

# Sequential Bayesian Model Selection of Regular Vine Copulas

Lutz Gruber\* and Claudia Czado†

**Abstract.** Regular vine copulas can describe a wider array of dependency patterns than the multivariate Gaussian copula or the multivariate Student’s  $t$  copula. This paper presents two contributions related to model selection of regular vine copulas. First, our pair copula family selection procedure extends existing Bayesian family selection methods by allowing pair families to be chosen from an arbitrary set of candidate families. Second, our method represents the first Bayesian model selection approach to include the regular vine density construction in its scope of inference. The merits of our approach are established in a simulation study that benchmarks against methods suggested in current literature. A real data example about forecasting of portfolio asset returns for risk measurement and investment allocation illustrates the viability and relevance of the proposed scheme.

**Keywords:** dependence models, graphical models, reversible jump MCMC, multivariate statistics, multivariate time series, portfolio risk forecasting.

## 1 Introduction

The use of copulas in statistics allows for the dependence of random variables to be modeled separately from the marginal distributions. This property makes copulas a very convenient tool to be used by statistical modelers (Nelsen (2006); McNeil et al. (2005); Kurowicka and Cooke (2006); Kurowicka and Joe (2010)). While many classes of bivariate copulas, also called pair copulas, are known (Joe (2001)), there is only a very limited number of multivariate copulas available with a closed-form analytical expression. Additionally, these only cover limited patterns of dependence. Regular vine copulas provide a solution to this problem by offering a construction method to design multivariate copula densities as products of only bivariate (conditional) copula densities (Joe (1996); Bedford and Cooke (2001)).

A  $d$ -dimensional regular vine copula is set up in two steps. A sequence of  $d - 1$  linked trees  $\mathcal{V} = (T_1, \dots, T_{d-1})$ , called the regular vine, functions as the building plan for the pair copula construction. Each of the  $d - j$  edges of tree  $T_j$ ,  $j = 1:(d - 1)$ , corresponds to a bivariate copula density that is conditional on  $j - 1$  variables. A copula family is selected for each of these (conditional) bivariate building blocks from a set of bivariate (parametric) candidate families  $\mathbf{B}$ . The mapping of the pair copula families to the regular vine is denoted by  $\mathcal{B}_{\mathcal{V}}$ , and the parameters, which depend on the choice of the pair copula families  $\mathcal{B}_{\mathcal{V}}$ , are denoted by  $\theta_{\mathcal{V}}$ .

---

\*Center for Mathematics, Technical University of Munich, Munich, Germany, [gruber@ma.tum.de](mailto:gruber@ma.tum.de)

†Center for Mathematics, Technical University of Munich, Munich, Germany

Model selection of regular vine copulas is a difficult task, given that there exist  $\frac{d!}{2} \times 2^{\binom{d-2}{2}}$  different  $d$ -dimensional regular vine tree structures alone (Morales-Napoles (2011)). To obtain the number of possible regular vine copulas on  $d$  dimensions, the number of possible regular vine tree structures must be multiplied by the number of possible combinations of pair copula families,  $|\mathbf{B}|^{\frac{d(d-1)}{2}}$ . In higher dimensions, there are too many possible models to analyze all of them to select the suitable few. To reduce the complexity of model selection, Dißmann et al. (2013) suggested a tree-by-tree approach, which selects the trees  $T_1, \dots, T_{d-1}$  of the regular vine  $\mathcal{V}$  sequentially. We present a combination of Dißmann et al. (2013)'s tree-by-tree strategy of complexity reduction with a proper Bayesian model selection scheme.

Existing research on Bayesian model selection of vine copulas is restricted to two relatively small subclasses of regular vine copulas, D-vine copulas and C-vine copulas. Smith et al. (2010) developed a model indicator-based approach to select between the independence copula and one alternative copula family at the pair copula level for D-vine copulas. Min and Czado (2010) and Min and Czado (2011) discuss a more flexible approach to estimate the pair copula families of D-vine copulas that is based on reversible jump Markov chain Monte Carlo (MCMC) (Green (1995)). Our proposed method provides two substantial contributions to Bayesian selection of vine copulas: firstly, our method applies to the general class of regular vine copulas and is capable of selecting the pair copula families  $\mathcal{B}_{\mathcal{V}}$  from an arbitrary set of candidate families  $\mathbf{B}$ , which is beyond the scope of Smith et al. (2010); Min and Czado (2010, 2011) and contains their selection procedures as special cases; secondly, our method is the first Bayesian approach to estimating the regular vine  $\mathcal{V}$  of a regular vine copula along with the pair copula families  $\mathcal{B}_{\mathcal{V}}$ . The latter innovation eliminates an unrealistic assumption all previous Bayesian selection procedures rest on—that the regular vine  $\mathcal{V}$  is already known.

The remainder is organized as follows. Section 2 formally introduces regular vine copulas to the extent required. In Section 3, we present our new approach to Bayesian model selection for regular vine copulas using reversible jump Markov chain Monte Carlo. Section 4 presents the results of a simulation study to help establish the validity of our model selection algorithm. Section 5 presents a real data example using our model selection procedure to improve forecasting of risk metrics of financial portfolios. We conclude with further remarks in Section 6.

