

Copulas selection in pairwise Markov chain

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Abstract. The Hidden Markov Chain (HMC) model considers that the process of unobservable states is a Markov chain. The Pairwise Markov Chain (PMC) model however considers the couple of processes of observations and states as a Markov chain. It has been shown that the PMC model is strictly more general than the HMC one, but retains the ease of processings that made the success of HMC in a number of applications. In this work, we are interested in the modeling of class-conditional densities appearing in PMC by bi-dimensional copulas and the mixtures estimation problem. We study the influence of copula shapes on PMC data and the automatic identification of the right copulas from a finite set of admissible copulas, by extending the general “Iterative Conditional Estimation” parameters estimation method to the context considered. A set of systematic experiments conducted with eight families of one-parameters copulas parameterized with Kendall’s tau is proposed. In particular, experiments show that the use of false copulas can degrade significantly classification performances.

Keywords. Hidden Markov Chain, Pairwise Markov chain, Copulas, Iterative Conditional Estimation, Unsupervised classification.

1 Introduction

Let $\mathbf{x}_{1:N} = (x_1, \dots, x_N)$ and $\mathbf{y}_{1:N} = (y_1, \dots, y_N)$ be two series of data. Each x_n takes its value in the finite set $\Omega = \{1, \dots, K\}$ and each y_n in the set of real numbers \mathbb{R} . When looking for the unobservable data series $\mathbf{x}_{1:N}$ from the observable one $\mathbf{y}_{1:N}$, and when there is no deterministic link between them, probability theory provides a rigorous framework to lead to results that are generally effective and sometimes spectacular. The couple $(\mathbf{x}_{1:N}, \mathbf{y}_{1:N})$ is considered as a realization of two random processes $\mathbf{X}_{1:N} = (X_1, \dots, X_N)$ and $\mathbf{Y}_{1:N} = (Y_1, \dots, Y_N)$ and the stochastic links between the two series are modeled by a law $p(\mathbf{x}_{1:N}, \mathbf{y}_{1:N})$ of couple $(\mathbf{X}_{1:N}, \mathbf{Y}_{1:N})$. Despite the lack of deterministic relationship between $\mathbf{x}_{1:N}$ and $\mathbf{y}_{1:N}$, it is possible to propose optimal

methods for finding $\mathbf{x}_{1:N}$, in mean or in long-term, when dealing with the problem a “large number” of time.

However, it is impossible, when N increases, to consider the general law $p(\mathbf{x}_{1:N}, \mathbf{y}_{1:N})$ because of the high algorithmic complexity, and we are led to consider specific laws. Among these the most spread law is the “Hidden Markov Chain” (HMC), which writes

$$p(\mathbf{x}_{1:N}, \mathbf{y}_{1:N}) = p(x_1) p(y_1 | x_1) p(x_2 | x_1) p(y_2 | x_2) \dots p(x_N | x_{N-1}) p(y_N | x_N). \quad (1)$$

This model was later generalized to “Pairwise Markov Chain” (PMC) [14]:

$$p(\mathbf{x}_{1:N}, \mathbf{y}_{1:N}) = p(x_1, y_1) p(x_2, y_2 | x_1, y_1) \dots p(x_N, y_N | x_{N-1}, y_{N-1}). \quad (2)$$

HMC model is very effective and commonly used, but the PMC model, which allows the same processing as the HMC, can improve performances significantly, even in an unsupervised way [3].

Consider a PMC such that the law $p(x_{n-1}, y_{n-1}, x_n, y_n)$ of $(X_{n-1}, Y_{n-1}, X_n, Y_n)$ does not depend on $n = 1, \dots, N - 1$. Law $p(\mathbf{x}_{1:N}, \mathbf{y}_{1:N})$ is then entirely characterized by

$$p(x_1, y_1, x_2, y_2) = p(x_1, x_2) p(y_1, y_2 | x_1, x_2). \quad (3)$$

Our work deals with the modeling of laws $p(y_1, y_2 | x_1, x_2)$ by means of copulas [11]. Copulas are used for a long time in the field of economy and finance without considering Markovianity) [5, 6, 12], and only more recently in signal processing without markovianity [10, 8] and with markovianity [2, 1].

The first work that combined copulas and Markov model was proposed in [2], where the process $\mathbf{X}_{1:N}$ is a Markov chain (such a model is called a HMC “with dependent noise”). In addition, a method for parameters estimation has been proposed, allowing unsupervised processings. Note that both HMC and copulas are known and used for several decades. It may then seem surprising that the two concepts have been considered in the same model only recently. This is likely due to the fact that in traditional models (1) the noise is “independent”, which implies that $p(y_1, y_2 | x_1, x_2) = p(y_1 | x_1) p(y_2 | x_2)$, and therefore the problem of modeling the dependence of random variables Y_1 and Y_2 conditional on (X_1, X_2) does not arise. However, as discussed in this article, this dependence can have a significant influence on the processings.

In this paper we extend work [2] in two directions. First, we consider general PMC, in which $\mathbf{X}_{1:N}$ is no more necessarily a Markov chain. Second we consider the problem of generalized mixtures estimation : for all $(i, j) \in \Omega^2$, the copula associated with $p(y_1, y_2 | x_1 = i, x_2 = j)$ is unknown and is automatically searched for in a finite set of eligible copulas, from $\mathbf{Y}_{1:N} = \mathbf{y}_{1:N}$ only. The experiments performed allow to affirm the importance of choosing the true copula. They also show the effectiveness of automatic identification method of copulas, based on the Bayesian selection method proposed in [7].

The remainder of the paper is organized as follows. Section 2 provides a brief overview of the PMC model and its various special cases, and the notion of copula. Section 3 is devoted to highlighting the importance of using the right copula for supervised restoration. The method of generalized mixture estimation, which is an extension of the general “Iterative Conditional Estimation” (ICE) method [13], and the results of several Bayesian unsupervised restorations are proposed in Section 4. The final section contains conclusions and perspectives.

