Statistical Elucidation of Latent Structures via Copulas

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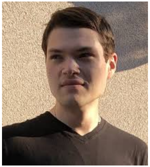
Outline

Copulas for serially correlated data with hidden structures

This project was done in collaboration with



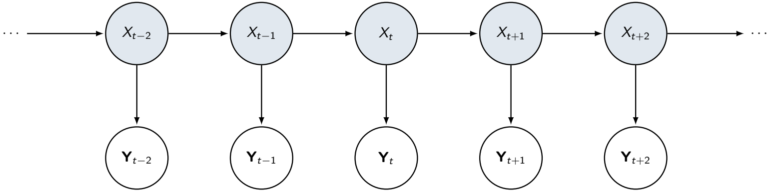
Robert Zimmerman (Imperial College London)

Vianey Leos Barajas (Toronto)

Paper: Copula Modelling of Serially Correlated Multivariate Data with Hidden Structures (JASA, 2024).

Hidden Markov Models: Briefly put

- 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.

Fusion of Multiple Data Sources

- In real-world applications (sports, stock exchange, animal movement, etc), 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 $\mathbf{Y}_t = (Y_{t,1}, \ldots, Y_{t,d})$ 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?

Occupancy Data

- The ability to detect whether a room is occupied using sensor data (such as temperature and CO_2 levels)
- 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), as well as binary indicators for whether the room was occupied or not at the time of measurement

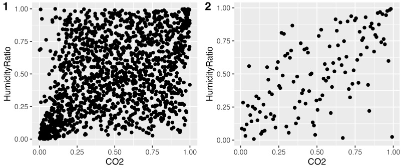


Figure: Pseudo-observations computed from unoccupied (Panel 1) and occupied (Panel 2) subsets.

Copulas: The Joys

- Copulas are mathematical devices used to model dependence between random variables regardless of their marginals.
- Copulas are useful for data fusion/integration as they lead to coherent joint models, even when the marginals are in different families or of different types.
- Copulas unlock information contained in the dependence part of the distribution (second-order) that complements the information in the marginals.
- Copulas extend statistical methods beyond the use of a multivariate Gaussian or Student.

At the root of it all, a theorem

- Copulas are distribution functions on $[0,1]^d$ that model dependence between continuous random variables.
- Sklar's Theorem: If $Y_1, Y_2, \dots Y_d$ are continuous r.v.'s with distribution functions (df) $F_1, \dots, F_d$, there exists an unique copula function $C : [0,1]^d \to [0,1]$ such that

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

- The copula bridges the marginal distributions of $Y_1, \dots, Y_d$ 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:

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

Copulas Within HMMs

- Here we consider a HMM $\{(\mathbf{Y}_t, X_t)\}_{t\geq 1} \subseteq \mathbb{R}^d \times \mathcal{X}$ in which the state-dependent distributions use 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, 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:

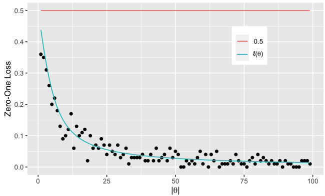


Figure: Zero-one losses for independent margins (red dots) and true model (blue dots)

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

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

Computation for HMMs Via the EM Algorithm

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

New problems

- The EIFM algorithm is not an GEM algorithm

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

does not imply

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

- 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).

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, $\epsilon = 0.29$	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.

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.

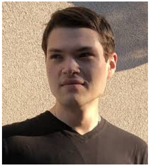
Occupancy Data

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.

Latent Variable Models with Copulas

This project is currently developed in collaboration with



Robert Zimmerman (Imperial College London)

Latent Variables (LV)

- The variable of interest W is sometimes impossible to measure directly
  - State of the economy
  - Traffic in a city
  - State of your health
  - State of a complex disease
- Instead, one measures
  - $\mathbf{Y} = (Y_1, \ldots, Y_k)^T$ whose components are surrogates of W and each provide partial information about W
  - Covariate $\mathbf{X} \in \mathbb{R}^p$
- We are often interested in the explanatory power of $\mathbf{X}$ for W.