## 2 Regular Vine Copulas

A copula describes a statistical model's dependence behavior separately from its marginal distributions (Sklar (1959)). The copula associated with a  $d$ -variate cumulative distribution function (cdf)  $F_{1:d}$  with univariate marginal cdfs  $F_1, \dots, F_d$  is a multivariate distribution function  $C: [0, 1]^d \rightarrow [0, 1]$  with *Uniform(0,1)* margins that satisfies

$$F_{1:d}(\mathbf{x}) = C(F_1(x_1), \dots, F_d(x_d)), \mathbf{x} \in \mathbb{R}^d.$$

### 2.1 Model Formulation

Joe (1996) presented the first construction of a multivariate copula using (conditional) bivariate copulas. Bedford and Cooke (2001) developed a more general construction method of multivariate densities and introduced regular vines to organize different pair copula constructions. The definitions and results stated in remainder of this section follow Bedford and Cooke (2001), if not stated otherwise.

**Definition 1** (Regular vine tree sequence). *A set of linked trees  $\mathcal{V} = (T_1, T_2, \dots, T_{d-1})$  is a regular vine on  $d$  elements if*

1.  $T_1$  is a tree with nodes  $N_1 = \{1, \dots, d\}$  and a set of edges denoted by  $E_1$ .
2. For  $k = 2, \dots, d - 1$ ,  $T_k$  is a tree with nodes  $N_k = E_{k-1}$  and edge set  $E_k$ .
3. For  $k = 2, \dots, d - 1$ , if  $a = \{a_1, a_2\}$  and  $b = \{b_1, b_2\}$  are two nodes in  $N_k$  connected by an edge, then exactly one of the  $a_i$  equals one of the  $b_i$  (Proximity condition).

Regular vines serve as the building plans for pair copula constructions. When each edge of the regular vine is interpreted as a (conditional) bivariate copula in the pair copula construction, the resulting copula is a regular vine copula. We use the following notation in the formal definition: the complete union  $A_e$  of an edge  $e = \{a, b\} \in E_k$  in tree  $T_k$  of a regular vine  $\mathcal{V}$  is defined by

$$A_e = \{v \in N_1 \mid \exists e_i \in E_i, i = 1, \dots, k - 1, \text{ such that } v \in e_1 \in \dots \in e_{k-1} \in e\}.$$

The conditioning set associated with edge  $e = \{a, b\}$  is defined as  $D(e) := A_a \cap A_b$  and the conditioned sets associated with edge  $e$  are defined as  $i(e) := A_a \setminus D(e)$  and  $j(e) := A_b \setminus D(e)$ , where  $A \setminus B := A \cap B^c$  and  $B^c$  is the complement of  $B$ . The conditioned sets can be shown to be singletons (see, for example, Kurowicka and Cooke (2006)). In graphs we label an edge  $e$  by the derived quantities  $i(e), j(e); D(e)$ , which suggests a probabilistic interpretation. Figure 1 shows a 6-dimensional regular vine to illustrate this notational convention.

**Definition 2** (Regular vine copula). *Let  $\mathcal{V} = (T_k = (N_k, E_k) \mid k = 1, \dots, d - 1)$  be a regular vine on  $d$  elements. Let*

$$\mathcal{B}_k := (\mathcal{B}_e \mid e \in E_k) \text{ and } \boldsymbol{\theta}_k := (\boldsymbol{\theta}_e \mid e \in E_k)$$

*be the pair copula families and parameters of level  $k$ , where the parameter vector  $\boldsymbol{\theta}_e$  depends on the pair copula family  $\mathcal{B}_e$  of edge  $e$ . The pair copula families of all levels  $k = 1:(d - 1)$  are collected in  $\mathcal{B}_{\mathcal{V}} := \mathcal{B}_{1:(d-1)} := (\mathcal{B}_1, \dots, \mathcal{B}_{d-1})$ . The same notational convention extends to the parameters  $\boldsymbol{\theta}_{\mathcal{V}}$ .*

*The regular vine copula  $(\mathcal{V}, \mathcal{B}_{\mathcal{V}}, \boldsymbol{\theta}_{\mathcal{V}})$  has the density function*

$$c(\mathbf{u}; \mathcal{V}, \mathcal{B}_{\mathcal{V}}, \boldsymbol{\theta}_{\mathcal{V}}) = \prod_{T_k \in \mathcal{V}} \prod_{e \in E_k} c_{\mathcal{B}_e}(u_{i(e)|D(e)}, u_{j(e)|D(e)}; \boldsymbol{\theta}_e), \tag{1}$$

