Bayesian Inference for Conditional Copulas using Gaussian Process Single Index Models

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Abstract

Parametric conditional copula models allow the copula parameters to vary with a set of covariates according to an unknown calibration function. In this paper we develop flexible Bayesian inference for the calibration function of a bivariate conditional copula. We construct a prior distribution over the set of smooth calibration functions using a sparse Gaussian process (GP) prior for the single index model (SIM). The estimation of parameters from the marginal distributions and the calibration function is done jointly via Markov Chain Monte Carlo sampling from the full posterior distribution. We introduce a new Conditional Cross Validated Pseudo-Marginal (CCVML) criterion that is used to perform copula selection and is modified using a permutation-based procedure to assess data support for the simplifying assumption. The performance of the estimation method and model selection criteria is studied via a series of simulations using correct and misspecified models with Clayton, Frank and Gaussian copulas and a numerical application involving red wine features.

Keywords: Conditional Copula, Cross Validated Marginal Likelihood, Gaussian Process, Simplifying Assumption, Single Index Model.

1 Introduction and Motivation

Copulas are useful in modelling the dependent structure in the data when there is interest in separating it from the marginal models or when none of the existent multivariate distributions are

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suitable. For continuous multivariate distributions, the elegant result of Sklar (1959) guarantees the existence and uniqueness of the copula \( C : [0, 1]^p \rightarrow [0, 1] \) that links the marginal cumulative distribution functions (cdf) and the joint cdf. Specifically,
\[
H(Y_1, \ldots, Y_p) = C(F_1(Y_1), \ldots, F_p(Y_p)),
\]
where \( H \) is the joint cdf, and \( F_i \) is the marginal cdf for variable \( Y_i \), for \( 1 \leq i \leq p \), respectively.

The extension to conditional distributions via the conditional copula was used by Lambert and Vandenhende (2002) and subsequently formalized by Patton (2006) so that
\[
H(Y_1, \ldots, Y_p | X) = C_X(F_1|X(Y_1 | X), \ldots, F_p|X(Y_p | X)),
\]
where \( X \in \mathbb{R}^q \) is a vector of conditioning variables, \( C_X \) is the conditional copula that may change with \( X \) and \( F_i|X \) is the conditional cdf of \( Y_i \) given \( X \) for \( 1 \leq i \leq p \). A parametric model for the conditional copula assumes \( C_X = C_{\theta(X)} \) belongs to a family of copulas and only the parameter \( \theta \in \Theta \) varies as a function of \( X \). In the remaining of this paper we assume that there exists a known one-to-one function \( g : \Theta \rightarrow \mathbb{R} \) such that \( \theta(X) = g^{-1}(\eta(X)) \) with the calibration function \( \eta : \mathbb{R} \rightarrow \mathbb{R} \) in the inferential focus.

There are a number of reasons one is interested in estimating the conditional copula. First, in regression models with multivariate responses, one may want to determine how the dependence structure among the components of the response varies with the covariates. This model will ultimately impact the performance of model-based prediction. For instance, for a bivariate response in which one component is predicted given the other, the conditional density takes the form
\[
h(y_1 | y_2, x) = f(y_1 | x)c_{\theta(x)}(F_1|_x(y_1 | x), F_2|_x(y_2 | x)),
\]
where \( c_{\theta(x)} \) is the density of the conditional copula \( C_{\theta(x)} \). Hence, in addition to the information contained in the marginal model, in equation (2) we use for prediction also the information in the other responses.

Second, when specifying a general multivariate distribution, the conditional copula is an essential ingredient. For instance, if \( U_1, U_2, U_3 \) are three Uniform(0, 1) variables then their joint density is
\[
c(u_1, u_2, u_3) = c_{12}(u_1, u_2)c_{23}(u_2, u_3)c_{\theta(u_2)}(P(U_1 \leq u_1 | u_2), P(U_3 \leq u_3 | u_2) | u_2).
\]
Finally, a conditional copula with predictor values \( X \in \mathbb{R}^q \) in which \( \eta(X) \) is constant, may exhibit non-constant patterns when some of the components of \( X \) are not included in the model. 

This point will be revisited in section 5.1.

When estimation for the conditional copula model is contemplated, one must consider that there are multiple sources of error and each will have an impact on the model. Even in the simple case in which the estimation of the marginals and copula suffer from errors that depend only on \( x \) one obtains

\[
c_{\theta(x) + \delta_1(x)}(F_{1|x}(y_1|x) + \delta_1(x), F_{2|x}(y_2|x) + \delta_2(x)) = c_{\theta(x)}(F_{1|x}(y_1|x), F_{2|x}(y_2|x)) + O(|\delta(\gamma||\xi)|)
\]

where \( c^{(1,0,0)} \), \( c^{(0,1,0)} \) and \( c^{(0,0,1)} \) are the partial derivatives of \( c_{\gamma}(x,y) \) w.r.t. \( x \) and \( y \), respectively. 

The right hand term in equation (3) marks the correct term joint likelihood while (4)-(6) show the biases incurred due to errors in estimating the first and second marginal conditional cdf’s and the copula calibration function, respectively. It becomes apparent that in order to keep the estimation error low, one must consider flexible models for the marginals and the copula.

Depending on the strength of assumptions we are willing to make about \( \eta(X) \), a number of possible approaches are available. The most direct is to assume a known parametric form for the calibration function, e.g. constant or linear, and estimate the corresponding parameters by maximum likelihood estimation (Genest et al., 1995). This approach relies on knowledge about the shape of the calibration function which, in practice, can be unrealistic. A more flexible approach uses non-parametric methods (Acar et al., 2011; Veraverbeke et al., 2011) and estimate the calibration function using smoothing methods. For univariate \( X \), Craiu and Sabeti (2012a) devised Bayesian inference based on a flexible cubic spline model and for multivariate \( X \), Sabeti et al. (2014), Chavez-Demoulin and Vatter (2015) and Klein and Kneiß (2015) avoid the curse of dimensionality that appears even for moderate values of \( q \), say \( q > 3 \), by specifying an additive model structure for the calibration function. Few alternatives to the additive structure exist. One exception is Hernández-Lobato et al. (2013) who used a sparse Gaussian Process (GP) prior for estimating the calibration function and subsequently used the same construction for vine copulas.
estimation in Lopez-Paz et al. (2013). However, when the dimension of the predictor space is even moderately large the curse of dimensionality prevails and it is expected that the $q$-dimensional GP used for calibration estimation will not capture important patterns for sample sizes that are not very large. Moreover, the full efficiency of the method proposed in Hernández-Lobato et al. (2013) is difficult to assess since their model is build with uniform marginals, which in a general setup is equivalent to assuming exact knowledge about the marginal distributions. In fact, when the marginal distributions are estimated it is of paramount importance to account for the resulting variance inflation due to error propagation in the copula estimation as reflected by equations (3)-(6). The Bayesian model in which joint and marginal components are simultaneously considered will appropriately handle error propagation as long as it is possible to study the full posterior distribution of all the parameters in the model, be they involved in the marginals or copula specification.

Great dimension reduction of the parameter space is achieved under the so-called simplifying assumption (SA) that assumes $C_X = C$ for all $X$, i.e. the conditional copula is constant (Gijbels et al., 2015). The SA condition can significantly simplify the vine copula estimation (for example, see Aas et al., 2009), but it is known to lead to bias when the model ignores its violation (Acar et al., 2012). Therefore, for conditional copula models it is of practical interest to assess whether the data supports or not SA. A first step towards a formal test for SA can be found in Acar et al. (2013). The reader is referred to Derumigny and Fermanian (2016) for an excellent review of work on SA, and ideas for future work.

This paper’s contribution is two-fold: on one hand we consider Bayesian joint analysis of the marginal and copula models using flexible GP models. Our emphasis is placed on the estimation of the calibration function $\eta(x)$ which is assumed to have a GP prior that is evaluated at $\beta^T X$ for some normalized $\beta$, thus coupling the GP-prior construct with the single index model (SIM) of Choi et al. (2011) and Gramacy and Lian (2012). The GP-SIM is more flexible than a canonical linear model and computationally more manageable than a full GP with $q$ variables. The proposed model can be used for large covariate dimension $q$ and for large samples. Both marginal means will be fitted using sparse GP approaches so that large data sets can be computationally manageable. The dimension reduction of the SIM approach has been noted also by Fermanian and Lopez (2015).
but their method differs in fundamental aspects from the one proposed here. So far, GP-SIM’s have been used mostly in regression settings where the algorithm of Gramacy and Lian (2012) can be used to efficiently sample the posterior distribution. However, the GP-SIM model for conditional copulas involves a non-Gaussian likelihood which requires a new sampling algorithm.

A second contribution of the paper deals with model selection issues that are particularly relevant for the conditional copula construction. We consider of importance the choice of copula family and identifying whether the simplifying assumption (SA) is supported by the data. For the former task we develop a conditional cross-validated marginal likelihood (CCVML) criterion and also examine the performance of the Watanabe Information Criterion (Watanabe, 2010), while for determining whether the data supports the SA assumption or not we construct a permutation-based variant of the CVML that shows good performance in our numerical experiments. Finally, we identify an important link between SA and missing covariates in the conditional copula model. To our knowledge, this connection has not been reported elsewhere.

In the next section we review the GP-SIM formulation and introduce the notation. The construction of the conditional copula model, the computational algorithm and the model selection procedures are covered in Section 3. In Section 4 we illustrate the efficiency of the method via simulation and a numerical analysis of wine data. All the contributions relevant to the important issue of SA are included in Section 5. The paper ends with conclusions and directions for future work.

