Bivariate vine copula based quantile regression

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Abstract

The statistical analysis of univariate quantiles is a well developed research topic. However, there is a profound need for research in multivariate quantiles. We tackle the topic of bivariate quantiles and bivariate quantile regression using vine copulas. They are graph theoretical models identified by a sequence of linked trees, which allow for separate modelling of marginal distributions and the dependence structure. We introduce a novel graph structure model (given by a tree sequence) specifically designed for a symmetric treatment of two responses in a predictive regression setting. We establish computational tractability of the model and a straightforward way of obtaining different conditional distributions. Using vine copulas the typical shortfalls of regression, as the need for transformations or interactions of predictors, collinearity or quantile crossings are avoided. We illustrate the copula based bivariate quantiles for different copula distributions and provide a data set example. Further, the data example emphasizes the benefits of the joint bivariate response modelling in contrast to two separate univariate regressions or by assuming conditional independence, for bivariate response data set in the presence of conditional dependence.

Keyword: multivariate quantiles, bivariate response, bivariate conditional distribution functions

1 Introduction

The topic of predicting quantiles of a response variable conditioned on a set of predictor variables taking on fixed values, continuously attracts interest. The statistical analysis of such univariate quantiles is a well developed research topic (Koenker and Bassett 1978; Koenker 2005). Since the introduction of the linear quantile regression by Koenker and Bassett (1978) many extensions have been developed for the case of a univariate response variable. A short summary of developments in quantile regression modelling is given in Koenker (2017).

One of the most recent approaches for quantile regression are vine copula based quantile regression methods (Kraus and Czado 2017; Tepegjozova et al. 2022; Chang and Joe 2019; Zhu et al. 2021). Copulas allow for separate modelling of the marginal distributions and the dependence structure in the data, while vine copulas allow the multivariate copula to be constructed using bivariate building blocks only, a so-called pair copula construction. This way, a very flexible model, without assuming homoscedasticity, or a linear relationship between the response and the predictors, is constructed. Thus, vine based quantile regression methods overcome two drawbacks of the standard quantile regression methods. First, by construction quantile crossings and collinearity are avoided, and second, there is no need for transformations or interactions of variables (Kraus and Czado 2017). There are several different vine copula tree structures that can be considered, resulting in the most general regular (R-)vine copulas, or its subsets as drawable (D-vines whose tree structure is a sequence of paths) and canonical (C-vines whose tree

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structure is a sequence of stars) vines. Kraus and Czado (2017) developed a parametric D-vine based quantile regression method by optimizing the conditional log-likelihood and adding predictors until there is no improvement, thus introducing an automatic forward variable selection method. This approach was extended in Tepegojzova et al. (2022) where a nonparametric D- and C-vine copula based quantile regression was introduced. They also follow the approach to maximize the conditional log likelihood, but introduce an additional step to check for future improvement of the conditional log likelihood, a so called two-step ahead approach. Chang and Joe (2019) introduced an R-vine based quantile regression by first finding the optimal R-vine structure among all predictors and then adding the response variable to each tree in the vine structure as a leaf node. Another R-vine based regression was introduced in Zhu et al. (2021) by optimizing the R-vine structure which gives the largest sum of the absolute value of the partial correlations in each step of the forward extension with predictor variables, while keeping the response as a leaf node. This approach is motivated by the algorithm and results from Zhu et al. (2020). All these selected structures allow to express the conditional density of the response given the predictors without integration.

Despite the great attention univariate quantiles have received, the extension to multivariate response quantiles is not trivial nor well-defined. Several theoretical notions of multivariate quantiles have been introduced, but there is no consensus which one is the corresponding generalization of the univariate quantiles. These include geometric quantiles based on halfspace depth contours with different concepts of statistical depth (e.g. see Tukey (1975), Chaudhuri (1996), Hallin et al. (2010), Chernozhukov et al. (2017)), vector quantiles (see Carlier et al. (2016) and Carlier et al. (2017)), spatial quantiles (see Abdous and Theodorescu (1992)). Our goal is to define bivariate quantiles in terms of copulas and to introduce a vine based regression method able to handle bivariate responses.

The first heuristic for a vine based quantile regression with multiple responses is given in Zhu et al. (2021), but the question of multivariate response quantiles is not tackled. The suggested heuristic for the bivariate response case is limited to modelling only, but not predicting the bivariate quantiles. Further, this approach has an asymmetric treatment of the response variables. This might lead to different performance of the regression methods when the order of the response variables is exchanged. Thus, there is still a need for: (1.) a valid definition of (unconditional and conditional) multivariate quantiles linked to the usage of copulas; (2.) a vine based quantile regression method with a symmetric treatment of the responses; (3.) a numerical method for obtaining the multivariate (unconditional and conditional) quantiles from the estimated vine based model and evaluating predictions from it.

Our methodology deals with the case of a bivariate response variables, i.e. bivariate (unconditional and conditional) quantiles defined by sets that can be characterised as curves. For the conditional case we choose the multivariate vine copulas class since they allow modelling of complex dependence patterns including asymmetric tail dependencies. For (1.) we extend the definition of bivariate unconditional and conditional quantiles in terms of a copula distribution function. Further, we illustrate the bivariate unconditional quantiles for known bivariate copula distributions and the bivariate conditional quantiles for a 3-dimensional vine copula distribution. For (2.), we propose a novel tree structure for vines, called Y-vine tree sequence, which is contained in the set of regular vine tree sequences. It is designed to allow for a symmetric treatment of the responses. Moreover, we show that using the Y-vine tree sequence the associated bivariate conditional density is analytically expressible as a product of all pair copula terms involving one or both of the response variables. In the case of more than one conditioning variable (predictor) we develop a forward selection method. For this we propose an appropriate fit measure for the predictors to prevent overfitting and remove non-significant predictors. For (3.) we develop a numerical method to evaluate the bivariate unconditional and conditional quantile sets. In advance, for applicability of the proposed method we develop a prediction method that can be also used for simulating multivariate data from a Y-vine. Finally, we give an application involving a data set with minimal and maximal daily temperatures together with other weather variables. For this application we show that the conditional dependence cannot be ignored and that it is non-Gaussian, thus requiring the full class of pair copula families.
The remainder of the paper is organized as follows. First, we introduce the necessary vine copula concepts for our approach in Section 2. Then, in Section 3 we define bivariate quantiles in terms of copulas and develop the numerical method used for their evaluation. In Section 4 we introduce the Y-vine copula based quantile regression model for bivariate responses. For application purposes, in Section 5 we present the prediction method for Y-vine copulas. For the demonstration of the usefulness of our method we include a real data example in Section 6 that contains dependent bivariate responses. We highlight the advantages of bivariate response modelling over standard univariate models or models that assume conditional independence. Finally, in Section 7 we give conclusions and areas of future research.

2 Theoretical background

Consider any continuous d-dimensional random vector \( \mathbf{X} = (X_1, \ldots, X_d)^T \) with observed values \( \mathbf{x} = (x_1, \ldots, x_d)^T \). We use capital letters for random variables and lowercase letters for their observed values, i.e., we write \( X_i = x_i \) for \( i = 1, \ldots, d \). Let \( \mathbf{X} \) have joint distribution function \( F \), joint density \( f \) and marginal distributions \( F_{X_i}, i = 1, \ldots, d \). Following Sklar’s theorem (Sklar 1959), we can express the multivariate distribution function \( F \) in terms of the marginal distributions, \( F_{X_i} \), and the d-dimensional copula \( C \) as

\[
F(x_1, \ldots, x_d) = C(F_{X_1}(x_1), \ldots, F_{X_d}(x_d)).
\]

The copula \( C : [0, 1]^d \rightarrow [0, 1] \) corresponds to the distribution of the random vector \( \mathbf{U} = (U_1, \ldots, U_d)^T \), with the components of \( \mathbf{U} \) being the probability integral transforms (PITs or u-scale) of the components of \( \mathbf{X} \) (x-scale), \( U_i = F_{X_i}(X_i) \) for \( i = 1, \ldots, d \). Each \( U_i \) is uniformly distributed and their joint distribution function \( C \) is the copula associated with \( \mathbf{X} \). If all marginal distributions \( F_{X_i} \) are continuous, then by Sklar’s Theorem it is implied that \( C \) is unique. Also, if derivatives of the marginal distributions \( F_{X_i} \) exist, the density \( f \) can be derived as

\[
f(x_1, \ldots, x_d) = c(F_{X_1}(x_1), \ldots, F_{X_d}(x_d)) \cdot \prod_{i=1}^{d} f_{X_i}(x_i),
\]

where \( c \) is the d-dimensional density corresponding to the copula \( C \) and \( f_{X_1}, \ldots, f_{X_d} \) are the univariate marginal densities. However, Equations (1) and (2) both incorporate a possibly complicated multivariate copula distribution and density. As shown by Joe (1996), a d-dimensional copula density can be decomposed into \( d(d-1)/2 \) bivariate copula densities. This decomposition is not unique, but a large number of possible decompositions exist. The elements of these decompositions, the bivariate copula densities can be chosen completely independent of each other. A graphical model introduced by Bedford and Cooke (2002), called regular vine copulas (R-vines), organizes all such decompositions that lead to a valid density. Thus, the estimation of a d-dimensional copula density is subdivided into the estimation of \( d(d-1)/2 \) two-dimensional copula densities. A regular vine copula on \( d \) uniformly distributed random variables \( U_1, \ldots, U_d \), consists of a regular vine tree sequence, denoted by \( \mathcal{V} \), a set of bivariate copula families (also known as pair copulas) \( \mathcal{B}(\mathcal{V}) \), and a set of parameters corresponding to the bivariate copula families \( \Theta(\mathcal{B}(\mathcal{V})) \). The vine tree sequence or tree structure \( \mathcal{V} \) consists of a sequence of linked trees, \( T_k = (N_k, E_k), k = 1, \ldots, d-1 \), satisfying the following conditions:

(i) \( T_1 \) is a tree with node set \( N_1 = \{U_1, \ldots, U_d\} \) and edge set \( E_1 \).

(ii) (Proximity condition) For \( k \geq 2 \), two nodes of the tree \( T_k \) can be connected by an edge if the corresponding edges of \( T_{k-1} \) have a common node.

(iii) For \( k \geq 2 \), \( T_k \) is a tree with node set \( N_k = E_{k-1} \) and edge set \( E_k \).

If the vine tree sequence consists of paths only, then we call it a drawable vine (D-vine), and if it consists of stars, it is called a canonical vine (C-vine) (Bedford and Cooke 2002). The tree sequence
uniquely specifies which bivariate (conditional) copula densities occur in the decomposition. Each edge \( e \in E_k \) for \( k = 1, \ldots, d - 1 \) is associated with a bivariate copula family \( c_{U_{j e}, U_{k e}} : U_{D_e} \in \mathcal{B}(\mathcal{V}) \), and a corresponding set of parameters \( \theta_{j e, k e} : \Theta(\mathcal{B}(\mathcal{V})) \). \( U_{j e} \) and \( U_{k e} \) are the conditioned variables and \( U_{D_e} \) represents the conditioning set corresponding to edge \( e \), \( U_{D_e} = (U_l)_{i \in D_e} \). Denote the conditional distribution of \( U_{j e} | U_{D_e} = u_{D_e} \) with \( C_{U_{j e} | U_{D_e}} \). We define the so-called pseudo copula data \( u_{j e} | D_e \) as \( u_{j e} | D_e := C_{U_{j e} | U_{D_e}} (u_{j e} | u_{D_e}) \). Similarly, \( u_{k e} | D_e \) is defined. Then, \( c_{U_{j e}, U_{k e} | U_{D_e}} \) denotes the density of the copula between the pseudo copula data \( u_{j e} | D_e \) and \( u_{k e} | D_e \). The corresponding distribution function is denoted as \( C_{U_{j e}, U_{k e} | U_{D_e}} \).

Bedford and Cooke (2002) have shown that the graphical model of regular vines, leads to a natural decomposition of the joint copula density \( c \) using the pair-copulas defined through the tree sequence as

\[
c(u_1, \ldots, u_d) = \prod_{k=1}^{d-1} \prod_{e \in E_k} c_{U_{j e}, U_{k e} | U_{D_e}} \left( C_{U_{j e} | U_{D_e}} (u_{j e} | u_{D_e}), C_{U_{k e} | U_{D_e}} (u_{k e} | u_{D_e}) | u_{D_e} \right).
\]

(3)

Using Equation (3) we can decompose any given regular vine copula density. However, the individual pair copulas, \( c_{U_{j e}, U_{k e} | U_{D_e}} \) in Equation (3) are dependent on \( u_{D_e} \). This represents the different conditional dependencies between \( U_{j e} \) and \( U_{k e} \) for different conditioning values of \( u_{D_e} \). To improve computational tractability, it is customary to ignore this influence and simplify Equation (3) to:

\[
c(u_1, \ldots, u_d) = \prod_{k=1}^{d-1} \prod_{e \in E_k} c_{U_{j e}, U_{k e} | U_{D_e}} \left( C_{U_{j e} | U_{D_e}} (u_{j e} | u_{D_e}), C_{U_{k e} | U_{D_e}} (u_{k e} | u_{D_e}) \right).
\]

(4)

This simplification is known as the simplifying assumption (more in Haff et al. (2010) and Stoebber et al. (2013)). In this case, we talk about pair copula constructions (PCC) of multivariate densities.

