Copula modelling of serially correlated multivariate data with hidden structures

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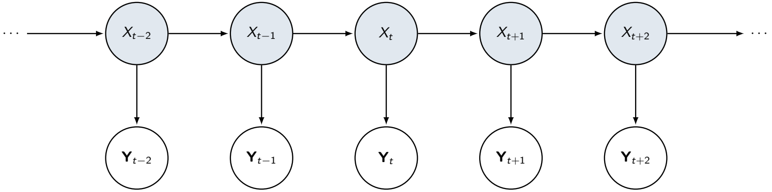
Hidden Markov Models: A Primer

- A hidden Markov model (HMM) pairs an observed time series $\{\mathbf{Y}_t\}_{t\geq 1} \subseteq \mathbb{R}^d$ with a Markov chain $\{X_t\}_{t\geq 1}$ on some state space $\mathcal{X}$, such that the distribution of $\mathbf{Y}_s \mid X_s$ is independent of $\mathbf{Y}_t \mid X_t$ for $s \neq t$:



- $\mathbf{Y}_{t,h}|\{X_t = k\} \sim f_{k,h}(\cdot|\lambda_{k,h})\ \forall h = 1, \ldots, d$
- $\{X_t\}$ is a Markov process (finite state space $\mathcal{X}$) with initial probability mass distribution $\{\pi_i\}_{i\in\mathcal{X}}$ and transition probabilities $\{\gamma_{i,j}\}_{i,j\in\mathcal{X}}$

Inferential aims for HMMs

- Typically, the chain $\{X_t\}_{t\geq 1}$ is partially or completely unobserved.
- The hidden states can correspond to a precise variable (occupancy data) or might be postulated (psychology, ecology, etc)
- Aim 1: Model the data generating mechanism Nasri et al. (2020)
- Aim 2: Decode (i.e., classify) or predict the X_t's from the observed data.

Examples

- A tri-axial accelerometer captures a shark's acceleration with respect to three positional axes depending on the shark's activity (resting, hunting, attacking). For short periods some of the sharks are filmed.
- Stock exchanges keep track of real-time prices for hundreds of stocks within an industry, depending on market conditions/states (stagnant, growing, shrinking).
- In-game team statistics like shots on goal and ball touches in a ~~soccer~~ football match are changing with the "momentum" of the team (defensive, offensive, passive) Ötting et al. (2021)

Fusion of Multiple Data Sources

- In the real-world applications above, various sensors capture multiple streams of data, which are "fused" into a multivariate time series $\{\mathbf{Y}_t\}_{t\geq 1}$

- In such situations, the components of any $\mathbf{Y}_t = (Y_{t,1}, \dots, Y_{t,d})$ cannot be assumed independent (even conditional on X_t)

- The corresponding assumption for HMMs – that of contemporaneous conditional independence Zucchini et al. (2017) – is often violated

- Instead, it is common to assume that $\mathbf{Y}_t$ follows a multivariate Gaussian distribution, but this places limits on marginals and dependence structures

- What if the strength of dependence between the components of $\mathbf{Y}_t$ could be informative about the underlying state X_t?

Copulas

- Copula functions are used to model dependence between continuous random variables.

- If $Y_1, Y_2, \ldots Y_d$ are continuous r.v.'s with distribution functions (df) $F_1, \ldots, F_d$, there exists an unique copula function $C : [0,1]^d \to [0,1]$ such that

$$H(t_1, \ldots, t_d) = \mathbb{P}(Y_1 \leq t_1, \ldots, Y_d \leq t_d) = C(F_1(t), \ldots, F_d(t_d)).$$

- The copula bridges the marginal distributions of $Y_1, \ldots, Y_d$ with the joint distribution. It corresponds to a distribution on $[0,1]^d$ with uniform margins.

