Estimating Discrete Markov Models From Various Incomplete Data Schemes

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Abstract

The parameters of a discrete stationary Markov model are transition probabilities between states. Traditionally, data consist in sequences of observed states for a given number of individuals over the whole observation period. In such a case, the estimation of transition probabilities is straightforwardly made by counting one-step moves from a given state to another. In many real-life problems, however, the inference is much more difficult as state sequences are not fully observed, namely the state of each individual is known only for some given values of the time variable. A review of the problem is given, focusing on Monte Carlo Markov Chain (MCMC) algorithms to perform Bayesian inference and evaluate posterior distributions of the transition probabilities in this missing-data framework. Leaning on the dependence between the rows of the transition matrix, an adaptive MCMC mechanism accelerating the classical Metropolis-Hastings algorithm is then proposed and empirically studied.

Keywords: Bayesian inference, industrial reliability, missing data, Markov models, adaptive MCMC, Gaussian copulas.

1. Introduction

When facing situations where a variable of interest $Z$ takes time-dependent values within a finite (discrete) set $S = \{s_1, s_2, \ldots, s_r\}$ of $r$ classes (let us call them states), a decision-maker is most often interested in estimating the probability $p_A(t)$ for $Z$ to be in a given set of states $A \subset S$ as a function of time $t$. For instance, these states can correspond to failure states in reliability analysis, thus $1 - p_A(t)$ is the reliability function of the system under investigation $\Sigma$ at time $t$. Another function of interest could be the expected number of states $N_A$ before $\Sigma$ reaches $A$. To do so, the decision-maker first has to estimate the transition probabilities from one state to another, i.e. estimate the transition matrix $\psi$. The vector $p(0)$ of the initial probabilities $p_1(0), \ldots, p_r(0)$ for the system to be in states $s_1, \ldots, s_r$ respectively, at $t = 0$, is usually assumed known in real-life applications; therefore, the knowledge of the transition matrix $\psi$ allows to evaluate, for a given time $t$, the probabilities for being in each of the $r$ states, i.e. the vector:

$$p(t) = p(0) \cdot \psi^t. \quad (1)$$

Given some data $z$ under the form of observed sequences of states, the statistical estimation of these probabilities is traditionally facilitated by a time-homogeneous, first-order Markov station-
arity assumption about the process $\Lambda$ which generates the data. In other words, the transition probability $\psi_{i,j}$ from any state $s_i$ to any other state $s_j$ ($i$ possibly equals to $j$) is assumed to be independent of time and of the past trajectories before reaching $s_i$. As noted by [Jones (2005)], this assumption can seem somewhat restrictive regarding the external knowledge about the process, but “using (possibly more appropriate) higher-order processes increases the complexity and data requirements quite substantially, and may not be feasible with only a limited time series”, which is often the case in practice. Such situations are encountered in a wide range of application domains, as we discuss now.

To start with, the applications of Markov models in engineering practice are numerous. In reliability engineering and safety analysis, discrete Markov schemes, the states of which correspond to gradually degraded operating conditions, have for instance been used to assess the reliability of programmable electronic systems ([Bukowski and Globe 1995]), cogeneration plants ([El-Nashar 2008]), machineries of oil refineries ([Cochran et al. 2001]), water meters ([Pasanisi and Parent 2004]), piping systems of power plants ([Cronvall and Männistö 2009]) and welded structures submitted to fatigue damage ([Lassen 1991]). In this paper, the example treated in Section 2.5 provides a real industrial use-case where a Markov model is used to assess the reliability of rotating machines. Examples of application in hydrology and water resources engineering concern the modeling of river inflows ([Parent et al. 1991]), lake inflows ([Duckstein and Bogardi 1979]), water supply reservoir states ([Vogel 1987]) or pollutants propagations ([Ang and Täng 1984; Zhang and Dai 2007]). In biomedical survey, Markov chains can model the health condition of patients affected by infectious or viral diseases like in [Gentleman et al. 1994]. These models are also applied to capture-recapture problems ([Dupuis 1995; Dupuis and Schwartz 2007]), used to describe the dynamics of an animal population. As a last example, the financial world makes a wide use of first-order Markov transition matrices to explain the migration of credit ratings ([Jones 2005; Fuertes and Kalotychou 2007]) or to model loan defaults ([Grimshaw and Alexander 2011]).

In an ideal framework, the data $z$ consist in $m$ time series of observed states for $m$ identical individuals $\Sigma$ that are assumed independent. If no data is missing, the estimation of $\psi$ is relatively straightforward. In many applied problems, however, part of data is missing. Such problems can often be divided in two classes.

(i) We call an incomplete sequence problem the estimation of $\psi$ when $z$ are observed trajectories of states:

$$
\begin{align*}
&z_{(1,1)} \bullet \ldots \ z_{(1,T-1)} \ z_{(1,T)} \\
&\bullet \quad z_{(2,2)} \ldots \ z_{(2,T-1)} \ z_{(2,T)} \\
&\vdots \quad \vdots \quad \vdots \quad \vdots \\
&z_{(m,1)} \bullet \ldots \ z_{(m,T-1)} \bullet,
\end{align*}
$$

containing random missing items (random successions of unknown states symbolized by “$\bullet$”), assuming the initial state is known. This occurs typically when the $m$ individuals are checked at deterministic times $t = 1, \ldots, T$, independently from $\Lambda$, as noted by [Dupuis 1995] or when the survey of all individuals at the same time is impossible (e.g. only a given proportion of the machineries can be inspected simultaneously, in order to avoid stopping the industrial production).

(ii) We call an aggregate data problem the estimation of $\psi$ when the sequential data $z$ are reduced to the numbers of individuals $n_i(t)$ being in a given state $s_i$ at a given time $t$ (i.e. $n_i(t) = \sum_{j=1}^{m} 1\{z_{(j,t)} = s_i\}$). Such data are frequently ([Gouno et al. 2011]) the only ones
being at disposal of the analyst, because, for instance, the full trajectories of individuals represented too much information or were not considered of primary importance during the survey process.

Our first aim in this paper is to give in Section 2 a short review of the main computational methods dedicated to the estimation task in the complete data scheme, as well as in both missing data schemes described above, in a Bayesian statistical framework that we defend as being the most convenient. Monte Carlo Markov Chains (MCMC) [Robert and Casella, 2004] are used to deal with such missing data schemes. More specifically, we address ourselves to the reader who is interested in reducing the computational cost, which appears as a practical difficulty when the number of degrees of freedom is high and/or when the Markov model is part of a larger, encompassing model. Simulated experiments help us give some guidelines to select a variant of these methods in the common case where, for each individual, the state at just one time step has been observed.

In Section 3 we consider the time-consuming aspects of numerical computation. Two adaptation mechanisms, which explore the correlations between the transition probabilities, are proposed to accelerate the convergence of the Metropolis-Hastings algorithm towards the posterior distribution. A series of numerical experiments based on a class of transition matrices largely encountered in reliability analysis is led in Section 4. Although they remain relatively basic, we show that our proposals can help reduce the computation time significantly. Finally, a discussion section sums up the main results and advices arising from both main parts of the paper, and highlights several promising research avenues, especially in the theoretical description of adaptive MCMC.

2. Bayesian estimation of transition probabilities: a review

This section provides a review of Bayesian inference techniques for the estimation of the transition matrix $\psi$ under the obvious conditions:

$$0 \leq \psi_{i,j} \leq 1, \quad \sum_{j=1}^{r} \psi_{i,j} = 1. \quad (2)$$

This estimation problem has thus $r(r - 1)$ degrees of freedom. As stated hereinbefore, we voluntarily chose a Bayesian viewpoint. Besides the more theoretical issues pointed by [Robert, 2001], we motivate our choice, in an industrial context, by the possibility to explicitly (and relatively easily) quantify, via predictive simulation [Girard and Parent, 2004], the uncertainty affecting some quantities of practical interest for the reliability engineer (e.g. the probability for the system to be in a failure state for a given time $t$, or the mean time before the system reaches one of the failure states). Moreover, from a strictly computational point of view, the Bayesian framework allows here to deal with some issues that can be quite burdensome in frequentist inference, without any particular additional difficulty. These include the intractability of the likelihood expression in missing data schemes, the respect of constraints (2), the difficulty to obtain a probability distribution for the estimators $\hat{\psi}$, which requires using (possibly costly) bootstrap approaches [Fuhl, 1993]. Besides, the validity of such distributions remains usually asymptotic. Finally, even if this point has not been investigated, using an informative prior could maybe solve some identifiability problems [Allman et al., 2009], when the dimension of $\psi$ is high and/or data are poorly informative [Puolamäki and Kaski, 2009].
A convenient prior for the transition matrix $\psi$ can be obtained as the product of $r$ independent Dirichlet distributions, one for each row $\psi_i$ of $\psi$:

$$
\pi(\psi_i) \propto \prod_{j=1}^{r} \psi_i^{\gamma_{i,j} - 1}.
$$

(3)

As the Dirichlet density is null outside the standard $(r-1)$-simplex, it is particularly suited as a prior distribution of probabilities vectors, that must fulfil conditions (2). Another well-known rationale for choosing a Dirichlet prior is that it can be seen as the reference posterior for a multinomial parameter given some virtual data of state-occupancy, whose sizes $\gamma_{i,j} - 1$ can be interpreted as measures of the prior’s strength (Minka, 2003). However, in absence of precise expert opinion in the remainder of this paper, uniform priors ($\gamma_{i,j} = 1$, $\forall i,j$) were used for the examples shown hereinafter, following the recent recommendations from Tuyl et al. (2009) based on symmetry requirements of posterior predictive distributions.

