

Dependence Calibration in Conditional Copulas: A Nonparametric Approach

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The study of dependence between random variables is a mainstay in statistics. In many cases, the strength of dependence between two or more random variables varies according to the values of a measured covariate. We propose inference for this type of variation using a conditional copula model where the copula function belongs to a parametric copula family and the copula parameter varies with the covariate. In order to estimate the functional relationship between the copula parameter and the covariate, we propose a nonparametric approach based on local likelihood. Of importance is also the choice of the copula family that best represents a given set of data. The proposed framework naturally leads to a novel copula selection method based on cross-validated prediction errors. We derive the asymptotic bias and variance of the resulting local polynomial estimator, and outline how to construct pointwise confidence intervals. The finite-sample performance of our method is investigated using simulation studies and is illustrated using a subset of the Matched Multiple Birth data.

DS: Copula parameter; Copula selection; Covariate adjustment; Local likelihood; Local polynomials; Prediction error.

1. Introduction

Understanding dependence is an important, yet challenging, task in multivariate statistical modeling. One often needs to specify a complex joint distribution of random variables to have a complete view of the dependence structure. The challenge of constructing such multivariate distributions can be significantly reduced if one uses a copula model to separate the marginal components of a joint distribution from its dependence structure. Sklar's theorem (1959) is central to the theoretical foundation needed for the use of copulas as it states that a multivariate distribution can be fully characterized by its marginal distributions and a copula, that is, a multivariate distribution function having uniform $[0, 1]$ marginals.

In what follows, we focus on the bivariate case only for simplicity, the arguments being extendable to more than two dimensions. Let Y_1 and Y_2 be continuous random variables of interest with joint distribution function H and marginal distributions F_1 and F_2 , respectively. Sklar's theorem ensures the existence of a unique copula $C : [0, 1]^2 \rightarrow [0, 1]$, which satisfies $H(y_1, y_2) = C\{F_1(y_1), F_2(y_2)\}$, for all $(y_1, y_2) \in \mathbb{R}^2$.

In the last 20 years, copulas have been widely used in a variety of applied work. We refer the reader to Embrechts, McNeil, and Straumann (2002); Cherubini, Luciano, and Vecchiato (2004); and Frees and Valdez (1998) for applications specific to finance and insurance. In survival analysis, Clayton (1978), Shih and Louis (1995), Wang and Wells (2000), and the monograph by Hougaard (2000) present the copula techniques to model multivariate time-to-event data and competing risks. As a direct result of their wide applicability, a large number of parametric families of copulas, typically indexed by a real-valued parameter θ , have been proposed in the literature to represent different dependence patterns. While the copula family describes the functional form, within each family it

is the copula parameter, θ , that controls the strength of the dependence. A comprehensive introduction on copulas and their properties can be found in Nelsen (2006) and the connections between various copulas and dependence concepts are discussed in detail by Joe (1997). If a parametric form is assumed for the copula function, estimation can be achieved using maximum likelihood estimation for the single copula parameter (Genest, Ghoudi, and Rivest, 1995; Joe, 1997). Alternatively, estimation can be performed fully nonparametrically by using kernel estimators (Fermanian and Scaillet, 2003; Chen and Huang, 2007).

Although copulas have been in use in the applied statistical literature for more than 20 years, the covariate adjustment for copulas has been considered only recently. The extension of Sklar's theorem for conditional distributions (Patton, 2006) allows us to adjust for covariates. For instance, if, in addition to Y_1 and Y_2 , we have information on a covariate X , then the influence of X on the dependence between Y_1 and Y_2 can be modeled by the conditional copula $C(\cdot | X)$, which is the joint distribution function of $U_1 \equiv F_{1|X}(Y_1 | x)$ and $U_2 \equiv F_{2|X}(Y_2 | x)$ given $X = x$, where $Y_k | X = x$ has cdf $F_{k|X}(\cdot | x)$, $k = 1, 2$. Patton (2006) showed that for each x in the support of X , the joint conditional distribution is uniquely defined by

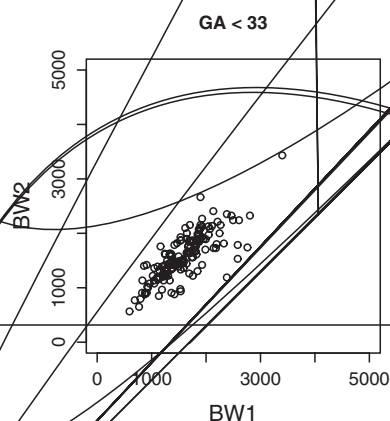
$$H_X(y_1, y_2 | x) = C\{F_{1|X}(y_1 | x), F_{2|X}(y_2 | x) | x\}, \quad (1) \\ \text{for all } (y_1, y_2) \in \mathbb{R}^2.$$

Conditional copulas have been used mostly in the context of financial time series to allow for time-variation in the dependence structure via likelihood inference for ARMA models (Jondeau and Rockinger, 2006; Patton, 2006; Bartram, Taylor, and Wang, 2007).

The main contribution of the current work is to provide a nonparametric procedure to estimate the functional relationship between the copula parameter and the covariate(s). Our motivation is to relax the parametric assumptions about this relationship. Since a parametric model will only find features in the data that are already incorporated a priori in the model, parametric approaches might not be adequate if the dependence structure does not fall into a preconceived class of functions.

In Section 4, we investigate the impact of gestational age on the dependence between twin birth weights using a subset of the Matched Multiple Birth Data Set. Among the twin live births, we consider those who were delivered between 28 and 42 weeks of gestation and in which both twins survived for the first year of life. Our initial investigation, shown in Figure 1, indicates a relatively stronger dependence between the birth weights (in grams) of the preterm (28–32 weeks) and postterm (38–42 weeks) twins compared to the twins delivered at term (33–37 weeks). This suggests the need of such nonparametric approach as an exploratory tool for detecting the underlying functional relationship between the copula parameter and the covariate.

Smoothing methods for function estimation have been substantially studied for various problems. In this article, we use the local polynomial framework (see Fan and Gijbels, 1996, for a comprehensive review) for the covariate adjusted copula estimation via local likelihood-based models (Tibshirani and Hastie, 1987). In practice, all inferential methods for copulas must be accompanied by a strategy to select among a number of copula families the one that best approximates the data at hand. Choosing an appropriate family of copulas to fit a given set of data is challenging and has recently attracted considerable interest. Some methods for copula selection include goodness-of-fit tests based on the empirical copula (Durrleman, Nikoghbali, and Roncalli, 2000), on the Kendall process (Genest and Rivest, 1993; Wang and Wells, 2000; Genest, Rémillard, and Beaudoin, 2007), and on kernel density estimation (Fermanian, 2005; Craiu and Craiu, 2008). Our estimation procedure naturally leads to a novel copula selection method based on cross-validated prediction errors (CVPE). Besides being data-adaptive, the proposed selection criterion makes comparisons across copula families possible due to its general applicability.



The article is organized as follows. In Section 2, we present the proposed estimation procedure, discuss aspects related to copula selection, and derive the asymptotic bias and variance of the nonparametric estimator used for constructing pointwise confidence bands. Section 3 contains our simulation studies and in Section 4 we use the Matched Multiple Birth Data Set to investigate the influence of the gestational age on the strength of dependence between the twin birth weights. Discussion and conclusions are presented in Section 5. Technical details and additional simulated and real data examples can be found in the Web Appendix.

