

Dependence modeling and computational algorithms: A surprising symbiosis

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Two themes

- ▶ Methods for modelling dependence patterns in the data so we can:
 - ▶ Fuse different data streams (today)
 - ▶ Extend the range of statistical models to capture complex generative processes
 - ▶ Improve inference (prediction, estimation, etc) (today)
 - ▶ **Modelling dependence is accompanied by computational challenges.** (today)
- ▶ Design of efficient computational algorithms for sampling or optimization.
 - ▶ Sampling is of paramount importance to Bayesian statisticians
 - ▶ Optimization is important to everyone
 - ▶ Introducing dependence in the design of sampling algorithms can improve performance (today)
 - ▶ **Coming up with the "right" dependence is challenging.**

Outline

Serially correlated data with hidden structures

Hidden Markov Models with Multivariate Observations

Copula Generalization

Estimation and Computation

A unified approach to antithetic sampling

The Antithetic Swindle

Antithetic Sampling techniques

Desirable properties

Sampling on Segments

Numerical Illustration

Copulas for serially correlated data with hidden structures

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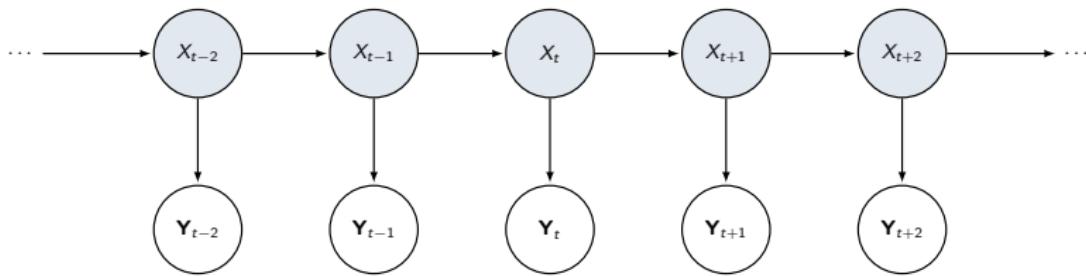
Paper: Copula Modelling of Serially Correlated Multivariate Data with Hidden Structures (JASA, 2024).

Hidden Markov Models: An Example

- ▶ We observe a system in time, e.g. the evolution of several stocks, the humidity and temperature in a room, the number of people late for work in Toronto, etc.
- ▶ We believe that these measurements are informative about variables that are not observed directly (they are hidden):
 - ▶ Stocks —> State of Economy
 - ▶ Room H and T —> State of occupancy
 - ▶ People late —> Traffic level
 - ▶ The hidden variables are not constant, but they also change in time.

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 $s \neq t$:



- ▶ $\mathbf{Y}_{t,h} | \{X_t = k\} \sim f_{k,h}(\cdot | \lambda_{k,h}) \quad \forall h = 1, \dots, d$
- ▶ $\{X_t\}$ 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 $\mathbf{Y}_t = (Y_{t,1}, \dots, Y_{t,d})$ cannot be assumed independent (even conditional on X_t)
- ▶ 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

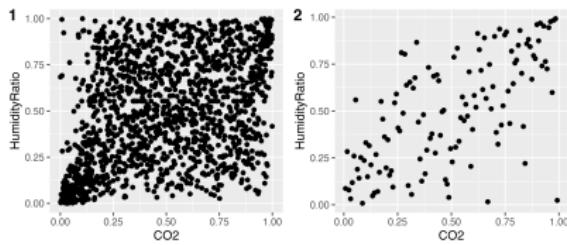


Figure: Pseudo-observations computed from unoccupied (Panel 1) and occupied (Panel 2) subsets.

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 $C : [0, 1]^d \rightarrow [0, 1]$ such that

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

- ▶ 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.