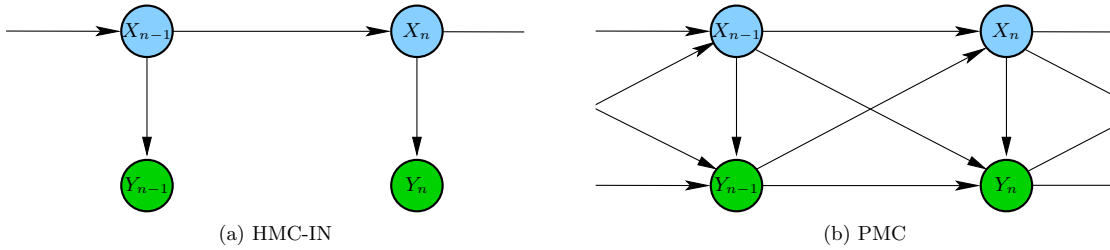


Figure 1: Oriented dependence graphs for the HMC-IN and the PMC models.

2 Copulas and PMC

The aim of this Section is to present the Pairwise Markov Chain (PMC) model with copulas, including both supervised and unsupervised Bayesian data restoration according to this model.

PMC basics

Let $\mathbf{Z}_{1:N} = (Z_1, \dots, Z_N)$ with $\mathbf{Z}_n = (X_n, Y_n)$ for all $n = 1, \dots, N$. The process $\mathbf{Z}_{1:N}$ is said to be a “Pairwise Markov Chain” (PMC) [14], if it is a Markov chain:

$$p(\mathbf{z}_{1:N}) = p(x_1, y_1) p(x_2, y_2 | x_1, y_1) \dots p(x_N, y_N | x_{N-1}, y_{N-1}). \quad (4)$$

Transition probabilities can write in the following way

$$p(z_n | z_{n-1}) = p(x_n, y_n | x_{n-1}, y_{n-1}) = p(x_n | x_{n-1}, y_{n-1}) p(y_n | x_{n-1}, y_{n-1}, x_n). \quad (5)$$

In PMC, the law $p(\mathbf{x}_{1:N} | \mathbf{y}_{1:N})$ is always Markovian, allowing the estimation of $\mathbf{X}_{1:N}$ from $\mathbf{Y}_{1:N} = \mathbf{y}_{1:N}$, while $\mathbf{X}_{1:N}$ being Markovian or not. A particular case of special interest is given by the so-called “Hidden Markov Chain with Independent Noise” (HMC-IN) in which $p(x_n | x_{n-1}, y_{n-1}) = p(x_n | x_{n-1})$ and $p(y_n | x_{n-1}, y_{n-1}, x_n) = p(y_n | x_n)$, so that transitions in eq. (5) write

$$p(x_n, y_n | x_{n-1}, y_{n-1}) = p(x_n | x_{n-1}) p(y_n | x_n). \quad (6)$$

Process $\mathbf{X}_{1:N}$ is then a Markov chain and random variables Y_1, \dots, Y_N are independent conditionally to $\mathbf{X}_{1:N}$. This classical model is traditionally called the hidden Markov chain.

In this work, we will only consider the general PMC model given by eq. (5) and classical HMC-IN model given by eq. (6). Oriented dependence graphs for the HMC-IN and the general PMC model are reported in Fig. 1. Note also that the PMC model in eq. (4) can be evaluated online at url www.fresnel.fr/perso/hmcext/index.php. Furthermore, in the following, we consider Stationary and Reversible PMCs (SR-PMC). The first hypothesis means that $p(z_n, z_{n+1})$ does not depend on $n = 1, \dots, N - 1$ and the second one means that the two families of conditional laws $p(z_{n+1} | z_n)$ and $p(z_n | z_{n+1})$ are identical. We then get the following result, whose demonstration within a general framework can be consulted in [9]:

Proposition Let $\mathbf{Z}_{1:N}$ be a SR-PMC, then the three following conditions are equivalent: (i) $\mathbf{X}_{1:N}$ is a Markov chain; (ii) $p(y_2 | x_1, x_2) = p(y_2 | x_2)$; (iii) $p(y_n | x_{1:N}) = p(y_n | x_n)$, for all $n = 1, \dots, N$.

Given eq. (4), eq. (6) and previous proposition, we can assess how the PMC generalizes the HMC-IN model. Note that this greater generality can result in greater efficiency in unsupervised image segmentation: as experimented in [3], the error rate can be halved. The main purpose of this paper is to study various models for laws $p(y_1, y_2 | x_1, x_2)$ in eq. (4) with copulas. This problem has been addressed in the case of an HMC with correlated noise in [2]. Results obtained in unsupervised image segmentation are very encouraging. Here, we extend this study in two directions: (i) We consider the general case of SR-PMC, abbreviated by PMC, where $\mathbf{X}_{1:N}$ is not necessarily Markovian; (ii) We study the estimation of $p(z_1, z_2)$, including the automatic choice of copulas within a finite set of admissible copulas.

Copulas in PMC

From $p(z_2 | z_1) = p(z_1 | z_2)$, and so $p(x_1, x_2) = p(x_2, x_1)$ and $p(y_1 | x_1, x_2) = p(y_2 | x_2, x_1)$, a stationary and reversible PMC is characterized by (1) $K(K+1)/2 - 1$ joint *a priori* probabilities $p(x_1, x_2)$; (2) K^2 bi-dimensional densities $p(y_1, y_2 | x_1, x_2) = f_{x_1, x_2}(y_1, y_2)$ with only K^2 margins.