2. Methodology

2.1 Proposed Method

Let Y_1 and Y_2 be continuous variables of interest and X be a continuous variable that may affect the dependence between Y_1 and Y_2 . We consider the model (1) with the conditional density $h_X(Y_1, Y_2 | x; \theta, \alpha_1, \alpha_2)$ in which our main interest lies in the conditional copula parameter θ , while the conditional marginal densities $f_{1|X}$ and $f_{2|X}$ are characterized by α_1 and α_2 , respectively,

$$h_X(y_1, y_2 | x; \theta, \alpha_1, \alpha_2) = f_{1|X}(y_1 | x; \alpha_1) f_{2|X}(y_2 | x; \alpha_2) \times c(u_1, u_2 | x; \theta, \alpha_1, \alpha_2),$$

where $u_k = F_{k|X}(y_k | x; \alpha_k)$, $k = 1, 2$ and $c(u_1, u_2 | x; \theta, \alpha_1, \alpha_2)$ is the conditional copula density. Here, we impose a minimal requirement that the parameters that govern the marginals are different from the copula parameter. It is easy to see that such a requirement is not restrictive, for instance, in a regression setting, marginals may correspond to mean effects and the copula to covariance structure. Hence, the estimation can be performed in two stages, first for the marginal parameters and then for the copula. Then, by replacing the estimates $\hat{F}_{1|X}(y_1 | x)$ and $\hat{F}_{2|X}(y_2 | x)$ in (1), we can estimate the functional form of the copula parameter.

Since our main focus is on the dependence structure, we assume that the conditional marginal distributions $F_{1|X}$ and $F_{2|X}$ are known, and consider the following model:

$$(U_{1i}, U_{2i}) | X_i \sim C\{u_{1i}, u_{2i} | \theta(x_i)\},$$

where $\theta(x_i) = g^{-1}\{\eta(x_i)\}$, $i = 1, \dots, n$.

Here, $g^{-1} : \mathbb{R} \rightarrow \mathbb{R}$ is the known inverse link function, which ensures that the copula parameter has the correct range, and η is the unknown *calibration function* to be estimated. The term *calibration* emphasizes that the level of dependence is adjusted for the covariate effect on the copula parameter. Analogous to the generalized linear models one needs to choose an appropriate link function, since there is no guarantee that the estimate of θ is in the correct parameter range for the particular copula family under consideration. For instance, for the

represents best the data at hand. For the q th copula family, the bandwidth selection process yields the optimal bandwidth h_q^* . For each left-out sample point (U_{1i}, U_{2i}, X_i) , we obtain the estimate for the conditional copula's parameter $\hat{\theta}_{h_q^*}^{(-i)}$, which, in turn, leads to the *best candidate model* from the q th family, $C_q\{U_{1i}, U_{2i} | \hat{\theta}_{h_q^*}^{(-i)}(X_i)\}$, with $i = 1, \dots, n$, $q = 1, \dots, Q$. We use the conditional expectation formula to measure the predictive ability for each of the candidate models. Within family C_q , the *best conditional prediction* for U_{1i} is

$$\hat{E}_q^{(-i)}(U_{1i} | U_{2i}, X_i) = \int_0^1 U_{1c_q} \{U_{1i}, U_{2i} | \hat{\theta}_{h_q^*}^{(-i)}(X_i)\} dU_{1i}.$$

Then, the CVPE is used to define the model selection criterion

$$\text{CVPE}(C_q) = \sum_{i=1}^n \left[\{U_{1i} - \hat{E}_q^{(-i)}(U_{1i} | U_{2i}, X_i)\}^2 + \{U_{2i} - \hat{E}_q^{(-i)}(U_{2i} | U_{1i}, X_i)\}^2 \right]. \quad (4)$$

The copula family C_q , which yields the minimum $\text{CVPE}(C_q)$ value, is selected. This criterion can be justified as follows. If we denote M_0 the true copula family and M the working copula family, then the first part in (4) normalized by $1/n$ is an approximation of $E_{M_0}[\{U_1 - E_M(U_1 | U_2, X)\}^2 | U_2, X]$, which is minimized when the model M is correctly specified, that is, $M = M_0$. A similar result holds for the second part in (4).

2.3 Asymptotic Properties

Before presenting the main results, we will introduce some notation. Let $f_X(\cdot) > 0$ be the density function of the covariate X . Denote the moments of K and K^2 respectively by $\mu_j = \int t^j K(t) dt$ and $\nu_j = \int t^j K^2(t) dt$, and write the matrices $S = (\mu_{j+\ell})_{0 \leq j, \ell \leq p}$, $S^* = (\nu_{j+\ell})_{0 \leq j, \ell \leq p}$, the $(p+1) \times 1$ vectors ${}_p = (\mu_{p+1}, \dots, \mu_{2p+1})^T$, as well as the unit vector $e_1 = (1, 0, \dots, 0)^T$. For simplicity, we use $\ell(\theta, U_1, U_2) = \ln c(U_1, U_2 | \theta)$ for the log-copula density and denote its first and second derivatives with respect to θ by $\ell'(\theta, U_1, U_2) = \partial \ell(\theta, U_1, U_2) / \partial \theta$ and $\ell''(\theta, U_1, U_2) = \partial^2 \ell(\theta, U_1, U_2) / \partial \theta^2$, respectively. For a fixed point x lying in the interior of the support of f_X , define $\sigma^2(x) = -E(\ell''[g^{-1}\{\eta(x)\}, U_1, U_2] | X = x)$.

For our derivations, we require the assumptions given in the Appendix. The assumption (A1) is to ensure that the copula density satisfies the first- and second-order Bartlett identities. Further discussion on condition (A1) for certain copula families can be found in Hu (1998) and Chen and Fan (2006). The mild regularity conditions in (A2) are commonly adopted in nonparametric regression.

Typically, an odd-order polynomial fit is preferred to an even-order fit in local polynomial modeling, as the latter induces a higher asymptotic variance (see Fan and Gijbels, 1996, for details). Therefore, we consider only the odd-order fits in the asymptotic expressions for the conditional bias and variance. The following theorem summarizes the main results, denoting the collection of covariate/design variables $\{X_1, \dots, X_n\}$ by \mathbb{X} , while the technical details are deferred to the Web Appendix.

1: Assume that (A1) and (A2) hold, $h \rightarrow 0$ and $nh \rightarrow \infty$ as $n \rightarrow \infty$, for an odd-order local polynomial fit of

degree p ,

$$\begin{aligned} \text{Bias}(\hat{\eta}(x) | \mathbb{X}) &= e_1^T S^{-1} {}_p \frac{\eta^{(p+1)}(x)}{(p+1)!} h^{p+1} + o_p(h^{p+1}), \\ \text{var}(\hat{\eta}(x) | \mathbb{X}) &= \frac{1}{nh f(x) [(g^{-1})' \{\eta(x)\}]^2 \sigma^2(x)} e_1^T S^{-1} S^* S^{-1} e_1 \\ &\quad + o_p\left(\frac{1}{nh}\right). \end{aligned}$$

As a direct corollary of Theorem 1, we obtain the asymptotic conditional bias and variance of the copula parameter estimator, $\hat{\theta}(x) = g^{-1}\{\hat{\eta}(x)\}$.