2 Brief review of Bayesian inference for Sparse GP

Assume we observe $n$ independent observations $\{(x_i, y_i), \ i = 1 \ldots n\}$, where $Y_i \in \mathbb{R}$ is the response variable and $X_i \in \mathbb{R}^q$ is a vector of covariates. Suppose that the probability distribution of $Y_i$ has a known form and depends on $X_i$ through some unknown function $f$, e.g. $Y_i \overset{\text{ind}}{\sim} \mathcal{N}(f(X_i), \sigma^2)$. The goal is to estimate the unknown smooth function $f : \mathbb{R}^q \rightarrow \mathbb{R}$. A Gaussian Process (GP) prior on the function $f$ implies

$$
(f(X_1), f(X_2), \ldots, f(X_n))^T \sim \mathcal{N}(0, K(X, X; w)), \quad (7)
$$
where $\mathcal{N}(\mu, \Sigma)$ denotes a multivariate normal distribution with mean $\mu$ and variance covariance matrix $\Sigma$ and $K$ is a covariance matrix which depends on $X_1, \ldots, X_n$ and additional parameters.

In this paper we use the squared exponential kernel to model the matrix $K(X, X; \mathbf{w})$, i.e. its $(i, j)$ element is

$$k(X_i, X_j; \mathbf{w}) = e^{w_0} \exp \left[ -\sum_{s=1}^{s=q} \frac{(X_{is} - X_{js})^2}{e^{w_s}} \right]. \quad (8)$$

The unknown parameters $\mathbf{w} = (w_0, \ldots, w_q)$ that determine the strength of dependence in (8) are inferred from the data.

In the case in which the covariate dimension, $q$, is moderately large, an accurate estimation of $f$ will require a large sample size, $n$. Unfortunately, this desideratum is hindered by the computational complexity involved in fitting a GP model when $n$ is large, as the MCMC sampler designed to sample from the posterior require at each iteration the calculation and inversion of the matrix $K(X, X; \mathbf{w}) \in \mathbb{R}^{n \times n}$.

To make GP models applicable for larger data we follow the literature on sparse GP (more details can be found in Quiñonero-Candela and Rasmussen, 2005; Snelson and Ghahramani, 2005; Naish-Guzman and Holden, 2007) in which it is assumed that learning about $f$ can be achieved using a smaller sample of $m$ latent variables, called inducing variables, that channel the information contained in the covariates $\{x_1, \ldots, x_n\}$. To complete the description we consider the following notation: if the original covariates are $X = (x_1, \ldots, x_n)^T \in \mathbb{R}^{n \times q}$ and the inducing variables are $X^* = (x_1^*, \ldots, x_m^*)^T \in \mathbb{R}^{m \times q}$ then we denote $K(X, X^*; \mathbf{w}) \in \mathbb{R}^{n \times m}$ the matrix

$$K(X, X^*; \mathbf{w}) = \begin{bmatrix}
k(x_1, x_1^*; \mathbf{w}) & \cdots & k(x_1, x_m^*; \mathbf{w}) \\
\vdots & \ddots & \vdots \\
k(x_n, x_1^*; \mathbf{w}) & \cdots & k(x_n, x_m^*; \mathbf{w})
\end{bmatrix}, \quad (9)$$

where $k(x_i, x_j^*; \mathbf{w})$ is defined as in (8). We also define the following two matrices that will be used throughout the paper

$$A(X^*, X; \mathbf{w}) = K(X^*, X, \mathbf{w})K(X, X, \mathbf{w})^{-1},$$

$$B(X^*, X; \mathbf{w}) = K(X^*, X^*, \mathbf{w}) - K(X^*, X, \mathbf{w})K(X, X, \mathbf{w})^{-1}K(X^*, X, \mathbf{w})^T. \quad (11)$$

The ratio $m/n$ influences the trade-off between computational efficiency and statistical efficiency, as a smaller $m$ will favour the former and a larger $m$ will ensure no significant loss of the latter.
We assume $X_j^* = X_{u_j}$ for $j = 1, \ldots, m$ and the function values for the inducing points are
\[
\tilde{f} = (f(x_{u_1}), \ldots, f(x_{u_m}))^T = (f_{u_1}, \ldots, f_{u_m})^T. 
\]
The joint density of the response $Y$, the latent variable $\tilde{f}$ and the parameter $w$ can be expressed only in terms of the $m$-dimensional vector $\tilde{f}$ since
\[
P(Y, \tilde{f}, w | X, \tilde{X}) = P(Y | A(X, \tilde{X}; w) \tilde{f}) N(\tilde{f}; 0, K(\tilde{X}, \tilde{X}; w)) p(w),
\]
where $p(w)$ is the prior probability for the parameters $w$. The posterior distribution $\pi(\tilde{f}, w | D)$ is still not tractable, but sampling from it will be much less expensive since $K(X, \tilde{X}; w) \in \mathbb{R}^{n \times m}$ and $K(\tilde{X}, \tilde{X}; w) \in \mathbb{R}^{m \times m}$. So far we have assumed that the inducing inputs $\tilde{X}$ are selected from the samples collected. A data-driven alternative is to choose $x_{u_1}, \ldots, x_{u_m}$ as the centers of $m$ clusters created from the original covariates $X$ via a simple k-means algorithm [Bishop, 2006]. Intuitively, it makes sense to have more inducing points in regions that exhibit more variation in covariate values.

Finally, in order to reduce the dimensionality of the parameter space, we assume that
\[
\tilde{f}(x_i) = \tilde{f}(x_i^T \beta),
\]
and we set $\tilde{f} = (\tilde{f}(x_1^T \beta), \ldots, \tilde{f}(x_n^T \beta))^T$, where $\tilde{f} : \mathbb{R} \to \mathbb{R}$ is an unknown function that is part of inferential focus and $\beta \in \mathbb{R}^q$ is normalized, i.e. $\|\beta\| = 1$. Note that without normalization the parameter $\beta$ is not identifiable. The single index model (SIM) defined by (13) coupled with the sparse GP approach has the advantage that it casts the original problem of estimating a general function $f$ in $q$ dimensions based on $n$ observations into the estimation of $q$-dimensional parameter vector $\beta$ and of the one-dimensional map $\tilde{f}$ based on $m << n$ inducing points.

### 3 GP-SIM for Conditional copula

Suppose that the observed data $D = \{(Y_{1i}, Y_{2i}, x_i) \mid i = 1 \ldots n\}$ consists of triplets $(Y_{1i}, Y_{2i}, X_i)$ where $Y_{1i}, Y_{2i} \in \mathbb{R}$ and $X_i \in \mathbb{R}^q$. For notational convenience let $Y_1 = (Y_{11}, \ldots, Y_{1n})^T$, $Y_2 = (Y_{21}, \ldots, Y_{2n})^T$ and $X = (X_1, \ldots, X_n)^T$. We assume that the marginal distribution of $Y_{ji}$ ($j = 1, 2$) is Gaussian with mean $f_j(x_i)$ and constant variance $\sigma_j^2$. If we let $f_j = (f_j(x_1), \ldots, f_j(x_n))^T$ we can compactly write:
\[
P(Y_j | X) = N(f_j, \sigma_j^2 I_n) \quad j = 1, 2.
\]
We use a conditional copula to account for the fact that the dependence between the responses varies with covariate $X$. The likelihood is

$$P(Y_1, Y_2|X) = \prod_{i=1}^{n} \frac{1}{\sigma_1} \phi \left( \frac{Y_{1i} - f_{1i}}{\sigma_1} \right) \frac{1}{\sigma_2} \phi \left( \frac{Y_{2i} - f_{2i}}{\sigma_2} \right) \times c \left( \Phi \left( \frac{Y_{1i} - f_{1i}}{\sigma_1} \right), \Phi \left( \frac{Y_{2i} - f_{2i}}{\sigma_2} \right) | \theta(x_i) \right).$$  

(15)

Here $c$ denotes a parametric copula density function, while $\Phi$ and $\phi$ are the cumulative probability function and density function of a standard normal distribution, respectively. The parameter of a copula depends on the unknown function $\theta(x_i) = g^{-1}(f(x_i))$, where $f$ is assumed to take the form given in (13) and $g$ is a known invertible link function that allows an unrestricted parameter space for $f$. It is worth noting that the GP-SIM model used for estimating the copula parameter is invariant to the scale used. For instance, whether one chooses to estimate the calibration for the copula parameter, $\theta(X)$, or Kendall’s $\tau(X)$, the form given in (13) will be valid for both. However, this is not true in general for additive models, since a non-linear transformation will break the additivity.