- This can be extended to conditional distributions and copulas:

$$\mathbb{P}(Y_1 \leq t_1, \ldots, Y_d \leq t_d | X) = C(F_1(t|X), \ldots, F_d(t_d|X)|X).$$

Copulas Within HMMs

- Our model consists of an HMM $\{(\mathbf{Y}_t, X_t)\}_{t\geq 1} \subseteq \mathbb{R}^d \times \mathcal{X}$ in which the state-dependent distributions are copulas:

$$\mathbf{Y}_t \mid (X_t = k) \sim H_k(\cdot) = \underbrace{C_k\Big(F_{k,1}(\cdot\,; \lambda_{k,1}), \ldots, F_{k,d}(\cdot\,; \lambda_{k,d}) \Big| \theta_k\Big)}_{\text{depends on the hidden state value } k}.$$

- $C_k(\cdot, \ldots, \cdot \mid \theta_k)$ is a d-dimensional parametric copula
- $\{X_t\}_{t\geq 1}$ is a Markov process on finite state space $\mathcal{X} = \{1, 2, \ldots, K\}$ and K is known.
- In this model, virtually all aspects of the state-dependent distributions are allowed to vary between states

Information in the dependence

- For a range of $\theta \in [0, 100)$, we simulated a bivariate time series of length $T = 100$ from the 2-state HMM

$$\mathbf{Y}_t \mid (X_t = k) \sim C_{\text{Frank}} \left(\mathcal{N}(0,1), \mathcal{N}(0,1) \mid (-1)^k \cdot |\theta| \right), \quad k = 1, 2$$

and then separately assessed the accuracy of a standard decoding algorithm, first assuming independent margins and then the true model:

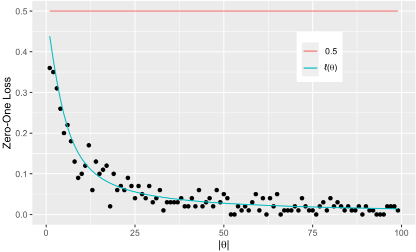


Figure: Zero-one losses for independent margins (red dots) and true model (blue dots)

Stronger Dependence Leads to Better Accuracy

- In fact, $\ell_{01}(\theta) = \frac{1}{2} - \frac{2}{\theta}\log\left(\cosh\frac{\theta}{4}\right) \to 0$ as $\theta \to \infty$
- Similar formulas hold for other radially symmetric copulas
- Much more generally, we have the following:

Theorem

Let $\nu_{t,k} = \mathbb{P}(X_t = k)$. The expected zero-one loss of the classifications made by local decoding is given by

$$\ell_{01}(\boldsymbol{\eta}) = 1 - \frac{1}{T}\sum_{t=1}^{T}\sum_{k=1}^{K}\nu_{t,k}\int_{\mathbb{R}^d}\mathbb{1}\left\{\frac{\nu_{t,k}\cdot h_k(\mathbf{y})}{\max_{j\neq k}\nu_{t,j}\cdot h_j(\mathbf{y})} > 1\right\}\mathrm{d}H_k(\mathbf{y}).$$

where $h_k(\mathbf{Y})$ is the joint density of $\mathbf{Y}|X = k$.

- Corollary: as the copula in any particular state approaches either of the Fréchet-Hoeffding bounds, the observations produced by that state will be detected with complete accuracy

Estimation with missing data

- Data consist in observed $\mathbf{Y}_{1:T}$ and missing $X_{1:T}$
- Parameters are $\eta = \{\lambda_{h,k}\}_{\substack{h=1:d \\ k=1:T}} \cup \{\theta_k\}_{k=1:T} \cup \{\gamma_{i,j}\}_{\substack{i=1:K \\ j=1:K}}$ $\cup\{\pi_j\}_{j=1:K}$.
- The complete-data log-likelihood for one trajectory of the copula HMM is given by

$$\ell_{\text{com}}\left(\boldsymbol{\eta} \mid \mathbf{y}_{1:T}, X_{1:T}\right) = \pi_{X_1} + \sum_{t=2}^{T} \log \gamma_{X_{t-1},X_t} + \sum_{h=1}^{d} \log f_{X_t,h}(y_{t,h}; \lambda_{X_t,h})$$
$$+ \sum_{t=1}^{T} \log c_{X_t}\left(F_{X_t,1}(y_{t,1}; \lambda_{X_t,1}), \ldots, F_{X_t,1}(y_{t,d}; \lambda_{X_t,d}) \mid \theta_{X_t}\right). \quad (1)$$

Inference for HMMs Via the EM Algorithm

- Without copula, the estimation is done via the EM algorithm (aka Baum-Welch)

E-step Compute $Q(\boldsymbol{\eta}|\boldsymbol{\eta}^{(s)}) = E[l_{com}(\boldsymbol{\eta}|\mathbf{Y}_{1:T}, X_{1:T})|\boldsymbol{\eta}^{(s)}, \mathbf{Y}_{1:T}]$