1: Assume that conditions of Theorem 1 holds,

then

$$\text{Bias}(\hat{\theta}(x) | \mathbb{X}) = e_1^T S^{-1} {}_p \frac{\eta^{(p+1)}(x)}{g' \{\theta(x)\} (p+1)!} h^{p+1} + o_p(h^{p+1}), \quad (5)$$

$$\text{var}(\hat{\theta}(x) | \mathbb{X}) = \frac{1}{nh f(x) \sigma^2(x)} e_1^T S^{-1} S^* S^{-1} e_1 + o_p\left(\frac{1}{nh}\right). \quad (6)$$

One can use the result of Corollary 1 to approximate the bias and variance of the estimated copula parameter. The unknown quantity $\sigma^2(x)$ in the variance expression can be approximated by

$$\hat{\sigma}^2(x) = - \int_0^1 \int_0^1 \ell''\{\hat{\theta}(x), U_1, U_2\} c\{U_1, U_2 | \hat{\theta}(x)\} dU_1 dU_2, \quad (7)$$

where $c(\cdot, \cdot)$ is the density corresponding to the underlying copula family. The approximate $100(1 - \alpha)\%$ pointwise confidence bands for the copula parameter are given by,

$$\hat{\theta}(x) - \hat{b}(x) \pm z_{1-\alpha/2} \hat{V}(x)^{1/2}, \quad (8)$$

where $\hat{b}(x)$ and $\hat{V}(x)$ are the estimated bias and variance based on (5) and (6), and $z_{1-\alpha/2}$ is the $100(1 - \alpha/2)$ th quantile of the standard normal distribution. In practice, estimating the bias can be difficult due to unknown higher order derivatives (see Fan and Gijbels, 1996, for further discussion on bias correction). Alternatively, when variability plays a dominant role in (8), one may use a smaller bandwidth to bring the bias down to negligible levels (Fan and Zhang, 2000).

In practice, the estimation of the conditional marginal distributions may have an impact on the inference of the copula parameter. If the marginal distributions can be adequately characterized by a parametric model, as in the example con-

the Web Appendix using the twin data set. It is not surprising that, due to the uncertainty in the nonparametric marginals, the bootstrap bands are wider than the asymptotic ones using (8). Thus in the absence of an adequate parametric marginal model, we suggest the use of the raw bootstrap approach. Nevertheless, the construction of more computationally efficient and theoretically justified inference procedures is of great importance and constitutes a central topic of our future efforts.

3. Simulation Study

This section illustrates the finite sample performance of the local copula parameter estimation and the copula selection method. We consider the Clayton, Frank, and Gumbel families of copulas in simulations. These choices cover a wide range of situations as the Clayton and Gumbel copulas are known to exhibit strong and weak lower tail dependence, respectively, while the Frank copula is symmetric and shows no tail dependence. Basic properties of these copulas can be found in the Appendix.

The inverse link functions are chosen as $g^{-1}(t) = \exp(t)$ for the Clayton copula, $g^{-1}(t) = t$ for the Frank copula, and $g^{-1}(t) = \exp(t) + 1$ for the Gumbel copula, so that the resulting copula parameter estimates will be in the correct range.

We generate the data $\{(U_{1i}, U_{2i} | X_i) : i = 1, \dots, n\}$ from the Clayton copula under each of the following models:

- (1) Linear calibration function : $\eta(X) = 0.8X - 2$

$$(U_1, U_2) | X \sim C\{u_1, u_2 | \theta = \exp(0.8X - 2)\} \\ \text{where } X \sim \text{Uniform}(2, 5),$$

- (2) Quadratic calibration function: $\eta(X) = 2 - 0.3(X - 4)^2$

$$(U_1, U_2) | X \sim C\{u_1, u_2 | \theta = \exp\{2 - 0.3(X - 4)^2\}\} \\ \text{where } X \sim \text{Uniform}(2, 5).$$

We first generate the covariate values X_i from Uniform $(2, 5)$. Then, for each $i = 1, \dots, n$, we obtain the copula parameter, $\theta_i = \exp\{\eta(x_i)\}$, imposed by the given calibration and link functions, and simulate the pairs $(U_{1i}, U_{2i}) | X_i$ from the Clayton copula with the parameter θ_i . The true copula parameter varies from 0.67 to 7.39 in the linear calibration model, and from 2.22 to 7.39 in the nonlinear one. Under each model, we conduct experiments with sample sizes $n = 200$ and $n = 500$, each replicated $m = 100$ times. Additional simulation results in which the true underlying model is based on the Frank copula are included in the Web Appendix.

To estimate the copula parameter, we perform the local linear estimation, with $p = 1$, under each family, as well as the parametric estimation in which η is assumed to be linear in X . By performing the estimation also under the Frank and Gumbel families, we investigate the impact of the copula (mis)specification. We compare our proposed approach with the parametric estimation when the underlying calibration function is correctly specified, as in the first model, and when it is misspecified, as in the second one. For the bandwidth parameter, we consider 12 candidate values, ranging from 0.33 to 2.96, equally spaced on a logarithmic scale. All results reported are based on the local estimates at the chosen optimum bandwidth, which is given by the cross-validated likelihood criterion (3).

Since the accuracy of the calibration estimation is not directly comparable across different copula families, we convert the copula parameters to a common scale provided by the Kendall's tau measure of association, a widely used approach in copula inference (Trivedi and Zimmer, 2007). The population version of Kendall's tau can be expressed in terms of a conditional copula function

$$\tau_C(x) = 4 \int_0^1 \int_0^1 C(u_1, u_2 | x) dC(u_1, u_2 | x) - 1.$$

For each of the three families, we report the connection between θ and Kendall's tau in the Appendix. Table 1 displays the Monte Carlo estimates of the integrated mean square error (IMSE) along with the integrated square Bias (IBIAS²) and integrated Variance (IVAR),

$$\begin{aligned} \text{IBIAS}^2(\hat{\tau}) &= \int_{\mathcal{X}} [E\{\hat{\tau}(x)\} - \tau(x)]^2 dx, \\ \text{IVAR}(\hat{\tau}) &= \int_{\mathcal{X}} E\{[\hat{\tau}(x) - E\{\hat{\tau}(x)\}]^2\} dx, \\ \text{IMSE}(\hat{\tau}) &= \int_{\mathcal{X}} E\{[\hat{\tau}(x) - \tau(x)]^2\} dx \\ &= \text{IBIAS}^2(\hat{\tau}) + \text{IVAR}(\hat{\tau}). \end{aligned}$$

From Table 1, we see that the parametric estimation performs better under the linear calibration model when it is using the correct functional form. However, when there is no known parametric model for the calibration function, the proposed nonparametric approach better captures the covariate effect on the copula parameter. The results also show that the performance of the estimation deteriorates as the properties of the used copula family significantly depart from the true one. Since the Frank copula, having no tail dependence, is closer to the Clayton copula than is the Gumbel copula, it yields better results in all simulation scenarios compared to Gumbel.

We also construct the approximate 90% pointwise confidence bands for the copula parameter under the correctly selected Clayton family, where the bias is much smaller than the variance as noticed in Table 1. We thus use half of the optimum bandwidth to assess $\sigma^2(x)$ in (7) while further reducing the bias to a negligible level (Fan and Zhang, 2000). To be consistent, for each Monte Carlo sample, the confidence intervals obtained for the copula parameter are converted to the Kendall's tau scale. Figure 2 displays the confidence bands for the Kendall's tau, averaged over 100 Monte Carlo samples ($n = 200$). For comparison, we present the Monte Carlo based confidence bands obtained from 100 estimates of Kendall's tau, which agree well with our proposal.

For the copula selection, we calculate the cross-validated prediction errors (4) and evaluate the performance by counting the number of times the Clayton copula is selected. The results show that we successfully identify the true copula family, 91% ($n = 200$) and 99% ($n = 500$) of the times under the linear calibration model; and 97% ($n = 200$) and 100% ($n = 500$) of the times under the quadratic calibration model.