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.**

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:

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

- $C_k(\cdot, \dots, \cdot \mid \theta_k)$ is a d -dimensional parametric copula
- $\{X_t\}_{t \geq 1}$ is a Markov process on finite state space $\mathcal{X} = \{1, 2, \dots, K\}$ 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

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

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

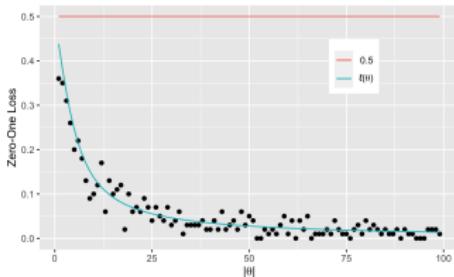


Figure: Zero-one losses for independent margins (red dots) and true model (blue dots)

Estimation with missing data

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

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

Computation for HMMs Via the EM Algorithm

- ▶ Without copula, the estimation is done via the EM algorithm
- ▶ The **E-Step** is straightforward
- ▶ The maximization required by the **M-Step** is unstable or plain unfeasible.
- ▶ The solution we found was to perform optimization in two steps:
 - ▶ First optimize the parameters of the marginal distributions
 - ▶ Second, optimize the parameters of the copulas after plugging in the marginal estimates obtained in the previous step.
- ▶ However, this approach changes the nature of the algorithm which is no longer "EM-like" so a proof of its validity is required.

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 $\boldsymbol{\eta} = (\mu_{1,1}, \dots, \mu_{2,d}, \theta_1, \theta_2)$ 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, $\epsilon = \|\eta - \hat{\eta}\|_2$
 - 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:

$\mathbf{Y}_i \mid (X_i = k) \sim C_k (SN(\cdot; \xi_{k,1}, \omega_{k,1}, \alpha_{k,1}), SN(\cdot; \xi_{k,2}, \omega_{k,2}, \alpha_{k,2}) \mid \tau_k),$
 for $k \in \{1, \dots, 4\}.$

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

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.

Living on the Edge: An Unified Approach to Antithetic Sampling

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Paper: Living on the Edge: An Unified Approach to Antithetic Sampling (Statistical Science, 2024).

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The Monte Carlo method

- ▶ The Monte Carlo method is at the core of model-based scientific exploration.
- ▶ It relies on approximating an integral of interest $I = \int f(\mathbf{x})\pi(\mathbf{x})d\mathbf{x}$ with $\hat{I}_d = \frac{1}{d} \sum_{i=1}^d f(\mathbf{X}_i)$ where
 - ▶ π is a probability density,
 - ▶ $f : \mathbb{R}^p \mapsto \mathbb{R}$ is a integrable function with respect to π
 - ▶ d is the Monte Carlo sample size
 - ▶ $\mathbf{X}_1, \dots, \mathbf{X}_d$ are iid samples from π .

The Antithetic Swindle

- ▶ Techniques needed to reduce the Monte Carlo sample size d , while maintaining the desired precision in estimation, are essential.
- ▶ *Variance reduction techniques* use statistical properties induced by the sampling design to reduce $\text{Var}(\hat{I}_d)$
- ▶ If the independence condition between samples X_1, \dots, X_d is dropped then

$$\mathbb{V}ar(\hat{l}_d) = \frac{1}{d^2} \sum_{i=1}^d \mathbb{V}ar(f(X_i)) + \frac{1}{d^2} \sum_{i \neq j} \mathbb{C}ov(f(X_i), f(X_j)).$$

- ▶ The antithetic swindle is executed when we are able to generate X_1, \dots, X_d so that the average covariance

$$\frac{1}{d^2} \sum_{i \neq j} \text{Cov}(f(X_i), f(X_j))$$

is negative.

Pairwise Construction

- ▶ The pairwise antithetic coupling introduced by [Hammersley and Morton \(1956\)](#) relies on $d/2$ (assume for a moment d is even) iid pairs of negatively correlated random variables (X_{1i}, X_{2i}) , $i = 1, \dots, d/2$.
- ▶ This is achieved by sampling using the quantile coupling:

$$X_{1i} \sim \pi, \quad X_{2i} = F_{\pi}^{-1}(1 - F_{\pi}(X_{1i})).$$

or

$$X_{1i} = F_{\pi}^{-1}(U), \quad X_{2i} = F_{\pi}^{-1}(1-U)$$

where $U \sim U(0, 1)$

- ▶ This procedure minimizes the correlation for any monotonic f in the case $d = 2$ and $p = 1$.
- ▶ However, the result doesn't hold for $d > 2$.