The GP-SIM is fully specified once we assign the GP priors to $f_1, f_2, f$ and the parametric priors for the remaining parameters, as follows:

$$f_1 \sim \mathcal{GP}(w_1), \quad f_2 \sim \mathcal{GP}(w_2), \quad f \sim \mathcal{GP}(w),$$

$$w_1 \sim N(0, 5I_{q+1}), \quad w_2 \sim N(0, 5I_{q+1}), \quad w \sim N(0, 5I_2),$$

$$\beta \sim U(S^q - 1), \quad \sigma_1^2 \sim IG(0.1, 0.1), \quad \sigma_2^2 \sim IG(0.1, 0.1).$$  

(16)

The $\mathcal{GP}(w)$ is a Gaussian Process prior with mean of 0, squared exponential kernel with parameters $w$, $U(S^q - 1)$ is a uniform distribution on the surface of the $q$-dimensional unit sphere and $IG(\alpha, \beta)$ denotes the inverse gamma distribution. Because the focus of the paper is on inference for the copula, we allow $f_1$ and $f_2$ to be evaluated on $\mathbb{R}^q$ while $f$ is on $\mathbb{R}$. In order to avoid computational problems that affect the GP-based inference when the sample size is large, the inference will rely on the Sparse GP method that was described in the previous section. Suppose $\tilde{X}_1$ are $m_1$ inducing inputs for function $f_1$, $\tilde{X}_2$ are $m_2$ inducing inputs for function $f_2$ and $\tilde{Z}$ are $m$ inducing inputs for function $f$. Also let $\tilde{f}_1$ be $f_1$ evaluated at $\tilde{X}_1$, $\tilde{f}_2$ be $f_2$ evaluated at $\tilde{X}_2$ and $\tilde{f}$ be $f$ evaluated at $\tilde{Z}$. 
Then the joint density of the observed data and parameters is proportional to:

\[
P(Y_1, Y_2, \tilde{f}_1, \tilde{f}_2, \tilde{f}, w_1, w_2, \sigma_1^2, \sigma_2^2, \beta | X, \tilde{X}_1, \tilde{X}_2, \tilde{Z}) \propto N(Y_1; f_1, \sigma_1^2 I_n)N(Y_2; f_2, \sigma_2^2 I_n) \times 
\]

\[
\times \prod_{i=1}^{i=n} \left( \Phi \left( \frac{Y_{1i} - f_{1i}}{\sigma_1} \right), \Phi \left( \frac{Y_{2i} - f_{2i}}{\sigma_2} \right) \right) \right) \times N(\tilde{f}_1; 0, K(\tilde{X}_1, \tilde{X}_1; w_1)) \times 
\]

\[
\times N(\tilde{f}_2; 0, K(\tilde{X}_2, \tilde{X}_2; w_2))N(\tilde{f}; 0, K(\tilde{Z}, \tilde{Z}; w))N(w_1; 0, 5I_{q+1}) \times 
\]

\[
N(w_2; 0, 5I_{q+1}) N(w; 0, 5I_2) IG(\sigma_1^2; 0, 0.1) IG(\sigma_2^2; 0, 0.1),
\]

where \( f_1 = A(X, \tilde{X}_1; w_1) \tilde{f}_1, \ f_2 = A(X, \tilde{X}_2; w_2) \tilde{f}_2 \) and \( f = A(X, \beta, \tilde{Z}; w) \tilde{f} \). The number of inducing inputs \( m_1 \), \( m_2 \) and \( m \) can all be different but in our applications we will choose their values to be significantly smaller than the sample size, \( n \). Ideally we need the number of inducing inputs to be as large as possible but at the same time make the MCMC implementation computationally feasible.

As suggested earlier we can define \( \tilde{X}_1 \) and \( \tilde{X}_2 \) as centers of \( m_1 \) and \( m_2 \) clusters of \( X \). So if \( m_1 \) is the same as \( m_2 \) then inducing inputs would also be the same. We cannot use the same strategy for \( \tilde{Z} \), since then we would need the centers for the clusters of the variable \( X^T \beta \) which are unknown. If we assume that each covariate \( x_{ij} \) is between 0 and 1 (this can be achieved easily if we subtract the minimum value and divide by range) then following the Cauchy-Schwartz inequality we obtain

\[
\|x^T \beta\| \leq \sqrt{\|x_i\|^2 \|\beta\|^2} \leq \sqrt{q} \quad \forall x_i, \beta.
\]

Hence we can choose \( \tilde{Z} \) to be \( m \) equally spaced points in the interval \([-\sqrt{q}, \sqrt{q}]\).

The contribution of the conditional copula model to the joint likelihood breaks the tractability of the posterior conditional densities and complicates the design of an efficient MCMC algorithm that can sample efficiently from the posterior distribution. The conditional joint posterior distribution of the latent variables \( (f) \) and parameters \( (w) \) given the observed data \( D \) does not have a tractable form and its study will require the use of Markov Chain Monte Carlo (MCMC) sampling methods. Specifically, we use Random Walk Metropolis (RWM) within Gibbs sampling for \( w \) (Craiu and Rosenthal, 2014; Rosenthal, 2009; Andrieu et al., 2003) while for \( f \) we will use the elliptical slice sampling (Murray et al., 2010) that has been designed specifically for GP-based models and does not require tuning of free parameters.
3.1 Computational Algorithm

Inference is based on the posterior distribution $\pi(\tilde{f}_1, \tilde{f}_2, \tilde{f}, w_1, w_2, w, \sigma_1^2, \sigma_2^2, \beta | D, \tilde{X}_1, \tilde{X}_2, \tilde{Z})$ which is not mathematically tractable, so the study of its properties will rely on Monte Carlo sampling.

In this section we provide the detailed steps of the MCMC sampler designed to sample from $\pi$.

The general form of the algorithm falls within the class of Metropolis-within-Gibbs (MwG) samplers in which we update in turn each component of the chain by sampling from its conditional distribution, given all the other components. The presence of the copula in the likelihood breaks the usual conditional conjugacy of the GP models so none of the components have conditional distributions that can be sampled directly.

Suppose we are interested in sampling a target $\pi(\theta_1, \ldots, \theta_k)$. A generic MwG sampler proceeds as follows:

**Step 1** Initialize the chain at $\theta^{(1)}_1, \theta^{(1)}_2, \ldots, \theta^{(1)}_k$.

**Step R** At iteration $t + 1$ run iteratively the following steps for each $j = 1, \ldots, k$:

1. Sample $\theta^*_j \sim q_j(\theta_j | \theta^{(t+1:t)}_{-j})$ where $\theta^{(t+1:t)}$ is the most recent state of the chain with the first $j - 1$ components updated already (hence the supraindex $t + 1$), the $j$th component removed and the remaining $n - j$ components having the values determined at iteration $t$ (hence the supaindex $t$).

2. Compute $r = \min \left\{ 1, \frac{\pi(\theta^{(t+1)}_1, \ldots, \theta^{(t+1)}_{j-1}, \theta^*_j, \theta^{(t)}_{j+1}, \ldots, \theta^{(t)}_k)}{\pi(\theta^{(t+1)}_1, \ldots, \theta^{(t+1)}_{j-1}, \theta^{(t+1)}_j, \theta^{(t)}_{j+1}, \ldots, \theta^{(t)}_k)} \right\}$.

3. With probability $r$ accept proposal and set $\theta^{(t+1)}_j = \theta^*_j$ and with $1 - r$ reject proposal and let $\theta^{(t+1)}_j = \theta^{(t)}_j$.

The proposal density $q_j(\cdot | \cdot)$ corresponds to the transition kernel used for the $j$th component.

Our algorithm uses a number of proposals corresponding to Random Walk Metropolis-within-Gibbs (RWMwG), Independent Metropolis-within-Gibbs (IMwG) and Elliptical Slice Sampling within Gibbs (SSwG) moves.

At the $t + 1$ step we use the following proposals to update the chain:

**$w_i$:** Use a RWM transition kernel: $w^* \sim \mathcal{N}(w^{(t)}_i, \sigma^2_{w_i})$. The constant $c_{w_i}$ is chosen so that the acceptance rate is about 30%, $i = 1, 2$. 

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w: Use the RWM: \(w^* \sim N(w^{(t)}, c_w I_2)\). The constant \(c_w\) is chosen so that the acceptance rate is about 30%.

\(\sigma_i^2\): Without the copula, the conditional posterior distribution of \(\sigma_i^2\) would be \(IG(0.1 + n/2, 0.1 + (Y_i - A_i \hat{f}_i^{(t)})^T(Y_i - A_i \hat{f}_i^{(t)}))\) where \(A_i = A(X, \tilde{X}_i; w^{(t+1)})\) for all \(i = 1, 2\). We will use this distribution as a proposal distribution in the IM transition kernel, i.e. the proposal is \((\sigma^2)_i^* \sim IG(0.1 + n/2, 0.1 + (Y_i - A_i \tilde{f}_i^{(t)})^T(Y_i - A_i \tilde{f}_i^{(t)}))\). The acceptance rate is usually in the range of \([0.25, 0.60]\) and the chain mixes better than it would under a RWM.

\(\beta\): Since \(\beta\) is normalized we will use RWM on unit sphere using ‘Von-Mises-Fisher’ distribution (henceforth denoted \(VMF\)). The VMF distribution has two parameters, \(\mu\) (normalized to have norm one) which represents the mean direction and \(\kappa\), the concentration parameter. A larger \(\kappa\) implies that the distribution will be more concentrated around \(\mu\). The density is symmetric in \(\mu\) and the argument and is proportional to \(f_{VMF}(x; \mu, \kappa) \propto \exp(\kappa x^T \mu)\).

The proposals are generated using \(\beta^* \sim VMF(\beta^{(t)}, \kappa), \) where \(\kappa\) is chosen so that the acceptance rate is around 30%.

\(\tilde{f}\)’s: For \(\tilde{f}_i, i = 1, 2\) and \(\tilde{f}\) we use the elliptical slice sampling proposed by Murray et al. (2010) which does not require the tuning of simulation parameters.

In our experience the efficiency of the algorithm benefits from initial values that are not too far from the posterior mode. Therefore we propose first to estimate the two independent regressions for \(Y_1\) and \(Y_2\) to get \((\tilde{f}_1, w_1, \sigma_1^2)^{(1)}\) and \((\tilde{f}_2, w_2, \sigma_2^2)^{(1)}\). Then run another MCMC fixing marginals and only sampling \((\tilde{f}, w)\). This procedure estimates \((\tilde{f}, w)^{(1)}\). These 3 short chains (100-200 iterations each) give point-estimates of true parameters and these estimates can be used as initial values for the joint MCMC. This simple approach shortens the time it would take for the original chain to find the regions of high mass under the posterior.