2.1. Complete sequence problem

Transition probabilities estimation can easily be performed when complete states time-series (often alternatively called panel data) are available for the $m$ individuals. The estimation is based on the calculation, for every couple of states $(s_i, s_j)$, of the number of observed one-step transitions from state $s_i$ to state $s_j$:

$$
w_{i,j} = \sum_{t=1}^{T} \sum_{k=1}^{m} \mathbb{1}\{z(k,t-1) = s_i, z(k,t) = s_j\}.
$$

(4)

Full data likelihood can be written as a function of the sufficient statistics $w_{i,j}$ by observing that conditional on the row vector $\psi_i = (\psi_{i,1}...\psi_{i,r})$, the vector $w_i = (w_{i,1}...w_{i,r})$ is multinomial with parameters $\psi_i$ and $\sum_{j=1}^{r} w_{i,j}$. Therefore, the likelihood $L(z|\psi)$ can be written as the product of $r$ multinomial terms:

$$
L(z|\psi) = \prod_{i=1}^{r} \left( \frac{\sum_{j=1}^{r} w_{i,j}}{w_{i,1}...w_{i,r}} \right) \psi_i^{w_{i,1}}...\psi_i^{w_{i,r}}.
$$

(5)

In a Bayesian framework, the estimation of transition probabilities given complete sequences is straightforward. The inference problem consists in computing the posterior probability distribution of model parameters $\pi(\psi|z)$ by updating the prior distribution $\pi(\psi)$ conditional to the observed data $z$, through the Bayes formula:

$$
\pi(\psi|z) = \frac{L(z|\psi) \pi(\psi)}{\int_{\Omega} L(z|\psi) \pi(\psi) \, d\psi},
$$

(6)

where $\Omega$ denotes the set of all possible values of $\psi$. From (6), it can be seen that the prior [3] of $\psi$ is conjugate, i.e. the posterior distributions of the $\psi_i$’s are also Dirichlet distributions, with parameter vectors equal to $(\gamma_{i,1} + w_{i,1}, \ldots, \gamma_{i,r} + w_{i,r})$. This is the well known Dirichlet-multinomial model.
2.2. Incomplete sequence problem, ignorable DCM

In the most general case of incomplete sequences problem, the estimation problem turns out to be more complicated. Throughout this study, we will mostly consider the case where the Data Collection Mechanism (DCM) is ignorable, which means, in practice, that it can be neglected in the statistical data analysis. Besides simplicity purposes, this choice is essentially motivated by the framework and the background of our study, which is reliability analysis. Some elements about the more general cases of non-ignorable DCM will be provided in the next section.

Let \( x(k,t) \) be an auxiliary binary variable (missingness indicator) which is one if the observation is missing, zero if the state has been observed. The DCM is described by a complementary statistical model specifying \( P(x(k,t)|z, z_{mis}, \eta) \), i.e. the probability for an observation to be missing, depending on observed and unobserved data and (possibly) some other parameters \( \eta \).

Fulfilling two conditions is sufficient for ignorability (Gelman et al., 2004): the first one states the independence between the parameters of the DCM and the main model (here \( \eta \) and \( \psi \) respectively), the second one asserts that the probability that an observation is missing does not depend on missing data (MAR: missing at random condition). The first condition is generally easily checked, while the second one highly depends on the context of the statistical study. For instance, in capture-recapture experiments the probability of recapture may depend or not on the state of the individual (e.g. younger animals can be more easily captured than older ones). In longitudinal medical surveys the health state of a patient can prevent him from going to a periodical visit (e.g. in case he/she is hospitalized). In an industrial reliability framework, and in particular in the specific context of EDF (Electricité de France), the presence of missing data is mainly due to the impossibility of simultaneously surveying the whole population of components for cost or system availability reasons. This motivates our choice to mainly focus on ignorable DCM situations.

Let us now come back to our estimation problem. In incomplete sequences problems, the likelihood has a highly complex expression. It is the product of \( m \) terms which are the probabilities to observe each one of the \( m \) sequences. Whilst writing the term related to an incomplete sequence, one must consider all possible values of the unknown observations. For example, the probability of the sequence \((s_1, s_1, \bullet, \bullet, s_3)\) must be written by taking into account all possible three-steps paths from state \( s_1 \) to state \( s_3 \):

\[
P(s_1, s_1, \bullet, \bullet, s_3) \propto \sum_{i=1}^{r} \left[ \psi_{1,i} \sum_{j=1}^{r} \psi_{i,j} \psi_{j,3} \right].
\]

Estimation methods dealing directly with the likelihood expression may be quite tricky to perform (Deltout et al., 1999). On the other hand, Bayesian inference can elegantly be performed by means of a Gibbs sampler.

This procedure is particularly adapted to the cases where the posterior distribution of model parameters would be more easily determined if data were fully observed. Missing data are considered as additional model parameters \( z_{mis}(k,t) \) and, within the Gibbs sampling, an additional step is performed to simulate them, thus completing the data set. This technique is usually known as data augmentation (Robert and Casella, 2004). Note that Gibbs sampling may be viewed as the Bayesian mirror of Stochastic Expectation-Maximization (SEM) algorithms based on a similar mechanism (Deltout et al., 1999).

In our case the augmented data set, say \( y \), is the set of the completed state sequences for all individuals:

\[ y(k,t) = z(k,t) \text{ if } z(k,t) \text{ is observed,} \]
and

\[ y(k,t) = z_{\text{mis}(k,t)} \text{ otherwise.} \]

The Gibbs sampler algorithm for the incomplete sequence problem can be viewed as a particular case of the more general method for the Arnason-Schwarz capture-recapture model (Marin and Robert, 2007). We first initialize the algorithm by arbitrarily completing state sequences. Then at each step \( h = 1, 2, \ldots \), we perform the following two-step procedure:

1. drawing new parameter values, conditional on the augmented data \( \mathbf{y}^{[h-1]} \):

   \[ \psi^{[h]} | \mathbf{y}^{[h-1]} \sim \text{Dir} \left( \gamma_{i,1} + w_{i,1}^{[h-1]}, \ldots, \gamma_{i,r} + w_{i,r}^{[h-1]} \right), \]

   where \( w_{i,j}^{[h-1]} \) are the sufficient statistics (4) evaluated from current completed sequences \( \mathbf{y}^{[h-1]} \);

2. drawing missing data \( z_{\text{mis}(k,t)}^{[h]} \) conditional to the current values \( \psi^{[h]} \) of model’s parameters (data augmentation step). This can be done by sampling from a conditional categorical distribution defined by the following probabilities:

   \[
   \mathbb{P} \left( y_{(k,1)}^{[h]} = s_j | y_{(k,2)}^{[h-1]} = s_i, \psi^{[h]} \right) \propto \psi_{j,i}^{[h]}, \text{ for } t = 1,
   \]

   \[
   \mathbb{P} \left( y_{(k,T)}^{[h]} = s_j | y_{(k,T-1)}^{[h]} = s_i, \psi^{[h]} \right) \propto \psi_{i,j}^{[h]}, \text{ for } t = T,
   \]

   and

   \[
   \mathbb{P} \left( y_{(k,t)}^{[h]} = s_j | y_{(k,t-1)}^{[h]} = s_i_1, y_{(k,t+1)}^{[h-1]} = s_i_2, \psi^{[h]} \right) \propto \psi_{i_1,j}^{[h]} \cdot \psi_{j,i_2}^{[h]}, \text{ otherwise.}
   \]

The computational method shown above is quite general and easy to implement. On the other hand, the more incomplete the sequences are, the more additional parameters are required and the more the data augmentation step becomes time-consuming. This issue will be illustrated later on in the example of Section 2.6. A technique to accelerate this step, consisting in simulating blocks of consecutive missing data instead of one datum at a time, is proposed by Dupuis and Schwartz (2007).

A particularly interesting case of incomplete sequence problem occurs when each individual is observed just once over the observation period. This can happen in industrial reliability when the data come from the first survey of operating machines, as in the real-world example of Section 2.5 or from destructive controls (Pasanisi and Parent, 2004). Then let \( t_k \) (with \( 1 < t_k < T \)) be the time when the individual \( k \) has been observed and \( s_j \) be the observed state. The state sequences takes the form:

\[ \bullet, \ldots, \bullet, s_j, \bullet, \ldots, \bullet. \]

In that case, it can be shown (proof in Appendix A) that the likelihood \( L(z|\psi) \) has the general expression:

\[
L(z|\psi) \propto \prod_{t=1}^{T} \prod_{j=1}^{r} p_j(t)^{n_j(t)}.
\]
In the formula above, $p_j(t)$ is the unconditional probability for the system to be in state $s_j$ at time $t$ and $n'_j(t) = \sum_{i=1}^{m} 1\{z_{i,t}=s_j\}$ is the number of times the state $s_j$ has been observed at time $t$ in the data sample $z$. It has to be noticed that the expression of the likelihood depends on sufficient statistics $n'_j(t)$ and the statistical problem is equivalent to the aggregate data problem considered hereinafter. In this particular case, Bayesian estimation can be performed using the Gibbs sampler described above or the Metropolis-Hastings procedure we carry out for the aggregate data problem in Section 2.4.

