z_{c,t+1} \in \Omega_Z} \beta_{c,t+1}^{(m)}(z_{c,t+1}) \times P_{y_{c,t}}^{(m)}(z, z_{c,t+1}) \times R^{(m)}(z_{c,t+1}, y_{c,t+1}).
\end{aligned}$$

We finally obtain the backward recursive expression:

$$\forall 1 \leq t \leq M - 1, \beta_{c,t}^{(m)}(z) = \sum_{z_{c,t+1} \in \Omega_Z} R^{(m)}(z_{c,t+1}, y_{c,t+1}) \beta_{c,t+1}^{(m)}(z_{c,t+1}) P_{y_{c,t}}^{(m)}(z, z_{c,t+1}).$$

### C.3.3. Expression of quantities $\rho$ and $\xi$ in terms of $\alpha$ and $\beta$ :

We have

$$\rho_{c,t}^{(m)}(z) = \mathbb{P}(Z_{c,t} = z | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}).$$

and we can express it as follows:

$$\rho_{c,t}^{(m)}(z) = \frac{\mathbb{P}(Z_{c,t} = z, Y_{c,0:M} = y_{c,0:M} | \theta^{(m)})}{\mathbb{P}(Y_{c,0:M} = y_{c,0:M} | \theta^{(m)})}.$$

In the same way, we have:

$$\xi_{c,t}^{(m)}(z', z') = \mathbb{P}(Z_{c,t-1} = z', Z_{c,t} = z' | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}),$$

which we can transform as follows:

$$\xi_{c,t}^{(m)}(z', z') = \frac{\mathbb{P}(Z_{c,t-1} = z', Z_{c,t} = z', Y_{c,0:M} = y_{c,0:M} | \theta^{(m)})}{\mathbb{P}(Y_{c,0:M} = y_{c,0:M} | \theta^{(m)})}.$$

First, we express the quantity  $\mathbb{P}(Y_{c,0:M} = y_{c,0:M} | \theta^{(m)})$ , which is the likelihood, in terms of  $\alpha$  and  $\beta$ . Let us denote  $P = \mathbb{P}(Y_{c,0:M} = y_{c,0:M} | \theta^{(m)})$ . We can decompose  $P$  as follows:

$$\begin{aligned} P &= \mathbb{P}(Y_{c,0:M} = y_{c,0:M} | \theta^{(m)}) \\ &= \sum_{z_{c,t} \in \Omega_Z} \mathbb{P}(Y_{c,0:M} = y_{c,0:M}, Z_{c,t} = z_{c,t} | \theta^{(m)}) \\ &= \sum_{z_{c,t} \in \Omega_Z} \mathbb{P}(Y_{c,0:M} = y_{c,0:M} | Z_{c,t} = z_{c,t}, \theta^{(m)}) \mathbb{P}(Z_{c,t} = z_{c,t} | \theta^{(m)}) \\ &= \sum_{z_{c,t} \in \Omega_Z} \mathbb{P}(Y_{c,0:t} = y_{c,0:t} | Z_{c,t} = z_{c,t}, \theta^{(m)}) \mathbb{P}(Y_{c,t+1:M} = y_{c,t+1:M} | Z_{c,t} = z_{c,t}, Y_{c,t} = y_{c,t} \theta^{(m)}) \\ &\quad \times \mathbb{P}(Z_{c,t} = z_{c,t}, Y_{c,t}, \theta^{(m)}) \\ &= \sum_{z_{c,t} \in \Omega_Z} \beta_{c,t}^{(m)}(z_{c,t}) \times \mathbb{P}(Y_{c,0:t} = y_{c,0:t} | Z_{c,t} = z_{c,t}, \theta^{(m)}) \mathbb{P}(Z_{c,t} = z_{c,t}, \theta^{(m)}) \\ &= \sum_{z_{c,t} \in \Omega_Z} \beta_{c,t}^{(m)}(z_{c,t}) \times \mathbb{P}(Y_{c,0:t} = y_{c,0:t}, Z_{c,t} = z_{c,t} | \theta^{(m)}) \\ &= \sum_{z_{c,t} \in \Omega_Z} \beta_{c,t}^{(m)}(z_{c,t}) \times \alpha_{c,t}^{(m)}(z_{c,t}). \end{aligned}$$