Empirically we have also found, that for faster convergence it is better to start with small \(w_1\) values (allowing for more variation in the calibration function). If the chain starts in large \(w_1\) values, it requires a large number of simulations before it moves to the correct region in the sample space.
3.2 Model Selection

The conditional copula model involves two types of selection. First one needs to choose the copula family from a set of possible candidates. Second, it is often of interest to determine whether a parametric simple form for the calibration is supported by the data. For instance, a constant calibration function indicates that the dependence structure does not vary with the covariates, a conclusion that may be of scientific interest in some applications. We investigate the performance of three measures of fit that can be estimated from the MCMC samples \( \omega(t) \ t = 1 \ldots M \) where \( \omega(t) \) is the vector of parameters and latent variables drawn at step \( t \) from the posterior corresponding to model \( M \).

3.3 Cross-Validated Pseudo Marginal Likelihood

The cross-validated pseudo marginal likelihood (CVML) (Geisser and Eddy 1979; Hanson et al. 2011) calculates the average (over parameter values) prediction power for model \( M \) via

\[
\text{CVML}(M) = \sum_{i=1}^{n} \log \left( P(Y_{1i}, Y_{2i}|\mathcal{D}_{-i}, \mathcal{M}) \right),
\]

where \( \mathcal{D}_{-i} \) is the data set from which the \( i \)th observation has been removed. An estimate of \( \text{CVML} \) can be obtained using posterior draws for all the parameters and latent variables in the model (see, for example, Sabeti et al. 2014). Specifically, if the latter are denoted by \( \omega \), then

\[
E \left[ P(Y_{1i}, Y_{2i}|\omega, \mathcal{M})^{-1} \right] = P(Y_{1i}, Y_{2i}|\mathcal{D}_{-i}, \mathcal{M})^{-1},
\]

where the expectation is with respect to conditional (posterior) distribution of \( \omega \) given full data \( \mathcal{D} \) and the model \( \mathcal{M} \). Based on the posterior samples we can estimate the CVML as

\[
\text{CVML}_{est}(\mathcal{M}) = -\sum_{i=1}^{n} \log \left( \frac{1}{M} \sum_{t=1}^{M} P(Y_{1i}, Y_{2i}|\omega^{(t)}, \mathcal{M})^{-1} \right).
\]

The model with the largest CVML is selected.

3.4 Conditional CVML criterion

The conditional copula construction is particularly useful in predicting one response given the other ones. We exploit this feature by computing the predictive distribution of one response given the rest of the data. The resulting conditional CVML (CCVML) is computed from the \( P(Y_{1i}|Y_{2i}, \mathcal{D}_{-i}) \)
and \( P(Y_{2i}|Y_{1i}, D_{-i}) \) via

\[
CCVML(\mathcal{M}) = \frac{1}{2} \left\{ \sum_{i=1}^{n} \log [P(Y_{1i}|Y_{2i}, \mathcal{D}_{-i}, \mathcal{M})] + \sum_{i=1}^{n} \log [P(Y_{2i}|Y_{1i}, D_{-i}, \mathcal{M})] \right\}.
\] (21)

Note that when the marginal distributions are uniform, then CCVML is the same as CVML. Using a technique similar to the one used in Sabeti et al. (2014) one can show that

\[
E[P(Y_{1i}|Y_{2i}, \omega, \mathcal{M})] = E[P(Y_{2i}|Y_{1i}, \omega, \mathcal{M})] = P(Y_{1i}|Y_{2i}, D_{-i}, \mathcal{M})^{-1}.
\] (22)

Based on (22) one can easily estimate CCVML from MCMC samples:

\[
CCVML_{est}(\mathcal{M}) = -\frac{1}{2} \sum_{i=1}^{n} \log \left( \frac{1}{M} \sum_{t=1}^{M} P(Y_{2i}|\omega^{(t)}, \mathcal{M}) \right) + \log \left( \frac{1}{M} \sum_{t=1}^{M} P(Y_{1i}|\omega^{(t)}, \mathcal{M}) \right) + \log \left( \frac{1}{M} \sum_{t=1}^{M} P(Y_{1i}|\omega^{(t)}, \mathcal{M}) \right).
\] (23)

3.5 Watanabe-Akaike Information Criterion

The Watanabe-Akaike Information Criterion (WAIC, Watanabe, 2010) is an information-based criterion that is closely related to the CVML (see Gelman et al., 2014, for a discussion of the connection between CVML and WAIC).

The WAIC is defined as

\[
WAIC(\mathcal{M}) = -2\text{fit}(\mathcal{M}) + 2p(\mathcal{M}),
\] (24)

where the model fitness is

\[
\text{fit}(\mathcal{M}) = \sum_{i=1}^{n} \log E[P(y_{1i}, y_{2i}|\omega, \mathcal{M})]
\] (25)

and the penalty

\[
p(\mathcal{M}) = \sum_{i=1}^{n} \text{Var}[\log P(y_{1i}, y_{2i}|\omega, \mathcal{M})].
\] (26)

The expectation in (25) and the variance in (26) are with respect to the conditional distribution of \( \omega \) given the data and can be computed using the samples produced by the MCMC sampler that draws from \( \pi \). For instance, the Monte Carlo estimate of the fit is

\[
\hat{\text{fit}}(\mathcal{M}) = \sum_{i=1}^{n} \log \left( \frac{\sum_{t=1}^{M} P(y_{1i}, y_{2i}|\omega^{(t)}, \mathcal{M})}{M} \right),
\] (27)

and \( p(\mathcal{M}) \) can be estimated similarly using the posterior samples. The model with the smallest WAIC is preferred. In the next section we also investigate via simulations the performance of
CVML, CCVML and WAIC criteria when identifying data support for a constant calibration function.

4 Performance of the algorithms

4.1 Simulations

The purpose of the simulation study is to assess empirically: 1) the performance of the estimation method under the correct and misspecified models, as well as 2) the ability of the model selection criteria to identify the correct copula structure, i.e. the copula family and the parametric form of the calibration function. For the former aim we compute the integrated mean square for various quantities of interest, including the Kendall’s \( \tau \). In order to facilitate estimation performance across different copula families, we estimate the calibration function on the Kendall’s \( \tau \) scale. The latter is given by

\[
\tau(X) = 4 \left( \int \int C(U_1, U_2 | X) c(U_1, U_2 | X) dU_1 dU_2 \right) - 1.
\]

We will compare 3 copulas: Clayton, Frank and Gaussian under the general GP-SIM model and the Clayton with constant calibration function. To fit the model with constant copula, we still use MCMC but instead of \( f, \tilde{f}, w \) and \( \beta \) in calibration we have a constant scalar copula parameter, \( \theta \). The RWMwG transition is used to sample \( \theta \), as the proposal distributions for marginals’ parameters and latent variables remain the same.

Table 1 provides inverse-link functions \( g^{-1} \) used for calibration and the functional relationship between Kendall’s \( \tau \) and copula parameters. In addition of Kendall’s \( \tau \) we use also the conditional

<table>
<thead>
<tr>
<th>Copula</th>
<th>Inv-Link function</th>
<th>Kendall’s ( \tau ) formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clayton</td>
<td>( \theta = \exp(f) - 1 )</td>
<td>( \tau = \frac{\theta}{\theta + 2} )</td>
</tr>
<tr>
<td>Frank</td>
<td>( \theta = f )</td>
<td>No closed form</td>
</tr>
<tr>
<td>Gaussian, T</td>
<td>( \theta = \frac{\exp(f) - 1}{\exp(f) + 1} )</td>
<td>( \tau = \frac{2}{\pi} \arcsin \theta )</td>
</tr>
<tr>
<td>Gumbel</td>
<td>( \theta = \exp(f) + 1 )</td>
<td>( 1 - \frac{1}{\theta} )</td>
</tr>
</tbody>
</table>

Table 1: Inverse-link functions and the functional relationship between Kendall’s \( \tau \) and the copula parameter.
mean of $Y_1$ given $Y_2$ and $X$ for assessing the estimation. Such conditional means can be useful in prediction when one of the responses is more expensive to measure than the other. The calculation is mathematically straightforward

$$E(Y_1|Y_2 = y_2, X = x) = f_1(x) + \sigma_1 \int_0^1 \Phi^{-1}(z) c \left( z, \Phi \left( \frac{y_2 - f_2(x)}{\sigma_2} \right); \theta(x) \right) dz. \quad (28)$$

If we assume that marginal distributions are uniform then we have the simpler expression:

$$E(U_1|U_2 = u_2, X = x) = \int_0^1 c(z, u_2; \theta(x)) dz. \quad (29)$$

The integrals in (28) and (29) are usually not tractable, but can be easily estimated via numerical integration since they are one-dimensional and defined on the closed interval $[0, 1]$.

### 4.2 Simulation Details

We generate samples of size $n = 400$ from each of the next 6 scenarios using the Clayton copula. The covariates are generated independently from Uniform$(0, 1)$ distribution. The covariate dimension $q$ in Scenario 3 is 10, in all other scenarios it is 2.