An example

- Cardiotocography (CTG) is a medical procedure that monitors the fetal heart rate.
- The LV is the fetus' underlying state of health during birth, W.
- Our surrogate response is the bivariate vector (Q, Y) where
  - Q is the number of peaks (acceleration followed by a deceleration of heart beats) for the signal recorded by the CTG
  - Y is the log of mean short-term "beat-to-beat" variability (MSTV) where the short-term variability (STV) is obtained by measuring the time between successive R waves (cardiac systoles) of the fetus' electrocardiogram.
- The covariates are `FM` (fetal movement) and `UC` (uterine contraction), two continuous variables monitored during birth.

Conditional independence LV model

- A canonical LV model, given $W_i = X_i\beta + \epsilon$, is

$$
\begin{aligned}
&Y_i \perp Q_i | W_i \\
&Y_i \sim N(\mu_c + \lambda_c W_i, \sigma^2) \\
&Q_i \sim Poisson(\exp(\mu_d + \lambda_d W_i))
\end{aligned}
$$

- This implies that the two marginal regressions share a common random effect so they are marginally dependent (and conditionally independent)

- The induced dependence is not analytically available.

Conditional independence is a Copula LV

- The copula alternative is, conditional on W_i,

$$H(Y_i, Q_i|W_i) = C_{\theta_i}(F_Y(Y_i|W_i), F_Q(Q_i|W_i)), \;\; \theta_i = \kappa^{-1}(\xi_0 + \xi_1 W_i)$$
$$Y_i \sim N(\mu_c + \lambda_c W_i, \sigma^2); \; Q_i \sim Poisson(\exp(\mu_d + \lambda_d W_i))$$

- The whole joint distribution of (Y, Q) is varying with W not just the marginals.
- The copula captures the residual dependence on W after the marginal effects have been accounted for.
- The previous model is obtained when the copula is the independence copula.

Why the Conditional Copula?

- $Y_i|x \sim N(f_i(x), \sigma_i)$ $x \in \mathbb{R}^2$
- True marginal means:
  - $f_1(x) = 0.6\sin(5x_1) - 0.9\sin(2x_2)$
  - $f_2(x) = 0.6\sin(3x_1 + 5x_2)$
  - $\sigma_1 = \sigma_2 = 0.2$, $X_1 \perp X_2$.
- Copula: Frank with $\theta(x) = 0.71$
- Suppose x_2 is not observed so inference is based only on x_1

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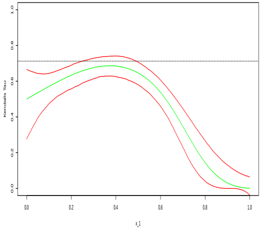


(Levi and Craiu, 2018)

CTG: The LV Copula Model

- $(Q_i, Y_i)|W_i$ has joint density

$$f_{(Q,Y)}(q,y) = f_c(y) \cdot \left[C_{d|c}\left(F_d(q), F_c(y)\right) - C_{d|c}\left(F_d(q-), F_c(y)\right)\right],$$

where

$$C_{d|c}(u_d, u_c) = \frac{\partial}{\partial u_c} C(u_d, u_c).$$

- Data Augmentation: Introduce latent variable Z such that

$$Q \stackrel{d}{=} F_d^-(F_Z(Z)),$$

- The copula between (Y, Z) is the same as the copula between (Y, Q)
- We can choose the distribution of Z to help the computation.
- For instance if we use a Gaussian copula, it helps to have $Z \sim N(0,1)$
- Craiu and Sabeti (2012); Smith and Khaled (2012).