Therefore, we have

$$\mathbb{P}(Y_{c,0:M} = y_{c,0:M} | \theta^{(m)}) = \sum_{z_{c,t} \in \Omega_Z} \alpha_{c,t}^{(m)}(z_{c,t}) \beta_{c,t}^{(m)}(z_{c,t}).$$

- **Expression of  $\rho$ :**

Let us denote  $A = \mathbb{P}(Z_{c,t} = z_{c,t}, Y_{c,0:M} = y_{c,0:M} | \theta^{(m)})$ . We can decompose  $A$

as follows:

$$\begin{aligned}
A &= \mathbb{P}(Y_{c,0:M} = y_{c,0:M} | Z_{c,t} = z_{c,t}, \theta^{(m)}) \mathbb{P}(Z_{c,t} = z_{c,t} | \theta^{(m)}) \\
&= \mathbb{P}(Y_{c,0:t} = y_{c,0:t} | Z_{c,t} = z_{c,t}, \theta^{(m)}) \mathbb{P}(Y_{c,t+1:M} = y_{c,t+1:M} | Z_{c,t} = z_{c,t}, Y_{c,t} = y_{c,t}, \theta^{(m)}) \\
&\quad \times \mathbb{P}(Z_{c,t} = z_{c,t}, \theta^{(m)}) \\
&= \beta_{c,t}^{(m)}(z_{c,t}) \times \mathbb{P}(Y_{c,0:t} = y_{c,0:t} | Z_{c,t} = z_{c,t}, \theta^{(m)}) \mathbb{P}(Z_{c,t} = z_{c,t}, \theta^{(m)}) \\
&= \beta_{c,t}^{(m)}(z_{c,t}) \times \mathbb{P}(Y_{c,0:t} = y_{c,0:t}, Z_{c,t} = z_{c,t} | \theta^{(m)}) \\
&= \beta_{c,t}^{(m)}(z_{c,t}) \alpha_{c,t}^{(m)}(z_{c,t}).
\end{aligned}$$

Therefore, we deduce:

$$\rho_{c,t}^{(m)}(z) = \frac{\alpha_{c,t}^{(m)}(z) \beta_{c,t}^{(m)}(z)}{\sum_{z \in \Omega_Z} \alpha_{c,t}^{(m)}(z) \beta_{c,t}^{(m)}(z)}.$$

- **Expression of  $\xi$ :**

Let us denote  $A' = \mathbb{P}(Z_{c,t-1} = z_{c,t-1}, Z_{c,t} = z_{c,t}, Y_{c,0:M} = y_{c,0:M} | \theta^{(m)})$ . We can



decompose  $A'$  as follows:

$$\begin{aligned}
A' &= \mathbb{P}(Y_{c,0:t-2} = y_{c,0:t-2}, Y_{c,t:M} = y_{c,t:M} | Z_{c,t-1} = z_{c,t-1}, Z_{c,t} = z_{c,t}, Y_{c,t-1} = y_{c,t-1}, \theta^{(m)}) \\
&\quad \times \mathbb{P}(Z_{c,t-1} = z_{c,t-1}, Z_{c,t} = z_{c,t}, Y_{c,t-1} = y_{c,t-1} | \theta^{(m)}) \\
&= \mathbb{P}(Y_{c,0:t-2} = y_{c,0:t-2} | Y_{c,t-1} = y_{c,t-1}, Z_{c,t-1} = z_{c,t-1}, \theta^{(m)}) \\
&\quad \times \mathbb{P}(Z_{c,t-1} = z_{c,t-1}, Y_{c,t-1} = y_{c,t-1} | \theta^{(m)}) \mathbb{P}(Y_{c,t:M} = y_{c,t:M} | Z_{c,t} = z_{c,t}, \theta^{(m)}) \\
&\quad \times \mathbb{P}(Z_{c,t} = z_{c,t} | Z_{c,t-1} = z_{c,t-1}, Y_{c,t-1} = y_{c,t-1}, \theta^{(m)}) \\
&= \mathbb{P}(Y_{c,0:t-1} = y_{c,0:t-1}, Z_{c,t-1} = z_{c,t-1} | \theta^{(m)}) \mathbb{P}(Y_{c,t:M} = y_{c,t:M} | Z_{c,t} = z_{c,t}, \theta^{(m)}) \\
&\quad \times P_{y_{c,t-1}}(z_{c,t-1}, z_{c,t}) \\
&= \alpha_{c,t-1}^{(m)}(z_{c,t-1}) P_{y_{c,t-1}}^{(m)}(z_{c,t-1}, z_{c,t}) \mathbb{P}(Y_{c,t} = y_{c,t} | Z_{c,t} = z_{c,t}, \theta^{(m)}) \\
&\quad \times \mathbb{P}(Y_{c,t+1:M} = y_{c,t+1:M} | Z_{c,t} = z_{c,t}, Y_{c,t} = y_{c,t}, \theta^{(m)}) \\
&= \alpha_{c,t-1}^{(m)}(z_{c,t-1}) P_{y_{c,t-1}}^{(m)}(z_{c,t-1}, z_{c,t}) R^{(m)}(z_{c,t}, y_{c,t}) \beta_{c,t}^{(m)}(z_{c,t}).
\end{aligned}$$

We finally obtain:

$$\xi_{c,t}^{(m)}(z_{c,t-1}, z) = \frac{\alpha_{c,t-1}^{(m)}(z_{c,t-1}) P_{y_{c,t-1}}^{(m)}(z_{c,t-1}, z) R^{(m)}(z, y_{c,t}) \beta_{c,t}^{(m)}(z)}{\sum_{z \in \Omega_Z} \alpha_{c,t}^{(m)}(z) \beta_{c,t}^{(m)}(z)}.$$

#### C.4. Step $M$ - Solving the maximization problem

We want to solve the following problem of maximization :

$$\theta^{(m+1)} = \arg \max_{\theta} Q(\theta | \theta^{(m)}),$$

under the following constraints:

- $\sum_{z_t \in \Omega_Z} P_{y_{c,t-1}}(z_{t-1}, z_t) = 1$  ;
- $\sum_{y_t \in \Omega_Y} R(z_{c,t}, y_t) = 1$ .

(We recall that we do not estimate  $\pi(\cdot)$ .)

C.4.1. *Writing the Lagrangian of problem*

We write the Lagrangian of the problem  $\mathcal{L}$ :

$$\begin{aligned}
\mathcal{L} &= \sum_{c=1}^C \sum_{z_{c,0} \in \Omega_Z} \ln(\pi(z_{c,0})) \mathbb{P}(Z_{c,0} = z_{c,0} | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) - \eta_1 \left( \sum_{z_0 \in \Omega_Z} \pi(z_0) - 1 \right) \\
&+ \sum_{c=1}^C \sum_{t=1}^M \sum_{(z_{c,t}, z_{c,t-1}) \in \Omega_Z^2} \ln(P_{y_{c,t-1}}(z_{c,t-1}, z_{c,t})) \mathbb{P}(Z_{c,t-1} = z_{c,t-1}, Z_{c,t} = z_{c,t} | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \\
&- \eta_2(y_{c,t-1}, z_{c,t-1}) \left( \sum_{z' \in \Omega_Z} P_{y_{c,t-1}}(z_{c,t-1}, z') - 1 \right) \\
&+ \sum_{c=1}^C \sum_{t=0}^M \sum_{z_{c,t} \in \Omega_Z} \ln(R(z_{c,t}, y_{c,t})) \mathbb{P}(Z_{c,t} = z_{c,t} | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) - \eta_3(z_{c,t}) \left( \sum_{y \in \Omega_Y} R(z_{c,t}, y) - 1 \right)
\end{aligned}$$