To derive the conditional distributions in Equation (4), we use the recursion formula from Joe (1996). It defines a recursion for conditional distributions of a regular vine over its tree sequence. Let \( l \in D_e \) and \( D_{-l} := D_e \setminus \{l\} \). Further, let \( h_{U_{j e} | U_{l}; U_{D_{-l}}} (\cdot | \cdot) \) denote the so-called h-function associated with the pair copula \( c_{U_{j e}, U_{l}; U_{D_{-l}}} \), defined as \( h_{U_{j e} | U_{l}; U_{D_{-l}}} (u_{j e} | u_l) := \frac{\partial}{\partial u_l} C_{U_{j e}, U_{l}; U_{D_{-l}}} (u_{j e}, u_l) \). Then the following recursion is valid

\[
C_{U_{j e} | U_{D_e}} (u_{j e} | u_{D_e}) = h_{U_{j e} | U_l; U_{D_{-l}}} \left( C_{U_{j e} | U_{D_{-l}}} (u_{j e} | u_{D_{-l}}), C_{U_l | U_{D_{-l}}} (u_l | U_{D_{-l}}) \right).
\]

(5)

3 Bivariate quantiles

We look at the extension of univariate quantiles, defined as cut points that divide the range of a univariate distribution into intervals with given probabilities, to bivariate quantiles. Expanding on the definition of the univariate quantile function by Koenker and Bassett (1978), we define the bivariate quantiles as cut curves dividing the range of a bivariate distribution into areas with given probabilities. Bivariate quantiles are curves rather than points as the domain of bivariate distributions is a two-dimensional space. The notion of multivariate quantiles we use is linked to the usage of copulas. Since we are interested in a regression setting, we define both bivariate unconditional quantiles, meaning that we have no predictors in the model, the so-called null regression model, and bivariate conditional quantiles, which are quantiles conditioned over a set of predictors.

3.1 Bivariate unconditional quantiles

Let \( Y_1 \) and \( Y_2 \) be two continuous random variables with observed values \( y_1, y_2 \) and a joint distribution function \( F_{Y_1, Y_2}(y_1, y_2) \).
**Definition 3.1.** The bivariate quantile function for \( \alpha \in (0,1) \) and continuous random variables \( Y_1, Y_2 \) is a curve in \( \mathbb{R}^2 \) defined by the set
\[
Q^\alpha_Y := \{(y_1, y_2) \in \mathbb{R}^2 ; F_{Y_1,Y_2}(y_1, y_2) = \alpha \}.
\]

Define the probability integral transforms of the random variable \( Y_j \) as \( V_j := F_{Y_j}(Y_j) \) for \( j = 1, 2 \). Applying Sklar’s Theorem (Equation (1)) to the joint distribution function of \( Y_1, Y_2 \), we obtain \( F_{Y_1,Y_2}(y_1, y_2) = C(F_{Y_1}(y_1), F_{Y_2}(y_2)) = C_{V_1,V_2}(v_1, v_2) \). So we rewrite the bivariate quantile function from Definition 3.1 in terms of copulas, \( Q^\alpha_Y = \{(F^{-1}_{Y_1}(v_1), F^{-1}_{Y_2}(v_2)) \in \mathbb{R}^2 ; C_{V_1,V_2}(v_1, v_2) = \alpha \} \). We can also define the bivariate quantile function of the probability integral transformed variables on the unit square \([0,1]^2\) as
\[
Q^\alpha_V := \{(v_1, v_2) \in [0,1]^2 ; C_{V_1,V_2}(v_1, v_2) = \alpha \}.
\]

The difference between \( Q^\alpha_Y \) and \( Q^\alpha_V \) is that \( Q^\alpha_Y \) is defined on \( \mathbb{R}^2 \), while \( Q^\alpha_V \) is defined on \([0,1]^2\). The connection between the two is given as \( Q^\alpha_Y = \{(F^{-1}_{Y_1}(v_1), F^{-1}_{Y_2}(v_2)) \in \mathbb{R}^2 ; (v_1, v_2) \in Q^\alpha_V \} \). The Sklar’s Theorem implies that a transformation of the bivariate quantile curves between the x- and u-scale is obtained using the univariate marginal distributions \( F^{-1}_{Y_1}, F^{-1}_{Y_2} \), rather than the bivariate joint distribution \( F_{Y_1,Y_2} \).

### 3.2 Bivariate conditional quantiles

Let \( Y = (Y_1, Y_2)^T \) and \( X = (X_1, \ldots, X_p)^T, \ p \geq 1 \), be two continuous random vectors, with the corresponding marginal distribution functions \( Y_j \sim F_{Y_j} \), for \( j = 1, 2 \) and \( X_i \sim F_{X_i} \), for \( i = 1, \ldots, p \). Our interest is the bivariate conditional quantile of \( Y|X \) and we define this conditional quantile similarly as in Section 3.1. Denote the conditional distribution function of \( Y_1, Y_2|X = x \) as \( F_{Y_1,Y_2|X}(y_1, y_2|x) \).

**Definition 3.2.** The bivariate conditional quantile function for \( \alpha \in (0,1) \) and a continuous bivariate vector \( Y = (Y_1, Y_2)^T \) given the outcome of a p-dimensional random vector \( p \geq 1 \), \( X = x \) is a curve in \( \mathbb{R}^2 \) defined by the set
\[
Q^\alpha_Y(x) := \{(y_1, y_2) \in \mathbb{R}^2 ; F_{Y_1,Y_2|X}(y_1, y_2|x) = \alpha \}.
\]

In order to derive the quantile function in terms of copulas, we need to express the conditional distribution of \( Y_1, Y_2|X \) in terms of a copula distribution function.

**Proposition 3.3.** The conditional distribution of \( Y = (Y_1, Y_2)^T \) given \( X = (X_1, \ldots, X_p)^T \), with corresponding PITs \( V_j := F_{Y_j}(Y_j) \), \( j = 1, 2 \) and \( U_i := F_{X_i}(X_i) \), \( i = 1, \ldots, p \) can be expressed in terms of a copula distribution as
\[
F_{Y_1,Y_2|X}(y_1, y_2|x) = C_{V_1,V_2|U}(F_{Y_1}(y_1), F_{Y_2}(y_2)|F_{X_1}(x_1), \ldots, F_{X_p}(x_p)).
\]

Proof of Proposition 3.3 is given in Appendix B.1. Thus, the bivariate quantile function \( Q^\alpha_Y(x) \) can be rewritten as \( Q^\alpha_Y(x) = \{(F^{-1}_{Y_1}(v_1), F^{-1}_{Y_2}(v_2)) \in \mathbb{R}^2 ; C_{V_1,V_2|U}(v_1, v_2|u) = \alpha \} \), where \( u = (u_1, \ldots, u_p)^T \) are realizations of \( U = (U_1, \ldots, U_p)^T \). Similarly, we define the bivariate conditional quantile function of the probability integral transformed variables on the unit square \([0,1]^2\) as
\[
Q^\alpha_V(u) := \{(v_1, v_2) \in [0,1]^2 ; C_{V_1,V_2|U}(v_1, v_2|u) = \alpha \}.
\]
3.3 Confidence regions

Definition 3.4. The $100 \times (1 - \alpha) \%$ bivariate confidence region for an $\alpha \in (0, 1)$ and a continuous bivariate vector $\mathbf{Y} = (Y_1, Y_2)^T$ given the outcome of a $p$-dimensional random vector $\mathbf{X} = \mathbf{x}$ is the set of points in $\mathbb{R}^2$ enclosed by the quantile curves $Q_{\alpha/2}^Y(x)$ and $Q_{1-\alpha/2}^Y(x)$, i.e.

$$CI_{\alpha}^Y := \left\{ (w_1, w_2) \in \mathbb{R}^2 \mid \exists (y_1^1, y_2^1) \in Q_{\alpha/2}^Y(x), (y_1^2, y_2^2) \in Q_{1-\alpha/2}^Y(x) \text{ such that } y_1^1 \leq w_1 \leq y_1^2 \text{ and } y_2^1 \leq w_2 \leq y_2^2 \right\}.$$ 

As before, in a similar manner we can define the $100 \times (1 - \alpha) \%$ confidence region for the vector $(V_1, V_2)^T$ on the unit square, as the set enclosed by the curves $Q_{\alpha/2}^V(u)$ and $Q_{1-\alpha/2}^V(u)$.

3.4 Numerical evaluation of bivariate quantiles

Let $C(a, b)$ be a bivariate (conditional) distribution defined on the unit square $[0, 1]^2$ with no closed form solution for the bivariate quantile function. Assume that $C(a, b)$ can be evaluated at all points $(a, b) \in [0, 1]^2$. The goal is to obtain a numerical estimate of the set defining the (conditional) bivariate quantile curve, given in Equation (6) (or Equation (7) for the conditional case). Given a granularity argument $m \in \mathbb{N}^+$ and $\alpha \in (0, 1)$ we employ the following procedure:

1. The set $M = \{w_1, \ldots, w_m\}$ is initialized as $m$ equidistant points in the interval $[0, 1]$.

2. We define the set of lines $L$ as follows:

$$L = \{(((0, 0), (w_1, 1)) \mid \forall w_1 \in M\} \cup \{((0, 0), (1, w_1)) \mid \forall w_1 \in M\}.$$ 

3. Each line $l_s \in L$ is treated as a separate optimization problem and a line search procedure is employed to obtain the point $(a_s, b_s) \in l_s$ for which $C(a_s, b_s) = \alpha$. Consider any line $l_s$ and two points on the line, denoted as $(a_1, a_2)$ and $(b_1, b_2)$, s.t. $a_1 \leq b_1$ and $a_2 \leq b_2$. Then, $P(V_1 \leq a_1, V_2 \leq a_2) \leq P(V_1 \leq b_1, V_2 \leq b_2)$ holds. This implies that values of $C(\cdot, \cdot)$ along any line $l_s$ going from $(0, 0)$, are increasing. In addition, $C$ is a bivariate distribution function and is continuous. Therefore, for each $l_s \in L$ a line search is guaranteed to converge to a solution. (The same arguments hold for the conditional copula distribution function as well.)

4. Finally, the points $(a_s, b_s)$ for $s = 1, \ldots, 2m$ are smoothed to obtain a curve representing an estimate of the (conditional) bivariate quantile curve for a given $\alpha$.

The algorithms used for this numerical evaluation of bivariate quantiles are given in the supplementary material to this manuscript. The bivariate distribution function $C(a, b)$ is equivalent to $C_{V_1,V_2}(v_1, v_2)$ (or $C_{V_1,V_2}|U(v_1, v_2|u)$) if unconditional (or conditional) bivariate quantile curves are evaluated. In Figure 1 we show a graphical representation of the numerical procedure for evaluating bivariate quantiles. On the unit square $[0, 1]^2$ in panel (a), shown are 5 exemplary lines, $l_1 = ((0,0), (w_1, 1))$, $l_2 = ((0,0), (w_2, 1))$, $l_3 = ((0,0), (1, 1))$, $l_4 = ((0,0), (1, w_2))$, $l_5 = ((0,0), (1, w_1))$ on which a line search is employed to find the pair $(a^*, b^*)$ such that $C(a^*, b^*) = \alpha$ holds. The dotted lines represent the solution of the line search, in our case, the bivariate quantile lines for $\alpha = 0.1, 0.5, 0.9$. In panel (b) we illustrate the binary line search for line $l_1 = ((0,0), (w_1, 1))$. First, the desired function is evaluated at the middle of the line $l_1$, at $C(\frac{w_1}{4}, \frac{1}{2})$. Here it holds $C(\frac{w_1}{4}, \frac{1}{2}) > \alpha$, so the middle of the line $((0,0), (\frac{w_1}{4}, \frac{1}{2}))$ is evaluated next, $C(\frac{w_1}{4}, \frac{1}{4}) < \alpha$, so the middle of the line $((\frac{w_1}{4}, \frac{1}{2}), (\frac{w_1}{2}, \frac{1}{2}))$ is evaluated next, $C(\frac{3w_1}{8}, \frac{3}{8})$. Here $C(\frac{3w_1}{8}, \frac{3}{8}) > \alpha$, so we consider the middle of the line $((\frac{w_1}{4}, \frac{1}{2}), (\frac{3w_1}{8}, \frac{3}{8}))$ and iteratively continue until the algorithm converges to a solution. The red dot (star), say $(a^*, b^*)$ is the point at which $C(a^*, b^*) = \alpha$. 

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3.5 Illustration of bivariate quantiles on the unit square

We illustrate the bivariate unconditional quantiles for known pair-copula distributions and the bivariate conditional quantiles for a 3-dimensional vine structure. They correspond to the case of no predictors or 1 predictor in a regression setting, respectively. In Figure 2 we explore plots of the unconditional quantile curves on the unit square for the bivariate Gauss, Student-t, Clayton and Gumbel copulas (rows) with different strengths of dependency, expressed through Kendall’s τ (Kendall 1938), with τ = 0.25, 0.5, 0.75 (columns). The theoretical quantiles of a bivariate random vector \((V_1, V_2)^T\) with bivariate distribution function \(C_{V_1, V_2}(v_1, v_2; \theta)\) are derived using Equation (6) for a given \(\alpha\) and are depicted with thick black lines. Further, we estimate the bivariate quantiles for the given pair-copulas. For this we simulate data from the given copula and based on the simulated data, a pair copula is estimated. The gray points are 300 data points simulated from the given copulas. Subsequently, quantile curves are evaluated and plotted. The coloured lines represent the corresponding estimated quantile curves. In the supplementary material to this manuscript, we give a detailed description on how the theoretical and the estimated quantile curves are obtained for each of the four copula families. The figures showcase bivariate quantile curves for \(\alpha = 0.05, 0.1, 0.25, 0.5, 0.75, 0.9, 0.95\).