CTG: The Augmented LV Copula Model

- The dependence between Y, Z and Q is defined by their joint conditional distribution

$$f_{(Q,Z,Y)|W}(q,z,y \mid w) = h(z,y \mid w, \mu_c, \lambda_c, \boldsymbol{\psi}_c, \boldsymbol{\xi}) \cdot \mathbb{1}_{F_Z^{-1}(F_d(q-|\varphi_d(\mu_d,\lambda_d,w))) \leq z < F_Z^{-1}(F_d(q|\varphi_d(\mu_d,\lambda_d,w)))}.$$

- Let $\boldsymbol{\xi} = (\xi_0, \xi_1) \in \mathbb{R}^2$ and $A(w) = \xi_0 + \xi_1 \cdot w$. Then we set

$$\theta(w, \boldsymbol{\xi}) = \frac{e^{A(w)} - e^{-A(w)}}{e^{A(w)} - e^{-A(w)}}$$

  as the correlation parameter of the bivariate Gaussian conditional copula of $(Y,Z)|W = w$.

- Parameters are a priori independent

Model Selection: WAIC

- The WAIC is defined as

$$\mathrm{WAIC}(\mathcal{M}) = -2\mathrm{fit}(\mathcal{M}) + 2\mathrm{p}(\mathcal{M}), \tag{3}$$

where the model fitness is

$$\mathrm{fit}(\mathcal{M}) = \sum_{i=1}^{n} \log\left(\mathbb{E}\left[\Pr(y_i, q_i|\omega, \mathcal{M})\right]\right) \tag{4}$$

and the penalty

$$\mathrm{p}(\mathcal{M}) = \sum_{i=1}^{n} \mathrm{Var}\left(\log\left(\Pr(y_i, q_i|\omega, \mathcal{M})\right)\right), \tag{5}$$

where ω contains all the parameters and latent variables in the model.

Spotlight on dependence: A conditional WAIC

- We use the following two conditional WAICs (Levi and Craiu, 2018)

$$\mathrm{CWAIC}_{Y|Q}(\mathcal{M}) = -2\sum_{i=1}^{n}\log\left(\mathbb{E}\left[\Pr(y_i|q_i,\omega,\mathcal{M})\right]\right) + \\ +2\sum_{i=1}^{n}\mathrm{Var}\left(\log\left(\Pr(y_i|q_i,\omega,\mathcal{M})\right)\right),$$

$$\mathrm{CWAIC}_{Q|Y}(\mathcal{M}) = -2\sum_{i=1}^{n}\log\left(\mathbb{E}\left[\Pr(q_i|y_i,\omega,\mathcal{M})\right]\right) + \\ +2\sum_{i=1}^{n}\mathrm{Var}\left(\log\left(\Pr(q_i|y_i,\omega,\mathcal{M})\right)\right),$$

- $\frac{1}{2}(\mathrm{CWAIC}_{1|2} + \mathrm{CWAIC}_{2|1})$ is asymptotically equivalent to the following CCV for the marginal (conditional) distribution

$$\mathrm{CCV}(\mathcal{M}) = \frac{1}{2}\left\{\sum_{i=1}^{n}\log\left(\Pr(y_i|q_i,\mathcal{D}_{-i},\mathcal{M})\right) + \sum_{i=1}^{n}\log\left(\Pr(q_i|y_i,\mathcal{D}_{-i},\mathcal{M})\right)\right\}.$$

Simulation Experiment

- Generate data using a Gaussian copula

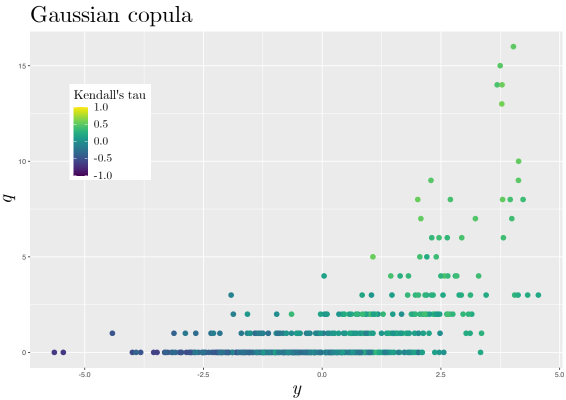


Figure: Bivariate scatterplot of the generated data with Gaussian copula, and Poisson and normal marginals