M-step Set $\boldsymbol{\eta}^{(s+1)} = \arg\max_{\eta} Q(\boldsymbol{\eta}|\boldsymbol{\eta}^{(s)})$

- The complete-data log-likelihood is written in terms of the state membership indicators $U_{k,t} = \mathbb{1}_{X_t=k}$ and $V_{j,k,t} = \mathbb{1}_{X_{t-1}=j, X_t=k}$
- In the **E-Step**, these indicators are estimated by the conditional probabilities $\hat{u}_{k,t} = \mathbb{P}(X_t = k \mid \mathbf{Y}_{1:T} = \mathbf{y}_{1:T})$ and $\hat{v}_{j,k,t} = \mathbb{P}(X_{t-1} = j, X_t = k \mid \mathbf{Y}_{1:T} = \mathbf{y}_{1:T})$, which are computed based on current parameter estimates
- This only requires evaluating the state-dependent densities at each of the observations $\mathbf{y}_1, \ldots, \mathbf{y}_T$ (this is "OK")

The M-Step Is Hard

- In the **M-Step**, the resulting complete-data log-likelihood is maximized with respect to all parameters in the model simultaneously
  - Only for the simplest univariate models do the state-dependent MLEs exist in closed form; otherwise, one must resort to numerical methods (this is hard and unstable!)
  - Evaluating a copula density $c_k(\cdot, \dots, \cdot \mid \theta_k)$ in high dimensions is slow
  - When the state-dependent distributions in an HMM are copulas, performing the M-Step directly requires the evaluation of

$$\underset{\{\theta_k\},\{\lambda_{k,h}\}}{\operatorname{argmax}} \left\{ \sum_{k=1}^{K} \sum_{t=1}^{T} \hat{u}_{k,t} \left[\log c_k\left(F_{k,1}(y_{t,1}; \lambda_{k,1}), \dots, F_{k,d}(y_{t,d}; \lambda_{k,d}) \,\middle|\, \theta_k \right) + \sum_{h=1}^{d} \log f_{k,h}(y_{t,h}; \lambda_{k,h}) \right] \right\}$$

  - This is very unstable (and slow)

Inference Functions for Margins

- Likelihood-based inference for copulas is easier when the goal is to estimate θ alone in the presence of known margins

- Why not perform inference on the marginal distributions first, and then on the copula itself?

- In the context of iid data, this is exactly the inference functions for margins (IFM) approach of Joe and Xu (1996):
  - First estimate each λ_h by its "marginal MLE" $\hat{\lambda}_h$ given $\{Y_{t,h}\}_{t\geq 1}$, for $h \in \{1, \ldots, d\}$
  - Then estimate θ assuming fixed marginals $F_1(\cdot; \hat{\lambda}_1), \ldots, F_d(\cdot; \hat{\lambda}_d)$

- One can show that the IFM estimator is consistent and asymptotically normal (although relatively less efficient than the MLE)

IFM Step

- For each $j \in \mathcal{X}$, estimate the initial distribution and transition probabilities:

$$\delta^{(s+1)} = (\hat{u}_{1,1}^{(s)}, \dots, \hat{u}_{K,1}^{(s)})$$

and

$$\gamma_{j,\cdot}^{(s+1)} = \left(\frac{\sum_{t=2}^{T} \hat{v}_{j,1,t}^{(s)}}{\sum_{k=1}^{K} \sum_{t=2}^{T} \hat{v}_{j,k,t}^{(s)}}, \dots, \frac{\sum_{t=2}^{T} \hat{v}_{j,K,t}^{(s)}}{\sum_{k=1}^{K} \sum_{t=2}^{T} \hat{v}_{j,k,t}^{(s)}} \right).$$

- For each $k \in \{1, \dots, K\}$ and $h \in \{1, \dots, d\}$, estimate the marginal parameters

$$\lambda_{k,h}^{(s+1)} = \arg\sup_{\lambda} \sum_{t=1}^{T} \hat{u}_{k,t}^{(s+1)} \cdot \log\left(f_{k,h}(y_{t,h}; \lambda)\right).$$