Differences can be spotted between, both estimated and theoretical, Clayton and Gumbel quantile curves at \(\alpha = 0.05\) and 0.95. The Clayton copula curve has a significantly smaller surface below the \(\alpha = 0.05\) quantile curve caused by its heavy lower tail (expected realizations are closer to the lower diagonal as compared to a lighter lower tail copula). On the other hand, the heavy upper tail of the Gumbel copula is causing a bigger surface above the \(\alpha = 0.95\) curve compared to the Clayton copula. In contrast, the Gaussian copula has no tails at all and the Student-t copula has a symmetric tail dependence governed by a single parameter. Their surface below the \(\alpha = 0.05\) curve is greater than the corresponding quantile surface in the lower heavy-tailed Clayton copula, and the surface above the \(\alpha = 0.95\) curve is smaller than the upper heavy-tailed Gumbel copula. Considering the \(\alpha = 0.5\) quantile curve, the greatest surface below it has the Gumbel copula, due to it upper heavy tail, and the smallest surface below the \(\alpha = 0.5\) curve has the Clayton copula, again due to the heavy lower tail. This holds for all Kendall’s \(\tau\) values. Also, as the dependence between the variables increases, the data is more centered around the diagonal, so the curves have sharper curvature around the diagonal. The shape of dispersion of the simulated points from the vine (the gray points in Figure 2) show that the quantile lines indeed represent a valid division of the distribution function into areas with given probabilities. Further, in Appendix A we show the associated bivariate distribution functions in a 3-dimensional plot in which the set defining
Figure 2: x-axis: $V_1$, y-axis: $V_2$. Gray points: simulated data from copula (n=300). Black curves: theoretical quantile curves. Colored curves: estimated quantile curves. Depicted are quantile curves for $\alpha = 0.05, 0.1, 0.25, 0.5, 0.75, 0.90, 0.95$ (left bottom to right top in each panel) for Gaussian, Student-t ($df = 5$), Clayton and Gumbel copulas (top to bottom) and $\tau = 0.25, 0.5, 0.75$ (left to right).
the quantile curve is shown for given \( \alpha \) levels. Basically, the bivariate quantile set for some given \( \alpha \) is the level set of the bivariate distribution (Di Bernardino et al. 2013).

Next we consider conditional bivariate quantiles arising from a 3-dimensional regular vine distribution \( D_3 \). Let \( (V_1, V_2, U_1)^T \sim D_3 \) with vine tree sequence and pair-copulas of \( D_3 \) given by Figure 3:

![Vine Tree Sequence](image)

**Figure 3:** Vine tree sequence of \( D_3 \) with the pair-copula families and Kendall’s \( \tau \) corresponding to parameters.

The corresponding parameters to the copulas are \( \theta_{V_1, U_1} = 3, \theta_{U_1, V_2} = 5 \) and \( \theta_{V_1, V_2, U_1} = 1.33 \). To obtain theoretical quantiles from \( D_3 \) we employ the following procedure. First, to evaluate \( C_{V_1, V_2|U_1} \) at a specific point \( (\tilde{v}_1, \tilde{v}_2) \) conditioned on \( U_1 = \tilde{u}_1 \) we use

\[
C_{V_1, V_2|U_1} (\tilde{v}_1, \tilde{v}_2|\tilde{u}_1) = \int_{0}^{\tilde{v}_1} \int_{0}^{\tilde{v}_2} c_{V_1, V_2|U_1} (v_1', v_2'|\tilde{u}_1) \, dv_2' \, dv_1' \\
= \int_{0}^{\tilde{v}_1} \int_{0}^{\tilde{v}_2} c_{V_2|U_1} (v_2'|\tilde{u}_1) \cdot c_{V_1|V_2, U_1} (v_1'|v_2', \tilde{u}_1) \, dv_2' \, dv_1' \\
= \int_{0}^{\tilde{v}_2} c_{V_2|U_1} (v_2'|\tilde{u}_1) \left[ \int_{0}^{\tilde{v}_1} c_{V_1|V_2, U_1} (v_1'|v_2', \tilde{u}_1) \, dv_1' \right] \, dv_2' \\
= \int_{0}^{\tilde{v}_2} c_{V_2|U_1} (v_2'|\tilde{u}_1) C_{V_1|V_2, U_1} (\tilde{v}_1|v_2', \tilde{u}_1) \, dv_2'.
\]

(8)

We can also condition on \( V_1 \) instead of \( V_2 \). The corresponding conditional quantile curve is evaluated using the numerical evaluation procedure from Section 3.4 and Equation (8). We are also interested in the estimated conditional quantiles. To obtain them, we simulate a data set \( W \in [0, 1]^{504 \times 3} \) from \( D_3 \) and split \( W \) into \( W_{\text{train}} \in \mathbb{R}^{500 \times 3} \) and \( W_{\text{test}} \in \mathbb{R}^{4 \times 3} \). On the training set \( W_{\text{train}} \) we fit a vine model \( \hat{D}_3 \) with the same graph structure and order of the variables as the data generator \( D_3 \). By order we mean the order from left to right in which the variables appear in the first tree of the sequence. Precise definitions of the order for C-vines and D-vines can be found in Tepegjozova et al. (2022). The estimated pair-copulas are \( \hat{C}_{V_1, U_1} \sim \text{Clayton} (\hat{\tau} = 0.57, \hat{\theta}_{V_1, U_1} = 2.65) \), \( \hat{C}_{U_1, V_2} \sim \text{Gumbel} (\hat{\tau} = 0.79, \hat{\theta}_{U_1, V_2} = 4.92) \), \( \hat{C}_{V_1, V_2, U_1} \sim \text{Clayton} (\hat{\tau} = 0.40, \hat{\theta}_{V_1, V_2, U_1} = 1.34) \). The corresponding conditional quantile curves of \( \hat{D}_3 \) are obtained using the numerical evaluation procedure from Section 3.4 and evaluating \( \hat{C}_{V_1, V_2|U_1} \) in a similar manner as in Equation (8), using the estimates of each term. Note that the estimated and the data-generating vine are approximately very close, due to the use of the same tree structure in both data generation and estimation. But in practice this is not the case, as the underlying tree structure is unknown. We turn back to this question later.

Figure 4 shows the theoretical and the estimated bivariate quantiles for 4 conditioning values of \( u_1 \). The values of \( u_1 \) are chosen from \( W_{\text{test}} \). The quantile curves depend on the conditioning value. If the value of \( u_1 \) is low (top-left and bottom-right plot) the quantiles are more restricted to the lower left corner. For greater values of \( u_1 \) (top-right and bottom-left plot) the quantile curves are more restricted to the top right corner. These occurrences can be explained by the high positive dependence of the pairs \( (V_1, U_1) \) and \( (V_2, U_1) \) in the first tree of the vine structure, meaning that low values of \( u_1 \) correspond to low values of both \( v_1, v_2 \).
However, the question remains how can we estimate the bivariate quantiles when the pair copulas or/and the vine structure are not known? What can we do when we have not only one predictor as the case in our conditional illustration, but many of them? Which vine tree sequence we can use and with which ordering of the variables? These questions will be treated next.

4 Vine copula based bivariate quantile regression

Having defined the bivariate unconditional and conditional quantiles in terms of copula distributions, one can estimate them using a bivariate copula based quantile regression model. Consider the variables $(Y_1, Y_2)^T$ as a 2-dimensional response vector and $X = (X_1, \ldots, X_p)^T$ as the $p$-dimensional predictor vector. Let $X_{-i}$ be a $(p - 1)$-dimensional vector defined as $X_{-i} : = (X_1, \ldots, X_{i-1}, X_{i+1}, \ldots X_p)^T$ and let $X_{i:i+k}$ be a $(k + 1)$-dimensional vector defined as $X_{i:i+k} : = (X_i, \ldots, X_{i+k})^T$. Similar definitions hold for the vectors $x_{-i}, u_{-i}, u_{-i}$, and for $x_{i:i+k}, u_{i:i+k}, u_{i:i+k}$, respectively.

The main interest of the bivariate vine based quantile regression is to predict the $\alpha \in (0, 1)$ quantile of the response variables $Y = (Y_1, Y_2)^T$ given the outcome of some predictor variables $X = x$. This can be achieved by joint modelling of $(Y, X)^T$ and subsequently using the bivariate conditional quantile function defined in Definition 3.2. The same can be achieved by joint modelling of the PIT values of the responses $V = (V_1, V_2)^T$, the predictors $U = (U_1, \ldots, U_p)^T$, and the bivariate conditional quantile function in Equation (7). The connection between the both is the following

$$Q^Y_\alpha(x) = \{(F^{-1}_{Y_1}(v_1), F^{-1}_{Y_2}(v_2)) \in \mathbb{R}^2 : C_{Y_1, Y_2|x}(v_1, v_2|x) = \alpha \}$$

$$= \{(F^{-1}_{Y_1}(v_1), F^{-1}_{Y_2}(v_2)) \in \mathbb{R}^2 : (v_1, v_2) \in Q^V_\alpha(u) \}.$$ (9)
Using Equation (9), in order to model the bivariate conditional quantile function, we need to estimate the marginal distributions \( F_{V_j}, F_{X_i} \) for \( j = 1, 2, \ i = 1, \ldots, p \), and the bivariate conditional distribution \( C_{V_j, V_k|U} \). To obtain the later, we need to estimate the \( p + 2 \) dimensional copula \( C_{V_1, V_2|U} \) describing the joint distribution of \((V_1, V_2, U)\). Estimating the univariate marginal distributions is a fairly simple task. Following Kraus and Czado (2017), Noh et al. (2013), we estimate the marginals nonparametrically and predictor variables.

Following Kraus and Czado (2017), Noh et al. (2013), we estimate the marginals nonparametrically to reduce the bias caused by model misspecification. Examples of nonparametric univariate estimators are the continuous kernel smoothing estimator (Parzen 1962) and the transformed local likelihood estimator (Geenens 2014). A more complex task is estimating the \( p + 2 \) dimensional copula \( C_{V_1, V_2|U} \) and subsequently, deriving the bivariate conditional distribution from the copula. We propose to model the copula \( C_{V_1, V_2|U} \) using regular vine copulas. However, we also have to take care that deriving the bivariate conditional distribution \( C_{V_1, V_2|U} \) remains analytically tractable. Thus, to obtain the joint conditional distribution of the response variables using the recursion formula in Equation (5), additional constraints are required. The constraint for a univariate vine regression is that the node containing the response in the conditioned set is a leaf node in each tree of the tree sequence, as shown by Kraus and Czado (2017) for D-vines and by Tepegjozova et al. (2022) for C-vines. Following these results, the constraint for the bivariate vine regression model is that the two response variables are exactly the conditioned set of the edge of the last tree in the vine tree sequence, as also used by Zhu et al. (2021). Therefore, we propose a new vine tree structure specifically designed for bivariate quantile regression modelling.

### 4.1 Y-vine copula model

**Definition 4.1.** Given the marginal PIT transformed response variables \( V_1, V_2 \) and predictor variables \( U_1, \ldots, U_p \), we define the \( p + 1 \) trees of the Y-vine tree sequence for bivariate quantile regression as the following:

- **\( T_1 \)** with \( N_1 = \{ V_1, V_2, U_1, \ldots, U_p \} \) and \( E_1 = \{ (V_1, U_1), (V_2, U_1) \} \cup \bigcup_{i=1}^{p-1} (U_i; U_{i+1}).

- **\( T_2 \)** with \( N_2 = \{ V_1 U_1, V_2 U_1, U_1 U_2, \ldots, U_{p-1} U_p \} \) and 

  \[ E_2 = \{ (V_1 U_1, U_1 U_2), (V_2 U_1, U_1 U_2) \} \cup \bigcup_{i=1}^{p-2} (U_i U_{i+1}, U_{i+1} U_{i+2}). \]

- **\( T_k \)** for \( 3 \leq k \leq p \) with \( N_k = \bigcup_{j=1,2} \{ V_j U_{k-1}; U_{1:k-2} \} \bigcup_{i=1}^{p-k} \{ U_i U_{i+k-1}; U_{i+1:i+k-2} \} \) and 

  \[ E_k = \bigcup_{j=1,2} \{ (V_j U_{k-1}; U_{1:k-2}, U_1 U_k; U_{2:k-1}) \} \cup \bigcup_{i=1}^{p-k} \{ (U_i U_{i+k-1}; U_{i+1:i+k-2}, U_{i+1} U_{i+k}; U_{i+2:i+k-1}) \}. \]

- **\( T_{p+1} \)** with \( N_{p+1} = \bigcup_{j=1,2} \{ V_j U_p; U_{1:p-1} \} \) and \( E_{p+1} = \{ (V_j U_p; U_{1:p-1}, V_2 U_p; U_{1:p-1}) \}. \)

The newly proposed Y-vine tree sequence is graphically illustrated in Figure 5. In each tree of the vine tree sequence the nodes containing the predictor variables in the conditioned set are arranged in a path, while the nodes containing the response variables in the conditioned set are added as leaves of the path on one end. The subset of the sequence that contains a single response and all predictors forms a D-vine tree sequence. In addition, this tree structure allows for symmetric treatment of the response variables, especially important since an asymmetric treatment might lead to different performances of the regression models on different responses. Next, we prove that the proposed Y-vine tree sequence satisfies the regular vine tree sequence conditions.

**Theorem 1.** The Y-vine tree sequence from Definition 4.1, satisfies the regular vine tree sequence conditions (i)-(iii) from Section 2 and thus, represents a valid regular vine tree sequence.

The proof of Theorem 1 is given in Appendix B.2.