Table 1
Integrated Squared Bias (IBIAS²), Integrated Variance (IVAR), and Integrated Mean Square Error (IMSE, multiplied by 100) of the Kendall's tau estimator. The last column shows the averages of the bandwidths h^ selected using (3).*

| Linear calibration model | | | | | | | | |
|--------------------------|-----|-----------------------|-------|-------|--------------------|-------|-------|-------|
| | | Parametric estimation | | | Local estimation | | | h^* |
| | n | IBIAS ² | IVAR | IMSE | IBIAS ² | IVAR | IMSE | |
| Clayton | 200 | 0.024 | 0.305 | 0.329 | 0.017 | 0.553 | 0.570 | 2.183 |
| | 500 | 0.018 | 0.136 | 0.154 | 0.020 | 0.228 | 0.248 | 2.283 |
| Frank | 200 | 0.490 | 0.596 | 1.086 | 0.044 | 0.963 | 1.007 | 1.848 |
| | 500 | 0.479 | 0.265 | 0.744 | 0.060 | 0.437 | 0.497 | 1.644 |
| Gumbel | 200 | 3.739 | 1.115 | 4.660 | 3.704 | 1.716 | 5.389 | 2.095 |
| | 500 | 3.499 | 0.429 | 3.928 | 3.510 | 0.556 | 4.066 | 2.385 |

| Quadratic calibration model | | | | | | | | |
|-----------------------------|-----|-----------------------|-------|-------|--------------------|-------|-------|-------|
| | | Parametric estimation | | | Local estimation | | | h^* |
| | n | IBIAS ² | IVAR | IMSE | IBIAS ² | IVAR | IMSE | |
| Clayton | 200 | 0.414 | 0.129 | 0.543 | 0.040 | 0.288 | 0.328 | 1.392 |
| | 500 | 0.423 | 0.046 | 0.469 | 0.027 | 0.113 | 0.140 | 0.910 |
| Frank | 200 | 0.324 | 0.276 | 0.600 | 0.123 | 0.504 | 0.627 | 1.779 |
| | 500 | 0.357 | 0.090 | 0.447 | 0.114 | 0.188 | 0.302 | 1.238 |
| Gumbel | 200 | 4.914 | 0.696 | 5.610 | 4.808 | 1.301 | 6.109 | 1.977 |
| | 500 | 4.862 | 0.246 | 5.108 | 4.761 | 0.497 | 5.258 | 1.676 |

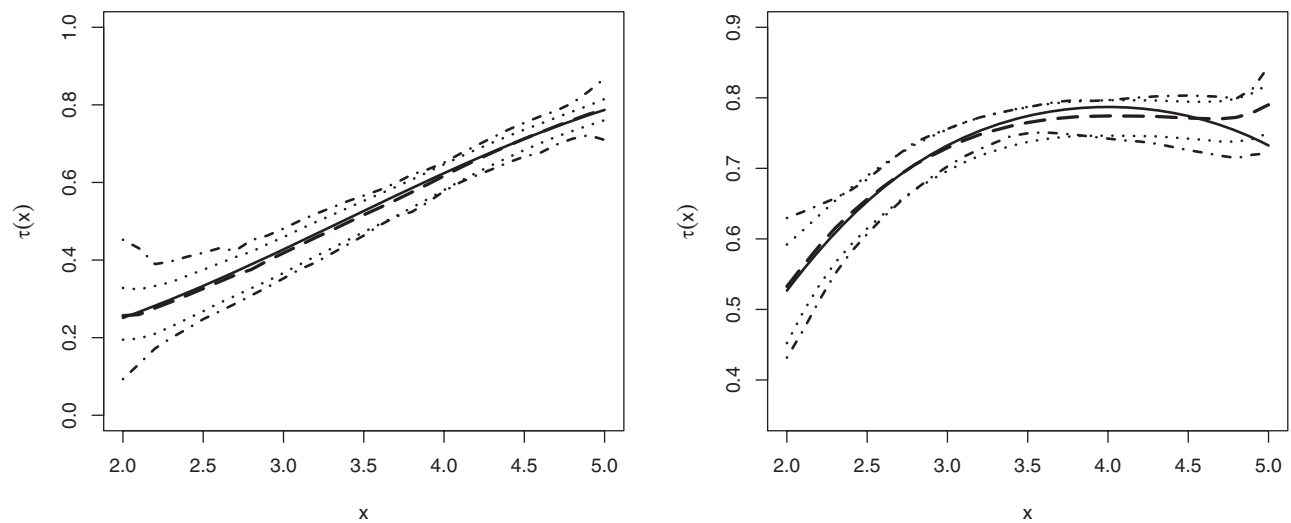


Figure 2. Simulation study: 90% confidence intervals for the Kendall's tau under the Clayton copula with the linear (left panel) and quadratic (right panel) calibration models: truth (solid line), averaged local linear estimates (dashed line), approximate confidence intervals (dotted line), and Monte Carlo confidence intervals (dotdashed line).

4. Data Example: Gestational Age-Specific Birth Weight Dependence in Twins

We now apply our proposed method to a subset of the Matched Multiple Birth Data Set. The data containing all twin births in the United States from 1995 to 2000 enable detailed investigation of twin gestations. In our application, we consider the twin live births in which both babies survived their first year of life with mothers of age between 18 and 40. Of interest is the dependence between the birth weights of twins (in grams), denoted by BW_1 and BW_2 , respectively. The gestational age, GA, is an important factor for prenatal

growth and is therefore chosen as the covariate. We consider a random sample of 30 twin live births for each gestational age (in weeks) between 28 and 42.

The scatterplot and histograms of the birth weights, for $n = 450$ twin pairs, are given in Figure 3a, from which the marginals are seen to be fitted well by parametric cubic regression models with normal noise, shown in Figure 3c and 3d. The resulting coefficients, all significant at 1% level, are plugged into $U_{ki} = [\{BM_i = \hat{\mu}_{ki}(GA)\}/\hat{\sigma}_k], k = 1, 2, i = 1, \dots, n$, to transform the response variables to uniform scale, where $\hat{\mu}_k$ are the cubic fit and $\hat{\sigma}_k$ are the estimated standard