- For each $k \in \{1, \dots, K\}$, estimate the copula parameters

$$\tilde{\theta}_{k}^{(s+1)} = \arg\sup_{\theta} \sum_{t=1}^{T} \hat{u}_{k,t}^{(s+1)} \cdot \log\left(c_k \left(F_{k,1}(y_{t,1}; \lambda_{k,1}^{(s+1)}), \dots, F_{k,d}(y_{t,d}; \lambda_{k,d}^{(s+1)}) \,\middle|\, \theta \right) \right).$$

New problems

- The EIFM algorithm is not an GEM algorithm

$$\sum_{t=1}^{T} \hat{u}_t \cdot \log\left(f_h(y_{t,h}; \lambda_h^{(s)})\right) \leq \sum_{t=1}^{T} \hat{u}_t \cdot \log\left(f_h(y_{t,h}; \lambda_h^{(s+1)})\right), \qquad h \in \{1, \dots, d\} \qquad (2)$$

does not imply

$$\begin{aligned} & \sum_{t=1}^{T} \hat{u}_t \cdot \log\left(c\left(F_1(y_{t,1}; \lambda_1^{(s)}), \dots, F_d(y_{t,d}; \lambda_d^{(s)}) \,\middle|\, \theta^{(s)}\right)\right) \\ \leq \; & \sum_{t=1}^{T} \hat{u}_t \cdot \log\left(c\left(F_1(y_{t,1}; \lambda_1^{(s+1)}), \dots, F_d(y_{t,d}; \lambda_d^{(s+1)}) \,\middle|\, \theta^{(s)}\right)\right). \end{aligned}$$

- The EIFM algorithm will converge (to a local or global maximum).
- The estimator is consistent and asymptotically normal (under mild regularity conditions).
- EIFM as a version of the ES algorithm of Elashoff and Ryan (2004).
- Use asymptotic theory of M-estimators for HMMs Jensen (2011).

Implementation of EIFM

- K is assumed known
- An initial clustering algorithm may be used in which the observed multivariate data follow vine copulas (Sahin and Czado, 2022)
- We consider the k-means algorithm for clustering.
- Initial parameter values for the copula(s) are obtained using a Gaussian copula
- If marginals are Gaussian this means fitting a multivariate normal for each cluster.

Does This Work?

- For $T \in \{100, 1000, 5000\}$ and $d \in \{2, 5, 10\}$, we simulated a d-dimensional time series of length T from the 2-state HMM

$$\mathbf{Y}_t \mid (X_t = 1) \sim C_{\text{Frank}}\left((\mathcal{N}(\mu_{1,h} = -h, 1))_{h=1}^{d} \mid \theta_1 = 3\right)$$
$$\mathbf{Y}_t \mid (X_t = 2) \sim C_{\text{Clayton}}\left((\mathcal{N}(\mu_{2,h} = h, 1))_{h=1}^{d} \mid \theta_2 = 3\right)$$

  and estimated $\boldsymbol{\eta} = (\mu_{1,1}, \ldots, \mu_{2,d}, \theta_1, \theta_2)$ using both approaches

- Applied to the basic EM algorithm, R's `optim` with `L-BFGS-B` (i.e., quasi-Newton with box constraints) typically fails as soon as $d \geq 3$
  - The procedure is extremely sensitive to initial values and requires $\hat{\boldsymbol{\eta}}^{(0)} \approx \boldsymbol{\eta}$ just to avoid overflow
  - This kind of tuning is very tedious or impossible in high dimensions

Does This Work?

- We keep track of the time (in seconds) until the algorithm converges, and the L_2 error of the resulting estimate, $\epsilon = \|\boldsymbol{\eta} - \hat{\boldsymbol{\eta}}\|_2$
  - We used the `lbfgsb3c` package, which is more stable than `optim`

	$d = 2$	$d = 5$	$d = 10$
$T = 100$	111.9 s, $\epsilon = 0.14$	123.4 s, $\epsilon = 299.98$	111.8 s, $\epsilon > 10^9$
$T = 1000$	166.6 s, $\epsilon = 0.63$	169.5 s, $\epsilon > 10^{11}$	418.23 s, $\epsilon = 725.06$
$T = 5000$	?	?	?