A regular vine copula associated with a Y-vine tree sequence together with a set of bivariate copulas \( B(V) \) and the corresponding pair copula parameters \( \Theta(B(V)) \) is called a Y-vine copula and we denote it
Figure 5: Y-vine tree sequence on the u-scale.
by $Y$. The joint density $f_{Y_1,Y_2,X}$ using a $Y$-vine tree sequence can be expressed by Equation (4) as

$$f_{Y_1,Y_2,X} (y_1, y_2, x) = \prod_{k=1}^{p-1} \left[ \prod_{i=1}^{p-k} c_{U_i,U_{i+k},U_{i+1:i+k-1}} \left( F_{X_i|x_{i+1:i+k-1}} \right) \left( x_i|x_{i+1:i+k-1} \right) \right]$$

$$\cdot \prod_{j=1,2} \left[ \prod_{i=1}^{p} c_{V_j,U_i,U_{i-1}} \left( F_{Y_j|x_{1:i-1}} \right) \left( y_j|x_{1:i-1} \right), F_{X_i|x_{1:i-1}} \left( x_i|x_{1:i-1} \right) \right]$$

$$\cdot c_{V_1,V_2,U} \left( F_{Y_1|x} \left( y_1|x \right), F_{Y_2|x} \left( y_2|x \right) \right) \cdot \prod_{j=1,2} f_{Y_j}(y_j).$$

(10)

**Theorem 2.** The joint conditional density of $(Y_1,Y_2)$ given the predictors $X=(X_1,\ldots,X_p)^T$ denoted by $f_{Y_1,Y_2|X}$ in a $Y$-vine copula is given as

$$f_{Y_1,Y_2|X} (y_1, y_2|x) = \prod_{i=1}^{p} \left[ \prod_{j=1,2} c_{V_j,U_i,U_{i-1}} \left( F_{Y_j|x_{1:i-1}} \right) \left( y_j|x_{1:i-1} \right), F_{X_i|x_{1:i-1}} \left( x_i|x_{1:i-1} \right) \right]$$

$$\cdot c_{V_1,V_2,U} \left( F_{Y_1|x} \left( y_1|x \right), F_{Y_2|x} \left( y_2|x \right) \right) \cdot \prod_{j=1,2} f_{Y_j}(y_j).$$

(11)

Proof of Theorem 2 is given in Appendix B.3.

In order to determine the joint and the bivariate conditional densities, $c_{V_1,V_2,U}$ and $c_{V_1,V_2|U}$, we only need to set the marginals to uniform densities, i.e. $f_{Y_j}(y_j) = 1, \ j = 1, 2$ and $f_{X_i}(x_i) = 1, i = 1, \ldots, p$ in Equation (10) and Equation (11) respectively. Thus, with the proposed $Y$-vine copula we can express the conditional bivariate density as a product of pair copula densities occurring in the Y-vine tree sequence that contain a response in the conditioned set, and the marginal densities of the responses. No integration is needed.

In addition to the analytic form of the joint conditional density $f_{Y_1,Y_2|X}$, from the Y-vine we can also derive other conditional densities in an analytic form.

**Corollary 1.** From the Y-vine copula associated with the Y-vine tree sequence of Definition 4.1, we can derive the following conditional densities:

a. for $j = 1, 2$ it holds

$$f_{Y_j|x} (y_j|x) = f_{Y_j}(y_j) \prod_{i=1}^{p} c_{V_j,U_i,U_{i-1}} \left( F_{Y_j|x_{1:i-1}} \right) \left( y_j|x_{1:i-1} \right), F_{X_i|x_{1:i-1}} \left( x_i|x_{1:i-1} \right);$$

(12)

b. for $j, k \in \{1,2\}$ with $j \neq k$, it holds

$$f_{Y_k|x,Y_j} (y_k|x,y_j) = \prod_{i=1}^{p} c_{V_k,U_i,U_{i-1}} \left( F_{Y_k|x_{1:i-1}} \right) \left( y_k|x_{1:i-1} \right), F_{X_i|x_{1:i-1}} \left( x_i|x_{1:i-1} \right) \right]$$

$$\cdot c_{V_1,V_2,U_1:p} \left( F_{Y_1|x_{1:p}} \left( y_1|x \right), F_{Y_2|x} \left( y_2|x \right) \right) \cdot f_{Y_k}(y_k).$$

(13)

Proof of Corollary 1 is given in Appendix B.4. For the associated univariate conditional densities $c_{V_1|U} (v_1|u)$, $c_{V_2|U} (v_2|u)$, and $c_{V_1,U,V_2} (v_1,u,v_2)$, $c_{V_2|U,V_1} (v_2|u,v_1)$, we set $f_{Y_j}(y_j) = 1, j = 1, 2$, in Equation (12) and Equation (13) respectively.
The univariate conditional distribution functions \( C_{V_1|U} \), \( C_{V_2|U} \), and \( C_{V_1|U,V_2} \), \( C_{V_2|U,V_1} \) can be obtained through integration of these associated conditional densities. The bivariate conditional distribution function \( C_{V_1,V_2|U_{1:p}} \) is obtained similar as in Equation (8) as:

\[
C_{V_1,V_2|U_{1:p}} (v_1,v_2|u_{1:p}) = \int_0^{v_2} c_{V_2|U_{1:p}} (v_2'|u_{1:p}) \cdot C_{V_1|V_2,U_{1:p}} (v_1|v_2'|u_{1:p}) dv_2'.
\]  

(14)

One can also condition on \( V_1 \) instead of \( V_2 \) in Equation (14).

### 4.2 Sequential forward selection of predictors

Until now, we ordered the predictors as \( X_1 \) to \( X_p \), however other permutations are possible. Let’s denote the associated permutation of the Y-vine \( Y \) from Figure 5 by \( \mathcal{O}(Y) := (1,2,\ldots,p-1,p) \). It is the order in which the predictors appear in \( T_1 \) of the tree sequence. One can choose the order of the predictors randomly, but the predictive power of the fit greatly depends on the chosen order. Different orders will produce different Y-vine fits, as the influence over the two responses varies with the predictors. There are \( p \) possible permutations of this order, computing and comparing each of them is not feasible and the optimal permutation is in general unknown. Thus, we propose an algorithm that automatically constructs a Y-vine by sequentially ordering predictors. In addition, we apply a stopping criteria to prevent overfitting, meaning that the least influential predictors will not be considered in the model. This way we obtain an automatic forward selection of predictors for the bivariate regression model. Similar ordering approaches are introduced in Kraus and Czado (2017) for univariate D-vine quantile regression and in Tepegjozova et al. (2022) for C-vine and D-vine copulas with an additional step to check for possible future improvement.

#### 4.2.1 Joint conditional log-likelihood

The goal is to find the order of the predictors that has the greatest explanatory power. To compare and quantify the explanatory power of different bivariate regression models we propose a log-likelihood approach. Inspired by the one dimensional vine based quantile regression (Kraus and Czado 2017), we would like to associate the fit measure with the target function of the bivariate vine based quantile regression. A suitable choice is the log-likelihood of \( c_{V_1,V_2|U_{1:p}} \), since \( c_{V_1,V_2|U_{1:p}} \) is the corresponding density of the target function. However, before deciding on the fit measure we take a more precise look at the proposed log-likelihood. Following Killiches et al. (2018), the conditional copula density \( c_{V_j|U_{1:p}} \) can be rewritten as a product of all pair-copulas that contain the response \( V_j \) in a D-vine copula. In the bivariate response case using Y-vines, we can express \( c_{V_1,V_2|U_{1:p}} \) as a product of all pair-copulas that contain the responses \( V_1 \) and \( V_2 \), as shown in Equation (11) by setting the marginals to uniform densities. Thus, the log-likelihood of \( c_{V_1,V_2|U_{1:p}} \) associated with a Y-vine, can be written as

\[
\ell (c_{V_1,V_2|U_{1:p}}) = \ell (c_{V_1,V_2,U_{1:p}}) + \ell (c_{V_1|U_{1:p}}) + \ell (c_{V_2|U_{1:p}}) \\
= \ell (c_{V_1,V_2|U_{1:p}}) + \sum_{j=1,2} \ell (c_{V_j,U_1}) + \sum_{k=2}^p \ell (c_{V_j,U_k,U_{1:k-1}}) \]

where \( \ell(f) \) denotes the log-likelihood associated to a statistical model with density \( f \) and a given independent and identically distributed sample. Here we used the predictor order as given in Figure 5.

The pair-copula density \( c_{V_j,U_k,U_{1:k-1}} \) represents the behaviour between \( U_k \) and \( V_j \) given that the effects of the conditioning values \( U_1,\ldots,U_{k-1} \) are adjusted. Therefore, a large value of the log-likelihood \( \ell (c_{V_j,U_k,U_{1:k-1}}) \) indicates an influence of \( U_k \) on the response \( V_j \). This implies that the log-likelihoods associated with the pair copulas \( c_{V_j,U_k,U_{1:k-1}} \) are suitable for a fit measure since we can interpret an increase in the fit measure as an increase in influence from a certain predictor. But what importance
does the copula between the responses given the predictors $c_{V_1,V_2;U_{1:k-1}}$ have on the predictive power of the model is a valid question for $k = 2, \ldots, p$. The term $c_{V_1,V_2;U_{1:k}}$ represents the behaviour between $V_1$ and $V_2$ given that the effects of $U_1, \ldots, U_k$ are adjusted. This implies that neither an increase nor a decrease in the log-likelihood $\ell(c_{V_1,V_2;U_{1:k}})$ can be interpreted as an increase in influence for a single predictor. Thus, $c_{V_1,V_2;U_{1:k}}$ for $k = 2, \ldots, p$ fails to quantify the marginal effect of any predictor on the responses and we exclude it from our proposed fit measure. Finally, we formally introduce the adjusted conditional log-likelihood as our fit measure.

**Definition 4.2.** The adjusted conditional log-likelihood of a bivariate Y-vine based quantile regression model, denoted by $acll$, with PIT transformed response and predictor variables $V_1, V_2, U_1, \ldots, U_p$, is defined as

$$acll(Y) := \ell(c_{V_1,V_2|U_1}) - \ell(c_{V_1,V_2|U_2})$$

$$= \sum_{j=1,2} \left[ \ell(c_{V_j,U_1}) + \sum_{k=2}^p \ell(c_{V_j,U_k|U_{1:k-1}}) \right]. \tag{15}$$

Since we are interested in forward selection of predictors, we need to easily compare nested models with one predictor difference. Let $Y_{p-1}$ and $Y_p$ be two nested Y-vine based regression models with response variables $V_1, V_2$, where $Y_{p-1}$ includes the predictors $U_1, \ldots, U_{p-1}$ in that order and $Y_p$ includes the predictors $U_1, \ldots, U_{p-1}, U_p$. Then the connection between the adjusted conditional log-likelihoods of those nested models is given as

$$acll(Y_p) = \ell(c_{V_1,U_p|U_{1:p-1}}) + \ell(c_{V_2,U_p|U_{1:p-1}}) + acll(Y_{p-1}), \tag{16}$$

and we use this result for forward selection of predictors.

### 4.2.2 Automatic forward selection algorithm

Assume we start with the PIT transformed response and predictors $V_1, V_2, U_1, \ldots, U_p$, and their observations $v_n = (v_1^n, v_2^n)^T$, $u_n = (u_1^n, \ldots, u_p^n)^T$, for $n = 1, \ldots, N$. We would like to fit a Y-vine copula model to the data, given that $V_1, V_2$ are the responses. First, we build a Y-vine copula model with one predictor only. To see which predictor needs to be on the first place in the order, we fit all possible one-predictor Y-vines. We derive their adjusted conditional log-likelihoods using Equation (15), and the predictor that maximizes it, say $U_{r_1}$ becomes the first predictor in the order of the Y-vine model. Let’s denote the fitted Y-vine model with one predictor as $\hat{Y}_1$ with order $O(\hat{Y}_1) = (r_1)$. In the next step, we need to choose the second predictor to be added to the model. To do so, we fit the additional pair-copulas that need to be estimated for the adjusted conditional log-likelihood. Following Equation (16), we need to estimate two more copulas for each of the remaining predictors, derive the adjusted conditional log-likelihoods and the predictor that maximizes it, say $r_2$ becomes the second predictor in the order. Thus, at the end of the second step we have a fitted Y-vine model with two predictors denoted as $\hat{Y}_2$ with order $O(\hat{Y}_2) = (r_1, r_2)$. We continue this forward selection algorithm until we order all predictors or if none of the remaining predictors is able to increase the conditional log-likelihood of the model, similar as in (Kraus and Czado 2017). The full estimation procedure and the pseudo code for the algorithm is given in Appendix C.