2.3. Incomplete sequence problem, non-ignorable DCM

Let us now consider the more general case where DCM is non ignorable. This problem has been studied in detail (Little and Rubin, 1987, Chapters 6-10) in particular within the framework of longitudinal medical surveys: indeed, for different reasons, patients can leave the study permanently (dropout) or temporarily (intermittent missing). Using the same notation as in the previous subsection, let $y_k$ be a complete data sequence for the individual $k$ (while $z_k$ denotes the actually observed sequence). The different ways for coping with MNAR (missing not at random) observations rely, from a technical point of view, on the way the full-data likelihood $L(y_k, x_k | \psi, \eta)$ is factorized. Three types of factorization are usually proposed:

$$L(y_k | x_k, \psi) \cdot L(x_k | \eta) \quad \text{(pattern mixture model)},$$

$$L(y_k | \psi) \cdot L(x_k | y_k, \eta) \quad \text{(selection model)},$$

and

$$\int L(y_k | x_k, v_k, \psi) \cdot L(x_k | v_k, \eta) \cdot f(v_k | \lambda) \, dv_k \quad \text{(shared parameter model)}.$$

The formulations above can be complexified, by considering the influence of covariates in both the main and the missingness models.

In the pattern mixture framework (Little, 1993), the analyst models the conditional distribution of the observable outcome, given its observation pattern, and the distribution of the different patterns. As a matter of fact, the data are stratified (each pattern determines a stratum) and the main parameters $\psi$ are estimated in each stratum.

The selection factorization, first introduced by Rubin (1976), instead, focuses on the dependence between the missingness and the actual value of the observable variable (in our case the state of the individual). This scheme explicitly copes with the distribution of the complete data $y$ conditional on the main parameter of the model, here $\psi$. The DCM parameters $\eta$ are easy to interpret and provide additional valuable information to the analyst.

In the shared-parameter scheme (Wu and Carroll, 1988), the missing mechanism is indirectly related to the observable variable through a latent variable $v$, depending on some additional parameters $\lambda$.

In the particular framework of the estimation of transition probabilities, Cole et al. (2005) considered categorical quality-of-life data in cancer clinical trials, using a selection factorization. Transition probabilities $\psi_{i,j}$ and missingness probabilities $\eta_i = P(x_{k,t} = 1 | y_{(k,t)} = s_i)$ both depend on observable covariates.

The Arnason-Schwarz model (Dupuis, 1995; Marin and Robert, 2007), also based on a selection factorization, provides an elegant Bayesian solution in the case where the $\eta_i$‘s do not depend on covariates. In this case, a natural choice of the prior for each one of the $\eta_i$‘s is a Beta pdf: $\text{Be}(\alpha_i, \beta_i)$.
The Gibss algorithm for estimating the posterior of \((\eta, \psi)\) is straightforward as, conditional on the complete data \(y\), both posterior distributions of \(\eta\) and \(\psi\) are explicit. The detailed description of the two steps of the algorithm (data augmentation and parameters estimation) is given in Appendix B.

### 2.4. Aggregate data problem

In many real-life problems, we do not follow individuals passing from state to state and the only available data for estimating transition probabilities are aggregate data \(n\), i.e. the number of individuals \(n_i(t)\) being in a given state \(s_i\) at a given time \(t\). Any track of individual trajectories is lost. That may occur in practice when a population of \(m\) individuals has been followed over an observation period but the original aim of the survey was simply having the fractions of the population in particular states. State sequences have thus been considered as raw data and discarded. Examples in sociology and population dynamics were highlighted by Bartholomew (1973) and Pollard (1973), among others. Applications in credit rating were recently studied by Jones (2005).

The inference problem has been formalized by Lee et al. (1968). Conditional on the probability vector \(p(t) = p(0) \cdot \psi^t\), the data vector \(n(t) = (n_1(t), n_2(t), \ldots, n_r(t))\) is multinomial with parameters \(p(t)\) and \(\sum_{j=1}^{r} n_j(t)\). The likelihood \(L(n|\psi)\) can then be written as the product of \(T\) independent terms:

\[
L(n|\psi) = \prod_{t=1}^{T} \left( \frac{\sum_j n_j(t)}{n_j(t)!} \right)^r \prod_{j=1}^{r} p_j(t)^{n_j(t)}. \tag{8}
\]

Lee et al. (1968) focused on obtaining point estimates of the matrix \(\psi\) and in particular the posterior mode of \(\pi(\psi|n)\) by maximizing the product of the likelihood (8) and \(r\) independent Dirichlet priors (3), one for each row of \(\psi\).

In the same frequentist context, MacRae (1977) then Kalbfleisch and Lawless (1984) were among the main authors who developed generalized least square estimators to remedy the difficulty of the maximum likelihood estimation, because of the untractability of \(L(n|\psi)\). Under mild conditions on the stationary matrix \(\psi\), Kalbfleisch and Lawless (1984) obtained general consistency results and asymptotic \(r(r-1)\)-variate normality (in \(T\) and \(N = \sum_{j=1}^{r} n_j(t)\)) for the estimated vector \(\psi_{row}\) of entries in \(\psi\) written rowwise, i.e. \(\psi_{row} = (\psi_{1,1}, \ldots, \psi_{1,r-1}, \psi_{2,1}, \ldots, \psi_{r,r-1})\). Lawless and McLeish (1984) gave conditions on functions of interest for which the information loss due to aggregation is asymptotically negligible with respect to the estimation based on complete sequences. In a specific reliability framework, Gouno et al. (2011) recently provided a methodology to estimate such functions of interest (e.g. survival probability, sojourn time in a state).

In a Bayesian context, the inference problem can be solved by using a Metropolis-Hastings (MH) algorithm to construct a sample of matrices of \(\Omega\) : \(\psi^{[0]}, \psi^{[1]}, \ldots, \psi^{[h]}, \ldots\), asymptotically drawn from the posterior \(\pi(\psi^n|n)\), by sampling at each step \(h\) a candidate vector \(\psi^{[h]}\) from a given distribution function \(J(\cdot|\psi^{[h-1]})\). The candidate is accepted with probability:

\[
\rho(\psi^{[h]}|\psi^{[h-1]}) = 1 \wedge \frac{\pi(\psi^{[h]}|n)}{\pi(\psi^{[h-1]}|n)} \cdot \frac{J(\psi^{[h]}|\psi^{[h-1]})}{J(\psi^{[h]}|\psi^{[h-1]})}, \tag{9}
\]

i.e. the acceptance of the candidate is the result of a Bernoulli trial of probability \(\rho(\psi^{[h]}|\psi^{[h-1]})\). The instrumental density function \(J(\cdot|\psi^{[h-1]})\) allows a random exploration of the space of parameters. The convergence of the chain to the target distribution is proved for any arbitrary function \(J(\cdot)\) which satisfies mild regularity conditions (Robert and Casella 2004). In the present
case, a comfortable instrumental function is the product of $r$ independent Dirichlet distributions $\text{Dir}(d_i \cdot \varphi_i^{[h-1]})$, where $d_i$ is a positive (scalar) constant. This is a usual case of controlled MCMC (Andrieu and Thoms 2008). As the Dirichlet density is null outside the standard $(r-1)$-simplex, all candidates drawn by the instrumental functions automatically respect constraints [2]. Obviously the support of $J$ contains the support of the posterior distribution and the chain is a reversible jump MCMC.

It can easily be seen that the mean of each of the $r$ Dirichlet instrumental densities is $\varphi_i^{[h-1]}$, i.e. the candidate matrix is sampled from a probability function which is “centered” on the last retained matrix. The variance terms of the covariance matrix, equal to $\varphi_{i,j}^{[h-1]}(1 - \varphi_{i,j}^{[h-1]})/(d_i + 1)$, depend on the shape parameters $d_i$ which can be interpreted as tuning coefficients that rule the distance of exploration from the current state of the MCMC chain to the next proposed one.

We notice that, as the expressions of the likelihoods (7) and (8) are formally the same, up to a proportionality constant, the MH procedure described above can also be used in the interesting case of incomplete sequences when each individual has been observed only once. Such examples are treated in the next paragraphs.

2.5. Real industrial case-study: survey of power station turbines

In the example shown hereby, a discrete Markov model has been used to describe the propagation of transverse cracks on steam turbine shafts. This phenomenon has been first observed on EDF facilities in late 90’s and since then periodical non-destructive controls are made to measure crack depths. For a description of the technical problem and available survey data, see (Garnero and Montgomery 2006). The most important identified explanatory variable is the time spent by the turbine in hot shutdown condition. For the purpose of our study, the time has been discretized in equally long intervals. Cracks depths are classified in four states $s_1\ldots s_4$ associated to growing crack lengths. The modelling of cracks growth by discrete Markov schemes is quite common, e.g. (Roh and Xi 2000).

We assume that the process is irreversible, which is physically correct as crack lengths cannot decrease. Thus, the transition matrix is upper-triangular and consequently, $\psi_{1,4} = 1$.

We made the hypothesis that all turbines are in state $s_1$ when putting-into-service at the beginning of the study. Manufacture and acceptance controls justify this hypothesis. A set of data collected between 1998 and 2001 has been analyzed. The data come from 68 turbines from 24 EDF power plants. Each turbine is observed only once for a given value of $t$ between 2 and 7. Given the uniformity of EDF French generation facilities (same design, operating conditions and maintenance policy for all units), we can assume that observed data are i.i.d.