**Sc1** $f_1(x) = 0.6 \sin(5x_1) - 0.9 \sin(2x_2),$

$$f_2(x) = 0.6 \sin(3x_1 + 5x_2),$$

$$\tau(x) = 0.7 + 0.15 \sin(15x^T \beta)$$

$$\beta = (1, 3)^T / \sqrt{10}, \sigma_1 = \sigma_2 = 0.2$$

**Sc2** $f_1(x) = 0.6 \sin(5x_1) - 0.9 \sin(2x_2)$

$$f_2(x) = 0.6 \sin(3x_1 + 5x_2)$$

$$\tau(x) = 0.3 \sin(5x^T \beta)$$

$$\beta = (1, 3)^T / \sqrt{10}, \sigma_1 = \sigma_2 = 0.2$$

**Sc3** $\beta = (1, 10, -3, 6, 1, -6, 3, 7, -1, -5)^T / \sqrt{267}, \sigma_1 = \sigma_2 = 0.2$

$$f_1(x) = \cos(x^T \beta)$$

$$f_2(x) = \sin(x^T \beta)$$

$$\tau(x) = 0.7 + 0.20 \sin(5x^T \beta)$$

**Sc4** $f_1(x) = 0.6 \sin(5x_1) - 0.9 \sin(2x_2)$

$$f_2(x) = 0.6 \sin(3x_1 + 5x_2)$$
\[ \tau(x) = 0.5 \]
\[ \sigma_1 = \sigma_2 = 0.2 \]

**Sc5**
\[ f_1(x) = 0.6 \sin(5x_1) - 0.9 \sin(2x_2) \]
\[ f_2(x) = 0.6 \sin(3x_1 + 5x_2) \]
\[ \eta(x) = 1 + 0.7 \sin(3x_1^3) - 0.5 \cos(6x_2^2) \]
\[ \sigma_1 = \sigma_2 = 0.2 \]

**Sc6**
\[ f_1(x) = 0.6 \sin(5x_1) - 0.9 \sin(2x_2) \]
\[ f_2(x) = 0.6 \sin(3x_1 + 5x_2) \]
\[ \eta(x) = 1 + 0.7x_1 - 0.5x_2^2 \]
\[ \sigma_1 = \sigma_2 = 0.2 \]

**Sc1** and **Sc2** have calibration functions for which the SIM model is true for Kendall’s \( \tau \) and, consequently, also for the copula parameter. **Sc1** corresponds to large dependence (\( \tau \) greater than 0.5) while **Sc2** has small dependence (\( \tau \) is between \(-0.3\) and 0.3). **Sc3** also has SIM form for calibration function the covariate dimension is \( q = 10 \), so this scenario is important to evaluate how well the algorithms scale up with dimension. **Sc4** corresponds to the covariate-free dependence (\( \tau = 0.5 \)) and allows us to verify the power to detect simple parametric forms for the calibration.

Scenarios **Sc5** and **Sc6** do not have SIM form, but have additive calibration function (as in Sabeti et al., 2014). They will be useful to evaluate the effect of model misspecification on the inference.

Note that **Sc6** has almost SIM calibration when \( x_2 \in [0, 1] \). For all scenarios we use \( m = 30 \) inducing inputs for all the sparse GP procedures (marginals and copula).

The MCMC samplers were run for 40000 iterations for **Sc3**, and 10000 iterations for all other scenarios. Simulations for **Sc3** require larger Monte Carlo runs because the parameter space is 32-dimensional compared to 8-dimensional in all other scenarios. The first half of the MCMC sample is discarded as burn-in and the second half is used for inference. As noted earlier, starting values were found by running two GP regressions separately to estimate marginal parameters and one MCMC sampler was run in order to estimate calibration parameters. All three samplers were run for only 100 iterations.
4.2.1 Proof of concept based on one Replicate

The simulation results show that \textbf{Sc1} and \textbf{Sc2} performed similarly. Since the calibration function in \textbf{Sc1} is more complicated, for the sake of reducing the paper’s length we present only results for that scenario. The trace-plots, autocorrelation functions and histograms of posterior samples of $\beta$, $\sigma^2_1$ and $\sigma^2_2$ are shown in Figure 1 when the fitted copula belongs to the correct Clayton family (red line is the true value). Next we show predictions for the marginals means with 95% credible intervals. Since these are 2-dimensional we estimate ‘slices’ from this surface at values 0.2 and 0.8, so that we first fix $x_1 = 0.2$ then $x_1 = 0.8$ and similarly for $x_2$. The results are in Figure 2 (black is true, green is estimation, red are credible intervals).

One of the inferential goals is the prediction of calibration function or, equivalently, Kendall’s $\tau$ function. In this case we are dealing with only two covariates so their joint effect can be visualized via the calibration surface. In Figure 3 we show the true calibration surface on the left panel and the fitted one on the right. The accuracy is remarkable and we are hard put to see major differences between the two panels.

Since the visual comparison of the three-dimensional true and fitted surfaces may be misleading, we also estimate one dimensional slices at values 0.2 and 0.8 and the results, shown in Figure 4.
Figure 2: **Sc1**: Estimation of marginal means. The leftmost 2 columns show the accuracy for predicting $Y_1$ and the rightmost 2 columns show the results for predicting $Y_2$. The black and green lines represent the true and estimated relationships, respectively. The red lines are the limits of the pointwise 95% credible intervals obtained under the true Clayton family.

Figure 3: **Sc1**: Estimation of Kendall’s $\tau$ dependence surface. The true surface (left panel) is very similar to the estimated one (right panel).

Another way to evaluate how well the model makes predictions is to fix 4 covariate points and estimate corresponding Kendall’s $\tau$ values: $\hat{\tau}(0.2, 0.2), \hat{\tau}(0.2, 0.8), \hat{\tau}(0.8, 0.2), \hat{\tau}(0.8, 0.8)$. At each MCMC iteration these predictions are calculated and histograms (Figure 5) are constructed (red lines are true value of $\tau$). The same estimates are presented in Figure 6 when the Gaussian copula is used for inference. One can notice that the estimates are biased in this instance, thus emphasizing
Figure 4: **Sc1**: Estimation of Kendall’s τ one-dimensional projections when $X_1 = 0.2$ or 0.8 (top panels) and when $X_2 = 0.2$ or 0.8 bottom panels. The black and green lines represent the true and estimated relationships, respectively. The red lines are the limits of the pointwise 95% credible intervals obtained under the true Clayton family.

Figure 5: **Sc1**: Histogram of predicted Kendall’s τ values obtained under the true Clayton copula.

the importance of identifying the right copula family. Similar patterns have been observed when using the Frank copula.

We also show how well the algorithm estimates calibration function when covariate dimension is large. Figure 7 shows one dimensional slices of Kendall’s τ function for **Sc3** which is estimated by Clayton GP-SIM model. Each plot is produced by varying one coordinate from 0 to 1 while fixing all other coordinates at $x = 0.5$. We observe that even in this case the estimated curves are very close to true Kendall’s τ function.

Finally, we focus on the accuracy of CVML, CCVML and WAIC in selecting the correct model.
Figure 6: **Sc1**: Histogram of predicted $\tau$s (Gaussian copula)

Figure 7: **Sc3**: Estimation of Kendall’s $\tau$ one-dimensional projections for each coordinate fixing all other coordinates at 0.5 levels. The black and green lines represent the true and estimated relationships, respectively. The red lines are the limits of the pointwise 95% credible intervals obtained under the true Clayton family.

Table 2 shows the values for each scenario and model. Bold values indicate largest CVML/CCVML and smallest WAIC values for each scenario. Observe that all bold values for **Sc1, Sc2, Sc3, Sc5, Sc6**, point to the Clayton family, while for **Sc4** they indicate the Clayton family with a constant calibration. We note that the correct copula is selected even when the generative calibration model is additive.
<table>
<thead>
<tr>
<th>Scenario 1</th>
<th>Scenario 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clayton</td>
<td>496 417  −994</td>
</tr>
<tr>
<td>Frank</td>
<td>435 362  −870</td>
</tr>
<tr>
<td>Gaussian</td>
<td>405 329  −817</td>
</tr>
<tr>
<td>Clayton-Const</td>
<td>455 378  −910</td>
</tr>
<tr>
<td>Scenario 2</td>
<td>Scenario 5</td>
</tr>
<tr>
<td>Clayton</td>
<td>166 103  −333</td>
</tr>
<tr>
<td>Frank</td>
<td>144 82   −289</td>
</tr>
<tr>
<td>Gaussian</td>
<td>146 84   −293</td>
</tr>
<tr>
<td>Clayton-Const</td>
<td>121 60   −243</td>
</tr>
<tr>
<td>Scenario 3</td>
<td>Scenario 6</td>
</tr>
<tr>
<td>Clayton</td>
<td>613 536  −1237</td>
</tr>
<tr>
<td>Frank</td>
<td>562 491  −1126</td>
</tr>
<tr>
<td>Gaussian</td>
<td>494 417  −1002</td>
</tr>
<tr>
<td>Clayton-Const</td>
<td>537 462  −1076</td>
</tr>
</tbody>
</table>

Table 2: CVML, CCVML and WAIC values for each Scenario and Model

4.2.2 Simulation Results based on multiple Replicates

So far, the results reported were based on a single implementation of the method. In order to facilitate interpretation, we perform 50 independent replications under each of the six scenarios described previously. However, since the focus of the inference is on the copula, we shorten the simulation time by assuming that the marginals are uniform.

The MCMC sampler was run for 20000 iterations for Sc3 and 5000 iterations for other scenarios. As before, the first half of iterations was ignored as a burn-in period. For each data set, 4 estimations were done with Clayton, Frank, Gaussian and constant Clayton copulas. For Sc5 and Sc6 we also fitted the Clayton copula with an additive model a la [Sabeti et al. (2014)] for each data set. The goal is to estimate integrated squared Bias (IBias$^2$), Variance (IVar) and mean squared error (IMSE) of Kendall’s $\tau$ evaluated at covariates $X = (x_1, \ldots, x_n)^T$. To calculate these quantities for any scenario and any model we do the following: for each data set, point estimations are produced $\hat{\tau}_r(x_i)$ where $r$ runs from 1 up to number of replicates ($R$) and $i = 1 \ldots n$. The
formulas for \( \text{IBias}^2 \), \( \text{IVar} \) and \( \text{IMSE} \) are given by:

\[
\text{IBias}^2 = \sum_{i=1}^{n} \left( \frac{\sum_{r=1}^{R} \hat{r}_r(x_i)}{R} - \tau(x_i) \right)^2 /n, \\
\text{IVar} = \sum_{i=1}^{n} \text{Var}_r(\hat{r}_r(x_i))/n, \\
\text{IMSE} = \text{IBias}^2 + \text{IVar}.
\]

We will apply these concepts not only for Kendall’s \( \tau \) but also for \( E(U_1|U_2 = u_2, X = x) \) for different \( u_2 \) and \( x \) combinations. Here we use \( U \)'s instead of \( Y \)'s to indicate that we assume uniform marginal distributions.