Beyond pairs: Latin Hypercube Sampling

- ▶ A popular procedure applicable to the general $d \geq 2, p \geq 1$ is the Latin Hypercube sampling ([McKay et al., 1979](#)).
- ▶ Given a standard uniform d -dimensional random vector \mathbf{V} and $\mathcal{D}^\sigma = (\sigma(0), \dots, \sigma(d-1))^T$, a permutation of $\{0, 1, \dots, d-1\}$ independent of \mathbf{U} , set

$$\mathbf{U} = \frac{1}{d} (\mathcal{D}^\sigma + \mathbf{V}). \quad (2)$$

► $d = 2$ and $D^\sigma = (0, 1)$:

$$U_1 = \frac{V_1}{2} \in \left(0, \frac{1}{2}\right), \quad U_2 = \frac{1+V_2}{2} \in \left(\frac{1}{2}, 1\right).$$

► $d = 3$ and $D^\sigma = (2, 0, 1)$:

$$U_1 = \frac{2+V_3}{3} \in \left(\frac{2}{3}, 1 \right), \quad U_2 = \frac{V_1}{3} \in \left(0, \frac{1}{3} \right), \quad U_3 = \frac{1+V_2}{3} \in \left(\frac{1}{3}, \frac{2}{3} \right).$$

Concordance Order

- ▶ Let \mathbf{X} and \mathbf{Y} be random vectors with CDFs F and G , respectively.
- ▶ \mathbf{Y} is more concordant than \mathbf{X} (written $\mathbf{X} \prec_C \mathbf{Y}$) if

$$F(x) \leq G(x), \quad \forall x \in \mathbb{R}^d.$$

- ▶ If $\mathbf{X}, \mathbf{Y} \in \mathbb{R}^d$ satisfy $\mathbf{X} \prec_C \mathbf{Y}$ then

$$\mathbb{V}ar \left(\sum_{h=1}^d b_h f(X_h) \right) \leq \mathbb{V}ar \left(\sum_{h=1}^d b_h f(Y_h) \right), \quad \forall \mathbf{b} \in \mathbb{R}^d$$

Countermonotonicity

- ▶ Consider a random vector $\mathbf{U} \in \mathbb{R}^d$ with uniform marginals
- ▶ \mathbf{U} is said to be d -countermonotonic (d -CTM), if there exists a family $\{g_h\}_{1 \leq h \leq d}$ of strictly increasing continuous functions $[0, 1] \mapsto \mathbb{R}$ and some $k \in \mathbb{R}$ such that:

$$\sum_{h=1}^d g_h(U_h) = k \text{ a.s.} \quad (3)$$

- ▶ It has been shown that the set of d -CTM vectors is contained in the subset of elements minimal in concordance order [Lee et al. \(2017\)](#)
- ▶ Bottom line: construct $\mathbf{U} \in \mathbb{R}^d$ with uniform marginals such that $\sum_{l=1}^d g_l(U_l) = \text{const}$ (often $g_l(u_l) = u_l$)
- ▶ Note that the LH vector \mathbf{U} is d -CTM iff \mathbf{V} is d -CTM.