The results of MCMC estimation, using the Gibbs sampler described in Section 2.2 (second half run of 10000 iterations), are shown in Table 1 (left). The application of the MH algorithm described above leads to the same results.

The data set has been enriched between 2001 and 2004 with new crack measures ($t$ between 2 and 7). 38 turbines among the 68 previously observed were inspected for the second time and two for the first time. Some of the collected data are redundant: this happens when for the first and the second observation the corresponding times spent in hot shutdown condition fall into the same interval. Finally, 17 new exploitable observations can be added to the data set. The estimation of transition probabilities gives the results shown in Table 1 (right).

We can notice that in this case the posterior variance has been very lightly reduced by incorporating the information conveyed by the new data. Given the posterior samples of transition probabilities, some quantities of practical interest in industrial reliability have been sampled: the unconditional probabilities of the four states, as a function of time, and the expected number of
steps before the system reaches the absorbing state $s_4$. As $s_4$ can be interpreted as a “failure” condition, the expected time to absorption is here the classical MTTF (Mean Time To Failure). Notice that here the term “failure” just means that the crack has reached a given length, arbitrarily chosen for the purposes of this paper.

The calculation of state probabilities using Equation (1) is straightforward. To evaluate the MTTF we made use of a well known property of absorbing Markov chains (Grinstead and Snell, 1997, chap. 11). If we consider the matrices:

\[
\zeta = \begin{pmatrix}
\psi_{1,1} & \psi_{1,2} & \psi_{1,3} \\
0 & \psi_{2,2} & \psi_{2,3} \\
0 & 0 & \psi_{3,3}
\end{pmatrix}
\quad \text{and} \quad
I = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix},
\]

the matrix $I - \zeta$ has an inverse and each component $t_i^*$ of the row vector

\[
t^* = (1, 1, 1) \cdot (I - \zeta)^{-1}
\]

is the expected number of steps before absorption, given that the initial state was $s_i$. In our case the MTTF is then the first component of the vector $t^*$.

Figure 1 shows the 95% credibility intervals of the predictive state probabilities for discretized time $t$ extended up to 15 and the histogram of 5000 samples from the predictive distribution of MTTF. Concerning state probabilities, we can notice that $p_1$ credibility intervals are narrower than other state probabilities as, according to our hypotheses of an irreversible process and initial state $s_1$, $p_1(t) = \psi_{1,1}^t$ which mean that the uncertainty over $p_1$ only depends on uncertainty over $\psi_{1,1}$ (and no other transition probability). The long tail in the MTTF distribution (which is even longer than shown in the figure) is due to the high values (close to 1) of the posterior distribution of $\psi_{3,3}$.

Remark. We stress that, even if the data come from real surveys, the study shown hereinbefore is given for exemplary purposes only and neither results nor methodology must be extrapolated to make any general conclusion about EDF risk assessment policies.

2.6. A four-dimensional simulated case study

The purpose of the previous example was to give a practical use-case of application of the estimation algorithms in a poorly informative data context. The next example will deal with more
general computational issues. In particular, we will compare the performances of Gibbs and MH algorithms in the case where individuals are observed only once. Following a case-study from Lee et al. (1968), we consider the following transition matrix:

\[
\Psi_0 = \begin{pmatrix}
0.6 & 0.4 & 0 & 0 \\
0.1 & 0.5 & 0.4 & 0 \\
0 & 0.1 & 0.7 & 0.2 \\
0 & 0 & 0.1 & 0.9
\end{pmatrix}
\]  \hspace{1cm} (10)

First, complete state sequences for \(m \in \{10, \ldots, 1200\}\) individuals have been generated for \(T = 20\) observation periods, under the hypothesis that at \(t = 0\) the initial vector probability is \((3/4, 1/4, 0, 0)\). Then, given complete sequences, a single observation per individual has been randomly selected, thus obtaining incomplete sequences. Finally, for each \(m\) we used the Gibbs and the Metropolis-Hastings algorithms described above. The convergence has been checked using the Brooks-Gelman statistic (Brooks and Gelman, 1998) computed on three parallel chains and a visual inspection of the chains. A classic rule of thumb (RT) is to suppose quasi-stationarity once the statistic stably remains under 1.1 (Brooks and Gelman, 1998). The precision in estimation was measured using the relative absolute error matrix between the elements of \(\Psi_0\) and a progressive Monte Carlo posterior estimate of \(\Psi\). In each case, it has been obtained by using the second half run of Metropolis-Hastings iterations and Gibbs iterations after the burn-in periods determined by Brooks-Gelman RT respectively. Parameters \(d_i\) were sampled uniformly in \([100, 2500]\). For a same estimation error of at most 5% per element, the CPU time observed on a 2.8 GHz CPU (Xeon) machine before the RT is fulfilled has been plotted in Figure 2 as a function of \(m\). Plots are smoothed over 30 repetitions of the algorithms. Clearly, the increasing number of missing data makes Gibbs less competitive than MH: after \(m = 700\), conditional sampling of individuals requires more CPU time than our basic MH. The number of missing data to be simulated increases linearly with the total number \(m\) of individuals, as individuals could be observed only once throughout their lifespan. This explains the linear behavior of the Gibbs CPU time.
The efforts of the practitioner should then concentrate on improving the mixing of Gibbs and MH algorithms to diminish their burn-in period. The development of acceleration methods has been the subject of a large number of works, reviewed in (Gilks and Roberts, 1996; Mira and Sargent, 2003; Gentle, 2004). Techniques such as blocking (Roberts and Sahu, 1997), which consists in updating multivariate blocks of (often highly correlated) parameters, were shown to be efficient to accelerate Gibbs algorithms in conjugate models (Ischwaran and James, 2001; Accoto, 2009), although their implementation often remains case-specific (Sargent et al., 2000) and can sometimes slow the sampler’s convergence (Roberts and Sahu, 1997). Alternatively, the multi-move Gibbs sampler (Carter and Kohn, 1994), which was developed for Markov switching state-space models, proved to be more efficient than the single-move Gibbs sampling, although its filtering aspects might be time-consuming (Früwirth-Schnatter, 2006, chap. 11, pp. 342-344). More recently, cheaper approximations of the Gibbs sampler using best linear predictors have been carried out (Nott and Kohn, 2005).

In the specific case of MH algorithms, the slow mixing and the computational cost are less due to the dimension of the problem than the difficulty of eliciting instrumental distributions to efficiently explore the parameter space. The remainder of this article is specifically dedicated to an empirical exploration of adaptive approaches aiming to improve this feature.

![Figure 2: Case study of Lee et al. (1968). Mean CPU time needed to reach quasi-stationarity (in the sense of the Brooks-Gelman rule of thumb) as a function of the number \( m \) of individuals (one individual being associated to a single true observation). Data have been generated according to the four-state transition matrix (10).](image)

### 3. Accelerating the MH algorithm using adaptive approaches

Heuristically, implementing an adaptive MCMC consists in sequentially tuning the transition kernel using the knowledge of past iterations, in an automated way during the simulation, in order to improve the mixing rate (Andrieu and Thoms, 2008). In the particular case of our class of MH algorithms, this means modifying the product of Dirichlet densities chosen as the instrumental distribution \( J \) for the MH algorithm introduced in Section 2.4. Each successive instrumental distribution is ideally selected such that parallel sampling can explore a large part of the parameter space, especially in the first steps of the algorithm.
Recently, a rich literature has been dedicated to these approaches, and is especially focused on the preservation of the ergodicity of the adaptive chains towards the stationary distribution, which is not automatically ensured by automated tunings. Seminal works on this subject are due to Roberts and Rosenthal (2007, 2009) and Andrieu et al. (Andrieu and Mouniès 2006; Andrieu and Atchadé 2007; Andrieu and Thoms 2008). These theoretical works also led to interesting software developments (Rosenthal 2007; Vihola 2010).

Assuming $\Gamma_i$ are indices chosen in some collection $\mathcal{Y}$ based on past algorithm output, we denote by $K_{\Gamma_i}$ the transition kernel updating $\psi^{[i]}$ to $\psi^{[i+1]}$:

$$K_{\Gamma_i}(\psi, \psi') = \rho_{\Gamma_i}(\psi, \psi') J_{\Gamma_i}(\psi' | \psi) + \int (1 - \rho_{\Gamma_i}(\psi, \epsilon)) J_{\Gamma_i}(\epsilon | \psi) d\epsilon \delta_\psi(\psi'),$$

where $\delta_\psi$ is the Dirac measure in $\psi$ and

$$\rho_{\Gamma_i}(\psi, \psi') = 1 \wedge \frac{\pi(\psi' | z) J_{\Gamma_i}(\psi | \psi')}{\pi(\psi | z) J_{\Gamma_i}(\psi' | \psi')}.$$}

Basically, the ergodicity and stationarity properties of an adaptive MH algorithm can be ensured if the amount of adapting progressively diminishes, in the sense that the kernel parameters are modified by smaller and smaller quantities, or if the probability of adaptation $\rho_{\Gamma_i}$ decreases towards zero as $i \to \infty$ (Roberts and Rosenthal 2007, Theorem 5). In the framework considered here, such adaptations could be based on eliciting vanishing adaptations for the parameters $(d_i)_{1 \leq i \leq r}$. These approaches would however be limitative since each $d_i$ characterizes the marginal distribution of row $i$, hence they do not explore the correlations between the rows. Therefore, the approach proposed here focuses on this particular aspect.