### Results

\( \text{IBias}^2 \), \( \text{IVar} \) and \( \text{IMSE} \) for each scenario and each model are shown in Table 3 (bold values show smallest \( \text{IMSE} \) for each scenario). Note that the smallest \( \text{IMSE} \) is produced when fitting the correct model and copula family. For each simulated data set and each model, \( E(U_1|U_2 = u_2, X = x) \) were estimated. For all scenarios except for \( \text{Sc3} \) we let each \( x_1, x_2, u_2 \) to take values in the set \( \{0.2, 0.4, 0.6, 0.8\} \), making a total of 64 combinations. For \( \text{Sc3} \) we let \( u_2 \) to take values from \( \{0.2, 0.4, 0.6, 0.8\} \), while \( x \) can take 33 values scattered in \([0, 1]\)\(10\), making a total of 132 combinations. The results are presented in Table 4.

Focusing on \( \text{Sc5} \) and \( \text{Sc6} \), the estimated integrated bias, variance and MSE for Kendall’s \( \tau \) and \( E(U_2|U_2 = u_2, X = x) \) when fitting Clayton GP-SIM and true Clayton Additive model are shown in Table 5. We observe that even though Clayton GP-SIM has best IMSE among other copula families it performs worse than Clayton additive model which generated data sets.

Finally we show how well CVML and WAIC perform in choosing correct model. For selecting...
Clayton

Frank

Gaussian

Clayton Constant

Scenario $\sqrt{\text{IBias}}^2$ $\sqrt{\text{IVar}}$ $\sqrt{\text{IMSE}}$ $\sqrt{\text{IBias}}^2$ $\sqrt{\text{IVar}}$ $\sqrt{\text{IMSE}}$ $\sqrt{\text{IBias}}^2$ $\sqrt{\text{IVar}}$ $\sqrt{\text{IMSE}}$ $\sqrt{\text{IBias}}^2$ $\sqrt{\text{IVar}}$ $\sqrt{\text{IMSE}}$

Sc1 0.0088 0.0131 0.0137 0.0279 0.0132 0.0039 0.0338 0.0163 0.0175 0.0379 0.0237 0.0034 0.0240

Sc2 0.0034 0.0145 0.0149 0.0290 0.0311 0.0403 0.0226 0.0184 0.0292 0.0644 0.0084 0.0649

Sc3 0.0068 0.0148 0.0163 0.0117 0.0175 0.0211 0.0320 0.0187 0.0292 0.0198 0.0024 0.0240

Sc4 0.0015 0.0070 0.0072 0.0265 0.0076 0.0072 0.0347 0.0250 0.0034 0.0237 0.0034 0.0070 0.0240

Sc5 0.0170 0.0192 0.0257 0.0347 0.0250 0.0417 0.0384 0.0192 0.0420 0.0219 0.0050 0.0225

Sc6 0.0076 0.0158 0.0176 0.0018 0.0095 0.0176 0.0384 0.0192 0.0420 0.0219 0.0050 0.0225

Table 4: Estimated $\text{IBias}^2$, $\text{IVar}$ and $\text{IMSE}$ of $E(U_1 | U_2, X)$ for each Scenario and Model

Kendall’s Tau

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Clayton GP-SIM $\sqrt{\text{IBias}}^2$</th>
<th>Clayton Additive $\sqrt{\text{IBias}}^2$</th>
<th>Clayton GP-SIM $\sqrt{\text{IVar}}$</th>
<th>Clayton Additive $\sqrt{\text{IVar}}$</th>
<th>Clayton GP-SIM $\sqrt{\text{IMSE}}$</th>
<th>Clayton Additive $\sqrt{\text{IMSE}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sc5</td>
<td>0.0712 0.0742 0.1029</td>
<td>0.0528 0.0469 0.0707</td>
<td>0.0620 0.0562 0.1067</td>
<td>0.0562 0.0505 0.0732</td>
<td>0.0707 0.0649 0.1067</td>
<td></td>
</tr>
<tr>
<td>Sc6</td>
<td>0.0286 0.0602 0.0667</td>
<td>0.0669 0.0390 0.0396</td>
<td>0.0707 0.0649 0.1067</td>
<td>0.0562 0.0505 0.0732</td>
<td>0.0707 0.0649 0.1067</td>
<td></td>
</tr>
</tbody>
</table>

$E(U_2 | U_1, X)$

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Clayton GP-SIM $\sqrt{\text{IBias}}^2$</th>
<th>Clayton Additive $\sqrt{\text{IBias}}^2$</th>
<th>Clayton GP-SIM $\sqrt{\text{IVar}}$</th>
<th>Clayton Additive $\sqrt{\text{IVar}}$</th>
<th>Clayton GP-SIM $\sqrt{\text{IMSE}}$</th>
<th>Clayton Additive $\sqrt{\text{IMSE}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sc5</td>
<td>0.0170 0.0192 0.0257</td>
<td>0.0136 0.0105 0.0172</td>
<td>0.0100 0.0076 0.0095</td>
<td>0.0095 0.0070 0.0097</td>
<td>0.0172 0.0105 0.0172</td>
<td></td>
</tr>
<tr>
<td>Sc6</td>
<td>0.0076 0.0158 0.0176</td>
<td>0.0018 0.0095 0.0097</td>
<td>0.0100 0.0076 0.0095</td>
<td>0.0095 0.0070 0.0097</td>
<td>0.0172 0.0105 0.0172</td>
<td></td>
</tr>
</tbody>
</table>

Table 5: Estimated $\sqrt{\text{IBias}}^2$, $\sqrt{\text{IVar}}$ and $\sqrt{\text{IMSE}}$ of Kendall’s $\tau$ and $E(U_1 | U_2, X)$ for GP-SIM and Additive models

between different copula families or to check whether dependence is covariate-free we just pick the model with largest CVML or smallest WAIC. Table 6 shows how often Clayton model is selected over other models using CVML and WAIC for Sc1, Sc2, Sc3, Sc5 and Sc6. Similarly, Table 7 shows how often Clayton-constant is selected over other models for Sc4.

We can conclude that both selection measures perform similarly for all scenarios. Also, selection results show that choosing between copula families is easy, while CVML and WAIC do not perform exceptionally well in selecting between different forms of calibration function (GP-SIM and SA). Since Sc5 and Sc6 where simulated with Clayton additive calibration, we show how often Clayton Additive model is selected over Clayton GP-SIM using different criteria (Table 5). Again CVML and WAIC perform similarly. The poor performance of criteria for Sc6 is not that surprising since the additive calibration in this scenario has almost SIM form as functions $y = x$ and $y = x^2$ are
Table 6: The percentage of correct decisions for each selection criterion when comparing the correct Clayton model with a non-constant calibration with all the other models: Frank model with non-constant calibration, Gaussian model with non-constant calibration, Clayton model with non-constant calibration. Notice that the CCVML and the CVML criteria are exactly equal in the case in which the marginals are uniform.

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Frank</th>
<th>Gaussian</th>
<th>Clayton Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sc1</td>
<td>100%</td>
<td>100%</td>
<td>98%</td>
</tr>
<tr>
<td>Sc2</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>Sc3</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>Sc4</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>Sc5</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>Sc6</td>
<td>100%</td>
<td>100%</td>
<td>90%</td>
</tr>
</tbody>
</table>

Table 7: The percentage of correct decisions for each selection criterion when comparing the correct Clayton model with a constant calibration with all the other models: Clayton model with non-constant calibration, Frank model with non-constant calibration and the Gaussian model with non-constant calibration. Notice that the CCVML and the CVML criteria are exactly equal in the case in which the marginals are uniform.

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Clayton</th>
<th>Frank</th>
<th>Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sc4</td>
<td>78%</td>
<td>78%</td>
<td>100%</td>
</tr>
<tr>
<td>Sc5</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>Sc6</td>
<td>70%</td>
<td>70%</td>
<td>70%</td>
</tr>
</tbody>
</table>

Table 8: The percentage of correct decisions for each selection criterion when comparing the correct additive model with GP-SIM with non-constant calibration similar for $x \in [0, 1]$.

4.3 Red Wine Data

We consider the data of [Cortez et al. (2009)](http://example.com) consisting of various physicochemical tests of 1599 red variants of the Portuguese "Vinho Verde" wine. Acidity and density are properties closely associ-
ated with the quality of wine and grape, respectively. Of interest here is to study the dependence pattern between ‘fixed acidity’ \( Y_{fa} \) and ‘density’ \( Y_{de} \) and how it changes with values of other variables: ‘volatile acidity’, ‘citric acid’, ‘residual sugar’, ‘chlorides’, ‘free sulfur dioxide’, ‘total sulfur dioxide’, ‘pH’, ‘sulphates’ and ‘alcohol’, denoted \( X_{va}, X_{ca}, X_{rs}, X_{ch}, X_{fs}, X_{ts}, X_{ph}, X_{su}, X_{al} \), respectively. Response variable are linearly transformed to have mean 0 and standard deviation of 1, similarly covariates where transformed to be between 0 and 1.

To select the appropriate copula family, we fit GP-SIM with ‘Clayton’, ‘Frank’, ‘Gaussian’, ‘Gumbel’ and ‘T-3’ (student T with 3 degrees of freedom) dependencies. For each model the MCMC was run for 10000 iterations with 5000 burn-in period. We used 30 inducing inputs for the marginals and calibration function estimation \( (m_1 = m_2 = m = 30) \). The resulting CVML, CCVML and WAIC values are shown in Table 9.