## 5 Prediction for bivariate quantile regression

Assume we have fitted a bivariate Y-vine regression model $\hat{Y}$ on a bivariate response vector $(V_1, V_2)^T$ with order of predictors $O(\hat{Y}) = (1, \ldots, p)$. The fitted vine has a tree sequence and pair-copula family sets denoted by $\hat{V}$ and $\hat{B}(\hat{V})$, respectively. Given a new realization $u^{new} = (u_1^{new}, \ldots, u_p^{new})^T$, our target is to obtain the set of points $Q_{\alpha}^V(u^{new}) = \left\{ (v_1, v_2) \in [0,1]^2 \mid C_{V_1,V_2|U}(v_1, v_2|u^{new}) = \alpha \right\}$. To estimate
the set \( Q^V \) we employ the same numerical procedure as explained in Section 3.4. In addition, we need to be able to evaluate the function \( C_{V_i,V_j} \) at every integration point \( \mathbf{v}^{inp} = (v_1^{inp}, v_2^{inp})^T \in [0,1]^2 \) and determine the integral given in Equation (14). We apply the chosen adaptive quadrature algorithm for integration (see more in Piessens et al. (2012)), which requires the ability to evaluate the function under the integral at all points of the integration interval. Therefore, given a point \( \mathbf{v}^{inp} = (v_1^{inp}, v_2^{inp})^T \) we define the integrand, denoted by \( \text{IN}(z) \) for any \( 0 < z < v_2^{inp} \), as

\[
\text{IN}(z) := c_{V_2}(z \mid u_{\text{new}}) \cdot C_{V_1,V_2}(v_1^{inp} \mid z, u_{\text{new}}).
\]

(17)

The integration is carried out over the interval \((0, v_2^{inp})\). While the first term in Equation (17) is available analytically since it is the conditional density associated with the D-vine \( V_2 - U_1 - \ldots - U_p \), the second term needs further consideration. For this we define the pseudo copula data for \( u_{\text{new}} \) as the following

\[
u^i_{i-1} = h_{U_i \mid V_{i-1}}(u^{new}_{i-1}, u^{new}_{i-1}), \quad u^i_{i-1} = h_{U_{i-1} \mid V_i}(u^{new}_{i-1} \mid u^{new}_{i-1}) \quad \forall i = 2, \ldots, p,
\]

where the \( h \)-functions \( h_{U_i \mid U_{i-1}} \) and \( h_{U_{i-1} \mid V_i} \) are obtained from the pair copula \( c_{U_i,U_{i-1}} \in \hat{B}(\hat{V}) \). For any \( k = 2, \ldots, p-1 \) it holds

\[
u^i_{i-1\mid k-1; i-1} = h_{U_i \mid U_{i-1} \mid U_{i-k}; U_{i-k+1}; \ldots; U_{i-2}; U_{i-1} \mid U_{i-1}}(u^{new}_{i-1\mid k-1; i-1}, u^{new}_{i-1\mid k-1; i-1}) \quad \forall i = 2, \ldots, p,
\]

and similarly, \( u^i_{i-1\mid k-1; i-1} = h_{U_i \mid U_{i-1} \mid U_{i-k}; U_{i-k+1}; \ldots; U_{i-2}; U_{i-1}}(u^{new}_{i-1\mid k-1; i-1}, u^{new}_{i-1\mid k-1; i-1}) \). In addition, based on this pseudo-copula data estimated from the fitted Y-vine we introduce the following two matrices, \( W \in [0,1]^{p \times p} \) and \( W' \in [0,1]^{p \times p} \), as

\[
W(\mathbf{u}_{\text{new}}; \hat{B}(\hat{V})) := \\
\begin{pmatrix}
    u_{11}^{new} & u_{12}^{new} & u_{13}^{new} & \cdots & u_{1p}^{new} \\
    u_{21}^{new} & u_{22}^{new} & u_{23}^{new} & \cdots & u_{2p}^{new} \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    u_{p1}^{new} & u_{p2}^{new} & u_{p3}^{new} & \cdots & u_{pp}^{new}
\end{pmatrix}
\]

\[
W'(\mathbf{u}_{\text{new}}; \hat{B}(\hat{V})) := \\
\begin{pmatrix}
    u_{11}^{new} & u_{12}^{new} & u_{13}^{new} & \cdots & u_{1p}^{new} \\
    u_{21}^{new} & u_{22}^{new} & u_{23}^{new} & \cdots & u_{2p}^{new} \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    u_{p1}^{new} & u_{p2}^{new} & u_{p3}^{new} & \cdots & u_{pp}^{new}
\end{pmatrix}
\]

Using matrices \( W \) and \( W' \), we define the following pseudo copula data for \( j = 1, 2 \), \( u_{w1} \mid j = h_{V_j \mid U_1}(w \mid u_{w1}) \) and \( u_{w1} \mid j = h_{V_j \mid U_1}(w \mid u_{w1}) \), where \( h_{V_j \mid U_1} \) and \( h_{U_1 \mid V_j} \) are estimated from the pair copula \( c_{V_j,U_1} \in \hat{B}\). Further, for \( i = 2, \ldots, p \), define \( u_{vj} \mid i = h_{V_j \mid U_{i-1} \mid U_{i-1}}(u_{vj} \mid i-1 \mid u_{vj} \mid i-1) \) and \( u_{vj} \mid i-1 = h_{U_i \mid V_j \mid U_{i-1}}(u_{vj} \mid i-1 \mid u_{vj} \mid i-1) \). These \( h \)-function are estimated from the pair copula \( c_{V_j,U_i \mid U_{i-1}} \in \hat{B}\). Then, we also define the matrix \( W^2 \in [0,1]^{(p+1) \times 2} \) with \( j \in \{1, 2\} \) as

\[
W^2(w, j; W', W) := \\
\begin{pmatrix}
    w & w \\
    u_{w1} & u_{w1} \\
    u_{w1} & u_{w1} \\
    u_{vj} & u_{vj} \\
    u_{vj} & u_{vj} \\
    \vdots & \vdots \\
    u_{vp} & u_{vp} \\
    u_{vp} & u_{vp}
\end{pmatrix}
\]

For a fixed input \( v_1^{inp} \) we can evaluate \( C_{V_1,V_2}(v_1^{inp} \mid z_{\text{new}}, u_{\text{new}}) = h_{V_2 \mid V_1}(u_{v1} \mid p \mid u_{v2} \mid p) \), at \( z = z_{\text{new}} \), such that \( u_{v1} \mid p \) is obtained from \( W^2(w = v_1^{inp}, j = 1; W, W') \) and \( u_{v2} \mid p \) is obtained from

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$W^2 (w = z^{new}, j = 2; W, W')$. The h-function $h_{V_1|V_2;U}$ is estimated from the pair copula $c_{V_1,V_2;U} \in \hat{B}(\hat{V})$. $c_{V_2|U}$ is evaluated as

$$c_{V_2|U} (z^{new}|u^{new}) = \frac{c_{V_2,U_2}}{c_U} = c_{V_2,U_1} (z^{new}, u^{new}_1) \prod_{i=2}^{p} c_{V_2,U_i;U_{1:i-1}} (u^{new}_{v_2|1:i-1}, u^{new}_{i|i-1}),$$

where $c_{V_2,U_1}, c_{V_2,U_i;U_{1:i-1}} \in \hat{B}(\hat{V})$ for $i = 1, \ldots, p$. Therefore, the integrand in Equation (17) can be evaluated with no further calculations from the Y-vine as

$$IN (z^{new}) = c_{V_2,U_1} (z^{new}, u^{new}_1) \prod_{i=2}^{p} c_{V_2,U_i;U_{1:i-1}} (u^{new}_{v_2|1:i-1}, u^{new}_{i|i-1}) \cdot h_{V_1|V_2;U} (u_{v_1|1:p}, u_{v_2|1:p}).$$

To summarize, given the integration point $v^{inp} = (v_1^{inp}, v_2^{inp})^T$, the integrand $IN (z^{new})$ at a point $z^{new} \in (0, v_2^{inp})$ conditioned on $u^{new}$, can be computed using the matrices $W, W'$, $W^2 (w = z^{new}, j = 2; W, W')$, $W^2 (w = v_1^{inp}, j = 1; W, W')$ and h-functions obtained from the pair copulas defined by $\hat{B}(\hat{V})$. This implies that we can efficiently evaluate the function $C_{V_1,V_2|U}$ using Equation (18). In addition, the newly introduced matrices $W, W'$ and $W^2$ can be used to simulate $(p + 2)$-dimensional data from the fitted Y-vine copula. More details on simulation from general R-vines can be found in (Dißmann 2010, Chapter 5).

5.1 Prediction method for conditionally independent responses

If the two responses are conditionally independent given the predictors, i.e., $F_{Y_1|X} (y|X) = F_{Y_1|X} (y_1|X) \cdot F_{Y_2|X} (y_2|X)$ holds, then we don’t need to use the involved prediction method previously developed. Instead, we can use specific prediction method for this case. The conditional independence doesn’t imply that the responses are independent, so our starting assumption that the responses are dependent still holds. Fitting two different regressions for each response variable doesn’t take into account the dependency between the responses, but our proposed method does. Recall that we can obtain the univariate conditional quantiles as the inverses of the marginal conditional distribution of each response given the predictors for a given value of $\alpha$, $\hat{v}_1 = F_{Y_1|X}^{-1} (\alpha|x) = F_{Y_1}^{-1} \left( C_{Y_1|U}^{-1} (\alpha|u) \right)$, $\hat{v}_2 = F_{Y_2|X}^{-1} (\alpha|x) = F_{Y_2}^{-1} \left( C_{Y_2|U}^{-1} (\alpha|u) \right)$. This boils down to the prediction case of two univariate D-vine quantile regressions, explained in Kraus and Czado (2017).

Then, in the conditionally independent case we can define the bivariate quantile curves for $\alpha \in (0, 1)$ as the union of the sets

$$Q^Y_{\alpha_2|Y_1|X} (x) := \left\{ (y_1, y_2) \in \mathbb{R}^2 ; \ F_{Y_1|X} (y_1|x) = \alpha_1, \ F_{Y_2|X} (y_2|x) = \frac{\alpha}{\alpha_1}, \ \alpha_1 \in (\alpha, 1) \right\},$$

$$\cup \left\{ (y_1, y_2) \in \mathbb{R}^2 ; \ F_{Y_1|X} (y_1|x) = \frac{\alpha}{\alpha_1}, \ F_{Y_2|X} (y_2|x) = \alpha_1, \ \alpha_1 \in (\alpha, 1) \right\}$$

Analogous definition holds for the case of bivariate quantiles on the unit square as well.

6 Data application

The implementation of the Y-vine quantile regression is done in the statistical software R (R Core Team 2021). As an application to real data we consider the Seoul weather data set, which contains two dependent responses, daily minimum and maximum air temperature. The data originates from the UCI machine learning repository (Dua and Graff 2019), it can be downloaded using https://archive.ics.uci.edu/ml/
datasets/Bias+correction+of+numerical+prediction+model+temperature+forecast and was first studied by Cho et al. (2020). It contains daily data for 25 weather stations in Seoul, South Korea between June 30th and August 30th in the period 2013-2017. Cho et al. (2020) use it for enhancing next-day maximum and minimum air temperature forecasts based on the Local Data Assimilation and Prediction System (LDAPS) model. To illustrate the proposed vine based bivariate quantile regression model, we consider the station located in central Seoul (station 25) and we ignore the temporal dependence between daily measurements. Disregarding geographical markers and precipitation measurements, we are left with a data set containing two response variables and 13 continuous predictors, with 307 data points representing summer days of the years 2013 to 2017. In the supplementary material we provide a description of the considered variables. We divide the data set into a training and testing set, consisting of 246 data points from 2013-2016, and 61 data points from 2017, respectively. In the supplement, we also show the empirical normalized contour plots for pairs of variables from the training set, which shows strong non-Gaussian dependence structure in the data, indicated by non-elliptical shapes. This shows that the data is suited for application of the proposed Y-vine copula class.

In the estimation of our Y-vine quantile regression model we model the marginals distributions using a nonparametric approach, while we model the pair copulas in a parametric approach, resulting in a semiparametric model. Modeling the marginals as well as the copulas parametrically might cause the resulting fully parametric estimator to be biased and inconsistent if one of the parametric models is misspecified Noh et al. (2013). Modeling them both using a nonparametric approach leads to a fully nonparametric approach that might overfit the data, because penalization is still an open research topic in the nonparametric case, as noted in Tepegjozova et al. (2022). Thus, we opt for a semiparametric approach. The marginals are estimated using a univariate nonparametric kernel density estimator implemented in the \texttt{R} package \texttt{kde1d} (Nagler and Vatter 2020), and the pair copulas are fitted using a parametric maximum-likelihood approach with the Akaike Information Criterion penalization (Akaike 1973) (AIC) implemented in the \texttt{R} package \texttt{rvinecopulib} (Nagler and Vatter 2021).

The response variables, minimum and maximum air temperature, are not independent of each other and are expected to rise and fall together. This dependence is emphasized by an estimated Kendall’s τ value of 0.45. We fit a pair copula to the two responses and the estimated pair copula is the Gaussian copula with a parameter of 0.64. This pair copula is used to estimate unconditional bivariate quantiles, as in Section 3.5. The estimated quantile curves are shown in Figure 6. Due to constraints of the weather system in question, the maximum temperature is always required to be greater than the minimum temperature. However, this ordering constraint does not imply an ordering constraint on the PITs on the u-scale.

![Figure 6](image-url) Black points: data from 2013-2016 (n=246). Colored curves: estimated unconditional quantile curves for $\alpha = 0.05, 0.1, 0.25, 0.5, 0.75, 0.90, 0.95$ (left bottom to right top).
For illustration see Figure 6, where the ordering is visible in panel (a), as all the data is below the diagonal, while this ordering is lost in panel (b). To obtain bivariate conditional quantile curves, a $Y$-vine model, denoted as $\hat{\mathcal{Y}}$, is fitted on the training set. More details on the fitted vine copulas is given in the supplementary material. The automatically chosen order of the predictors is given by

$$O(\hat{\mathcal{Y}}) = (\text{LDAPS}_{\text{Tmin lapse}}, \text{LDAPS}_{\text{Tmax lapse}}, \text{LDAPS}_{\text{RHmax}}, \text{LDAPS}_{\text{WS}}, \text{Present}_{\text{Tmin}}, \text{LDAPS}_{\text{CC1}}, \text{Present}_{\text{Tmax}}, \text{LDAPS}_{\text{LH}}, \text{LDAPS}_{\text{CC3}}, \text{LDAPS}_{\text{RHmin}}, \text{LDAPS}_{\text{CC4}}).$$

It orders the predictors by their influence over the responses. The fitted conditional pair copula between the responses given the 11 chosen predictors, $\hat{c}_{Y_1,Y_2|X}$ is a Clayton copula with a Kendall’s $\tau$ of 0.10. This implies that $Y_1 \perp Y_2|X$ does not hold. If there was conditional independence, the fitted pair copula has to be the independence copula, but that is not the case. Further, this conditional independence is derived not assuming multivariate Gaussianity, no asymptotic assumptions, but it is vine copula regression based (Bauer and Czado 2016).

Conditional quantile curves for days from the testing set are estimated using the fitted $Y$-vine model $\hat{\mathcal{Y}}$. Also, confidence regions defined as the areas between the respective quantile curves are obtained. The obtained quantile curves and confidence regions for 3 days of the testing set are given in Figure 7. The top row are estimates on the $u$-scale and the bottom row are on the $x$-scale. The ranges of the $x$-scale plots are the ranges of the minimum and maximum possible temperatures, $(22, 38)$ for the maximum temperature and $(16, 29)$ for the minimum temperature.