Densities $p(y_1, y_2 | x_1, x_2)$ can be parameterized using the theory of copulas [11]. This theory allows us to define a 2D density f from its two marginal densities $f^{(1)}$ and $f^{(2)}$, and a dependence structure c , called “copula”, $f(y_1, y_2) = f^{(1)}(y_1) f^{(2)}(y_2) c(F^{(1)}(y_1), F^{(2)}(y_2); \theta)$, where $F^{(\cdot)}$ denotes Cumulative Distribution Function (CDF) associated with $f^{(\cdot)}$ and θ denotes the set of parameters to characterize the parametric copula c . One can see that a copula is any bi-dimensional cumulative function with uniform marginals on $[0, 1]$. It is then possible to construct distributions over \mathbb{R}^2 by considering various marginal distributions (Gaussian, gamma, beta of first and second kinds. . .) and various copulas (Gaussian, Student’t, Clayton. . .) in an independent manner. A bi-dimensional Gaussian density is a particular case of Gaussian margins combined with a Gaussian copula.

For all experiments presented, we will consider the eight one-parameter copulas presented in Appendix 1, and the zero-parameter product copula which gives the independence case (see below). These copulas can all be parameterized by Kendall’s rank correlation (denoted by $\tau \in [-1, 1]$), allowing comparison between copula shapes with the same correlation. We will write either $c(\cdot, \cdot; \theta)$ or $c(\cdot, \cdot; \tau)$. Note that the range of possible value for τ is not the same for all copulas. Some of them do not allow $\tau = 0$, whereas some others do not allow $\tau < 0$. In the list considered here, Gaussian and Student’t copulas are the only ones which cover the entire range of possible values for τ .

To simplify notations, let for $x_1 = i$ and $x_2 = j$, $p(x_1, x_2) = p_{ij}$, $c_{x_n, x_{n+1}}(\cdot, \cdot; \theta_{x_n, x_{n+1}}) = c_{ij}(\cdot, \cdot; \tau_{ij})$, $f_{x_n, x_{n+1}}(\cdot, \cdot) = f_{ij}(\cdot, \cdot)$ (and so forth for marginal densities)

3 PMC supervised data restoration

The aim of this Section is to evaluate the influence of copula shapes in the supervised restoration of PMC data. We start by providing a method to simulate PMC data whatever the copula shapes involved. Then systematic results of data restoration are presented, with varying Kendall’s rank correlation and margin shapes.

Simulation and supervised restoration of PMC data

According to [3], PMC data can be generated using the following procedure. Starting data ($n = 1$) are simulated according to

$$p(x_1) = \sum_{x_2=1}^K p(x_1, x_2), \quad p(y_1) = \sum_{x_2=1}^K p(x_1 | x_2) f_{x_1, x_2}(y_1).$$

Simulation of y_1 requires a sampling from a mixture of, possibly non-Gaussian, 1D densities. Then, next data ($n > 1$) are generated by alternating the simulation of x_{n+1} (conditionally to $\mathbf{z}_n = (x_n, y_n)$) and the simulation of y_{n+1} (conditionally to \mathbf{z}_n and x_{n+1}) according to

$$\begin{aligned} p(x_{n+1} | x_n = i, y_n) &\propto p(i, x_{n+1}) f_{i, x_{n+1}}(y_n), \\ p(y_{n+1} | x_{n+1} = j, x_n = i, y_n) &= \frac{f_{ij}(y_n, y_{n+1})}{f_{ij}(y_n)} = f_{ji}(y_{n+1}) c_{ij}(F_{ij}(y_n), F_{ji}(y_{n+1}); \tau_{ij}) \end{aligned} \quad (7)$$

Note that inversion of indices in $f_{ji}(y_{n+1})$ and $F_{ji}(y_{n+1})$ in eq. (8) comes from the reversibility hypothesis of PMC models.

The simulation of y_{n+1} can be performed using the rejection principle, as presented in Appendix 2. Although very general, the method can be computer demanding since it involves an acceptance criterion which can result in many rejected draws for every accepted one (the rejection rate depends on the copula).

The Bayesian restoration of \mathbf{X} according to the MPM criterion writes

$$\forall n \in [1, N], \quad \hat{x}_n = \arg \max_{x_n \in \Omega} p(x_n | y_{1:N}), \quad (8)$$

with $p(x_n | y_{1:N}) = \alpha_n(x_n) \beta_n(x_n)$ the marginal *a posteriori* distributions computed from the forward-like $\alpha_n(x_n) = p(x_n, y_{1:n})$ and the backward-like $\beta_n(x_n) = p(y_{n+1:N} | x_n, y_n)$ probabilities suited to the PMC model. These probabilities can be computed recursively

$$\alpha_1(x_1) = p(x_1) p(y_1 | x_1), \quad \alpha_{n+1}(x_{n+1}) = \sum_{x_n \in \Omega} \alpha_n(x_n) p(z_{n+1} | z_n), \quad \text{for } 1 \leq n < N, \quad (9)$$

$$\beta_1(x_N) = 1, \quad \beta_n(x_n) = \sum_{x_{n+1} \in \Omega} \beta_{n+1}(x_{n+1}) p(z_{n+1} | z_n), \quad \text{for } 1 \leq n < N, \quad (10)$$

see [3] for details. Let us also define joint *a posteriori* probabilities $p(x_n, x_{n+1} | y_{1:N})$ which write

$$p(x_n, x_{n+1} | y_{1:N}) = \frac{\alpha_n(x_n) p(z_{n+1} | z_n) \beta_{n+1}(x_{n+1})}{\sum_{a \in \Omega} \sum_{b \in \Omega} \alpha_n(b) p(b, y_{n+1} | a, y_n) \beta_{n+1}(b)}. \quad (11)$$

Bayesian restoration according to the Maximum A Posteriori (MAP) criterion is also available for the PMC model [3] but will not be considered.