<table>
<thead>
<tr>
<th></th>
<th>Clayton</th>
<th>Frank</th>
<th>Gaussian</th>
<th>Gumbel</th>
<th>T-3</th>
</tr>
</thead>
<tbody>
<tr>
<td>CVML</td>
<td>-1858</td>
<td>-1816</td>
<td>-1788</td>
<td>-1829</td>
<td>-1810</td>
</tr>
<tr>
<td>CCVML</td>
<td>-582</td>
<td>-547</td>
<td>-522</td>
<td>-558</td>
<td>-534</td>
</tr>
<tr>
<td>WAIC</td>
<td>3713</td>
<td>3634</td>
<td>3572</td>
<td>3656</td>
<td>3621</td>
</tr>
</tbody>
</table>

Table 9: Red Wine data: CVML, CCVML and WAIC criteria values different models

All model selection measures indicate that among candidate copula families the most suitable one is the Gaussian one. The GP-SIM coefficients \( \beta \) fitted under the Gaussian copula family are shown in Table 10.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Posterior Mean</th>
<th>95% Credible Interval</th>
</tr>
</thead>
<tbody>
<tr>
<td>( X_{va} )</td>
<td>0.274</td>
<td>[0.154, 0.389]</td>
</tr>
<tr>
<td>( X_{ca} )</td>
<td>-0.336</td>
<td>[-0.413, -0.254]</td>
</tr>
<tr>
<td>( X_{rs} )</td>
<td>-0.076</td>
<td>[-0.278, 0.271]</td>
</tr>
<tr>
<td>( X_{ph} )</td>
<td>0.060</td>
<td>[-0.246, 0.259]</td>
</tr>
<tr>
<td>( X_{fs} )</td>
<td>0.276</td>
<td>[0.106, 0.410]</td>
</tr>
<tr>
<td>( X_{ts} )</td>
<td>0.402</td>
<td>[0.248, 0.608]</td>
</tr>
<tr>
<td>( X_{al} )</td>
<td>0.155</td>
<td>[0.054, 0.286]</td>
</tr>
<tr>
<td>( X_{su} )</td>
<td>0.501</td>
<td>[0.342, 0.601]</td>
</tr>
</tbody>
</table>

Table 10: Wine data: Posterior means and quantiles of \( \beta \)
The credible intervals suggest that not all covariates may be needed to model dependence between responses. For example, ‘residual sugars’ and ‘chlorides’ seem to not affect the calibration function so we consider a model in which they are omitted from the conditional copula model. In all models, we include all the covariates in the marginal distributions. For comparison, we have also fitted all Gaussian GP-SIM models with only one covariate, and with no covariates at all (constant). The computational algorithm to fit GP-SIM when the conditional copula depends on only one variable is very similar to the one described above. The main difference is that there is no $\beta$ variable and the inducing inputs (for calibration function) are evenly spread on $[0, 1]$. The testing results are shown in Table 11.

<table>
<thead>
<tr>
<th>Variables</th>
<th>CVML</th>
<th>CCVML</th>
<th>WAIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALL</td>
<td>1788</td>
<td>522</td>
<td>3572</td>
</tr>
<tr>
<td>$X_{va}, X_{ca}, X_{fs}, X_{ts}, X_{ph}, X_{su}, X_{al}$</td>
<td>1805</td>
<td>532</td>
<td>3608</td>
</tr>
<tr>
<td>$X_{va}$</td>
<td>-1823</td>
<td>552</td>
<td>3646</td>
</tr>
<tr>
<td>$X_{ca}$</td>
<td>-1815</td>
<td>541</td>
<td>3629</td>
</tr>
<tr>
<td>$X_{fs}$</td>
<td>-1849</td>
<td>582</td>
<td>3698</td>
</tr>
<tr>
<td>$X_{ts}$</td>
<td>-1842</td>
<td>578</td>
<td>3688</td>
</tr>
<tr>
<td>$X_{ph}$</td>
<td>-1852</td>
<td>584</td>
<td>3705</td>
</tr>
<tr>
<td>$X_{su}$</td>
<td>-1851</td>
<td>583</td>
<td>3700</td>
</tr>
<tr>
<td>$X_{al}$</td>
<td>-1841</td>
<td>571</td>
<td>3682</td>
</tr>
<tr>
<td>Constant</td>
<td>-1847</td>
<td>577</td>
<td>3697</td>
</tr>
</tbody>
</table>

Table 11: Wine data: CVML, CCVML and WAIC criteria values for variable selection in conditional copula

Based on the selection criteria results we conclude that all nine covariates are required to explain the dependence structure of two responses. Figure 8 shows 1-dimensional plots of Kendall’s $\tau$ calibration curve with 95\% credible as a function of covariates. The plots are constructed by varying one predictor while fixing all others at their mid-range values.

The plots clearly demonstrate that when covariates are fixed at their mid-range values, the conditional correlation between ‘fixed acidity’ and ‘density’ increases with ‘volatile acidity’, ‘free sulfur dioxide’, ‘total sulfur dioxide’, ‘pH’, ‘sulphates’ and ‘alcohol’, and decreases with levels of ‘citric acid’. These relationships can influence the preparation method of the wine.
Figure 8: Wine Data: Slices of predicted Kendall’s $\tau$ as function of covariates. Red curves represent 95% credible intervals.

Figure 9: Wine Data: Plots of ‘fixed acidity’ (blue) and ‘density’ (red) (linearly transformed to fit on one plot) against covariates.

In order to demonstrate the difficulty one would have in gauging the complex evolution of dependence between two responses as a function of covariates we plot in Figure 9 the response variables together as they vary with each covariate. It is clear that the model manages to identify a pattern that would be very difficult to distinguish without the help of a flexible mathematical
5 Simplifying Assumption

5.1 Model Misspecification and the Simplifying Assumption

Understanding whether the data support the SA or not is usually important for the subject matter analysis since a dependence structure that does not depend on the covariates can be of scientific interest. The SA has also a serious impact on the statistical analysis, because it has the potential to simplify greatly the estimation of the copula. There is however, an interesting connection between model misspecification and SA.

To illustrate the point, we consider two independent random variables, $X_1, X_2$ to serve as covariates in the Clayton copula model in which SA is satisfied, the sample size $n = 1500$ and

$$f_1(x) = 0.6 \sin(5x_1 + x_2),$$
$$f_2(x) = 0.6 \sin(x_1 + 5x_2),$$
$$\tau(x) = 0.5,$$
$$\sigma_1 = \sigma_2 = 0.2.$$

When we fit a GP-SIM model with the correct Clayton copula family, but with the $X_2$ covariate omitted from both marginal and copula models, the estimated Kendall’s $\tau(X_1)$ exhibits a clear non-constant shape, as seen in Figure 10. The CVML, CCVML and WAIC criteria, whose values are shown in Table 12 unanimously vote for a nonconstant calibration function.

<table>
<thead>
<tr>
<th>Variables</th>
<th>CVML</th>
<th>CCVML</th>
<th>WAIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_1$</td>
<td>-568</td>
<td>-174</td>
<td>1017</td>
</tr>
<tr>
<td>Constant</td>
<td>-570</td>
<td>-232</td>
<td>1140</td>
</tr>
</tbody>
</table>

Table 12: Missed covariate: CVML, CCVML and WAIC criteria values for model with conditional copula depends on one covariate and when it is constant.

While one may expect a nonconstant pattern when the two covariates are dependent, this residual effect of $X_1$ on the copula may be surprising when $X_1$ and $X_2$ are independent.
We can gain some understanding by considering a simplified example in which $Y_i|X_1, X_2 \sim N(f_i(X_1, X_2), 1)$ for $i = 1, 2$, and $\text{Cov}(Y_1, Y_2|X_1, X_2) = \text{Corr}(Y_1, Y_2|X_1, X_2) = \rho$, hence independent of $X_1$ and $X_2$. When considering marginal models that include only $X_1$, thus leading to residuals $W_i = Y_i - E[Y_i|X_1]$ for $i = 1, 2$, we are interested in understanding why $\text{Cov}(W_1, W_2|X_1)$ is not constant in $X_1$. Using the statistical properties of covariance along with the properties of conditional expectation one can show

$$\text{Cov}(W_1, W_2|X_1) = \text{Cov}(Y_1, Y_2|X_1),$$

(31)

and

$$\text{Cov}(Y_1, Y_2|X_1) = E[\text{Cov}(Y_1, Y_2|X_1, X_2)] + \text{Cov}(E[Y_1|X_1, X_2], E[Y_2|X_1, X_2])$$

$$= \rho + \text{Cov}(f_1(X_1, X_2), f_2(X_1, X_2)),$$

(32)

where the covariance in (32) is with respect to the distribution of $X_2$. Hence it is apparent that the conditional covariance $\text{Cov}(W_1, W_2|X_1)$ will generally not be constant in $X_1$. It should be noted that if the true means have additive form, i.e. $f_i(X_1, X_2) = \tilde{f}_i(X_1) + \hat{f}_i(X_2)$, for $i = 1, 2$, then the

Figure 10: Estimation of Kendall’s $\tau$ as a function of $x_1$ when only first covariate is used in estimation. The black and green lines represent the true and estimated relationships, respectively. The red lines are the limits of the pointwise 95% credible intervals obtained under the true Clayton family.
covariances in \( X_1 \) are indeed constant in \( X_1 \), but the estimated value of \( \text{Cov}(Y_1, Y_2|X_1) \) will be biased. Although here we focused on the covariance as a measure of dependence, the argument is extendable to copula parameters or Kendall’s tau, but the calculations are more involved.