In the following, assuming we are at step $h > 1$ of the MH algorithm, we propose two ways of building an adaptive instrumental distribution $\psi^{[h]} \sim J_h$ (denoting $J_{\Gamma_h} = J_h$ in the following for simplicity) taking advantage of a $\sigma$–algebra $\mathcal{F}_{h-1}$ generated by the succession of sampled parameter matrices $\psi^{[0]}, \ldots, \psi^{[h-1]}$. Both using a (small) fixed number $p$ of basic MH iterations, these approaches explore correlations between the rows in the instrumental sampling.

In our first approach (DCS-MH), we attempt to summarize the correlations within $(\psi_1, \ldots, \psi_r)$ by simply capturing the correlations between the diagonal elements of $\psi$.

In our second method (RCS-MH), we generalize the first method replacing the $r$–vector of diagonal elements by $r$ elements whose position is randomly sampled within each vector $\psi_i$. Doing so, we hope to capture more efficiently the dependency between the $\psi_i$ and accelerate the DCS-MH algorithm.

**Diagonal correlated sampling (DCS-MH).**

At iteration $h \gg p$ (large enough):

1. denote $\{\tilde{\psi}^{[1]}, \ldots, \tilde{\psi}^{[p]}\}$ the set of last $p$ non-identical sampled matrices in $(\psi^{[0]}, \ldots, \psi^{[h-1]});$  
2. for $i = 1, \ldots, r$
   (i) denote $\tilde{\psi}_{i,i} = (\tilde{\psi}_{i,i}^{[1]}, \ldots, \tilde{\psi}_{i,i}^{[p]})$ the $p$–vector of replicates of the $i$–th diagonal element;  
   (ii) compute $u_i = \tilde{F}_i(\tilde{\psi}_{i,i})$ where $\tilde{F}_i$ is the empirical marginal cdf of $\tilde{\psi}_{i,i}$  
3. estimate the Pearson correlation $R^{[h]}$ of $(u_1, \ldots, u_r);$  
4. sample a candidate vector $\psi^{[h]}_{\text{diag}}$ of diagonal elements $\psi^{[h]}_{1,1}, \ldots, \psi^{[h]}_{r,r}$ using:
   (i) a Gaussian copula, the parameter of which is $R^{[h]}$,
(ii) Beta marginal distributions Be\( \left( d_i \cdot \psi_i^{[h-1]}, d_i \left( 1 - \psi_i^{[h-1]} \right) \right) \);

5. for \( i = 1, \ldots, r \)

(i) sample \( \psi_i^{[h]} , \ldots, \psi_i^{[h-1]}, \psi_{i,i+1}^{[h]}, \ldots, \psi_{i,r}^{[h]} \) from:

\[
\text{Dir} \left( \frac{\psi_i^{[h-1]}}{1 - \psi_i^{[h-1]}}, \ldots, \frac{\psi_i^{[h-1]}}{1 - \psi_i^{[h-1]}}, \frac{\psi_{i,i+1}^{[h]}}{1 - \psi_{i,i+1}^{[h]}}, \ldots, \frac{\psi_{i,r}^{[h]}}{1 - \psi_{i,r}^{[h]}} \right);
\]

(ii) for \( j \neq i \), renormalize each \( \psi_{i,j}^{[h]} \) by multiplying with \( 1 - \psi_{i,i}^{[h]} \).

Randomized correlated sampling (RCS-MH).

At iteration \( h \gg p \) (large enough):

1. same as step 1 in DCS-MH;
2. sample (with replacement) a \( r \)–vector \( I \in \{1, \ldots, r\} \) of random indicators;
3. for \( i = 1, \ldots, r \)

   (i) denote \( \tilde{\psi}_{i,I_i} = (\tilde{\psi}_{i,I_i}^{[1]}, \ldots, \tilde{\psi}_{i,I_i}^{[p]} ) \) the \( p \)–vector of replicates of the \((i,I_i)\)–th matrix element;

   (ii) compute \( u_i = \hat{F}_i(\tilde{\psi}_{i,I_i}) \) where \( \hat{F}_i \) is the empirical marginal cdf of \( \tilde{\psi}_{i,I_i} \);

4. same as step 3 in DCS-MH;
5. sample a candidate vector \( \psi_{\text{rand}}^{[h]} \) of elements \( \psi_{1,I_1}^{[h]}, \ldots, \psi_{r,I_r}^{[h]} \) following the same main idea as in DCS-MH method
6. For \( i = 1, \ldots, r \)

   (i) sample \( \psi_i^{[h]} , \ldots, \psi_i^{[h-1]}, \psi_{i,i+1}^{[h]}, \ldots, \psi_{i,r}^{[h]} \) from:

\[
\text{Dir} \left( \frac{\psi_i^{[h-1]}}{1 - \psi_i^{[h-1]}}, \ldots, \frac{\psi_i^{[h-1]}}{1 - \psi_i^{[h-1]}}, \frac{\psi_{i,i+1}^{[h]}}{1 - \psi_{i,i+1}^{[h]}}, \ldots, \frac{\psi_{i,r}^{[h]}}{1 - \psi_{i,r}^{[h]}} \right);
\]

(ii) for \( j \neq i \), renormalize each \( \psi_{i,j}^{[h]} \) by multiplying with \( 1 - \psi_{i,i}^{[h]} \).

For a more general introduction to copulas, see for instance Nelsen (2006) or Genest and Favre (2007), as well as Kim et al. (2007) for more specific issues about copulas fitting.

In our experiments, we used a Gaussian copula to sample the new diagonal parameters, mainly because of its symmetric properties and its simplicity of calibration using a correlation matrix \( R \) (Marshall and Olkin 1988). Note that one has to consider and check up with great care the \( p \) previously simulated matrices \( \{\tilde{\psi}^{[1]}, \ldots, \tilde{\psi}^{[p]}\} \) to make sure that a robust empirical estimator of \( R \) can be defined, in the sense that its Cholesky decomposition is numerically stable during the sampling process (Marshall and Olkin 1988). The condition number can be used to do so (El Ghaoui 2002). Conditionally on correlated sampled parameters, Dirichlet distributions appear necessary to get coherent instrumental sampling of remaining elements within each row vector \( \psi_i^{[h]} \).


Theoretical behavior. Despite the large amount of existing work aiming to simplify the conditions ensuring ergodicity and stationarity of the target distribution (Nott and Kohn 2005; Roberts and Rosenthal 2007, 2009; Archadé et al. 2011), theoretical descriptions of kernels based on Dirichlet products compounded with Gaussian copulas turn out to be technically complex, and their study deserves a specific work which remains outside the scope of this article. Since our primary aim is to assess the interest of exploring the correlations between the rows of $\psi$, we adopt the simplest approach of a finite sampling scheme when choosing $J$, as proposed by Roberts and Rosenthal (2007): given a time $\tau < \infty$, $J_{\Gamma_n} = J_{\Gamma_\tau}$ for any $n \geq \tau$. This approach is carried out in this paper at each sweep of the algorithm after a given mixing period, selecting the final $J_{\Gamma_\tau}$ as the basic product of Dirichlet’s described hereinbefore. In substance, $\tau$ has the sense of an exploration time, and in practice is selected as the minimum time between the time required for a fixed number of iterations and the time until the Brooks-Gelman RT is fulfilled.

Nonetheless, this explorative study fits into recent schemes shared by several authors, who tested copula-based methods to improve the efficiency of their sampling algorithms. In their seminal work on the optimization of the adaptation, Haario et al. (2001) considered Gaussian copula instrumental distributions calibrated over the full past of the chains. See Andrieu and Thoms (2008) for a review of this particular major field of adaptive MCMC. Strid et al. (2010) used the sampling history to continuously calibrate a $t$-copula proposal distribution, in order to sample from dynamic stochastic equilibrium models. Finally, Craiu (2011) used products of bivariate copulas to tune MCMC during an initialization period only, in the same spirit as the finite sampling approach used in the present paper.

Illustration. Continuing the four-dimensional simulated example from Section 2.6, we applied the DCS-MH and RCS-MH methods with $p = 30$, still augmenting the number $m$ of individuals and using three parallel chains per experiment. Parameters $d_i$ remain similarly sampled at each iteration. Results are smoothed over 50 similar runs of algorithms. The comparison of Gibbs and MH burn-in periods in Figure 3, in the sense of the Brooks-Gelman RT, illustrates the improvement yielded by RCS-MH. On the other hand, in this case DCS-MH performs worse than basic MH and even Gibbs sampler. As we could expect, RCS-MH does clearly better than DCS-MH because of its widest exploration of the parameter space. RCS-MH strongly beats Gibbs even for relative low numbers of individuals.

The poor performance of DCS-MH is due to the computational cost of the selection of past matrices $\{\tilde{\psi}^{[1]}, \ldots, \tilde{\psi}^{[p]}\}$ sufficiently different to allow for a robust Cholesky inversion. This cost clearly increases with the progression towards stationarity since sampled matrices become more and more similar and many among them must be rejected in the calibration task of the instrumental distribution. The RCS-MH algorithm suffers of course from the same defect, but the much better mixing counterbalances the increase of the computational cost, with respect to the basic MH algorithm, in a significant way.