Impact of copula shapes on supervised PMC data restoration

In order to account for the numerical influence of the copula shapes only, we conducted the following experiment: (1) We simulated N PMC data with $K = 2$ classes ($\Omega = \{1, 2\}$), according

Table 1: Margins parameters used for PMC simulation and restoration with $K = [1, 2]$.

Gaussian margins $\mathcal{N}(\mu, \sigma)$ $p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$	$f_{11} \rightsquigarrow \mathcal{N}(0.0, 1.00)$; $f_{12} \rightsquigarrow \mathcal{N}(0.3, 1.60)$ $f_{21} \rightsquigarrow \mathcal{N}(1.1, 1.40)$; $f_{22} \rightsquigarrow \mathcal{N}(1.5, 1.00)$
Gamma margins $\mathcal{G}(\mu, \alpha, \theta)$ $p(x) = \frac{\theta^\alpha}{\Gamma(\alpha)} (x - \mu)^{\alpha-1} e^{-\theta(x-\mu)}$	$f_{11} \rightsquigarrow \mathcal{G}(0.0, 8.00, 0.13)$; $f_{12} \rightsquigarrow \mathcal{G}(0.3, 8.89, 0.18)$ $f_{21} \rightsquigarrow \mathcal{G}(1.1, 3.08, 0.46)$; $f_{22} \rightsquigarrow \mathcal{G}(1.5, 2.67, 0.38)$

Table 2: PMC model. Mean classification error rates using $\tau_{\#1} = 0.16$.

Copula	c^0	c^1	c^2	c^3	c^4	c^5	c^6
c^0	11.09 (0.9)	14.30 (1.2)	13.72 (1.3)	13.90 (1.2)	14.64 (1.2)	14.73 (1.2)	13.88 (1.2)
c^1	11.28 (0.9)	14.09 (1.2)	13.81 (1.4)	13.84 (1.2)	14.39 (1.3)	14.43 (1.3)	13.78 (1.3)
c^2	11.89 (0.9)	14.65 (1.2)	13.13 (1.3)	14.03 (1.2)	15.31 (1.3)	15.60 (1.2)	14.23 (1.3)
c^3	11.71 (0.9)	14.36 (1.2)	13.59 (1.3)	13.67 (1.2)	14.93 (1.3)	15.05 (1.2)	14.38 (1.3)
c^4	11.40 (1.0)	14.13 (1.2)	14.06 (1.4)	13.95 (1.2)	14.26 (1.3)	14.28 (1.3)	13.82 (1.3)
c^5	11.69 (1.0)	14.22 (1.2)	14.51 (1.4)	14.11 (1.2)	14.34 (1.3)	14.27 (1.2)	13.94 (1.3)
c^6	11.81 (1.0)	14.39 (1.2)	13.90 (1.4)	14.46 (1.2)	14.67 (1.3)	14.83 (1.3)	13.50 (1.3)

(a) Gaussian margins

Copula	c^0	c^1	c^2	c^3	c^4	c^5	c^6
c^0	8.54 (0.7)	10.58 (1.0)	10.89 (1.0)	10.95 (1.0)	10.87 (0.9)	10.82 (0.9)	10.46 (1.0)
c^1	8.75 (0.8)	10.26 (1.0)	10.78 (1.0)	10.75 (1.0)	10.41 (1.0)	10.33 (0.9)	9.93 (1.0)
c^2	9.12 (0.8)	10.65 (1.0)	10.18 (0.9)	10.92 (1.0)	11.04 (1.0)	11.07 (0.9)	10.12 (1.0)
c^3	8.78 (0.8)	10.36 (1.0)	10.58 (1.0)	10.57 (0.9)	10.65 (1.0)	10.63 (0.9)	10.24 (1.0)
c^4	8.81 (0.8)	10.29 (1.0)	10.86 (1.0)	10.81 (1.0)	10.33 (1.0)	10.24 (0.9)	9.93 (0.9)
c^5	8.89 (0.8)	10.33 (1.0)	11.09 (1.0)	10.88 (1.0)	10.38 (1.0)	10.22 (0.9)	9.98 (1.0)
c^6	9.17 (0.8)	10.48 (1.0)	10.73 (1.0)	11.23 (1.0)	10.69 (0.9)	10.65 (0.9)	9.73 (0.9)

(b) Gamma margins

to some *a priori* probabilities p_{ij} , to some given copulas c_{ij} with parameter τ_{ij} , and to some margins f_{ij} ; (2) Then we restored simulated observations according to MPM, using all simulation parameters except the copula shape which is replaced by one in the list in Appendix 1.

We set $K = 2$, $N = 2000$ and the same copula shape for the 4 copulas c_{ij} involved. Joint *a priori* probabilities were set to $p(1, 1) = 0.5$, $p(1, 2) = p(2, 1) = 0.05$ and $p(2, 2) = 0.4$. We conducted systematic experiments for all available copulas according to margin families (Gaussian and Gamma, see Table 1) and two Kendall's rank correlation values:

- $\tau_{\#1} = 0.16$. The set of eligible copulas is noted $\Pi_{\#1} = \{c^1, c^2, c^3, c^4, c^5, c^6\}$.
- $\tau_{\#2} = 0.70$. The set of eligible copulas is noted $\Pi_{\#2} = \{c^1, c^2, c^3, c^6, c^7, c^8\}$.

For all eligible copula shapes in $\Pi_{\#i}$, we simulated noisy data according to the corresponding PMC model. Then we restored data, providing all parameters used at simulation time, except the true copula shape which we replaced by one from $\Pi_{\#i}$. The error rates reported below are means of 300 independent experiments (standard deviation are reported between parenthesis). Experimental results are reported in Table 2 for $\tau_{\#1}$ and in Table 3 for $\tau_{\#2}$, using Gaussian and gamma margins. Comments can be summarized as follows:

- Whatever Kendall's correlation value and margins shapes, the restoration with the right copula always gives the lowest mean error rate;

Table 3: PMC model. Mean classification error rates using $\tau_{\#2} = 0.70$.