Simulation Experiment

- $\text{CWAIC}_{Y|Q}$ and $\text{CWAIC}_{Q|Y}$ selection criteria

Criteria\Copula	Gaussian	Frank	Gumbel	Clayton	Indep
$\text{CWAIC}_{Y\|Q}$	1627.36	1642.36	2395.17	1637.17	1606.31
$\text{CWAIC}_{Q\|Y}$	950.71	982.42	1673.57	976.05	997.43
Average	1289.04	1312.39	2034.37	1306.61	1301.87

Simulation Experiment

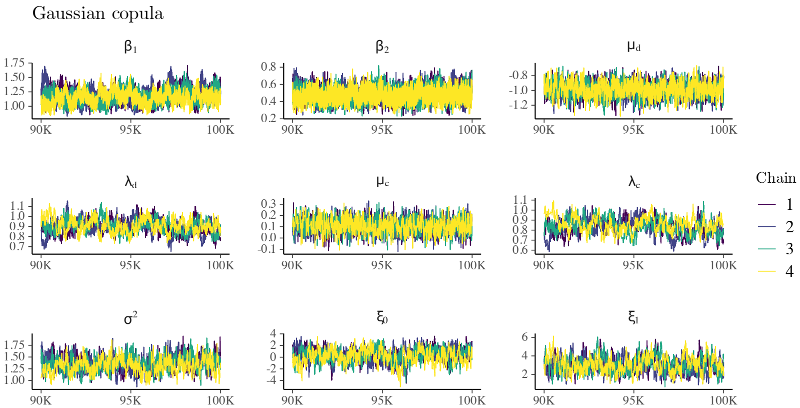
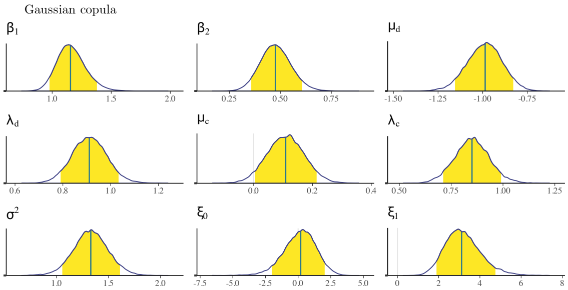


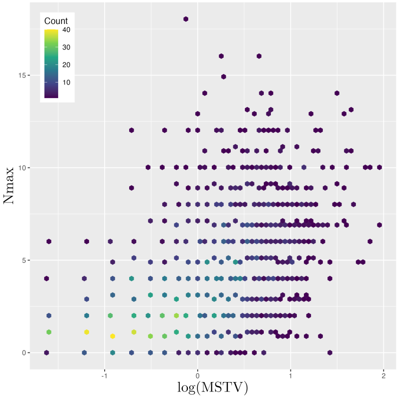
Figure: Traceplots for η's components.

Simulation Experiment



	β_1	β_2	λ_d	λ_c	ξ_1
Mean	1.18	0.48	0.90	0.84	3.10
True	1	0.5	1	1	3

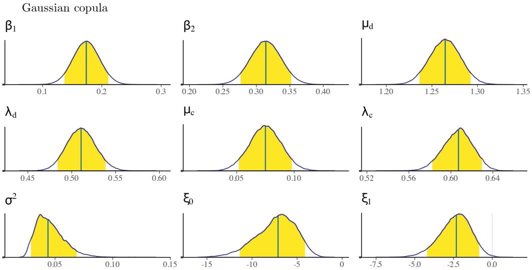
CTG: The data



CTG: Estimates

- $WAIC$, $WAIC_{Y|Q}$ and $WAIC_{Q|Y}$ all point to the Gaussian copula (over Gumbel, Frank, Clayton, Independence).
- The posterior means

	β_1 (FM)	β_2 (UC)	λ_d	λ_c	ξ_1
Mean	0.1744	0.3147	0.5101	0.6038	-2.3401



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