Figure 7: The plots correspond to the days 10.08.2017, 18.08.2017 and 25.08.2017 (left to right). Shown are estimated conditional quantile curves for $\alpha = 0.05, 0.1, 0.25, 0.5, 0.75, 0.90, 0.95$ (left bottom to right top) and corresponding 90%, 80% and 50% confidence region (light to dark grey shaded) on each panel. Row 1 are estimates on the $x$-scale and row 2 is on the $u$-scale. The black dot is the true value.
Comparing the 3 days shown in Figure 7, we can see very different quantile curves and confidence regions depending on the observed conditioning variables, i.e. predictors. For the day 10.08.2017 we observe that higher minimum and maximum temperatures are expected compared to the other days. The quantile curves on the $u$-scale show that the estimates for 10.08.2017 are more skewed to the upper tail, compared to the estimates for 25.08.2017, which are skewed towards the lower tail. Thus, the extreme case of very high maximum and minimum temperatures, is very likely on 10.08.2017 and highly unlikely on 25.08.2017. Opposite to this, the extreme case of a very small minimum temperature and high maximum temperatures is very likely on 25.08.2017 and highly unlikely on 10.08.2017. The estimates obtained for 18.08.2017 are very moderate and extreme values for both responses are highly unlikely on this date. The different shapes of the quantile curves for the three chosen days, coming from conditional distributions with different tail dependencies, also show that the dependence structure between the response variables does not follow an independence copula. Moreover, the dependence structure is not static and it changes based on the conditioning variables. Thus, ignoring this dependence can lead to a significant underestimation of extreme events, encoded in the tail dependencies of the joint conditional distribution of the responses.

6.1 Advantages of joint modelling of dependent responses

Next we compare the bivariate conditional quantile curves from the Y-vine regression and its corresponding confidence regions to differently obtained bivariate quantile curves and regions. For comparison purposes, we treat the response variables as independent in one case and as conditionally independent in the other. For the conditionally independent assumption we follow Section 5.1 and estimate the corresponding bivariate quantiles and quantile regions $\text{CI}^{Y_{1}, Y_{2} | X}_{\alpha}$, specified in Equation (19). For the independent case, the tasks of predicting maximal and minimal temperatures are treated as completely independent problems and univariate quantiles are estimated for both response variables. For this purpose, two univariate D-vine regression models with the same predictor order as the Y-vine regression are used. This way we can construct a bivariate quantile region from the univariate quantiles using the Bonferroni correction for multiple testing (Bonferroni 1936). We are interested in the bivariate quantiles at a $\alpha = 0.10$, meaning that the two univariate quantiles, from which we construct the bivariate quantiles, need to be evaluated at $\frac{\alpha}{2} = 0.05$. For better comparison, we use the predictions on the original scale, not the $u$-scale.

Figure 8 shows the bivariate confidence regions $\text{CI}^{Y_{1}, Y_{2} | X}_{0.10}$ (from Definition 3.4) for the three selected days, colored in grey in all 6 panels. The first row of Figure 8, additionally contains horizontal lines whose $y$-intercepts correspond to the 0.025 and 0.975 univariate quantiles obtained from the D-vine regression model with the minimal temperature as the response variable. Moreover, it contains vertical lines with $x$-intercepts corresponding to 0.025, 0.975 quantiles of the D-vine regression with the maximal temperature as the response variable. Further, the Cartesian product of the obtained univariate confidence intervals is shown in red. The second row of Figure 8 contains the bivariate confidence regions $\text{CI}^{Y_{1}, Y_{2} | X}_{0.10}$ colored in red, in the case that the response variables are treated as conditionally independent.

First, note the obvious difference in the obtained shapes of confidence regions arising from bivariate quantiles (dependent responses) and the Cartesian product based regions (independent responses). While the bivariate confidence regions are free to vary in shape, the regions obtained by the Cartesian product of univariate confidence intervals are bound to be rectangles.

Also, in each panel the Cartesian product of the univariate confidence intervals is a subset of the bivariate confidence regions obtained from the Y-vine regression. So, there is a whole range of points that are excluded from the bivariate quantile constructed from the univariate quantiles. In between those points are also the true observed values for the dates 18.08.2017 and 25.08.2017, while the true observed values falls into the bivariate confidence region from the bivariate regression. This is not a good indication of performance for the Cartesian product based quantiles. Also, they are quite low in volume and don’t capture any dependence between the responses. Thus, using univariate
Figure 8: The plots correspond to the days 10.08.2017, 18.08.2017 and 25.08.2017 (left to right). The black dot is the true value. Shown are conditional bivariate quantile curves $Q_{0.05}^{Y_0}(x)$ and $Q_{0.95}^{Y_0}(x)$ and the corresponding 90% confidence region $CI_{Y_0|X_{10}}$ (grey shaded). Additionally, in row 1 the estimated univariate quantiles for $\alpha = 0.025, 0.975$ for both response variables and the corresponding 90% confidence regions (in red) are shown. In row 2, the bivariate conditional quantiles when the responses are treated as conditionally independent and the associated 90% confidence regions $CI_{Y_1 \perp Y_2|X_{10}}$ (red shaded) are shown.

quantiles and the corresponding confidence regions fails to capture, not only the dependence, but also the multidimensional nature of the problem.

The second row illustrates the effect of disregarding tail dependence in the case where the response variables are treated as conditionally independent. We can see that the volume of the red (conditionally independent responses) confidence regions is considerably smaller than the volume of the grey (dependent responses) confidence regions. This difference in size is induced by bigger tail dependencies of a fitted non-independence copula compared to a independence copula. If the response variables do not exhibit conditional independence, this will lead to confidence regions that are too low in volume. In addition, the true value from the testing set is not contained in neither one of the confidence regions from the conditionally independent models (red regions), but contained when using the Y-vine based approach.

7 Conclusions and outlook

We studied the problem of bivariate (unconditional and conditional) quantiles using a very flexible class of models, vine copulas. They are multivariate distributions constructed from bivariate blocks (pair copulas) using conditioning. We develop a novel vine tree structure, the Y-vine tree structure, that is suitable for a regression problem containing bivariate response variables. Also, a forward selection of predictors
procedure gives the best suitable fitted Y-vine. In addition, the Y-vine tree structure enables an easy way of obtaining the bivariate conditional density. Our numeric method for evaluating the bivariate quantile sets enables us to evaluate and plot the bivariate quantile sets. This way a joint analysis of the dependence structure of the responses given the predictors is possible. This is a significant result especially when dealing with responses that are not (conditionally) independent. Also, we develop a prediction method for bivariate responses using the Y-vine quantile regression. This enables us to not only jointly model, but also predict bivariate response quantiles. Additionally, simulation from a Y-vine model is available. This is one of the very few methods that can generate multivariate data having two responses with possible tail dependence and asymmetric dependence structures. We apply our proposed model on a real life data set containing a bivariate response, minimal and maximal daily temperature. We analyse the data with our new approach for dependent responses and provide a joint vine copula model for the two responses. For this example, we also highlight the advantages of our joint bivariate modelling over independent and conditionally independent response modelling approaches with vine copulas.

For future possible applications we think of adding a spatial and/or temporal component to our Y-vine based quantile regression. It would be interesting to see how the response dependence changes when the spacial and/or temporal dependence component is also accounted for, but that is out of the scope of this paper. The standard lack of ability of copula based models to include discrete variables is also an ongoing research topic. Some results from the univariate vine based quantile regression are available (Schallhorn et al. 2017), but it becomes even more complicated in our case, because of the multidimensionality of the problem and the numerical method for obtaining the bivariate quantile sets. In addition, we can use the Y-vine tree structure for testing of conditional independence between two variables given a set of conditioning variables. The Y-vines provide a very symmetric treatment of the two variables whose conditional independence is being tested. Using this way of testing for conditional independence we do not need any asymptotic results, as we use a very flexible modelling approach. A similar approach was proposed in Bauer and Czado (2016) using D-vines, for non-Gaussian conditional independence testing in continuous Bayesian networks.

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Appendix

A Appendix A: Theoretical quantile curves of bivariate copula distributions

Figure 9: A 3-dimensional plot of bivariate copula distribution with theoretical quantile curves for $\alpha = 0.05, 0.1, 0.25, 0.5, 0.75, 0.90, 0.95$. Shown are Gaussian, Student-t ($\text{df} = 5$), Clayton and Gumbel copulas (top to bottom) and $\tau = 0.25, 0.5, 0.75$ (left to right).
B Appendix B: Proofs

B.1 Proof of Proposition 3.3

Proof.

\[ F_{Y_1, Y_2|X}(y_1, y_2| x) = \int_{-\infty}^{y_1} \int_{-\infty}^{y_2} f_{Y_1, Y_2|X}(y_1', y_2'| x) \, dy_2' \, dy_1' \]

\[ = \int_{-\infty}^{y_1} \int_{-\infty}^{y_2} \frac{f_{Y_1, Y_2|X}(y_1', y_2'| x)}{f_X(x)} \, dy_2' \, dy_1' \]

\[ = \frac{1}{f_X(x)} \int_{-\infty}^{y_1} \int_{-\infty}^{y_2} \partial^{p+2} \partial_{p} \partial_{\mathbf{y}}^{p+2} F_{Y_1, Y_2, X}(y_1, y_2, x) \bigg|_{y_1=y_1', y_2=y_2'} \, dy_2' \, dy_1' \]

\[ = \frac{1}{f_X(x)} \cdot \partial_{\mathbf{y}}^{p} \partial_{\mathbf{u}}^{p} C_{V_1, V_2|U}(F_{Y_1}(y_1), F_{Y_2}(y_2), F_{X_1}(x_1), \ldots, F_{X_p}(x_p)) \]

(\by Sklar’s theorem\)

\[ = \frac{1}{f_X(x)} \cdot \partial_{\mathbf{y}}^{p} \partial_{\mathbf{u}}^{p} C_{V_1, V_2|U}(v_1, v_2, u_1, \ldots, u_p) \bigg|_{v_1=F_{Y_1}(y_1), u_1=F_{X_1}(x_1)} \]

\[ = C_{V_1, V_2|U}(F_{Y_1}(y_1), F_{Y_2}(y_2)|F_{X_1}(x_1), \ldots, F_{X_p}(x_p)) \]

where \( C_{V_1, V_2|U}(F_{Y_1}(y_1), F_{Y_2}(y_2)|F_{X_1}(x_1), \ldots, F_{X_p}(x_p)) \) or shortly \( C_{V_1, V_2|U}(v_1, v_2|u) \) is the conditional distribution of \( V_1, V_2 \) given \( U = u \) and the joint copula distribution of \( Y_1, Y_2, X \) is denoted \( C_{V_1, V_2, U} \). \( \square \)

B.2 Proof of Theorem 1

Proof. We prove that a Y-vine tree sequence, \( \{T_1, \ldots, T_{p+1}\} \), satisfies conditions (i)-(iii) from Section 2. The first condition (i) is trivial and follows by definition of \( T_1 \). The next condition, the proximity condition, states that for \( k \geq 2 \) two nodes can be connected in \( T_k \) only if the corresponding edges in the previous tree \( T_{k-1} \) share a common node. Consider the part of the tree sequence that only contains the predictors \( \{X_1, \ldots, X_p\} \). By definition of the Y-vine tree sequence, the predictors are arranged in a D-vine tree sequence, which is a known regular vine tree sequence subset, implying that for the nodes containing only the predictors the proximity condition is satisfied. So, we consider the remaining nodes that contain the response variables in the conditioned set and the node that connects them to the D-vine of the predictors. For \( T_2 \), nodes \( V_1U_1, V_2U_1 \) are both connected to \( U_1U_2 \). For \( V_jU_1, j = 1, 2 \) the corresponding edge in \( T_1 \) is \( (V_jU_1) \) which shares the node \( U_1 \) with the corresponding edge of node \( U_1U_2 \). For \( j > 2 \) in \( T_k \) the nodes \( V_jU_k-1; U_{1:k-2} \) and \( V_2U_{k-1}; U_{1:k-2} \) are connected to \( U_1U_k; U_{2:k-1} \). In \( T_{k-1} \) the corresponding edge of node \( V_jU_k-1; U_{1:k-2} \) for \( j = 1, 2 \) is the edge \( (V_jU_k-2; U_{1:k-3}, U_1U_k-2; U_{1:k-3}) \) and for node \( U_1U_k; U_{2:k-1} \) the corresponding edge is \( (U_1U_k-2; U_{2:k-3}, U_2U_k; U_{3:k-1}) \). They share a common node \( U_1U_{k-2}; U_{2:k-3} \) in \( T_{k-1} \), thus the proximity condition is satisfied. The last condition requires that \( N_k = E_k-1 \forall k \geq 2 \). For \( k = 2 \), \( N_2 = \{V_1U_1, V_2U_1, U_1U_2, \ldots, U_{p-1}U_p\} = E_1 \) follows directly from Definition 4.1. To prove the statement for \( k > 2 \), we start with the edge set of tree \( T_{k-1} \), \( E_{k-1} \) given as

\[ E_{k-1} = \bigcup_{j=1,2} \{ (V_jU_k-2; U_{1:k-3}, U_1U_k-1; U_{2:k-2}) \} \]

\[ \bigcup_{i=1}^{p-k+1} \{ (U_iU_{i+k-2}; U_{i+1:i+k-3}, U_{i+1}U_{i+k-1}; U_{i+2:i+k-2}) \} . \]

The edge \( (V_jU_k-2; U_{1:k-3}, U_1U_k-1; U_{2:k-2}) \) is associated with the node \( V_jU_k-1; U_{1:k-2} \) in \( T_k \) for \( j = 1, 2 \) and the edge \( (U_iU_{i+k-2}; U_{i+1:i+k-3}, U_{i+1}U_{i+k-1}; U_{i+2:i+k-2}) \) is associated with the node \( U_iU_{i+k-1}; U_{i+1:i+k-2} \).
for \( i = 1, \ldots, p - k + 1 \) in \( T_k \). Therefore, by Definition 4.1, \( N_k = E_{k-1} \) holds for all \( k \) in the Y-vine tree sequence.