4. Numerical experiments

This section deals with simulation studies to test the potentialities of our adaptive proposals to a wide class of transition matrices commonly encountered in reliability and risk assessment (RRA). In RRA, it often occurs that the degradation of a system $\Sigma$ is described using $r$ separated states (for instance defined by a scale of crack sizes), ordered from minor defect to major failure (replacement cause). To be conservative, one may assume that potential repairs following a running failure are, at best, as bad as old, namely $\Sigma$ remains in the same state than before the failure. In other
Figure 3: Case study of Lee et al. (1968). Mean CPU time needed to reach quasi-stationarity as a function of the number $m$ of individuals (same simulations as Figure 2). With respect to the Figure 2, Gibbs and basic MH are also compared to DCS-MH and RCS-MH algorithms.

cases, one might assume these repairs bring actually more complications than real improvement (for instance if $\Sigma$ is old), so that $\Sigma$ is more deteriorated after the repair than before (worth than old repair). See Basile et al. (2007) for more details about these notions. Under a stationarity assumption, the transition matrix $\psi$ is necessarily upper triangular, with $\psi_r = (0, \ldots, 0, 1)$.

**Simulation features.** In the following experiments, we test the potentialities of Gibbs and the three MH algorithms described hereinbefore (basic, DCS-MH and RCS-MH) as a function of $r$. We vary the dimension $r$ between 2 and $r_{\text{max}}$ (in practice, we consider $r_{\text{max}} = 6$ to remain realistic). To start with, we need a rule to sample realistic matrices with decreasing dimension:

1. denote $\psi^{(r)}$ a $r \times r$ upper triangular matrix.
2. create $\psi^{(r-1)}$ matrix as follows: for $i = 1, \ldots, r - 1$, $$\psi^{(r-1)}_{i,j} = \psi^{(r)}_{i,j} \quad \text{for } j = 1, \ldots, r - 2$$ and $$\psi^{(r-1)}_{i,r-1} = \psi^{(r)}_{i,r-1} + \psi^{(r)}_{i,r}.$$ Doing so we automatically ensure that $\psi^{(r-1)}_{r-1} = (0, \ldots, 0, 1)$. The rationale for this construction is obviously to increase the probability of a major failure event when simplifying the model. Thus we simply need to sample $\psi^{(r_{\text{max}})}$ to get all other matrices considered for simulation tests. Pursuing our wish of realism, we assume that worth than old repairs are less probable than as bad as old ones. Therefore, for $i = 1, \ldots, r_{\text{max}} - 2$ and $k = 1, \ldots, r_{\text{max}} - i - 1$, we assume in the sampling:

$$\psi^{(r_{\text{max}})}_{i;i} > \psi^{(r_{\text{max}})}_{i;i+k} > \sum_{p=k+1}^{r_{\text{max}}-i} \psi^{(r_{\text{max}})}_{i;i+p},$$
and especially for \( i = r_{\text{max}} - 1 \), \( \psi^{(r_{\text{max}})}_{r_{\text{max}} - 1, r_{\text{max}} - 1} > \psi^{(r_{\text{max}})}_{r_{\text{max}} - 1, r_{\text{max}}} \) to ensure a constant decreasing of values \( \psi_{i,i}^{(r)} \), \( \psi_{i,i+1}^{(r)} \), \ldots, \( \psi_{i,r}^{(r)} \) for any \( r \leq r_{\text{max}} \). Finally, we selected matrices \( \psi^{(r_{\text{max}})} \) for which:

\[
\psi_{i,j}^{(r_{\text{max}})} \leq \psi_{i+1,j+1}^{(r_{\text{max}})}.
\]

This models the following case: the closer to a major failure state, the better (the more cautious) the repair. Notice that we do not take into account any of our simulation constraints in the following estimation procedures, except the presence of zeros beneath the diagonal of \( \psi \) (by reducing the length of Dirichlet distributed vectors in the instrumental sampling). We consider it as a minimal knowledge assumable in real case-studies (e.g. Section 2.5). Finally, per simulated matrix, a complete sequence for \( m = 1000 \) individuals was generated for \( T = 20 \) observation times. As we are always in the particular case of “a single observation per individual”, only one observation is retained in each sequence for the inference exercise.

**Estimation.** As in Section 2.6, each experiment for a given \( r \in [3, r_{\text{max}} = 6] \) consists in running three parallel chains for each method and monitoring them using the Brooks-Gelman statistic. Relative Euclidian errors on posterior means of matrix components (computed using 1000 iterations after a burn-in period determined by the Brooks-Gelman RT) are fixed at most at 5%, involving preliminary tests for fixing the total number of iterations. Again, parameters \( d_i \) are sampled uniformly in \([100, 2500]\). Finally, each experiment is repeated 100 times to average the results (each time a new family of matrices \( \psi^{(r_{\text{max}})}, \ldots, \psi^{(3)} \) being simulated).

**Results.** Boxplots and mean CPU times before quasi-stationarity (in the sense of the Brooks-Gelman RT) are plotted in Figures 4 and 5. Results obtained on the simulated example from Section 2.6 can be generalized: RCS-MH provides for all dimensions a significant improvement in mixing. Similar results have been obtained when carrying out an empirical approach to calibrate the mean acceptance rate to a standard nominal value of 50% then 25%.

5. Discussion

5.1. Main ideas and results

This article first aims to provide a general review and technical advises about the Bayesian estimation of finite-state transition matrices \( \psi \) in discrete Markovian models under various missing data schemes, which appear to be of particular interest in several domains, especially in engineering. Actually, reliability practitioners may frequently deal with classes of upper-triangular transition matrices that have been chosen for most of the experiments presented here. Depending on the nature of available data, the practitioner may have to choose between Gibbs or Metropolis-Hastings (MH) algorithms. The time-consuming features of these algorithms, depending on the size of missing data and the dimension of the problem, appear as limiting factors in practice. Therefore, the second part of this article focuses on a first exploration of two adaptive mechanisms (DCS-MH and RCS-MH) likely to accelerate the MH algorithms.

Numerical experiments have highlighted, on this specific class of examples, that using instrumental distributions based on Gaussian copulas to account for the correlations between the rows of \( \psi \) yields a better mixing of the chains, implying a significant reduction of the computational cost. The gap with basic MH strategies, based on the independent sampling of the rows of \( \psi \), increases with the number \( m \) of individuals or the number \( r \) of states. The simplicity of the approaches proposed here lets us think that any practitioner dealing with aggregate data could easily implement the DCS-MH and RCS-MH mechanisms and reduce the computational time.
Supplementary experiments have highlighted that the CPU time can be still diminished by using two “coarse” versions of the DCS-MH and RCS-MH mechanisms. They consist in estimating the copula parameter $R$ directly from the Pearson correlation of the matrix elements, namely removing the step 2.(ii) in each mechanism. These coarse approaches (we call them DCS-C-MH and RCS-C-MH) have been be compared to the previous ones in Figure 6. Here, the difference in CPU time is mainly due to the cost of empirical inversions in the DCS-MH and RCS-MH methods.

The adaptive schemes proposed here (especially the most powerful RCS-MH and RCS-C-MH), which remain only empirically studied, deserve a more specific study from both theoretical and applied viewpoints. This point is more widely discussed in the following subsection.

As a take-home message, in the most general case of incomplete data problems with several observations per individual, the Gibbs sampler based on the data augmentation technique seems to be the only possible alternative. In the particular case of a single observation per individual, the adaptive MH algorithms (and especially RCS-MH) are valid alternatives to the Gibbs sampler if the number of individuals is greater than a few hundred, say 200, and the number of states is greater than three. In low dimensional problems (two or three) the practical interest of adaptive MH methods, with respect to the simpler Gibbs sampler, is less obvious.

5.2. Directions of further research

The adaptation processes proposed here remain empirical, and theoretical studies are needed to build copula-based strategies ensuring the ergodicity and the stationarity of the chains less crudely than imposing a finite adaptation time, based on principles initiated by Roberts and Rosenthal (2007) and Andrieu and Moulines (2006). Indeed, fully adaptive MCMC should be build on infinite adaptations which continuously modify the choice of the transition kernel using the past values of $\psi$ along the chains, quasi-stationarity occurring when these kernel modifications become imperceptible. These adaptations should be led on both correlated and marginal features.
of the matrix elements. To this first aim, future studies could focus on the mechanism of state permutation, inspired by similar ones carried out in the framework of variable selection (Nott and Kohn, 2005), and on removing the strong assumption made by using a Gaussian copula to model correlations within the elements of \( \psi \). This choice can appear oversimplified since it does not take into account possible correlations between extreme values in the instrumental distribution of \( \psi \). Therefore a copula selection procedure should be carried out at different times of the adaptive chain, for instance using frequentist tests (e.g. Cramer-von Mises), based on distances between estimated and simulated copulas (Genest and Quessy, 2006; Nikoloulopoulos and Karlis, 2008) or Bayesian posterior odds (Huard et al., 2006). As those procedures remain time-consuming in dimensions \( r \geq 2 \), this approach was not implemented here in this exploratory work.

Furthermore, it is necessary that such more sophisticated adaptive Metropolis-Hastings algorithms be compared in practice to refined Gibbs algorithms, evoked at the end of Section 2.6, that could benefit from the stick-breaking properties of Dirichlet distributions.