Copula	c^0	c^1	c^2	c^3	c^6	c^7	c^8
c^0	11.06 (1.0)	26.27 (2.2)	25.77 (2.3)	26.27 (2.5)	27.50 (2.3)	25.63 (2.2)	25.71 (2.1)
c^1	41.55 (1.1)	14.95 (2.1)	17.84 (2.2)	17.13 (2.1)	19.43 (2.5)	16.90 (2.2)	16.70 (2.2)
c^2	36.16 (1.0)	16.01 (2.1)	16.86 (2.2)	15.69 (2.0)	17.07 (2.4)	16.27 (2.1)	15.97 (2.1)
c^3	40.50 (1.0)	18.14 (2.2)	18.98 (2.4)	12.43 (1.9)	29.37 (2.7)	20.48 (2.4)	15.78 (2.2)
c^6	44.41 (1.9)	21.09 (2.3)	21.84 (2.4)	27.97 (2.4)	6.31 (1.1)	18.68 (2.2)	24.21 (2.5)
c^7	37.97 (1.0)	16.56 (2.2)	17.64 (2.2)	19.12 (2.2)	13.62 (2.1)	15.25 (2.0)	17.55 (2.3)
c^8	39.25 (1.0)	16.59 (2.1)	17.80 (2.5)	13.71 (1.9)	24.98 (2.8)	17.94 (2.3)	14.99 (2.0)

(a) Gaussian margins

Copula	c^0	c^1	c^2	c^3	c^6	c^7	c^8
c^0	8.69 (0.7)	22.48 (2.0)	21.94 (2.2)	22.18 (2.1)	23.45 (2.3)	21.97 (2.2)	21.95 (2.2)
c^1	44.89 (2.0)	13.37 (1.8)	16.09 (2.0)	19.39 (2.2)	12.12 (1.7)	14.05 (1.9)	16.72 (1.9)
c^2	31.04 (2.0)	14.60 (1.8)	14.91 (2.0)	20.14 (2.1)	9.23 (1.3)	13.36 (1.7)	16.72 (1.9)
c^3	35.84 (1.1)	15.71 (1.9)	16.98 (2.1)	18.03 (2.1)	17.69 (2.2)	15.87 (2.0)	16.68 (1.9)
c^6	45.64 (2.9)	17.66 (2.0)	17.32 (1.9)	23.23 (2.1)	6.71 (1.1)	14.85 (1.8)	20.08 (2.1)
c^7	37.56 (2.0)	14.59 (1.8)	15.24 (1.9)	20.56 (2.1)	8.60 (1.2)	13.09 (1.7)	16.98 (1.9)
c^8	35.46 (1.4)	14.43 (1.8)	15.62 (2.0)	18.75 (2.2)	12.97 (1.7)	13.87 (1.8)	16.05 (1.9)

(b) Gamma margins

- When τ is low, the mean error rates can be very close (*e.g.* Table 2(a) row c^1 and Table 2(b) row c^5), showing that confusion can appear in experiments if correlation is low;
- When τ is large, the rates are very different. This is especially true for copula c^6 , where the rate is divided up to 4 when compared to copula c^3 in Table 3(a);

the main conclusion is that, when correlation is high, using a wrong copula can result in disastrous results.

4 Unsupervised PMC data restoration with copula selection

One of the very interesting properties of the PMC model is the ability to estimate parameters from observations only. Automatic parameters estimation has already been experimented in the “full-Gaussian” case in [3] (using ICE), and in the HMC-DN sub-model with Gaussian copulas and non-Gaussian margins (with SEM in [9]), with application in image and signal processing. Given the full PMC model, one would like to know if it is possible to automatically recover the proper shape of the copulas involved in simulated data. To that goal, we incorporated the Bayesian copula selection method introduced by Huard *et al* [7] in an ICE-based parameter estimation scheme, allowing to select the “best shape” for the K^2 copulas at each ICE iteration. Several experiments finally illustrate the nice behavior of the entire algorithm.

Bayesian copula selection

Bayesian identification of marginal and joint CDFs, and copula selection are the subjects of numerous recent papers, among them [6, 16]. In this work, we used the Bayesian copula selection method [7] (i) for its simplicity and low computational burden, and (ii) since all copulas considered can be parametrized by Kendall’s τ .

For short, given a set of 2D observations $\mathbf{y} = \{\mathbf{y}^1, \mathbf{y}^2\}$ with $\mathbf{y}^1 = \{y_1^1, \dots, y_N^1\}$ and $\mathbf{y}^2 = \{y_1^2, \dots, y_N^2\}$, the “best copula” c^s within a finite set of copula shapes $\Pi = \{c^1, \dots, c^R\}$ is selected according to

$$s = \arg \max_{r \in [1, R]} \frac{1}{\tau_M^r - \tau_m^r} \int_{\tau_m^r}^{\tau_M^r} \prod_{n=1}^N c^r (F^1(y_n^1), F^2(y_n^2); \tau) d\tau, \quad (12)$$

where F^1 and F^2 are the CDF of marginal data series \mathbf{y}^1 and \mathbf{y}^2 (their shapes are supposed known). Coefficients τ_m^r and τ_M^r for copula c^r represent the minimal and maximal admissible values for Kendall’s tau (see Table 5 for copulas considered here). One interesting specificity of the method is that it does not rely on the estimation of Kendall’s τ .