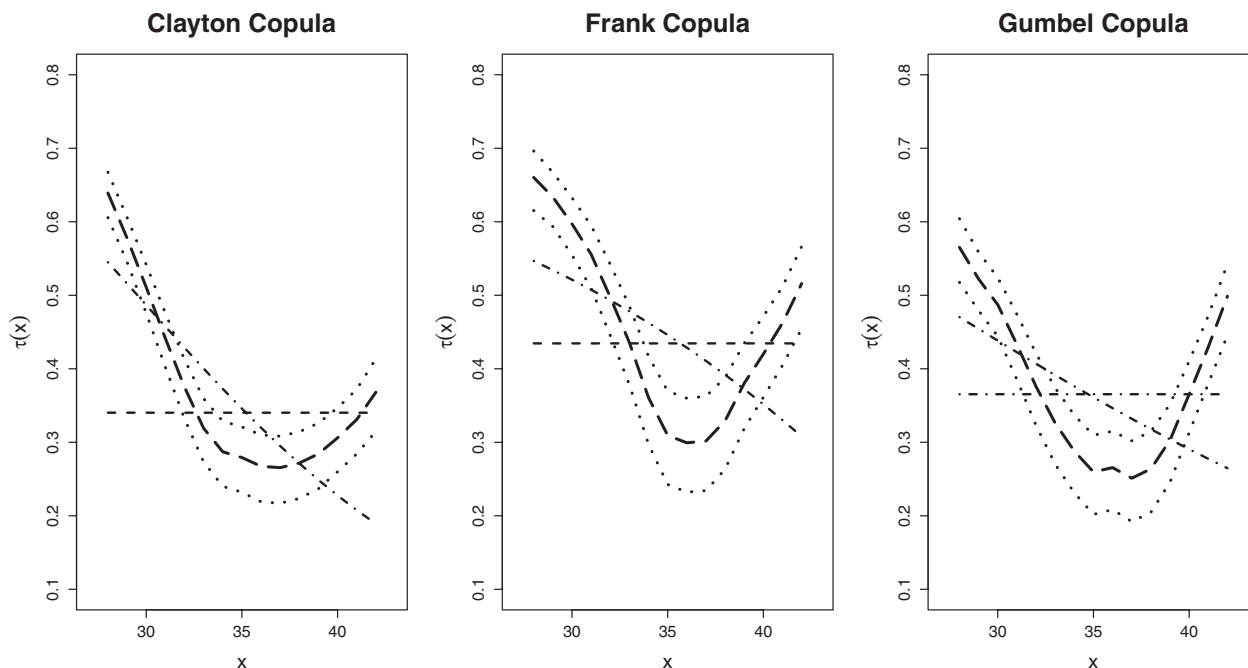


Figure 4. Twin birth data: the Kendall's tau estimates under three copula families: global constant estimate (dashed line), global linear estimates (dotdashed line), local linear estimates at the optimum bandwidth (longdashed line), and an approximate 90% confidence interval (dotted lines).

dependence and a measured covariate, we allow the copula parameter to change according to a *calibration function* of the covariate. Statistical inference for the calibration function is obtained using local polynomial estimation. The methodology proposed here leads to a novel conditional copula selection procedure, in which we use prediction accuracy to select, via cross-validation, among a number of copula families, the one that best approximates the data at hand.

Our simulation study conveys that (i) the nonparametric estimator of the calibration function is flexible enough to capture nonlinear patterns and (ii) the copula selection procedure performs well in the cases studied so far. The data analysis reveals a gestational age specific dependence pattern in the birth weights of twins that, to our knowledge, has not been detected before and may be of scientific interest.

Although in this article we focus our attention on bivariate copulas, it is possible to extend our method to more general multivariate copulas. In addition, if more covariates are of potential interest for the conditional copula model, then we recommend a careful selection of the variables prior to estimation of the calibration function, as the computational cost increases significantly with each covariate added to the model. We are currently working on extending the framework of the work presented here by considering mixtures of conditional copulas in order to increase the spectrum of applications that can be tackled using our approach.

6. Supplementary Materials

A Web Appendix containing technical details (referenced in Sections 2.1 and 2.3), and additional simulated and real data examples, is available under the Paper Information link at the *Biometrics* website <http://www.biometrics.tibs.org>.

A K D S

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A DI

Regularity Assumptions

Let $N(x)$ denote the neighborhood of an interior point x .

- (A1) $\ell'\{\theta(x), U_1, U_2\}$ and $\ell''\{\theta(x), U_1, U_2\}$ exist and are continuous on $N(x) \times (0, 1)^2$, and can be bounded by integrable functions of u_1 and u_2 in $N(x)$.
- (A2) The functions $f_X(\cdot), \eta^{(p+2)}(\cdot), g''(\cdot)$, and $\sigma^2(\cdot)$ are continuous in $N(x)$, and $\sigma^2(x') \geq c$ for $x' \in N(x)$ and some $c > 0$. Without loss of generality, the kernel density $K(\cdot)$ has a compact support $[-1, 1]$.

Copula Families Used in Our Implementations

The Clayton family has the copula function

$$C(u_1, u_2) = (u_1^{-\theta} + u_2^{-\theta} - 1)^{-\frac{1}{\theta}}, \quad \theta \in (0, \infty),$$

with Kendall's $\tau = \frac{\theta}{\theta + 2}$.

The Frank family has the copula function

$$C(u_1, u_2) = -\frac{1}{\theta} \ln \left\{ 1 + \frac{(e^{-\theta u_1} - 1)(e^{-\theta u_2} - 1)}{e^{-\theta} - 1} \right\},$$

$\theta \in (-\infty, \infty) \setminus \{0\}$,

with Kendall's $\tau = 1 + \frac{4}{\theta} \{D_1(\theta) - 1\}$, where $D_1(\theta) = \frac{1}{\theta} \int_0^\theta \frac{t}{e^t - 1} dt$ is the Debye function.

The Gumbel family has the copula function

$$C(u_1, u_2) = \exp \left[- \{(-\ln u_1)^\theta (-\ln u_2)^\theta\}^{\frac{1}{\theta}} \right], \quad \theta \in [1, \infty),$$

with Kendall's $\tau = 1 - \frac{1}{\theta}$.

Accepted Pre-proof
Dependence Characterization in Conditional Copulas
A Nonparametric Approach

Elif F. Acar, Radu V. Craiu, and Fang Yao

Appendix A: Technical Details

The score and hessian functions

The score vector $\nabla \mathcal{L}(\beta, \mathbf{z})$ and hessian matrix $\nabla^2 \mathcal{L}(\beta, \mathbf{z})$ used in the Newton-Raphson algorithm are given by, denoting $\mathbf{x}_{i,x} = (1, X_i - \mathbf{z}, \dots, (X_i - \mathbf{z})^p)^T$,

$$\begin{aligned} \nabla \mathcal{L}(\beta, \mathbf{z}) &= \frac{\mathcal{L}(\beta, \mathbf{z}, \mathbf{p}, \hat{\rho})}{\beta} \\ &= \sum_i^n \frac{1}{\beta} \left\{ \left(\mathbf{I}^{-1}(\mathbf{x}_{i,x}^T \beta), \mathbf{1}_i, \mathbf{2}_i \right) \right\} h(X_i - \mathbf{z}) \\ &= \sum_i^n \left\{ \left(\mathbf{I}^{-1}(\mathbf{x}_{i,x}^T \beta), \mathbf{1}_i, \mathbf{2}_i \right) \left[\left(\mathbf{I}^{-1} \right)'(\mathbf{x}_{i,x}^T \beta) \right] \mathbf{x}_{i,x} \right\} h(X_i - \mathbf{z}), \end{aligned} \tag{1}$$

$$\begin{aligned} \nabla^2 \mathcal{L}(\beta, \mathbf{z}) &= \frac{\nabla^2 \mathcal{L}(\beta, \mathbf{z}, \mathbf{p}, \hat{\rho})}{\beta^2} \\ &= \sum_i^n \frac{1}{\beta} \left\{ \left(\mathbf{I}^{-1}(\mathbf{x}_{i,x}^T \beta), \mathbf{1}_i, \mathbf{2}_i \right) \left[\left(\mathbf{I}^{-1} \right)'(\mathbf{x}_{i,x}^T \beta) \right] \mathbf{x}_{i,x} \right\} h(X_i - \mathbf{z}) \\ &= \sum_{i=1}^n \left\{ \left(\mathbf{I}^{-1}(\mathbf{x}_{i,x}^T \beta), \mathbf{1}_i, \mathbf{2}_i \right) \left[\left(\mathbf{I}^{-1} \right)'(\mathbf{x}_{i,x}^T \beta) \right]^2 \right. \\ &\quad \left. + \left(\mathbf{I}^{-1}(\mathbf{x}_{i,x}^T \beta), \mathbf{1}_i, \mathbf{2}_i \right) \left(\mathbf{I}^{-1} \right)''(\mathbf{x}_{i,x}^T \beta) \right\} \mathbf{x}_{i,x} \mathbf{x}_{i,x}^T h(X_i - \mathbf{z}) \end{aligned} \tag{2}$$