Another point of interest could be the adaptation of the methods reviewed here to the case of non stationary Markov chains. A simple way for doing this could be to stratify the data on the time \( t \) or on groups of values of \( t \) (Urabake et al., 1975; Sendi et al., 1999). The use of logit or proportional odds models (Cole et al., 2005; Grimshaw and Alexander, 2011) to include also the effect of additional covariates is another perspective for this work.

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Appendix A. Proof of expression (7)

The probability of a given sequence of $T+1$ states ($t$ from 0 to $T$) with only one observed state at $t = t_k$ can be written as the sum of $T$ sums fits into each other (with index from 1 to $r$), one for each unobserved state:

$$P(\cdots, s_j, \cdots, \cdots) \text{ is equal to}$$

$$\sum_{i_0} p_{i_0}(0) \left[ \sum_{i_1} \psi_{i_0,i_1} \left[ \sum_{i_2} \psi_{i_1,i_2} \cdots \left[ \sum_{i_{t_k-1}} \psi_{i_{t_k-2},i_{t_k-1}} \psi_{i_{t_k-1},j} \left[ \sum_{i_{t_k}} \psi_{i_{t_k},i_{t_k}} \cdots \left[ \sum_{i_T} \psi_{i_{T-1},i_T} \cdots \cdots \cdots \right] \right] \right] \right] \right]$$

In the expression above the sum of the first $t_k$ sums (indices from $i_0$ to $i_{t_k-1}$) is the unconditional probability $p_j(t_k)$ for the system to be in state $j$ at time $t_k$. That can be showed by developing the recursive formula (1):

$$p_j(t_k) = \sum_{g_1} p_{g_1}(t_k - 1) \cdot \psi_{g_1,j}$$

$$= \sum_{g_1} \sum_{g_2} p_{g_2}(t_k - 2) \cdot \psi_{g_2,g_1} \cdot \psi_{g_1,j}$$

$$= \sum_{g_1} \sum_{g_2} \sum_{g_3} p_{g_3}(t_k - 3) \cdot \psi_{g_3,g_2} \cdot \psi_{g_2,g_1} \cdot \psi_{g_1,j}$$

$$= \ldots$$

and renaming the index $g_1, g_2, g_3, \ldots$ as $i_{t_k-1}, i_{t_k-2}, i_{t_k-3}, \ldots$. The sum of the remaining sums in (??) is one as $\sum_j \psi_{i,j} = 1$. The probability of the sequence is then $p_j(t_k)$. Thus, the likelihood of
\[ m \text{ incomplete sequences where each individual is observed only once can be written:} \]
\[ \prod_{k=1}^{m} \prod_{j=1}^{r} \prod_{t=0}^{T} p_j(t) 1_{(t=t_{k,y(k,t)=s_j})} = \prod_{j=1}^{r} \prod_{t=0}^{T} p_j(t) \sum_k 1_{(t=t_{k,y(k,t)=s_j})} \]

which is, under the hypothesis that probabilities \( p_j(0) \) are known, the expression \([7]\) up to constant of proportionality.

**Appendix B. Gibbs sampler for MNAR data when missingness only depends on the actual state**

First initialize the algorithm by arbitrarily completing state sequences. Then at each step \( h = 1, 2, \ldots \), perform the following two-step procedure:

1. parameters estimation:

\[
\psi_{i}^{[h]} | \mathbf{y}^{[h-1]} \sim \text{Dir} \left( \gamma_{i1} + w_{i1,1}^{[h-1]}, \ldots, \gamma_{ir} + w_{1,r}^{[h-1]} \right)
\]

and

\[
\eta_{i}^{[h]} | \mathbf{y}^{[h-1]} \sim \text{Be} \left( \alpha_{i} + a_{i}^{[h-1]}, \beta_{i} + b_{i}^{[h-1]} \right),
\]

where \( a_{i}^{[h-1]} = \sum_{t=1}^{T} \sum_{k=1}^{m} 1_{\{y_{(k,t)} = s_{i}, x_{(k,t)} = 1\}} \), \( b_{i}^{[h-1]} = \sum_{t=1}^{T} \sum_{k=1}^{m} 1_{\{y_{(k,t)} = s_{i}, x_{(k,t)} = 0\}} \) and \( w_{i,j}^{[h-1]} \) are the same as in Section 2.2.

2. data augmentation: drawing \( z_{\text{mis}(k,t)}^{[h]} \) conditional on the following probabilities:

\[
\mathbb{P} \left( y_{(k,1)}^{[h]} = s_{j} | y_{(k,2)}^{[h-1]} = s_{i}, \psi_{i}^{[h]}, \eta^{[h]} \right) \propto \eta_{j}^{[h]} \cdot \psi_{i,j}^{[h]}, \text{ for } t = 1,
\]

\[
\mathbb{P} \left( y_{(k,T)}^{[h]} = s_{j} | y_{(k,T-1)}^{[h]} = s_{i}, \psi_{i}^{[h]}, \eta^{[h]} \right) \propto \eta_{j}^{[h]} \cdot \psi_{j,i}^{[h]}, \text{ for } t = T
\]

and

\[
\mathbb{P} \left( y_{(k,t)}^{[h]} = s_{j} | y_{(k,t-1)}^{[h]} = s_{i1}, y_{(k,t+1)}^{[h]} = s_{i2}, \psi_{i}^{[h]}, \eta^{[h]} \right) \propto \eta_{j}^{[h]} \cdot \psi_{i1,j}^{[h]} \cdot \psi_{j,i2}^{[h]}, \text{ otherwise.}
\]

**References**

Accoto, N., 2009. The hidden mixture Markov model with application to the analysis of electricity supply: a Bayesian perspective. Proceedings of the Complex Data Modeling and Computationally Intensive Statistical Methods for Estimation and Prediction (SCo 2009), Milan, 2009 September 14-16.

Allman, E.S., Matias, C., Rhodes, J.R., 2009. Identifiability of parameters in latent structure models with many observed variables. The Annals of Statistics 37, 3099-3132.

Andrieu, C., Moulines, E., 2006. On the ergodicity properties of some adaptive MCMC algorithms. Annals of Applied Probability 16, 1462-1505.
Andrieu, C., Atchadé, Y., 2007. On the efficiency of adaptive MCMC algorithms. Electronic Communications in Probability 12, 336-349.

Andrieu, C., Thoms, J., 2008. A tutorial on adaptive MCMC. Statistics and Computing 18, 343-373.

Ang, A.H.S., Tang, W.H., 1984. Probability Concepts in Engineering Planning and Design, volume 2. Wiley, New York.

Atchadé, Y.F., Fort, G., Moulines, E., Priouret, P., 2011. Adaptive Markov Chain Monte Carlo: Theory and Methods. In: Barber, D., Taylan Cemgil, A., Chiappa, S. (Eds). Bayesian Time Series Models, Cambridge University Press, 32-47.

Bartholomew, D.J., 1973. Stochastic Models for Social Processes, second edition. Wiley, New York.

Basile, O., Dehombreux, P., Riane, F., 2007. Evaluation of the uncertainty affecting reliability models, Journal of Quality in Maintenance Engineering 13, 137-151.

Brooks, S., Gelman, A., 1998. General Methods for Monitoring Convergence of Iterative Simulations. Journal of Computational and Graphical Statistics 47, 434-455.

Bukowski, J.V. Goble, W.M., 1995. Using Markov models for safety analysis of programmable electronic systems. ISA Transactions 34, 193-198.

Carter, C. K., Kohn, P., 1994. On Gibbs sampling for state space models. Biometrika 81, 541-553.

Cochran, J.K, Murugan, A., Krishnamurthy, V., 2001. Generic Markov models for availability estimation and failure characterization in petroleum refineries. Computers & Operations Research 28, 1-12.

Cole, B.F., Bonetti, M., Zaslavsky, A.M., Gelber, R.D., 2005. A multistate Markov chain model for longitudinal categorical quality-of-life data subject to non-ignorable missingness. Statistics in Medicine 24, 2317-2334.

Craiu, R., 2011. Tuning of Markov Chain Monte Carlo Algorithms using Copulas. UPB Scientific Bulletin Series A 73, 5-12.

Cronvall, O., Männistö, I., 2009. Combining discrete-time Markov processes and probabilistic fracture mechanics in RI-ISI risk estimates. International Journal of Pressure Vessels and Piping 86, 732-737.

Deltout, I., Richardson, S., Le Hersan, J.Y. (1999). Stochastic Algorithms for Markov Models Estimation with Intermittent Missing Data. Biometrics 55, 565-573.

Duckstein, L., Bogardi, I., 1979. Uncertainties in lake management. In: McBean, E.A., Hipel, K.W., Unn, T.E., (Eds.) Reliability in Water Resources Management, Water Resources Publications, Fort Collins, CO, 253-279.

Dupuis, J., 1995. Bayesian Estimation of Movement and Survival Probabilities from Capture-Recapture Data. Biometrika 82, 761-772.
Dupuis, J, Schwarz, C.J., (2007). A Bayesian approach to the Multistate Jolly-Seber capture-recapture model. Biometrics 63, 1015-1022.

El Ghaoui, L., 2002. Inversion error, condition number, and approximate inverses of uncertain matrices. Linear algebra and its applications 343, 171-193.

El-Nashar, A.M., 2008. Optimal design of a cogeneration plant for power and desalination taking equipment reliability into consideration. Desalination 229, 21-32.