\[ \tag{12} \]

\section*{B.3 Proof of Theorem 2}

\textit{Proof.} By definition of a conditional density it follows that \( f_{Y_1, Y_2 | X} = \frac{f_{Y_1, Y_2, X}}{f_X} \). The numerator \( f_{Y_1, Y_2, X} \) is expressed in Equation (10), and we need to derive the denominator \( f_X \) in terms of copulas. Consider the part of the Y-vine tree sequence after removing the PITs of the responses \( V_1 \) and \( V_2 \), i.e., the tree sequence consisting of only the PITs of the predictors \( (U_1, \ldots, U_p)^T \). By definition of the Y-vine tree structure, the predictors are arranged in a D-vine tree sequence with a specific order. Thus, the density of a D-vine with this given order (see more in Czado (2010)) can be expressed as

\[
\frac{f_{X}(x)}{\prod_{k=1}^{p} f_{X_k}(x_k) \cdot \prod_{k=1}^{p-1} \prod_{i=1}^{p-k} c_{U_i, U_{i+k}; U_{i+1:i+k-1}}(F_{X_i}|x_{i+1:i+k-1})} = \prod_{i=1}^{p-k} c_{U_i, U_{i+k}; U_{i+1:i+k-1}}(F_{X_{i+k}}|x_{i+1:i+k-1}),
\]

(20)

Canceling out all common terms in the expansions of the numerator and the denominator, given in Equation (10) and (20) respectively, we are left with the expression in Equation (11). All the required copulas in Equation (11) are already derived in the Y-vine tree sequence, \( c_{V_j, U_i; U_{1:i-1}} \in B(V) \) for \( j = 1, 2, i = 1, \ldots, p \) and \( c_{V_1, V_2; U} \in B(V) \) (these copulas can be seen as the copulas on the furthest left side of each tree in Figure 5).

\[ \tag{13} \]

\section*{B.4 Proof of Corollary 1}

\textit{Proof.} Let’s prove part a.) for \( j = 1 \). Due to symmetry the same proof follows for \( j = 2 \). By definition of a conditional density it follows that \( f_{Y_1 | X} = \frac{f_{Y_1, X}}{f_X} \). The denominator is expressed in Equation (20), while the numerator needs to be expanded. Consider the random vector \((V_1, U)^T\) in the tree sequence of the Y-vine, i.e. remove the node of the PIT of the response \( V_2 \) from the first tree \( T_1 \) and all the nodes in the further trees that will disappear by removing the variable \( V_2 \). By definition of the Y-vine, the variables \((V_1, U_1, \ldots, U_p)\) are arranged in a D-vine tree sequence with a specific order. Thus, the density of a D-vine with this given order (see more in Czado (2010)) is given as

\[
f_{Y_1, X}(y_1, y_2, x) = \prod_{k=1}^{p} f_{X_k}(x_k) \cdot f_{Y_1}(y_1) \cdot \prod_{k=1}^{p-1} \prod_{i=1}^{p-k} c_{U_i, U_{i+k}; U_{i+1:i+k-1}}(F_{X_i}|x_{i+1:i+k-1}),
\]

(21)

Cancelling common terms of the numerator, Equation (21), and the denominator, Equation (20), we are left with Equation (12) for \( j = 1 \). Now let’s prove part b.) for \((j, k) = (1, 2)\). Due to symmetry the same proof follows for \((j, k) = (2, 1)\). Use that \( f_{Y_2 | X, Y_1} = \frac{f_{Y_2, Y_1, X}}{f_{Y_1, X}} \) holds. The numerator is expressed in Equation (10), and the denominator is expressed as in the part a.) Equation (21). Considering the associated ratio and cancelling all common terms, we are left with Equation (13) for \((j, k) = (1, 2)\). Again, all the required copulas are already derived in the Y-vine tree sequence, \( c_{V_j, U_i; U_{1:i-1}} \in B(V) \) for \( j = 1, 2 \) and \( i = 1, \ldots, p \) and \( c_{V_1, V_2; U} \in B(V) \), which means we don’t require any additional calculations.
Algorithm 1: Bivariate vine based quantile regression algorithm

Input: Data set \( y_n = (y_{n1}^1, y_{n2}^2)^T, x_n = (x_{n1}, \ldots, x_{np})^T \), for \( n = 1, \ldots, N \)

Initialization:
\( acll_0 = 0 \)
\( NotChosenIndex = \{1, \ldots, p\} \)
\( ChosenIndex = \emptyset \)

1. Estimate marginals \( F_{Y_j}, F_{X_i}, j = 1, 2, i = 1, \ldots, p \), by a univariate kernel density estimator, implemented in \texttt{kde1d}.

2. Obtain pseudo copula data \( u_i^n := \hat{F}_{X_i}(x_i^n) \) for \( i = 1, \ldots, p \), \( v_1^n := \hat{F}_{Y_1}(y_1^n) \) and \( v_2^n := \hat{F}_{Y_2}(y_2^n) \).

for \( j = 1, \ldots, p \) do
  Calculate \( acll_j^1 \) as
  \[ acll_j^1 = acll_0 + \ell(cV_{1U_i}) + \ell(cV_{2U_i}) + \ell(cV_{1V2U_i}) \]
end

\( r_1 := \arg \max_{j=1, \ldots, p} acll_j^1 \)
\( NotChosenIndex = NotChosenIndex \setminus \{r_1\} \)
\( ChosenIndex = ChosenIndex \cup \{r_1\} \)
\( acll_1 := acll_1^{r_1} \)

for \( k = 2, \ldots, p \) do
  for \( t \in NotChosenIndex \) do
    Calculate \( acll_k^t \) as
    \[ acll_k^t = acll_{k-1}^t + \ell(cV_{1U_i};U_{r_1}, \ldots, U_{r_{k-1}}) + \ell(cV_{2U_i};U_{r_1}, \ldots, U_{r_{k-1}}) \]
  end
  \( r_k := \arg \max_{t \in NotChosenIndex} acll_k^t \)
  \( NotChosenIndex = NotChosenIndex \setminus \{r_k\} \)
  \( ChosenIndex = ChosenIndex \cup \{r_k\} \)
  \( acll_k := acll_k^{r_k} \)
end

return \( ChosenIndex = \{r_1, \ldots, r_p\} \), i.e. order of the predictors which uniquely determines the fitted bivariate quantile regression model.

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Bivariate vine copula based quantile regression: supplementary material

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1 Algorithms for numerical estimation

Algorithm 1: PseudoInverse

Input: m - granularity parameter (default = 1000),
      eq - function based on which $C(u,v)$ is to be evaluated,
      err - accuracy of algorithm,
      α - alpha level

Initialization:

\[ M = \bigcup_{i=1}^{m} \left\{ \frac{i}{m} \right\}, \]

\[ L = \{ \text{line}((0,0),(w_i,1)) | \forall w_i \in M \} \cup \{ \text{line}((0,0),(1,w_i)) | \forall w_i \in M \}, \]

\[ Points = \emptyset. \]

for $l_s \in L$ do

  \[ point = \text{BinaryLineSearch}(l_s, eq, err, \alpha) \]

  \[ Points = Points \cup point \]

end

return $Points$

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Algorithm 2: BinaryLineSearch

Input: l - line defined by two coordinates,
eq - function based on which \( C(u, v) \) is to be evaluated,
\( err \) - accuracy of algorithm,
\( \alpha \) - alpha level

Initialization:
Introduce notation \( l = \text{line} (p_{\text{start}} = (0, 0), p_{\text{end}} = (w, 1)) \).

\[ evl = \text{eq} \left( \frac{p_{\text{start}} + p_{\text{end}}}{2} \right) \]

\[ \text{diff} = \alpha - evl \]

while \( \text{diff} > err \) do
  if \( \text{diff} > 0 \) then
    \( p_{\text{start}} = \frac{p_{\text{start}} + p_{\text{end}}}{2} \)
  else
    \( p_{\text{end}} = \frac{p_{\text{start}} + p_{\text{end}}}{2} \)
  end
  \( evl = \text{eq} \left( \frac{p_{\text{start}} + p_{\text{end}}}{2} \right) \)
end

return \( \frac{p_{\text{start}} + p_{\text{end}}}{2} \)

2 Theoretical and estimated unconditional bivariate quantiles

2.1 Clayton copula

The distribution function of a bivariate Clayton copula with parameter \( \theta \) is

\[
C_{V_1, V_2}(v_1, v_2; \theta) = \left( v_1^{-\theta} + v_2^{-\theta} - 1 \right)^{-1/\theta}.
\]

By solving \( (v_1^\theta + v_2^\theta - 1)^{-1/\theta} = \alpha \) for \( v_2 \), we obtain the \( \alpha \) bivariate quantile curve as

\[
Q^V_\alpha := \left\{ (v_1, \left( \alpha^{-\theta} - v_1^{-\theta} + 1 \right)^{-1/\theta}) \mid \forall v_1 \in [0, 1] \right\}.
\]

2.2 Gumbel copula

The distribution function of a bivariate Gumbel copula with parameter \( \theta \) is

\[
C_{V_1, V_2}(v_1, v_2; \theta) = \exp \left\{ - \left[ (\ln v_1)^\theta + (\ln v_2)^\theta \right]^{1/\theta} \right\}.
\]

By solving \( \exp \left\{ - \left[ (\ln v_1)^\theta + (\ln v_2)^\theta \right]^{1/\theta} \right\} = \alpha \) for \( v_2 \), we obtain the \( \alpha \) bivariate quantile curve as

\[
Q^V_\alpha := \left\{ \left( v_1, \exp \left\{ - \left[ (\ln \alpha)^\theta - (\ln v_1)^\theta \right]^{1/\theta} \right\} \right) \mid \forall v_1 \in [0, 1] \right\}.
\]
2.3 Gaussian copula

In contrast to the Archimedean copulas as Clayton and Gumbel, for which there is a closed form solution of the quantile function, for the elliptical copulas, such as Gaussian and Student-t copula, there is no closed form solution for the quantile function. Thus, we use a numerical procedure to derive the theoretical quantiles.

The distribution function of the Gaussian pair copula is

\[ C_{V_1,V_2}(v_1,v_2; \theta) = \Phi_2 \left( \Phi^{-1}(v_1), \Phi^{-1}(v_2) \right) \]

\[ = \int_{-\infty}^{\Phi^{-1}(v_1)} \int_{-\infty}^{\Phi^{-1}(v_2)} \frac{1}{2\pi\sqrt{1-\theta^2}} \exp \left( -\frac{a^2 - 2\theta ab + b^2}{2(1-\theta^2)} \right) da \, db, \]

where \( \Phi \) and \( \Phi_2 \) are the univariate and bivariate standard normal distribution functions, respectively. As already stated, the equation

\[ \int_{-\infty}^{\Phi^{-1}(v_1)} \int_{-\infty}^{\Phi^{-1}(v_2)} \frac{1}{2\pi\sqrt{1-\theta^2}} \exp \left( -\frac{a^2 - 2\theta ab + b^2}{2(1-\theta^2)} \right) da \, db = \alpha \]

does not have a closed form solution. Thus, we evaluate \( C_{V_1,V_2} \) using the integral of its h-function given as

\[ h_{V_1|V_2}((v_1,v_2; \theta)) = \Phi \left( \frac{\Phi^{-1}(v_1) - \theta \Phi^{-1}(v_2)}{\sqrt{1-\theta^2}} \right). \]

The distribution function is then evaluated at the point \((\tilde{v}_1,\tilde{v}_2)\) as

\[ C_{V_1,V_2}(\tilde{v}_1,\tilde{v}_2; \theta) = \int_{0}^{\tilde{v}_2} h_{V_1|V_2}((\tilde{v}_1,v_2; \theta)) \, dv_2. \] (1)

Finally, the theoretical bivariate quantile curve is derived using the numerical evaluation defined in Section 3.4 of the manuscript and Equation (1).

2.4 Student-t copula

Similarly as with the Gaussian copula, the Equation \( C_{V_1,V_2}(v_1,v_2; \theta = (\theta,df)) = \alpha \) does not have a closed form solution. Again, we evaluate \( C_{V_1,V_2} \) using the integral of its h-function given as

\[ h_{V_1|V_2}((v_1,v_2; \theta = (\theta,df))) = t_{df+1} \left( \frac{t_{df}^{-1}(v_1) - \theta t_{df}^{-1}(v_2)}{\sqrt{(df+t_{df}^{-1}(v_2)^2)(1-\theta^2)}} \right), \]

where \( t_k \) is the distribution function of the Student-t distribution with \( k \) degrees of freedom. The distribution function is then evaluated at the point \((\tilde{v}_1,\tilde{v}_2)\) as

\[ C_{V_1,V_2}(\tilde{v}_1,\tilde{v}_2; \theta) = \int_{0}^{\tilde{v}_2} h_{V_1|V_2}((\tilde{v}_1,v_2; \theta)) \, dv_2. \] (2)

The theoretical bivariate quantile curve is derived using the numerical evaluation defined in Section 3.4 and Equation (2).
2.5 Estimated quantile curves

Let \( \{(v_i^1, v_i^2)\}_{i=1}^n \) be a set of \( n \) points randomly drawn from a bivariate copula distribution. Given an estimated parameter \( \hat{\theta} \) (together with family) obtained from this set of points we propose to evaluate \( \hat{C}_{V_1, V_2} \) at a point \((\tilde{v}_1, \tilde{v}_2)\) as

\[
\hat{C}_{V_1, V_2}(\tilde{v}_1, \tilde{v}_2) = \int_{0}^{\tilde{v}_1} \hat{C}_{V_2|V_1}(\tilde{v}_2|v'_1) \, dv'_1.
\]

(3)

The difference between the estimated and the theoretical quantiles for copulas for which the numerical inverse procedure is used is that in the theoretical case we use the theoretical h-function of a copula, while in the estimated case we use the estimated one. Basically, from the simulated data, we estimate a pair-copula, which has an h-function, and that estimated h-function is being used. The estimated bivariate quantile curves are obtained using the numerical evaluation defined in Section 3.4 and Equation (3).