Derivations of Asymptotic Bias and Variance

Let $\mathbf{W} = \text{diag}\{1, \dots, 1\}$, $\mathbf{W}_x = \text{diag}\{h(X_1 - \mathbf{x}), \dots, h(X_n - \mathbf{x})\}$,

$$X_x = \begin{pmatrix} 1 & X_1 - x & \cdots & (X_1 - x)^p \\ 1 & X_2 - x & \cdots & (X_2 - x)^p \\ \vdots & \vdots & & \vdots \\ 1 & X_n - x & \cdots & (X_n - x)^p \end{pmatrix}$$

Define $(p+1) \times (p+1)$ matrices $\mathbf{S}_n = \sum_{i=1}^n \mathbf{x}_{i,x} \mathbf{x}_{i,x}^T h(X_i - \mathbf{x})$ and $\mathbf{S}_n^* = \sum_{i=1}^n \mathbf{x}_{i,x} \mathbf{x}_{i,x}^T h^2(X_i - \mathbf{x})$, with entries $S_{n,j} = \sum_{i=1}^n (X_i - \mathbf{x})^j h(X_i - \mathbf{x})$ and $S_{n,j}^* = \sum_{i=1}^n (X_i - \mathbf{x})^j h^2(X_i - \mathbf{x})$.

The proofs of Theorem 1 and Corollary 1 rely on the following Taylor expansion

$$\mathbf{0} = \nabla \mathcal{L}(\hat{\beta}, \mathbf{x}) \approx \nabla \mathcal{L}(\beta, \mathbf{x}) + \nabla^2 \mathcal{L}(\beta, \mathbf{x}) \{\hat{\beta} - \beta\},$$

where $\beta = (\beta_0, \beta_1, \dots, \beta_p)^T$ is the vector of true local parameters and $\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p)^T$ is the local likelihood estimator, yielding

$$\hat{\beta} - \beta \approx -(\nabla^2 \mathcal{L}(\beta, \mathbf{x}))^{-1} \nabla \mathcal{L}(\beta, \mathbf{x})$$

Hence, the leading terms in the asymptotic conditional bias and variance can be written as

$$(\hat{\beta} | \mathbb{X}) - \beta \approx -(\nabla^2 \mathcal{L}(\beta, \mathbf{x}) | \mathbb{X})^{-1} (\nabla \mathcal{L}(\beta, \mathbf{x}) | \mathbb{X}), \quad (3)$$

$$\text{var}(\hat{\beta} | \mathbb{X}) \approx (\nabla^2 \mathcal{L}(\beta, \mathbf{x}) | \mathbb{X})^{-1} \text{var}(\nabla \mathcal{L}(\beta, \mathbf{x}) | \mathbb{X}) (\nabla^2 \mathcal{L}(\beta, \mathbf{x}) | \mathbb{X})^{-1} \quad (4)$$

In the following we approximate three terms appearing in (3) and (4). The expectation of the kernel weighted local score function is

$$(\nabla \mathcal{L}(\beta, \mathbf{x}) | \mathbb{X}) = \sum_{i=1}^n \{ \beta' (h^{-1}(\mathbf{x}_{i,x}^T \beta), \beta_{1i}, \beta_{2i}) | \mathbb{X} \} [h^{-1}(\mathbf{x}_{i,x}^T \beta)] \mathbf{x}_{i,x} h(X_i - \mathbf{x})$$

Since, for each $i = 1, 2, \dots, n$, we have $(\beta_{1i}, \beta_{2i}) | X_i \sim C(\beta_1, \beta_2 | h^{-1}(X_i))$, from the first order Bartlett's identity we have

$$\mathbf{0} = \{ \beta' (h^{-1}(X_i)), \beta_{1i}, \beta_{2i} | \mathbb{X} \} = \{ \beta' (h^{-1}(\mathbf{x}_{i,x}^T \beta + \boldsymbol{\tau}_i), \beta_{1i}, \beta_{2i}) | \mathbb{X} \},$$

by a p^{th} degree polynomial,

$$\nu_i = \sum_{j=p+1}^{\infty} \nu_j (X_i - \bar{x})^j = \nu_{p+1} (X_i - \bar{x})^{p+1} + o_p\{(X_i - \bar{x})^{p+1}\}$$

If η^{-1} is continuous and twice differentiable, then

$$\eta'(\eta^{-1}(X_i)), \nu_{1i}, \nu_{2i} \approx \eta'(\eta^{-1}(x_{i,x}^T \beta)), \nu_{1i}, \nu_{2i} + [\nu_i(\eta^{-1})'(x_{i,x}^T \beta)] \eta''(\eta^{-1}(x_{i,x}^T \beta)), \nu_{1i}, \nu_{2i},$$

and, after taking conditional expectations,

$$\{\eta'(\eta^{-1}(x_{i,x}^T \beta)), \nu_{1i}, \nu_{2i} | \mathbb{X}\} \approx -[\nu_i(\eta^{-1})'(x_{i,x}^T \beta)] \{\eta''(\eta^{-1}(x_{i,x}^T \beta)), \nu_{1i}, \nu_{2i} | \mathbb{X}\}$$

Hence, we obtain

$$(\nabla \mathcal{L}(\beta, \bar{x}) | \mathbb{X}) \approx - \{\eta''(\eta^{-1}(\bar{x})), \nu_{1}, \nu_{2} | \bar{x}\} [(\eta^{-1})'(\bar{x})]^2 X_x^T r,$$

where $r = (\nu_1, \nu_2, \dots, \nu_n)^T$.

Taking conditional expectation of the hessian matrix in (2) yields

$$(\nabla^2 \mathcal{L}(\beta, \bar{x}) | \mathbb{X}) \approx \{\eta''(\eta^{-1}(\bar{x})), \nu_{1}, \nu_{2} | \bar{x}\} [(\eta^{-1})'(\bar{x})]^2 \sum_{i=1}^n$$

The variance of the weighted local score function is

$$\nu(\nabla \mathcal{L}(\beta, \bar{x}) | \mathbb{X}) \approx [(\eta^{-1})'(\bar{x})]^2 \nu\{\eta'(\eta^{-1}(\bar{x})), \nu_{1}, \nu_{2} | \bar{x}\} \sum_{i=1}^n$$

The second order Bartlett's identity implies

$$\nu^2(\bar{x}) = - \{\eta''(\eta^{-1}(\bar{x})), \nu_{1}, \nu_{2} | \bar{x}\} = \nu\{\eta'(\eta^{-1}(\bar{x})), \nu_{1}, \nu_{2} | \bar{x}\}$$

Hence, we obtain

$$\begin{aligned} (\hat{\beta} | \mathbb{X}) - \beta &\approx \sum_{i=1}^n \eta^{-1} X_x^T r, \\ \nu(\hat{\beta} | \mathbb{X}) &\approx \frac{1}{[(\eta^{-1})'(\bar{x})]^2 \nu^2(\bar{x})} \sum_{i=1}^n \eta^{-1} \sum_{i=1}^n \eta^{-1} \end{aligned}$$

The approximations $\sum_{i=1}^n = n(\bar{x}) \sum_{i=1}^n \{1 + o_p(1)\}$ and $\sum_{i=1}^n = n^{1/2} \eta^{-1}(\bar{x}) \sum_{i=1}^n \{1 + o_p(1)\}$

are outlined in Fan and Gijbels (1996). The entries of $X_x^T r$ can be written as

$$\begin{aligned}
j &= \sum_{i=1}^n r_i (X_i - \mathbf{z})^j h(X_i - \mathbf{z}) \\
&= \sum_{i=1}^n \left\{ \sum_{m=p+1}^{\infty} m (X_i - \mathbf{z})^m \right\} (X_i - \mathbf{z})^j h(X_i - \mathbf{z}) \\
&= \sum_{m=p+1}^{\infty} n_{j+p+1} + o_p \{n^{\hat{\nu} j+p+1}\}
\end{aligned}$$

Letting $\mathbf{s}_n = (n_{n,p+1}, n_{n,p+2}, \dots, n_{n,2p+1})^T$, we obtain $X_x^T \mathbf{r} = \sum_{j=p+1}^{\infty} \mathbf{s}_n + o_p \{n^{\hat{\nu} p+1}\}$.