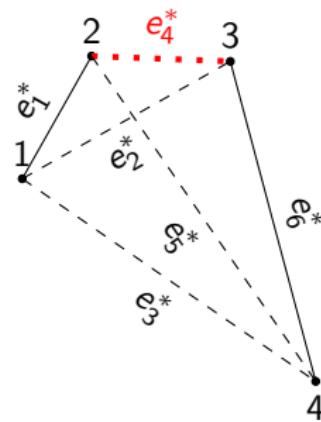
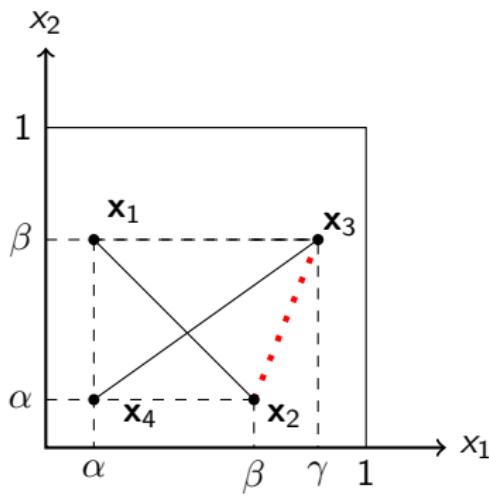
Sampling on segments

- ▶ Sampling with equal probability on a collection \mathcal{S} of line segments in the d -dimensional Euclidean space.
- ▶ Since each segment is uniquely characterized by its endpoints or vertexes, the collection \mathcal{S} can be equivalently represented by the set of vertex pairs that define the segments and their coordinates.
- ▶ This representation is efficient in large dimensions even when the segments share some of their vertexes.

Set up and notation

- ▶ Consider the vertex set $\mathcal{V} = \{1, \dots, n\}$ as a set of points in the d -dimensional hypercube
- ▶ The coordinates of the k -th vertex form the column vector $\mathbf{x}_k \equiv (x_{1k}, \dots, x_{dk})^T \in [0, 1]^d$
- ▶ The coordinate matrix $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ as the collection of vertex coordinates.
- ▶ There is an edge $e = (i, j)$ between i and j , with $i < j$, if there is a segment joining the two vertices i and j

Illustration



Consider the collection of segments in the left plot with coordinate matrix

$$\mathbf{X} = \begin{pmatrix} \alpha & \beta & \gamma & \alpha \\ \beta & \alpha & \beta & \alpha \end{pmatrix}, \quad (4)$$

where $\alpha < \beta \leq \gamma \in \mathbb{R}$. The edge set is: $\mathcal{E}^* = \{e_1^* = (1, 2), e_2^* = (1, 3), e_3^* = (1, 4), e_4^* = (2, 3), e_5^* = (2, 4), e_6^* = (3, 4)\}$

Sampling on segments

- ▶ The collection of segments is defined by the edge set $\mathcal{E} = \{(i, j) \in \mathcal{V} \times \mathcal{V}\}$.
- ▶ Then $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$ is an undirected graph and $\mathcal{S} = \{\mathcal{G}, \mathbf{X}\}$ is the collection of segments.
- ▶ The lexicographic order on vertex indexing induces an order on the edge set
- ▶ The map $\varphi_{\mathcal{E}} : \{1, \dots, |\mathcal{E}|\} \mapsto \mathcal{E}$, $k \rightarrow (i(k), j(k))$ associates the k -th element, $e_k \in \mathcal{E}$, to its couple of vertices.

Sampling on segments

1. Draw $V \sim \mathcal{U}[0, 1]$ and $W \sim \mathcal{U}[0, 1]$ independently;
2. Use W to choose with uniform probability on the edge set \mathcal{E} the edge e_K and obtain the random pair of vertices $(I, J) = (i(K), j(K))$ with $(i(K), j(K)) = \varphi_{\mathcal{E}}(K)$;
3. Obtain a random point on the segment joining vertices I and J with uniform probability

$$\begin{aligned} U_1 &= x_{1I}V + (1 - V)x_{1J}, \\ &\vdots \\ U_d &= x_{dI}V + (1 - V)x_{dJ}. \end{aligned} \tag{5}$$

Edge living and d-CTM

- d -CTM leads to:

$$\mathbb{E} \left[\sum_{j=1}^d U_j \right] = \sum_{j=1}^d \mathbb{E} [U_j] = \frac{d}{2}.$$