3 Data analysis supplementary material

In Table 1 given is a variable description, the unit of measurement and the range of possible values for the 2 predictors Next\(_\text{Tmax}\) or T\(_\text{max}\), Next\(_\text{Tmin}\) or T\(_\text{min}\) and the 13 possible continuous predictors we consider.

In Figure 1 shown are the empirical normalized contour plots for pairs of variables from the training set. On the lower diagonal, given are the normalized contour plots, where any deviance from elliptical shapes indicates a non-Gaussian dependence structure in the data. This is the case in almost all normalized contour plots and it supports our non-Gaussian approach with flexible vine copulas over any other modeling approach that assumes Gaussianity. On the upper diagonal, we see a scatter plot of the estimated u-data together with the corresponding empirical Kendall’s \( \hat{\tau} \). We notice quite high dependence between both the responses, inbetween the predictors and between each other. Thus, to model the data properly one needs to account for this dependence, and our approach can do so. On the diagonal, given are histograms of the fitted u-data, showing that the estimated PITs are properly transformed on the u-scale.

3.1 Fitted Y-vine regression model

The order of the fitted Y-vine model is

\[
O(\hat{Y}) = (\text{LDAPS\_Tmin\_lapse, LDAPS\_Tmax\_lapse, LDAPS\_RHmax, LDAPS\_WS, Present\_Tmin, LDAPS\_CC1, Present\_Tmax, LDAPS\_LH, LDAPS\_CC3, LDAPS\_RHmin, LDAPS\_CC4 }).
\]

The variables in the order we enumerate by their position in the fitted order plus 2, because the response \( T_{\text{max}} \) is enumerated with 1, \( T_{\text{max}} = 1 \), the response \( T_{\text{min}} \) is enumerated with 2, \( T_{\text{min}} = 2 \), then LDAPS\_Tmin\_lapse = 3 , LDAPS\_Tmax\_lapse = 4, LDAPS\_RHmax = 5, LDAPS\_WS = 6, Present\_Tmin = 7, LDAPS\_CC1 = 8, Present\_Tmax = 9, LDAPS\_LH = 10, LDAPS\_CC3 = 11, LDAPS\_RHmin = 12 and LDAPS\_CC4 = 13. Using that enumeration, in Tables 2 and 3 we show the parametric (conditional) pair copulas that were fitted by our Y-vine regression model. In each tree we give the pair copulas conditioned and conditioning sets, the estimated family, the rotation in degrees, the parameters and the Kendall’s \( \hat{\tau} \) values.
Table 1: Variable description, the unit of measurement and the range of possible values the considered variables can take.

| Variable name          | Description/unit                                      | Range       |
|------------------------|-------------------------------------------------------|-------------|
| Next_Tmax              | The next-day maximum air temperature (°C)            | 17.4 to 38.9|
| Next_Tmin              | The next-day minimum air temperature (°C)            | 11.3 to 29.8|
| Present_Tmax           | Maximum air temperature between 0 and 21 h on the present day (°C) | 20 to 37.6  |
| Present_Tmin           | Minimum air temperature between 0 and 21 h on the present day (°C) | 11.3 to 29.9|
| LDAPS_RHmin            | LDAPS model forecast of next-day minimum relative humidity (%) | 19.8 to 98.5|
| LDAPS_RHmax            | LDAPS model forecast of next-day maximum relative humidity (%) | 58.9 to 100  |
| LDAPS_Tmax_lapse       | LDAPS model forecast of next-day maximum air temperature applied lapse rate (°C) | 17.6 to 38.5|
| LDAPS_Tmin_lapse       | LDAPS model forecast of next-day minimum air temperature applied lapse rate (°C) | 14.3 to 29.6|
| LDAPS_WS               | LDAPS model forecast of next-day average wind speed (m/s) | 2.9 to 21.9 |
| LDAPS_LH               | LDAPS model forecast of next-day average latent heat flux (W/m²) | -13.6 to 213.4|
| LDAPS_CC1              | LDAPS model forecast of next-day 1st 6-hour split average cloud cover (0-5 h) (%) | 0 to 0.97  |
| LDAPS_CC2              | LDAPS model forecast of next-day 2nd 6-hour split average cloud cover (6-11 h) (%) | 0 to 0.97  |
| LDAPS_CC3              | LDAPS model forecast of next-day 3rd 6-hour split average cloud cover (12-17 h) (%) | 0 to 0.98  |
| LDAPS_CC4              | LDAPS model forecast of next-day 4th 6-hour split average cloud cover (18-23 h) (%) | 0 to 0.97  |
| Solar radiation        | Daily incoming solar radiation (wh/m²)               | 4329.5 to 5992.9|
Figure 1: Lower diagonal: normalized contour plots, upper diagonal: pairwise scatter plots with the associated empirical Kendall’s $\hat{\tau}$ values and on the diagonal: histograms of the u-data.
Table 2: For the fitted $T_1$ to $T_4$ given are the conditioned and conditioning sets of the pair copulas, the estimated family, the rotation in degrees, the parameters and the Kendall’s $\hat{\tau}$ values.

| tree | conditioned | conditioning | family  | rotation | parameters       | Kendall’s $\hat{\tau}$ |
|------|-------------|--------------|---------|----------|------------------|-------------------------|
| 1    | 1,8         | bb7          | 180     | 1.41, 1.02| 0.42             |
| 1    | 2,8         | bb1          | 180     | 0.63, 2.74| 0.72             |
| 1    | 7,8         | bb7          | 180     | 1.43, 0.91| 0.40             |
| 1    | 6,7         | frank        | 0       | -2.98    | -0.31            |
| 1    | 6,9         | clayton      | 180     | 0.27     | 0.12             |
| 1    | 4,9         | indep.       | 0       | 0        | 0                |
| 1    | 4,11        | joe          | 180     | 1.17     | 0.09             |
| 1    | 3,11        | gumbel       | 270     | 1.25     | -0.20            |
| 1    | 3,10        | student t    | 0       | 0.05, 5.88| 0.03             |
| 1    | 10,12       | joe          | 0       | 1.52     | 0.23             |
| 1    | 5,12        | bb7          | 180     | 1.42, 1.25| 0.45             |
| 1    | 5,12        | gauss        | 0       | 0.50     | 0.34             |
| 2    | 1,7         | 8            | inde.   | 0        | 0                |
| 2    | 2,7         | 8            | bb1     | 180      | 0.57, 1.81       | 0.57             |
| 2    | 6,8         | 7            | joe     | 180      | 1.24             | 0.12             |
| 2    | 7,9         | 6            | joe     | 90       | 1.25             | -0.12            |
| 2    | 4,6         | 9            | indep.  | 0        | 0                |
| 2    | 9,11        | 4            | joe     | 0        | 1.26             | 0.13             |
| 2    | 3,4         | 11           | gauss   | 0        | 0.70             | 0.49             |
| 2    | 10,11       | 3            | bb8     | 0        | 2.57, 0.89       | 0.35             |
| 2    | 3,12        | 10           | bb7     | 90       | 1.1, 0.13        | -0.11            |
| 2    | 5,10        | 12           | clayton | 180      | 0.28             | 0.12             |
| 2    | 12,13       | 5            | gauss   | 0        | 0.65             | 0.45             |
| 3    | 1,6         | 7,8          | clayton | 270      | 0.43             | -0.18            |
| 3    | 2,6         | 7,8          | student t| 0        | 0.15, 7.13       | 0.09             |
| 3    | 8,9         | 7,6          | frank   | 0        | 0.64             | 0.07             |
| 3    | 4,7         | 6,9          | gumbel  | 0        | 1.43             | 0.30             |
| 3    | 6,11        | 4,9          | gumbel  | 0        | 1.70             | 0.41             |
| 3    | 3,9         | 4,11         | indep.  | 0        | 0                |
| 3    | 4,10        | 3,11         | indep.  | 0        | 0                |
| 3    | 11,12       | 3,10         | gauss   | 0        | 0.30             | 0.2              |
| 3    | 3,5         | 10,12        | clayton | 270      | 0.24             | -0.11            |
| 3    | 10,13       | 5,12         | student t| 0        | -0.03, 4.95      | -0.02            |
| 4    | 1,9         | 6,7,8        | joe     | 180      | 1.11             | 0.06             |
| 4    | 2,9         | 6,7,8        | frank   | 0        | -1.68            | -0.18            |
| 4    | 4,8         | 6,7,9        | gauss   | 0        | 0.69             | 0.49             |
| 4    | 7,11        | 4,6,9        | bb8     | 90       | 2.29, 0.73       | -0.21            |
| 4    | 3,6         | 4,9,11       | frank   | 0        | -2.28            | -0.24            |
| 4    | 9,10        | 3,4,11       | joe     | 0        | 1.26             | 0.13             |
| 4    | 4,12        | 3,10,11      | joe     | 270      | 1.11             | -0.06            |
| 4    | 5,11        | 3,10,12      | frank   | 0        | 3.02             | 0.31             |
| 4    | 3,13        | 5,10,12      | gumbel  | 270      | 1.06             | -0.06            |
Table 3: For the fitted $T_5$ to $T_{12}$ given are the conditioned and conditioning sets of the pair copulas, the estimated family, the rotation in degrees, the parameters and the Kendall’s $\hat{\tau}$ values.

| tree | conditioned | conditioning | family   | rotation | parameters | Kendall’s $\hat{\tau}$ |
|------|-------------|--------------|----------|----------|------------|------------------------|
| 5    | 1,4         | 6,7,8,9      | frank    | 0        | 0.56       | 0.06                   |
| 5    | 2,4         | 6,7,8,9      | joe      | 0        | 1.25       | 0.12                   |
| 5    | 8,11        | 4,6,7,9      | joe      | 180      | 1.25       | 0.13                   |
| 5    | 3,7         | 4,6,9,11     | gumbel   | 180      | 1.15       | 0.13                   |
| 5    | 6,10        | 3,4,9,11     | gauss    | 0        | 0.28       | 0.18                   |
| 5    | 9,12        | 3,4,10,11    | joe      | 90       | 1.11       | -0.06                  |
| 5    | 4,5         | 3,10,11,12   | gauss    | 0        | 0.20       | 0.13                   |
| 5    | 11,13       | 3,5,10,12    | gumbel   | 270      | 1.08       | -0.07                  |
| 6    | 1,11        | 4,6,7,8,9    | indep.   | 0        | 0          | 0                      |
| 6    | 2,11        | 4,6,7,8,9    | joe      | 90       | 1.16       | -0.08                  |
| 6    | 3,8         | 4,6,7,9,11   | frank    | 0        | 1.55       | 0.17                   |
| 6    | 7,10        | 3,4,6,9,11   | joe      | 90       | 1.15       | -0.08                  |
| 6    | 6,12        | 3,4,9,10,11  | student t| 0        | -0.05, 4.64| -0.03                  |
| 6    | 5,9         | 3,4,10,11,12 | clayton  | 180      | 0.17       | 0.08                   |
| 6    | 4,13        | 3,5,10,11,12 | student t| 0        | -0.05, 7.98| -0.03                  |
| 7    | 1,3         | 4,6,7,8,9,11 | gumbel   | 0        | 1.05       | 0.05                   |
| 7    | 2,3         | 4,6,7,8,9,11 | joe      | 0        | 1.09       | 0.05                   |
| 7    | 8,10        | 3,4,6,7,9,11 | clayton  | 90       | 0.25       | -0.11                  |
| 7    | 7,12        | 3,4,6,9,10,11| gauss    | 0        | -0.47      | -0.31                  |
| 7    | 5,6         | 3,4,9,10,11,12| gumbel  | 0        | 1.38       | 0.28                   |
| 7    | 9,13        | 3,4,5,10,11,12| gauss  | 0        | 0.10       | 0.06                   |
| 8    | 1,10        | 3,4,6,7,8,9,11| gauss  | 0        | -0.14      | -0.09                  |
| 8    | 2,10        | 3,4,6,7,8,9,11| indep. | 0        | 0          | 0                      |
| 8    | 8,12        | 3,4,6,7,9,10,11| gauss | 0        | 0.26       | 0.17                   |
| 8    | 5,7         | 3,4,6,9,10,11,12| gauss | 0        | -0.30      | -0.19                  |
| 8    | 6,13        | 3,4,5,9,10,11,12| student t| 0        | -0.08, 6.18| -0.05                  |
| 9    | 1,12        | 3,4,6,7,8,9,10,11| gauss | 0        | -0.09      | -0.06                  |
| 9    | 2,12        | 3,4,6,7,8,9,10,11| joe    | 0        | 1.13       | 0.07                   |
| 9    | 5,8         | 3,4,6,7,9,10,11,12| gauss | 0        | 0.54       | 0.36                   |
| 9    | 7,13        | 3,4,5,6,9,10,11,12| indep. | 0        | 0          | 0                      |
| 10   | 1,5         | 3,4,6,7,8,9,10,11,12| indep. | 0        | 0          | 0                      |
| 10   | 2,5         | 3,4,6,7,8,9,10,11,12| student t| 0        | 0.13, 8.21| 0.08                   |
| 10   | 8,13        | 3,4,5,6,7,8,9,10,11,12| frank | 0        | -0.88      | -0.10                  |
| 11   | 1,13        | 3,4,5,6,7,8,9,10,11,12| joe    | 90       | 1.12       | -0.06                  |
| 11   | 2,13        | 3,4,5,6,7,8,9,10,11,12| gumbel | 90       | 1.07       | -0.07                  |
| 12   | 1,2         | 3,4,5,6,7,8,9,10,11,12,13| clayton | 0        | 0.21       | 0.10                  |