Hence, the bias and variance expressions become

$$\begin{aligned}
(\hat{\beta} | \mathbb{X}) - \beta &\approx \left(\sum_{j=p+1}^{\infty} \mathbf{s}_j \right)^{-1} \sum_{j=p+1}^{\infty} \mathbf{s}_j n^{\hat{\nu} j+p+1} \{1 + o_p(1)\}, \\
\text{var}(\hat{\beta} | \mathbb{X}) &\approx \frac{1}{n^{\hat{\nu}}} \frac{1}{(\mathbf{z})' [(-1)'(-1)]^2 (\mathbf{z})} \left(\sum_{j=p+1}^{\infty} \mathbf{s}_j \right)^{-1} \left(\sum_{j=p+1}^{\infty} \mathbf{s}_j \right)^* \left(\sum_{j=p+1}^{\infty} \mathbf{s}_j \right)^{-1} \{1 + o_p(1)\}
\end{aligned}$$

The result of Theorem 1 is obtained by considering the first entry in the above expressions.

Since

$$\hat{\nu}(\mathbf{z}) - \nu(\mathbf{z}) = (\hat{\nu}(\mathbf{z})) - (\nu(\mathbf{z})) \approx \nu'(\mathbf{z}) \{ \hat{\nu}(\mathbf{z}) - \nu(\mathbf{z}) \},$$

we reach the result of Corollary 1 by dividing the asymptotic bias and variance of the local calibration estimator by $\nu'(\mathbf{z})$ and $[\nu'(\mathbf{z})]^2$, respectively.

Appendix B  **Simulations** **Study** under the Frank Copula

This additional simulation study presents the results for the data $\{(\mathbf{z}_{1i}, \mathbf{z}_{2i} | X_i) : i = 1, 2, \dots, n\}$ generated from the Frank copula under each of the following models:

(1) Linear calibration function : $\nu(X) = 25 - 4/2 X$

$$(\mathbf{z}_1, \mathbf{z}_2) | X \sim C(\mathbf{z}_1, \mathbf{z}_2 | \nu = 25 - 4/2 X) \text{ where } X \sim \text{Uniform}(2, 5).$$

(2) Nonlinear calibration function: $\nu(X) = 12 + 8 \sin(0.4 X^2)$

$$(\mathbf{z}_1, \mathbf{z}_2) | X \sim C(\mathbf{z}_1, \mathbf{z}_2 | \nu = 12 + 8 \sin(0.4 X^2)) \text{ where } X \sim \text{Uniform}(2, 5)$$

The true copula parameter varies from 4 to 16.6 in the linear calibration model, and from 4 to 20 in the nonlinear one. Under each calibration model, we conduct $M = 100$ experiments with sample size $n = 200$. The local linear ($\nu = 1$) and parametric linear

estimation are performed to estimate the copula parameter under the Clayton, Frank and Gumbel copulas, and the results are converted to the Kendall's tau scale. Web Table 1 summarizes the performance of the Kendall's tau estimates in terms of integrated mean square error, integrated square bias and integrated variance.

[Web Table 1 about here.]

We construct approximate 90% pointwise condence bands for the copula parameter under the correctly selected Frank family, using half of the optimum bandwidth. Web Figure 1 displays the results in the Kendalls tau scale, averaged over 100 Monte Carlo samples. We also present the Monte Carlo based condence bands obtained from 100 estimates of the Kendalls tau.

[Web Figure 1 about here.]

Our copula selection method successfully identifies the Frank family 95% and 97% of the times under the linear and nonlinear calibration model, respectively.

e Appendix C Fr ingh e rt t dy

We analyze a subset of the Framingham Heart study to illustrate our proposed methodology. The data consist of 348 participants who had stroke incidence during the follow-up study and the clinical data was collected on each participant during three examination periods, approximately 6 years apart. Of interest is the dependence structure between the log-pulse pressures of the first two examination periods, $\log(\quad_1)$ and $\log(\quad_2)$. It is known that chronic malnutrition may occur after stroke, particularly in severe cases that result in eating difficulties. Conversely, some patients may gain weight as a side effect of medication. Therefore, as an indicator of health status, we consider the change in the body mass index (BMI) as the covariate.

For the initial investigation, we categorize the change in BMI, and focus on the three

extreme cases, namely quite stable ($-0.2 \leq \text{BMI} \leq 0.2$), highly increased ($\text{BMI} > 2$) and highly decreased ($\text{BMI} < -2$). From Web Figure 2, when there is a significant change in BMI in either direction, the dependence between the pulse pressures seems weaker compared to the case when BMI remains stable.

[Web Figure 2 about here.]

The scatterplot and histograms of the log-pulse pressures are given in Web Figure 3(a), from which the marginals are seen to be well-modeled by linear regression models assuming normal errors. We consider $j = ((\log(\text{PP}_j) - \hat{\mu}_j(\text{BMI})) / \hat{\sigma}_j)$ to transform the response variables to uniform scale, where $\hat{\mu}_j(\text{BMI})$ are obtained from fitting linear models, $\hat{\sigma}_j$ are the estimated standard errors in the linear regression models and Φ is the c.d.f. of $N(0, 1)$. Web Figure 3(b) gives the scatterplot and histograms of the transformed random variables $j, j' = 1, 2$.

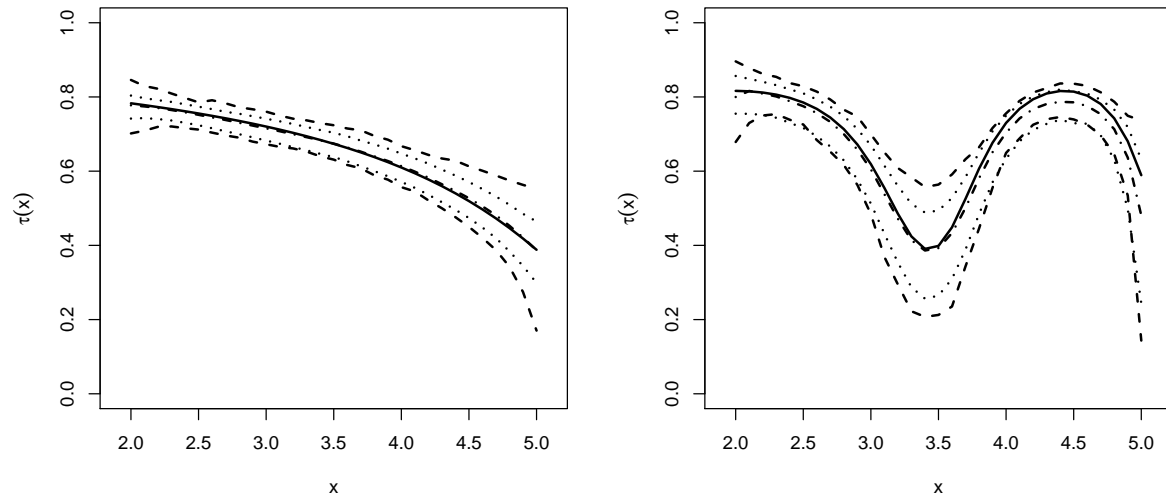
[Web Figure 3 about here.]