C.4.2. *Resolution*

- **For**  $P_y^{(m+1)}(z, z')$  :

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial P_y(z, z')} = 0 &\Leftrightarrow \frac{\sum_{c=1}^C \sum_{t=1}^M \mathbb{P}(Z_{c,t-1} = z, Z_{c,t} = z' | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \mathbf{1}_{(y=y_{c,t-1})}}{P_y(z, z')} = \eta_2(y, z) \\
&\Leftrightarrow \sum_{c=1}^C \sum_{t=1}^M \mathbb{P}(Z_{c,t-1} = z, Z_{c,t} = z' | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \mathbf{1}_{(y_{c,t-1}=y)} = \eta_2(y, z) \\
&\quad \times P_y(z, z') \\
&\Rightarrow \sum_{c=1}^C \sum_{t=1}^M \sum_{z' \in \Omega_Z} \mathbb{P}(Z_{c,t-1} = z, Z_{c,t} = z' | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \mathbf{1}_{(y_{c,t-1}=y)} = \eta_2(y, z) \\
&\quad \times \sum_{z' \in \Omega_Z} P_y(z, z') \\
&\Leftrightarrow \sum_{c=1}^C \sum_{t=1}^M \sum_{z' \in \Omega_Z} \mathbb{P}(Z_{c,t-1} = z, Z_{c,t} = z' | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \mathbf{1}_{(y_{c,t-1}=y)} = \eta_2(y, z)
\end{aligned}$$

Therefore, we obtain :

$$P_y^{(m+1)}(z, z') = \frac{\sum_{c=1}^C \sum_{t=1}^M \mathbb{P}(Z_{c,t-1} = z, Z_{c,t} = z' | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \mathbf{1}_{(y_{c,t-1}=y)}}{\sum_{c=1}^C \sum_{t=1}^M \sum_{z' \in \Omega_Z} \mathbb{P}(Z_{c,t-1} = z, Z_{c,t} = z' | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \mathbf{1}_{(y_{c,t-1}=y)}}.$$

- For  $R(z, y)^{(m+1)}$  :

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial R(z, y)} = 0 &\Leftrightarrow \frac{\sum_{c=1}^C \sum_{t=1}^M \mathbb{P}(Z_{c,t} = z | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \mathbb{1}_{(y_{c,t}=y)}}{R(z, y)} = \eta_3(z) \\
&\Leftrightarrow \sum_{c=1}^C \sum_{t=1}^M \mathbb{P}(Z_{c,t} = z | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \mathbb{1}_{(y_{c,t}=y)} = \eta_3(z) R(z, y) \\
&\Rightarrow \sum_{c=1}^C \sum_{t=1}^M \sum_{y \in \Omega_Y} \mathbb{P}(Z_{c,t} = z | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \mathbb{1}_{(y_{c,t}=y)} = \eta_3(z) \sum_{y \in \Omega_Y} R(z, y) \\
&\Leftrightarrow \sum_{c=1}^C \sum_{t=1}^M \mathbb{P}(Z_{c,t} = z | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \sum_{y \in \Omega_Y} \mathbb{1}_{(y_{c,t}=y)} = \eta_3(z) \\
&\Leftrightarrow \sum_{c=1}^C \sum_{t=1}^M \mathbb{P}(Z_{c,t} = z | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) = \eta_3(z)
\end{aligned}$$

Therefore, we have :

$$R(z, y)^{(m+1)} = \frac{\sum_{c=1}^C \sum_{t=1}^M \mathbb{P}(Z_{c,t} = z | y_{c,0:M} = y_{c,0:M}, \theta^{(m)}) \mathbb{1}_{(y_{c,t}=y)}}{\sum_{c=1}^C \sum_{t=1}^M \mathbb{P}(Z_{c,t} = z | Y_{c,0:M} = y_{c,0:M}, \theta^{(m)})}.$$