Automatic copula selection in ICE-based parameters estimation

Consider a stationary and reversible PMC whose law is given by $p_{\theta}(z_1, z_2)$, with θ a set of real parameters. When one wishes to estimate θ from $\mathbf{y}_{1:N}$, we can consider at least two general methods that produce series of estimates $\theta^0, \theta^1, \dots, \theta^q, \dots$:

- (i) “Expectation-Maximization” (EM) method: from θ^0 , θ^{q+1} is defined from θ^q using

$$\theta^{q+1}(\mathbf{y}_{1:N}) = \arg \max_{\theta} E \left[p_{\theta}(\mathbf{X}_{1:N}, \mathbf{Y}_{1:N}) | \mathbf{Y}_{1:N} = \mathbf{y}_{1:N}, \theta^q(\mathbf{y}_{1:N}) \right]. \quad (13)$$

- (ii) “Iterative Conditional Estimation” (ICE) method [13]: from θ^0 and an estimator $\hat{\theta}(\mathbf{x}_{1:N}, \mathbf{y}_{1:N})$ of θ from complete data $(\mathbf{x}_{1:N}, \mathbf{y}_{1:N})$, θ^{q+1} is defined from θ^q using

$$\theta^{q+1}(\mathbf{y}_{1:N}) = E \left[\hat{\theta}(\mathbf{X}_{1:N}, \mathbf{Y}_{1:N}) | \mathbf{Y}_{1:N} = \mathbf{y}_{1:N}, \theta^q(\mathbf{y}_{1:N}) \right]. \quad (14)$$

ICE is more general than EM since the estimator $\hat{\theta}(\mathbf{X}_{1:N}, \mathbf{Y}_{1:N})$ can be of any form, in particular it can be the maximum likelihood estimator or not [15]. In the case we are interested here, likelihood is difficult to handle and thus we choose to work with ICE.

When conditional expectation in eq. (14) is not computable for some components θ_m in θ , we estimate them by simulating L realizations $\mathbf{x}_{1:N}^1, \dots, \mathbf{x}_{1:N}^L$ of $\mathbf{x}_{1:N}$ according to

$$p_{\theta^q}(x_{n+1} | x_n, \mathbf{y}_{1:N}) = \frac{p_{\theta^q}(x_n, x_{n+1} | \mathbf{y}_{1:N})}{p_{\theta^q}(x_n | \mathbf{y}_{1:N})}, \quad (15)$$

see eq. (11), and by setting $\theta_m^{q+1}(\mathbf{y}_{1:N}) = \frac{\hat{\theta}_m(\mathbf{x}_{1:N}^1, \mathbf{y}_{1:N}) + \dots + \hat{\theta}_m(\mathbf{x}_{1:N}^L, \mathbf{y}_{1:N})}{L}$.

Let $p_{\theta}(z_1, z_2) = p_{\theta}(x_1, x_2) p_{\theta}(y_1, y_2 | x_1, x_2)$. As our main objective being to study the importance of copulas in the estimation of $\mathbf{x}_{1:N}$ from $\mathbf{y}_{1:N}$, we assume that the marginal distributions $p_{\theta}(y_1 | x_1, x_2)$ and $p_{\theta}(y_2 | x_1, x_2)$ are entirely known, *i.e.* both the laws family and their shape parameters are known. Laws $p_{\theta}(y_1, y_2 | x_1, x_2)$ are then determined by their copula. In order to simplify notations, let $p_{\theta}(x_1 = i, x_2 = j) = p_{ij}$ and τ_{ij} denotes the unique parameter for copula c_{ij} .

We solve the estimation problem using complete data $(\mathbf{x}_{1:N}, \mathbf{y}_{1:N})$ in the following way:

- Parameters p_{ij} can be estimated by the empirical estimate: $\hat{p}_{ij} = \frac{1}{N-1} \sum_{n=1}^{N-1} \mathbf{1}_{x_n=i, x_{n+1}=j}$.

Table 4: Results of automatic copula selection for experiment in Section 4. The integer value gives the number of times the right copula has been chosen for the 10 experiments. The mean Kendall's tau is given between parenthesis (true values are recalled in bold).

Experiment	c_{11}	c_{12}	c_{21}	c_{22}
#1	10 (0.69 - 0.70)	9 (0.29 - 0.40)	7 (0.32 - 0.40)	10 (0.71 - 0.70)
#2	10 (0.23 - 0.25)	9 (0.10 - 0.10)	9 (0.11 - 0.10)	10 (0.22 - 0.20)

- We divide the sample $\mathbf{y}_{1:N}$ in K^2 sub-samples $(\mathbf{y}_{1:N}^{ij})$, $i, j \in \Omega$ such that for $n = 1, \dots, N-1$, $y_n \in \mathbf{y}_{1:N}^{ij}$ if $(x_n, x_{n+1}) = (i, j)$. For all $(i, j) \in \Omega^2$, we select the “best copula” c_{ij}^s corresponding to $p_{\theta}(y_1, y_2 | x_1 = i, x_2 = j)$ among $\Pi_{ij} = \{c_{ij}^1, \dots, c_{ij}^P\}$, according to criterion in eq. (12), and then estimate its parameter τ_{ij}^s from $\mathbf{y}_{1:N}^{ij}$.

The principle of ICE is then applied according to:

- At first iteration ($q = 0$), we set initial values p_{ij}^0 for p_{ij} and initial copulas $c_{ij}^{s,0}$, based on a kmeans classification.

- For next iterations, p_{ij}^{q+1} are estimated from p_{ij}^q and $c_{ij}^{s,q}$ by taking the conditional expectation of \hat{p}_{ij} (see eq. (21) and (22) in [3]), whereas $c_{ij}^{s,q+1}$ are estimated using the complete data procedure described above, replacing $\mathbf{x}_{1:N}$ by $\mathbf{x}_{1:N}^q$.