- The constant sum condition can be written as a linear restriction on the coordinates of the vertices \mathbf{x}_k , that is

$$\sum_{h=1}^d U_h = \sum_{h=1}^d x_{hJ} + V \left[\sum_{h=1}^d x_{hI} - \sum_{h=1}^d x_{hJ} \right] = \frac{d}{2},$$

- This needs to be valid for all V and (I, J) so all vertices should be in the hyperplane of constant sum, i.e.

$$\sum_{h=1}^d x_{hk} = \sum_{h=1}^d \sum_{m=1}^{n_I} a_{h,m} \mathbb{I}_{\mathcal{M}_{h,m}}(k) = \frac{d}{2} \quad k = 1, \dots, n.$$

Additional remarks

- ▶ Sampling on segments can be guaranteed to produce uniform samples in the unit hypercube under certain verifiable assumptions (about the segments).
- ▶ We recover many existing antithetic constructions.
- ▶ The joint distribution of (U_1, \dots, U_d) is a copula (remember them?).
- ▶ This is a new copula family with some unusual properties (under study).

Probit regression

- ▶ The data represent the clinical characteristics summarized by two covariates of 55 patients, of which 19 were diagnosed with lupus.
- ▶ $Y_i \sim \text{Ber}(\Phi(\mathbf{x}_i^T \boldsymbol{\beta}))$ where Φ is the standard normal CDF and $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2)^T$ is the vector of parameters.
- ▶ We introduce latent variables $\psi_i \sim \mathcal{N}(\mathbf{x}_i^T \boldsymbol{\beta}, 1)$
- ▶ The sampling algorithm iterates between these two steps:
 - ▶ Sample $\boldsymbol{\beta} | \psi \sim \mathcal{N}\left(\tilde{\boldsymbol{\beta}}, (\mathbf{X}^T \mathbf{X})^{-1}\right)$ with $\tilde{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \psi$ with \mathbf{X} the data matrix whose i -th row is \mathbf{x}_i .
 - ▶ $\psi_i | \boldsymbol{\beta}, Y_i \sim \mathcal{T}\mathcal{N}(\mathbf{x}_i^T \boldsymbol{\beta}, 1, Y_i)$ where $\mathcal{T}\mathcal{N}(\mu, \sigma^2, Y)$ is a the normal distribution with mean μ and variance σ^2 , truncated to be positive if $Y > 0$ or negative otherwise.

Probit regression

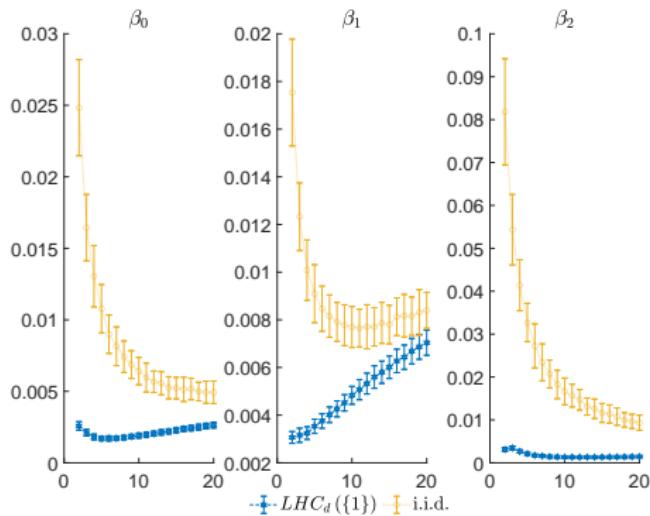


Figure: Monte Carlo variance of the posterior mean estimator (vertical axis) for different numbers of antithetic variates d (horizontal axis). In each plot: the average variance of antithetic Gibbs (blue dots) and of iid Gibbs (yellow dots) with their range (vertical segments). Note: all estimates are based on 100 independent experiments. In each experiment, the Gibbs sampler runs for 10 seconds.

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