Fuh, C.D., 1993. Statistical inquiry for Markov chains by bootstrap method. Statistica Sinica 3: 53-66.

Früwirth-Schnatter, S., 2006. Finite Mixture and Markov Switching Models. Springer, New York

Fuertes, A.M., Kalotychou, E., 2007. On sovereign credit migration: A study of alternative estimators and rating dynamics. Computational Statistics and Data Analysis 51, 3448-3469.

Garnero, M.A., Montgomery, N., 2006. Pronostic de la profondeur de fissuration d’un rotor de turbine (in French). In: Proceedings of the lambda-mu 15th congress, Lille, 2006 October 10-12.

Gelman, A., Carlin, J.B., Stern, H.S., Rubin, D.B., 2004. Bayesian data analysis, second edition. Chapman & Hall, Boca Raton, FL.

Gentle, J.E., Härdle, W., Mori, Y. (Eds.), 2004. Handbook of Computational Statistics. Springer-Verlag, Berlin.

Gentleman, R.C., Lawless, J.F., Lindsey J.C., Yan P., 1994. Multi-state Markov models for analyzing incomplete disease history data with illustration for HIV disease. Statistics in Medicine 13, 805-821.

Genest, C. Favre, A.C., 2007. Everything You Always Wanted to Know about Copula Modeling but Were Afraid to Ask. Journal of Hydrologic Engineering 12, 347-368.

Genest, C., Quesy, J.F., Rémillard, B., 2006. Goodness-of-fit procedures for copula models based on the probability integral transformation. Scandinavian Journal of Statistics 33, 337-366.

Gilks, W.R., Roberts, G.O. 1996. Strategies for improving MCMC. In: Gilks, W.R., Richardson, S., Spiegelhalter, D.J. (Eds.), Markov Chain Monte Carlo in Practice, Chapman & Hall, London, 89-114.

Girard, P., Parent, E., 2004. The deductive phase of statistical analysis via predictive simulations: test, validation and control of a linear model with autocorrelated errors representing a food process. Journal of Statistical Planning and Inference 124, 99-120.

Gouno, E., Courtrai, L., Fredette, M., 2011. Estimation from aggregate data. Computational Statistics and Data Analysis 55, 615-626.

Grimshaw, S.D., Alexander, W.P., 2011. Markov chain models for delinquency: Transition matrix estimation and forecasting. Applied Stochastic Models in Business and Industry 27, 267-279.

Grinstead, C.M., Laurie Snell, J., 1997. Introduction to Probability, second revised edition. American Mathematical Society Press, Providence RI.
Haario, H., Saksman, E., Tamminen, J., 2001. An adaptive Metropolis algorithm. Bernoulli 7, 223-242.

Huard, D., Évin, G., Favre, A.C., 2006. Bayesian copula selection. Computational Statistics and Data Analysis 51, 809-822.

Ishwaran, J., James, L.F., 2001. Gibbs sampling methods for stick-breaking priors. Journal of the American Statistical Association 96, 161-174.

Jones, M.T. 2005. Estimating Markov Transition Matrices using Proportions Data: An Application to Credit Risk. IMF Working Paper 2005/2219.

Kalbfleisch, J.D., Lawless, J.F., 1984. Least squares estimation of transition probabilities from aggregate data. Canadian Journal of Statistics 12, 169-182.

Kim, G., Silvapulle, M.J., Silvapulle, P., 2007. Comparison of semiparametric and parametric methods for estimating copulas. Computational Statistics and Data Analysis 51, 2836-2850.

Lassen, T., 1991. Markov modelling of the fatigue damage in welded structures under in-service inspection. International Journal of Fatigue 13, 17-422.

Lee, T.C., Judge, G.G., Zellner, A., 1968. Maximum Likelihood and Bayesian Estimation of Transition Probabilities. Journal of the American Statistical Association 63, 1162-1179.

Little, R.J.A., 1993. Pattern-Mixture models for multivariate incomplete data. Journal of American Statistical Association 88, 125-134.

Little, R.J.A., Rubin, D.B., 1987 Statistical analysis with missing data. Wiley, New York.

Lawless, J.F., McLeish, D.L., 1984. The information in aggregate data from Markov chains. Biometrika 71, 419-430.

MacRae, E.C., 1977. Estimation of Time-Varying Markov Processes with Aggregate Data. Econometrica 45, 183-198.

Marin, J.M., Robert, C.P., 2007. Bayesian Core: A Practical Approach to Computational Bayesian Statistics. Springer, New York.

Marshall, A.W., Olkin, I., 1988. Families of multivariate distributions. Journal of the American Statistical Association 83, 834-841.

Minka, T., 2003. Bayesian inference, entropy, and the multinomial distribution. Online tutorial Microsoft Research. http://research.microsoft.com/enu/um/people/minka/papers/multinomial.html.

Mira, A., Sargent, D.J., 2003. A new strategy for speeding Markov chain Monte Carlo algorithms. Statistical Methods and Applications 12, 49-60.

Nelsen, R.B., 2006. An Introduction to Copulas, second edition. Springer, New York.

Nikoloulopoulos, A.K., Karlis, D., 2008. Copula model evaluation based on parametric bootstrap, Computational Statistics and Data Analysis 52, 3342-3353.
Nott, D.J., Kohn, R., 2005. Adaptive sampling for Bayesian variable selection. Biometrika 92, 747-763.

Parent, E., Lebdi, F., Hurand, P., 1991. Stochastic modeling of a water resource system: analytical techniques versus synthetic approaches. In: Ganoulis, J. (Ed.), Water Resources engineering Risk Assessment. Springer-Verlag, Heidelberg, 415-434.

Pasanisi, A., Parent, E., 2004. Modélisation bayésienne du vieillissement des compteurs d'eau par mélange de classes d’appareils de différents états de dégradation (in French). Revue de Statistique Appliquée 52, 39-65.

Pollard, J.H., 1973. Mathematical Models for the Growth of Human Populations. Cambridge University Press, Cambridge.

Puolamäki, K., Kaski, S., 2009. Bayesian Solutions to the Label Switching Problem. In: Adams, N., Robardet, C., Siebes, A., Boulicaut, J.F (Eds.), Advances in Intelligent Data Analysis VIII, Proceedings of the 8th International Symposium on Intelligent Data Analysis, IDA 2009. Springer, Berlin, 381-392.

Robert, C.P., 2001. The Bayesian Choice: from Decision-Theoretic Motivations to Computational Implementation. Springer, New York.

Robert , C.P., Casella, G., 2004. Monte Carlo Statistical Methods, second edition. Springer, New York.

Roberts, G.O., Sahu, S.K., 1997. Updating schemes, correlation structure, blocking, and parametrisation for the Gibbs sampler. Journal of the Royal Statistical Society B 59, 291-317.

Roberts, G.O., Rosenthal, J.S., 2007. Coupling and Ergodicity of Adaptive MCMC. Journal of Applied Probabilities 44, 458-475.

Roberts, G.O., Rosenthal, J.S., 2009. Examples of Adaptive MCMC. Journal of Computational and Graphical Statistics 18, 349-367.

Roh, Y.S., Xi, Y., 2000. A general formulation for transition probabilities of Markov model and the application to fracture of composite materials. Probabilistic Engineering Mechanics 15, 241-250.

Rosenthal, J.S., 2007. AMCMC: An R interface for adaptive MCMC. Computational Statistics and Data Analysis 51, 5467-5470.

Rubin, D. B., 1976. Inference and missing data. Biometrika 63, 581-592.

Sargent, D.J., Hodges, J.S., Carlin, B.P., 2000. Structured Markov Chain Monte Carlo. Journal of Computational and Graphical Statistics 9, 217-234.

Sendi, P.P., Bucher, H.C., Craig, B.A., Pfluger, D., Battegay, M., 1999. Estimating AIDS-free survival in a severely immunosuppressed asymptomatic HIV-infected population in the era of antiretroviral triple combination therapy. Swiss HIV Cohort Study. Journal of acquired immune deficiency syndromes and human retrovirology 20, 376-381.
Strid, I., Giordani, P., Kohn, R., 2010. Adaptive hybrid Metropolis-Hastings samplers for DSGE models. Working Paper Series in Economics and Finance No. 724, Stockholm School of Economics.

Tuyl, P., Gerlach, R., Mengersen, K., 2009. Posterior predictive arguments in favor of the Bayes-Laplace prior as the consensus prior for binomial and multinomial parameters. Bayesian Analysis 4, 151-158.

Urakabe, S., Orita, Y., Fukuhara, Y., Ando, A., Ueda, N., Inque, M., Furukawa, T., Abe, H., 1975. Prognosis of chronic glomerulonephritis in adult patients estimated on the basis of the Markov process. Clinical Nephrology 3, 48-53.

Vogel, R.M., 1987. Reliability indices for water supply systems. Journal of Water Resources Planning and Management 113, 563-579.

Vihola, M., 2010. Grapham: Graphical models with adaptive random walk Metropolis algorithms. Computational Statistics and Data Analysis 54, 49-54.

Wu, M., Carroll, R., 1988. Estimation and comparison of changes in presence of informative right censoring by modelling the censoring process. Biometrics 44, 175-188.

Zhang, L., Dai, S., 2007. Application of Markov model to environmental fate of phenanthrene in Lanzhou Reach of Yellow River. Chemosphere 67, 1296-1299.