Finally, the K^2 best copulas $c_{ij}^{s,Q}$ involved in an estimated PMC model are the copulas selected when ICE has converged ($q = Q$).

Experiments on copula selection in PMC model

This section intends to evaluate the combination of ICE and Bayesian copula selection method for the reliable identification of copulas in a PMC mixture. For data simulation, common parameters of all experiments presented below are $K = 2$, $N = 2500$, $Q = 30$, and $p(1, 1) = 0.50$, $p(1, 2) = p(2, 1) = 0.05$, $p(2, 2) = 0.40$. Specific parameters used for the two experiments are:

- **Experiment #1** - Gaussian margins from Table 1 and

Set of admissible copulas: $\forall (i, j) \in \Omega^2, \Pi_{ij} = \Pi_{\#1} = \{c^1, c^3, c^6\}$.

$c_{11} = c^1$, $c_{12} = c^3$, $c_{21} = c^3$ and $c_{22} = c^6$ with $\tau_{11} = 0.7$, $\tau_{12} = 0.4$, $\tau_{21} = 0.4$, $\tau_{22} = 0.7$.

- **Experiment #2** - Gamma margins from Table 1 and

Set of admissible copulas: $\forall (i, j) \in \Omega^2, \Pi_{ij} = \Pi_{\#2} = \{c^2, c^3, c^5, c^6\}$.

$c_{11} = c^2$, $c_{12} = c^5$, $c_{21} = c^5$ and $c_{22} = c^6$ with $\tau_{11} = 0.25$, $\tau_{12} = 0.1$, $\tau_{21} = 0.1$, $\tau_{22} = 0.2$.

Regarding unsupervised restoration, all parameters involved in the PMC model are estimated except the marginal density families, *e.g.* Gaussian, Gamma, which are supposed known (but parameters of margins are also estimated). Table 4 gives the number of times the right copula were selected for the $K^2 = 4$ copulas on 10 independent simulations and unsupervised restorations for the two experiments. Note that parameters estimated for margin shapes are not reported. Whatever the margin and Kendall's tau involved, the right copulas are always selected for copulas c_{11} and c_{22} . One can note a few confusions for copulas c_{12} and c_{21} , which can be explained by the low number of samples available for copulas estimation (about $p(1, 2)N = p(2, 1)N = 0.05 * 2500 = 125$). Nevertheless, these few confusions have a limited impact on the mean of error rates for the 10 experiments: for experiment #1, the mean is 13.74% for the unsupervised case and 12.16% for the supervised case (*i.e.* without parameters

estimation, see Section 3); for experiment #2, the mean is 12.89% for the unsupervised case and 11.35% for the supervised case.

5 Conclusion

This paper examines the influence of copula shapes in the Pairwise Markov Chain model. We first present supervised restoration results when systematically interchanging copulas used for PMC data simulation with other copula families. All things being equal, the use of the false copula can degrade significantly segmentation results, both in the Markovian and non Markovian contexts. In the case of a noise with strong correlation, the use of an independent noise model can produce disastrous results. Finally, we also present an algorithm for the automatic selection of copulas involved in PMC within a finite set of admissible copulas. According to experiments, the method of copula identification and parameters estimation, based on the general ‘‘Iterated Conditional Expectation’’ (ICE) allows effective unsupervised classifications.

App 1 - Densities of copulas

Table 5 gives details about the one-parameter copulas considered for experiments: probability density function (pdf), range for parameter θ and its closed-form solution to Kendall’s tau. For the Student’s t copula (c^2) the degree of freedom ν is supposed to be known.

App 2 - Simulation of $Y_2 | Y_1 = y_1$

Let Y_1 and Y_2 be two real-valued random variables with probability density function $f^{(1)}(\cdot)$ and $f^{(2)}(\cdot)$, and cumulative distribution functions $F^{(1)}(\cdot)$ and $F^{(2)}(\cdot)$. Assuming a copula representation for $f(y_1, y_2)$, we can write $p(y_2 | y_1) = f_{y_1}(y_2) = f^{(2)}(y_2) c(F^{(1)}(y_1), F^{(2)}(y_2); \theta)$. Assuming a real number M and a density g such that $\forall x \in \mathbb{R}, f_{y_1}(x) \leq M g(x)$, the simulation of Y_2 conditionally to $Y_1 = y_1$ can be performed using the rejection algorithm [4]:

1. Sample $X = x$ according to g and $V = v$ according to $\mathcal{U}([0, 1])$, the uniform law.
2. Accept $y_2 = x$ if $v \leq \frac{f_{y_1}(x)}{M g(x)}$, else, go back to 1.

Choosing $g = f^{(2)}$ and $M = \max_{u_2 \in [0, 1]} c(u_1, u_2)$, previous equation writes $v \leq \frac{c(u_1, F^{(2)}(x))}{\max_{u_2 \in [0, 1]} c(u_1, u_2; \theta)}$ where $u_1 = F^{(1)}(y_1)$. So, it is possible to generate drawings from $Y_2 | Y_1 = y_1$ whatever the shape of the copula, once we know the pdf of the copula and how to generate a random variate for Y_2 . Algorithm efficiency, *i.e.* number of rejections before an acceptance occurs, depends on the value of M and so on the copula shape. When no closed-form solution is available, a numerical method to find the maximum value can be easily implemented.

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Table 5: One parameter (named θ) copulas $c^\rho(u_1, u_2; \theta)$ used in this report (FGM stands for Farlie-Gumbel-Morgenstern).