Table: EM Algorithm

	$d = 2$	$d = 5$	$d = 10$
$T = 100$	5.1 s, $\epsilon = 2.9$	3.0 s, $\epsilon = 0.94$	4.2 s, $\epsilon = 0.58$
$T = 1000$	34.4 s, $\epsilon = 0.57$	22.9 s, $\epsilon = 0.60$	34.4 s, $\epsilon = 0.80$
$T = 5000$	172.6 s, $\epsilon = 0.13$	106.2 s, $\epsilon = 0.12$	168.7 s, $\epsilon = 0.19$

Table: EFM Algorithm

Numerical Experiment I

- Generative model:

$$\mathbf{Y}_i \mid (X_i = k) \sim C_k \left(SN(\cdot; \xi_{k,1}, \omega_{k,1}, \alpha_{k,1}), SN(\cdot; \xi_{k,2}, \omega_{k,2}, \alpha_{k,2}) \mid \tau_k \right),$$

for $k \in \{1, \ldots, 4\}$.

State	Copula family	τ_k	$\xi_{k,1}$	$\omega_{k,1}$	$\alpha_{k,1}$	$\xi_{k,2}$	$\omega_{k,2}$	$\alpha_{k,2}$
1	Clayton	0.2	-4	1	5	-1	1	-3
2	B4	0.4	-2	1	3	2	1	-3
3	Gaussian	0.6	0	1	5	3	1	-5
4	$t_{(\nu=5)}$	0.8	2	1	3	4	1	-5

Table: True parameters for the state-dependent distributions.

Numerical Experiment I

T:		500	1000	2500	5000
Stopping Rule Tolerance:	0.01	14	24	23	15
	0.001	17	26	25	17
	0.0001	36	59	62	39
	0.00001	230	115	460	269
Classifier:	k-means	0.9020	0.9090	0.9200	0.9196
	Local state decoding	0.9640	0.9640	0.9696	0.9732

Table: For each $T \in \{500, 1000, 2500, 5000\}$: (Top rows) Number of iterations taken by the EIFM algorithm applied to $\mathbf{Y}_{1:T}$ before stopping using L_1-norm tolerances in $\{0.01, 0.001, 0.0001, 0.00001\}$. (Bottom rows) Classification accuracy of initial k-means clustering and local decoding with parameter estimates provided by the EIFM algorithm.

Numerical Experiment II

- The state-dependent distributions are Markov trees in which all conditional relationships are independent.

Figure: Markov trees for state 1 (left) and state 2 (right)

- The state-dependent distributions have densities supported on $\mathbb{R}^5$ given by

$$h_1(\mathbf{y}) = c_{1,12}(\Phi(y_1 - \mu_{1,1}), \Phi(y_2 - \mu_{1,2}) \mid \tau_{1,12}) \cdot c_{1,23}(\Phi(y_2 - \mu_{1,2}), \Phi(y_3 - \mu_{1,3}) \mid \tau_{1,23})$$

$$\cdot\, c_{1,34}(\Phi(y_3 - \mu_{1,3}), \Phi(y_4 - \mu_{1,4}) \mid \tau_{1,34}) \cdot c_{1,45}(\Phi(y_4 - \mu_{1,4}), \Phi(y_5 - \mu_{1,5}) \mid \tau_{1,45}) \cdot \prod_{h=1}^{5} \varphi(y_h - \mu_{1,h})$$

and

$$h_2(\mathbf{y}) = c_{2,14}(\Phi(y_1 - \mu_{2,1}), \Phi(y_4 - \mu_{2,4}) \mid \tau_{2,14}) \cdot c_{2,43}(\Phi(y_4 - \mu_{2,4}), \Phi(y_3 - \mu_{2,3}) \mid \tau_{2,43})$$

$$\cdot\, c_{2,35}(\Phi(y_3 - \mu_{2,3}), \Phi(y_5 - \mu_{2,5}) \mid \tau_{2,35}) \cdot c_{2,52}(\Phi(y_5 - \mu_{2,5}), \Phi(y_2 - \mu_{2,2}) \mid \tau_{2,52}) \cdot \prod_{h=1}^{5} \varphi(y_h - \mu_{2,h})$$