For comparison, the calibration function is estimated using both a parametric linear model and the proposed nonparametric model with local linear ($\eta = 1$) specification under the Clayton, Frank and Gumbel families. In the local linear estimation, the optimum bandwidths are chosen as 9.47, 6.72, and 4.25, for the Clayton, Frank and Gumbel copulas, respectively. We constructed approximate 90% confidence intervals under each family using half of these bandwidth values. Web Figure 4 displays the results converted to the Kendall's tau scale.

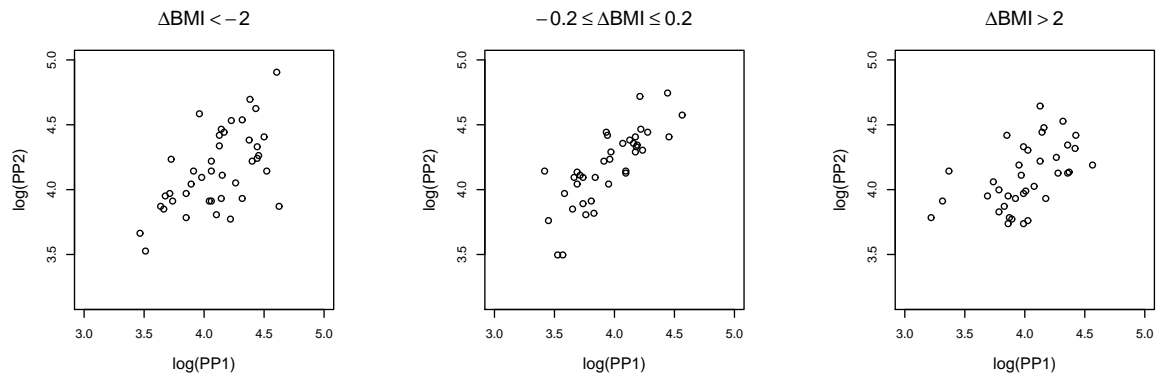
[Web Figure 4 about here.]

A natural interest in modeling the conditional dependence of log-pulse pressures at different periods is to predict the latter from the previous measurement. Therefore, in copula selection, we use the cross-validated prediction errors only for the second log-pulse pressure as the selection criterion which chooses the Frank copula family. Since, at a given change in BMI,

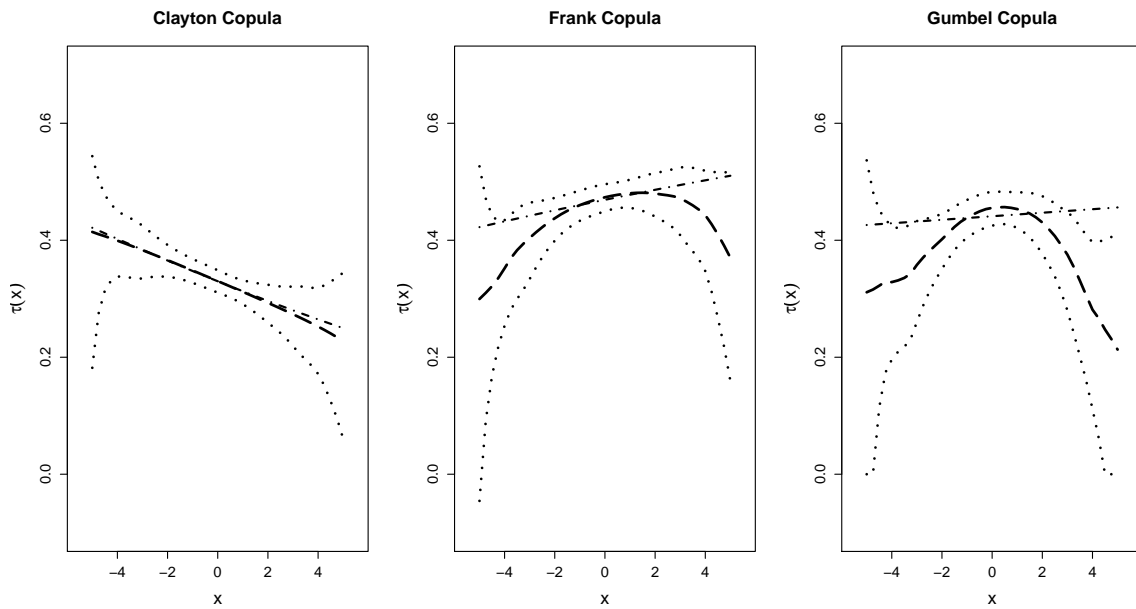
observing two high pulse pressures together or two low pulse pressures together would be equally likely, our choice of Frank copula model seems practically sensible. The results obtained using the nonparametric approach under the Frank copula indicates that the dependence between two log-pulse pressures is stronger when BMI remains stable, as reflected by a steady health status. However, the nonlinear pattern does not seem to be significant as the parametric linear fit in fact falls within the approximate 90% pointwise confidence bands, suggesting that the linear model may be already adequate.



e Fig re 90% confidence intervals for the Kendall's tau under the Frank copula with the linear (left panel) and quadratic (right panel) calibration models: truth (solid line), averaged local linear estimates (dashed line), approximate confidence intervals (dotted line), and Monte Carlo confidence intervals (dotdashed line)



e Fig re  Scatterplots of the log-pulse pressures at different covariate ranges.



e Fig re The Kendalls tau estimates under three copula families: global linear estimates (dot-dashed line), local linear estimates at the optimum bandwidth(long-dashed line), and an approximate 90% pointwise condence bands (dotted lines).

Web Table 1

Integrated Squared Bias, Integrated Variance and Integrated Mean Square Error of the Kendall's tau estimator (multiplied by 100) and the averages of the selected bandwidths \bar{h}^ .*

| Linear Calibration Model | | | | | | | |
|--------------------------|-----------------------|-------|-------|--------------------|-------|-------|-------------|
| | Parametric estimation | | | Local estimation | | | |
| | IBIAS ² | IVAR | IMSE | IBIAS ² | IVAR | IMSE | \bar{h}^* |
| Clayton | 8.611 | 1.125 | 9.736 | 8.334 | 1.514 | 9.848 | 2.056 |
| Frank | 0.006 | 0.316 | 0.322 | 0.006 | 0.444 | 0.450 | 2.206 |
| Gumbel | 1.887 | 0.478 | 2.365 | 1.793 | 0.746 | 2.539 | 2.133 |

| Nonlinear Calibration Model | | | | | | | |
|-----------------------------|-----------------------|-------|--------|--------------------|-------|--------|-------------|
| | Parametric estimation | | | Local estimation | | | |
| | IBIAS ² | IVAR | IMSE | IBIAS ² | IVAR | IMSE | \bar{h}^* |
| Clayton | 18.192 | 3.470 | 21.662 | 10.593 | 2.833 | 13.426 | 0.822 |
| Frank | 6.162 | 0.673 | 6.835 | 0.127 | 1.280 | 1.407 | 0.468 |
| Gumbel | 9.597 | 1.183 | 10.780 | 3.504 | 2.067 | 5.571 | 0.569 |