#p	Name	cdf C^ρ	pdf c^ρ	Kendall's τ	$[\tau_{\theta}, \tau_{\theta}^*]$
0	Product	$C^0 = u_1 u_2$	$c^0 = 1$	0	
1	Gauss ^a	$C^1 = \int_0^{u_1} \int_0^{u_2} \phi\left(\frac{\phi^{-1}(u_2) - \rho\phi^{-1}(u)}{\sqrt{1-\rho^2}}\right) du$	$c^1 = \frac{1}{\sqrt{1-\rho^2}} \exp\left(-\frac{1}{2}\xi^T(\rho - \mathbf{I})\xi\right)$	$\frac{2}{\pi} \text{asin } \theta$	$[-1, 1]$
		where $\xi_i = \phi^{-1}(u_i)$ with ϕ the standard normal distribution, $\rho = \begin{pmatrix} 1 & \theta \\ \theta & 1 \end{pmatrix}$ and \mathbf{I} are the 2×2 correlation and identity matrices.			
2	Student ^a	$C^2 = \int_0^{u_1} \int_0^{u_2} \frac{t_{\nu+1} \left(\sqrt{\frac{\nu+1}{\nu + (t_{\nu}^{-1}(u_1))^2 - \rho t_{\nu}^{-1}(u)}{\nu-1-\rho^2}}\right) du$	$c^2 = \frac{1}{\sqrt{1-\rho^2}} \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma^2(\frac{\nu+1}{2})} \left(1 + \frac{1}{\nu}\xi^T \rho^{-1} \xi\right)^{-\frac{\nu+1}{2}}$	$\frac{2}{\pi} \text{asin } \theta$	$[-1, 1]$
		where $\xi_i = t_{\nu}^{-1}(u_i)$ with t_{ν} the t distribution with ν degrees of freedom, $\rho = \begin{pmatrix} 1 & \theta \\ \theta & 1 \end{pmatrix}$ is the 2×2 correlation matrix and $\Gamma(\cdot)$ the Gamma function.			
3	Gumbel ^b	$C^3 = \exp\left(-\frac{1}{\theta}(U_1 + U_2)^{\frac{1}{\theta}}\right)$	$c^3 = \frac{U_1}{u_1 \ln(u_1)} \frac{U_2}{u_2 \ln(u_2)} (\theta - 1 + U_1 + U_2)^{\frac{1}{\theta}-2} \exp\left(-\frac{1}{\theta}(U_1 + U_2)^{\frac{1}{\theta}}\right)$	$1 - \frac{1}{\theta}$	$[0, 1]$
		where $U_i = (-\ln(u_i))^{\theta}$ and $U_2 = (-\ln(u_2))^{\theta}$.			
4	FGM	$C^4 = u_1 u_2 (1 + \theta(1 - u_1)(1 - u_2))$	$c^4 = 1 + \theta(1 - 2u_1)(1 - 2u_2)$	$\frac{2\theta}{9}$	$[-\frac{2}{9}, \frac{2}{9}]$
5	Cubic section	$C^5 = u_1 u_2 (1 + 2\theta(1 - u_1)(1 - u_2)(1 + u_1 + u_2 - 2u_1 u_2))$	$c^5 = 1 + 2\theta((1 - u_1)(1 - u_2)(-8u_2 u_1 + 2u_1 + 2u_2 + 1) + u_1(1 - u_2)(4u_2 u_1 - u_1 - 2u_2 - 1) + (1 - u_1)u_2(4u_2 u_1 - 2u_1 - u_2 - 1) + u_1 u_2(-2u_2 u_1 + u_1 + u_2 + 1))$	$\frac{2}{3}\theta - \frac{6}{225}\theta^2$	$[0, \frac{33}{200}]$
6	Clayton ^b	$C^6 = (u_1^{-\theta} + u_2^{-\theta} - 1)^{-\frac{1}{\theta}}$	$c^6 = (1 + \theta) u_1^{-1-\theta} u_2^{-1-\theta} (-1 + u_1^{-\theta} + u_2^{-\theta})^{-\frac{1}{\theta}-2}$	$\frac{\theta}{\theta+2}$	$]0, 1]$
7	Arch12 ^{b,c}	$C^7 = \left(1 + (U_1 + U_2)^{\frac{1}{\theta}}\right)^{-1}$	$c^7 = \frac{U_1}{u_1(u_1 - 1)} \frac{U_2}{u_2(u_2 - 1)} (\theta - 1 + (\theta + 1)(U_1 + U_2)^{\frac{1}{\theta}}) \frac{(U_1 + U_2)^{\frac{1}{\theta}-2}}{(1 + (U_1 + U_2)^{\frac{1}{\theta}})^3}$	$1 - \frac{2}{3\theta}$	$\left[\frac{1}{3}, 1\right]$
		where $U_i = \left(\frac{1}{u_i} - 1\right)^{\theta}$ and $U_2 = \left(\frac{1}{u_2} - 1\right)^{\theta}$			
8	Arch14 ^{b,c}	$C^8 = \left(1 + (U_1 + U_2)^{\frac{1}{\theta}}\right)^{-\theta}$	$c^8 = U_1 U_2 (U_1 + U_2)^{\frac{1}{\theta}-2} (1 + (U_1 + U_2)^{\frac{1}{\theta}})^{-2-\theta} \frac{\theta u_1 u_2 \left(\frac{1}{u_1^{\frac{1}{\theta}} - 1}\right) \left(\frac{1}{u_2^{\frac{1}{\theta}} - 1}\right)}{\left(\frac{\theta - 1 + 2\theta(U_1 + U_2)^{\frac{1}{\theta}}}{1 + (U_1 + U_2)^{\frac{1}{\theta}}}\right)}$	$1 - \frac{2}{3\theta}$	$\left[\frac{1}{3}, 1\right]$
		where $U_i = \left(u_i^{-\frac{1}{\theta}} - 1\right)^{\theta}$ and $U_2 = \left(u_2^{-\frac{1}{\theta}} - 1\right)^{\theta}$			

^aFamily of elliptical copulas.

^bFamily of Archimedean copulas.

^cCoin from the order of appearance in [11].

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