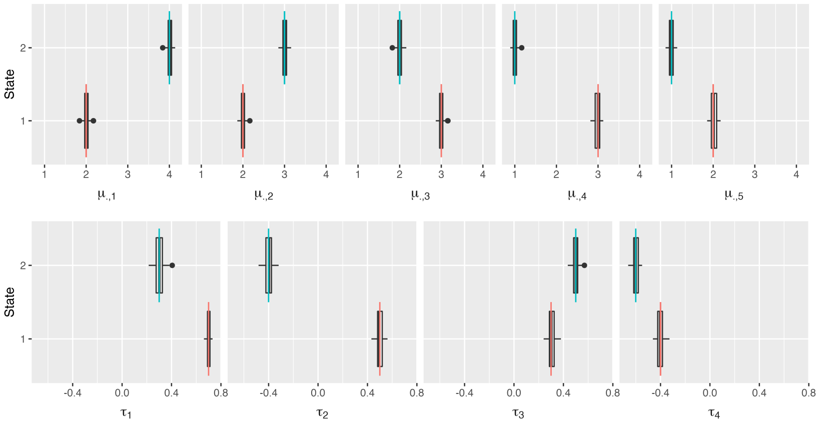


Figure: Parameter estimates based on 100 independent simulations and EIFM algorithm runs for the 5-dimensional 2-state HMMs

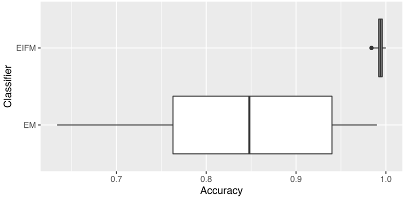


Figure: Accuracy across repetitions using initial independence model (bottom) and copula model (top)

Summary

- When using HMMs to model multivariate time series, ignoring the dependence between observed components can lead to...
  - Inaccurate state classifications
  - Failure to understand the true data-generating process
- The "copula-within-HMM" model integrates state-dependent copulas in order to capture joint information from the observed data, thereby addressing both problems
- The complexity of this model prohibits an application of the standard EM algorithm
- Our IFM-based refinement is faster and much more stable, but still produces estimators with desirable properties that perform as well or better in our experiments

Occupancy Data

- The ability to detect whether a room is occupied using sensor data (such as temperature and CO_2 levels) can potentially reduce unnecessary energy consumption by automatically controlling HVAC and lighting systems, without the need for motion detectors
- Consider three publicly-available labelled datasets presented by Candanedo and Feldheim (2016) which contain multivariate time series of four environmental measurements (light, temperature, humidity, CO_2) and one derived metric (the humidity ratio)
- Data contain binary indicators for whether the room was occupied or not at the time of measurement

Occupancy Data

- Several families of parametric copulas were tried

Family	AIC (State 1)	AIC (State 2)
Gauss	-370.786	-59.281
t	-437.542	-71.291
Clayton	-474.836	-66.087
Gumbel	-484.252	-72.437
Frank	-273.613	-66.497
Joe	-490.103	-64.995
Galambos	-295.549	-71.031
Hüsler-Reiss	-282.452	-61.547
BB1	-497.013	-70.509
BB6	-495.401	-70.435
BB7	**-518.923**	-68.207
BB8	-490.223	-66.738
Tawn (type 1)	-411.847	**-76.976**
Tawn (type 2)	-422.268	-55.382

Table: AICs for unoccupied (state 1) and occupied (state 2) classifications of the occupancy data.

Occupancy Data

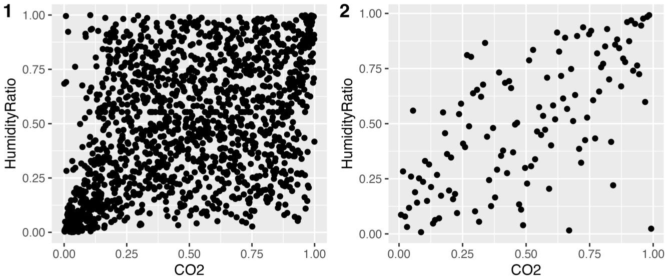


Figure: Pseudo-observations computed from unoccupied (Panel 1) and occupied (Panel 2) subsets.

Occupancy Data

Classifier	Train	Test 1
k-means clustering	0.865	0.818
Independence copulas within HMM	0.895	0.846
BB7/Tawn copulas within HMM	0.900	0.852

Table: Overall state classification accuracy for the training dataset and the test dataset, using *k*-means clustering and local decoding via the HMM with independent margins and the copula-within-HMM model.

Extensions and Future Work

- Can our algorithm be applied to models with continuous-time processes, and/or more general state spaces?
- How do we select the state-dependent copulas and/or the number of states in a fully unsupervised context?

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Paper available on my homepage: `http://www.utstat.toronto.edu/craiu/`