In conclusion, violation of the SA may be due to the omission of important covariates from the model. This phenomenon along with the knowledge that in general it is difficult to measure all the variables with potential effect on the dependence pattern, suggests that a non-constant copula is a prudent choice.

5.2 A Permutation-based Criterion to Detect Data Support for the Simplified Assumption

In this section we propose a to modify the CVML and the conditional CCVML method to identify data support for SA after the copula family is selected.

As was shown in previous sections, the selection criteria included in the paper do not perform well when true calibration is constant. This is in line with [Craiu and Sabeti (2012b)] who also noted that the traditional Bayesian model selection criteria, e.g. the Deviance information criterion (DIC) of [Spiegelhalter et al. (2002)], tend to prefer the more complex calibration model over a simple model with constant calibration even when the latter is actually correct. In addition of the simulations presented in the previous section, we add here that when the marginal distributions are estimated, the performance of the existing criteria worsens. To illustrate, we have simulated 50 replicates of sample sizes 1500 using Clayton copula from Sc1, Sc4 and Sc5. Each sample is fitted with the general model introduced here and a constant Clayton copula, while marginals are estimated using a general GP. Table 13 shows the proportion of correct decisions for the three scenarios and various selection criteria. These results show that even for a large sample size, the proportion of right decisions for Sc4, i.e. when SA holds, is quite low. One of the explanations is that the general model does a good job at capturing the constant trend of the calibration function and yields predictions that are not too far from the ones produced with the simpler (and correct) model. The modified CVML we propose is inspired by two desiderata: i) to separate the set of observations used for prediction from the set of observations used for fitting the model, and ii) to amplify the impact of the copula-induced errors in the CCVML calculation. The former will
reduce the implicit bias one gets when the same data is used for estimation and testing, while the latter is expected to increase the power to identify SA.

For i) we randomly partition the data into a training set \( \mathcal{D} = \{Y_{1i}, Y_{2i}, X_i\}_{i=1,...,n} \) and a test set \( \mathcal{D}^* = \{Y_{1i}^*, Y_{2i}^*, X_i^*\}_{i=1,...,n^*} \). In our numerical experiments we have kept two thirds of observations in the training set. In order to achieve ii) we note that permuting the response indexes will not affect the copula term if SA is indeed satisfied and will perturb the prediction when SA is not satisfied. However, one must cautiously implement this idea, since the permutation \( \lambda : \{1,...,n^*\} \rightarrow \{1,...,n^*\} \) will affect the marginal model fit, regardless of the SA status, as \( Y_{jM(i)}^* \) will be paired with \( X_i \), for all \( j = 1,2 \). Below we describe the permutation-based CVML criterion that combines i) and ii).

Assume that the fitted GP-SIM model yields posterior samples from the conditional distribution of latent variables and parameters \( w^{(t)} \sim w|\mathcal{D}, t = 1,...,M \). Then we define the observed data criterion as the predictive log probability of the test cases which can be easily estimated from posterior samples, as follows:

\[
CVML_{\text{obs}} = \sum_{i=1}^{n^*} \log P(Y_{1i}^*, Y_{2i}^*|\mathcal{D}, X_i^*) \approx \sum_{i=1}^{n^*} \log \left\{ \frac{1}{M} \sum_{t=1}^{M} P(Y_{1i}^*, Y_{2i}^*|w^{(t)}), X_i^* \right\} = \\
= \sum_{i=1}^{n^*} \log \left\{ \frac{1}{M} \sum_{t=1}^{M} \frac{1}{\sigma_1^{(t)}} \phi \left( \frac{Y_{1i}^* - f_{1i}^{(t)}}{\sigma_1^{(t)}} \right) \frac{1}{\sigma_2^{(t)}} \phi \left( \frac{Y_{2i}^* - f_{2i}^{(t)}}{\sigma_2^{(t)}} \right) \right\} \times \\
c \left\{ \Phi \left( \frac{Y_{1i}^* - f_{1i}^{(t)}}{\sigma_1^{(t)}} \right), \Phi \left( \frac{Y_{2i}^* - f_{2i}^{(t)}}{\sigma_2^{(t)}} \right) \right\}^{\theta_{i}^{(t)}}
\]

where \( f_{1i}^{(t)}, f_{2i}^{(t)}, \theta_{i}^{(t)} \) are the predicted values for the test cases produced by the GP-SIM model.

Consider \( J \) permutations of \( \{1...n^*\} \) which we denote as \( \lambda_1,...,\lambda_J \), and compute \( J \) permuted CVMLs as:

\[
CVML_j = \sum_{i=1}^{n^*} \log \left\{ \frac{1}{M} \sum_{t=1}^{M} \frac{1}{\sigma_1^{(t)}} \phi \left( \frac{Y_{1i}^* - f_{1i}^{(t)}}{\sigma_1^{(t)}} \right) \frac{1}{\sigma_2^{(t)}} \phi \left( \frac{Y_{2i}^* - f_{2i}^{(t)}}{\sigma_2^{(t)}} \right) \right\} \times \\
c \left\{ \Phi \left( \frac{Y_{1i}^* - f_{1i}^{(t)}}{\sigma_1^{(t)}} \right), \Phi \left( \frac{Y_{2i}^* - f_{2i}^{(t)}}{\sigma_2^{(t)}} \right) \right\}^{\theta_{i}^{(t)}}^{\lambda_j (i)}
\]

Note that \( CVML_{\text{obs}} \) differs from \( CVML_j \) only in the values of the copula parameters. While for the former we use \( \theta(X_i^*) \), in the latter we use \( \theta(X_{j\lambda_j(i)}) \) for the dependence between \( Y_{1i}^* \) and \( Y_{2i}^* \). If calibration is constant then \( CVML_{\text{obs}} \) and \( CVML_j \) should be similar, hence we define the evidence

\[
EV = 2 \times \min \left\{ \sum_{j=1}^{J} \mathbb{I} \{ CVML_{\text{obs}}<CVML_j \} \frac{J}{J} \sum_{j=1}^{J} \mathbb{I} \{ CVML_{\text{obs}}>CVML_j \} \frac{J}{J} \right\}
\]

(34)
Under the null model with constant calibration with known marginals and if we assume that $CVML_{obs}$ and $\{CVML_j : 1 \leq j \leq J\}$ are iid for each $j$, then each term inside the min function in (34) has a Uniform$(0,1)$ limiting distribution when $J \to \infty$. In that case it follows that $P(EV < 0.05) = 0.05$. In practice, the ideal situation just described is merely an approximation since the $\{CVML_j : 1 \leq j \leq J\}$ are not independent and we compute $EV$ using a fixed number of permutations. Nevertheless, the ideal setup can be used to build our decision that when $EV > 0.05$ the data support SA, and otherwise they do not.

A similar rule can be build using the CCVML criterion. For instance, its value for test data is

$$CCVML_{obs} = \frac{1}{2} \sum_{i=1}^{n^*} \log P(Y^*_1|D, X^*_i, Y^*_2) + \frac{1}{2} \sum_{i=1}^{n^*} \log P(Y^*_2|D, X^*_i, Y^*_1).$$

The permutation-based version of (35) can be obtained using the same principle as in (33) thus leading to the counterpart of (34) for CCVML.

Table 14 shows the proportion of correct decisions using proposed methods with 1000 and 500 samples in training and test set respectively, and $J = 500$ permutations. The results, especially those for Sc4, clearly show an important improvement in the rate of making the correct selection, with only a small decrease in the power to detect non-constant calibrations. We can also notice that CVML and CCVML performed similarly.

<table>
<thead>
<tr>
<th>Scenario</th>
<th>CVML</th>
<th>CCVML</th>
<th>WAIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sc1</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>Sc4</td>
<td>74%</td>
<td>78%</td>
<td>74%</td>
</tr>
<tr>
<td>Sc5</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
</tr>
</tbody>
</table>

Table 13: The percentage of correct decisions for each selection criterion and scenarios. GP-SIM and SA were fitted with Clayton copula, sample size is 1500

<table>
<thead>
<tr>
<th>Scenario</th>
<th>CVML</th>
<th>CCVML</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sc1</td>
<td>98%</td>
<td>96%</td>
</tr>
<tr>
<td>Sc4</td>
<td>92%</td>
<td>90%</td>
</tr>
<tr>
<td>Sc5</td>
<td>100%</td>
<td>100%</td>
</tr>
</tbody>
</table>

Table 14: The percentage of correct decisions for each selection criterion and scenario. Predicted CVML and CCVML values based on $n = 1000$ training and $n^* = 500$ test data, respectively. The calculation of $EV$ is based on a random sample of 500 permutations.
6 Conclusion and Future Work

The inclusion of a dynamic copula in the model comes with a significant computational price. The inclusion can be justified by the need for an exploration of dependence, or because it can improve the predictive accuracy of the model. The simplifying assumption is often used as a way to bypass the need for a conditional copula model. However, we have showed that even if the simplifying assumption holds for the true model, when we ignore the contribution of one covariate, fitted copula is no longer constant.

We have proposed a Bayesian procedure to estimate the calibration function of a conditional copula model jointly with the marginal distributions. In our attempt to move away from an additive model hypothesis we consider a sparse Gaussian process priors used in conjunction with a single index model. The resulting procedure reduces the dimensionality of the parameter space and can be used for small and moderate covariate dimension.

We have introduced a couple of selection criteria to help select the copula family from a set of candidates and to gauge data support in favour of the simplifying assumption. While the former task seems to be achieved by all criteria considered, the latter is a particularly difficult problem and we are excited about the good performance exhibited by our permutation-based version of the cross-validated marginal likelihood criterion. Its theoretical properties are the focus of our ongoing work and we plan to extend its use to identifying those covariates that do not influence the calibration function.

Acknowledgement

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References