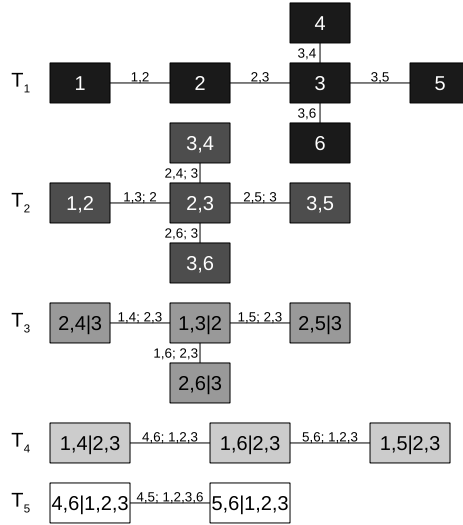


Figure 1: Six-dimensional regular vine copula. This copula corresponds to Scenario 1 of the simulation study of Section 4.

where  $c_{\mathcal{B}_e}(\cdot, \cdot; \boldsymbol{\theta}_e)$  denotes the density function of a bivariate copula of family  $\mathcal{B}_e$  with parameters  $\boldsymbol{\theta}_e$ . The arguments  $u_{i(e)|D(e)}$  and  $u_{j(e)|D(e)}$  of the bivariate copula density functions  $c_{\mathcal{B}_e}(\cdot, \cdot; \boldsymbol{\theta}_e)$  are the values of the conditional copula cdfs,

$$\begin{aligned} u_{i(e)|D(e)} &:= C_{i(e)|D(e)}(u_{i(e)}; T_{1:(k-1)}, \mathcal{B}_{1:(k-1)}, \boldsymbol{\theta}_{1:(k-1)} \mid \mathbf{u}_{D(e)}), \\ u_{j(e)|D(e)} &:= C_{j(e)|D(e)}(u_{j(e)}; T_{1:(k-1)}, \mathcal{B}_{1:(k-1)}, \boldsymbol{\theta}_{1:(k-1)} \mid \mathbf{u}_{D(e)}). \end{aligned} \quad (2)$$

The arguments  $u_{i(e)|D(e)}$  and  $u_{j(e)|D(e)}$  of a pair copula  $e \in E_k$  of level  $k$  depend only on the specification of the regular vine copula up to level  $k - 1$ .

Bedford and Cooke (2001) showed that the regular vine copula density function (see Definition 2) is a valid  $d$ -variate probability density function with uniform margins.

A regular vine copula is said to be *truncated at level  $K$*  if all pair copulas conditional on  $K$  or more variables are set to bivariate independence copulas (Brechmann et al. (2012)). In that case, the pair copula densities of trees  $T_{K+1}, \dots, T_{d-1}$  simplify to 1 and do not affect the density of the truncated regular vine copula anymore (see (1)). This means that the first  $K$  levels fully specify the truncated vine copula,

$$(\mathcal{V} = (T_1, \dots, T_K), \mathcal{B}_{\mathcal{V}} = (\mathcal{B}_1, \dots, \mathcal{B}_K), \boldsymbol{\theta}_{\mathcal{V}} = (\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_K)).$$

In general, regular vine copulas that differ in the tree structure or in at least one pair copula family have different copula densities. Notable exceptions from this rule include the multivariate Gaussian, Student's  $t$  or Clayton copula, whose densities can be represented by different pair copula constructions (cf. Stöber et al. (2013)).

## 2.2 Likelihoods

Definition 2 specifies regular vine copulas tree-by-tree. Similarly, we introduce likelihoods of individual trees and edges of a regular vine copula. The likelihoods are understood given data  $\mathbf{U} = (\mathbf{u}^1, \dots, \mathbf{u}^T) \in [0, 1]^{T \times d}$ . The likelihood of level  $k$  depends only on the specification of the regular vine copula up to level  $k$ . We write

$$L(\mathcal{B}_e, \boldsymbol{\theta}_e | \mathbf{U}) := \prod_{t=1:T} c_{\mathcal{B}_e}(u_{i(e)}^t |_{D(e)}, u_{j(e)}^t |_{D(e)}; \boldsymbol{\theta}_e) \text{ and}$$

$$L(T_k, \mathcal{B}_k, \boldsymbol{\theta}_k | \mathbf{U}) := \prod_{e \in E_k} L(\mathcal{B}_e, \boldsymbol{\theta}_e | \mathbf{U})$$

for the likelihood of edge  $e \in E_k$  and the likelihood of level  $k$ , respectively. The pair  $(u_{i(e)}^t |_{D(e)}, u_{j(e)}^t |_{D(e)})$  denotes the  $t$ -th transformed observation (see (2)). The likelihood of a regular vine copula is then calculated tree-by-tree

$$L(\mathcal{V}, \mathcal{B}_{\mathcal{V}}, \boldsymbol{\theta}_{\mathcal{V}} | \mathbf{U}) = \prod_{T_k \in \mathcal{V}} L(T_k, \mathcal{B}_k, \boldsymbol{\theta}_k | \mathbf{U}). \tag{3}$$

## 2.3 Pair Copula Families

Joe (2001, Chapter 5) provides a collection of parametric copula families for use in a pair copula construction. In our analyses, we will consider the Independence (I), Gaussian (N) and Student’s t (T) copula as well as all rotations of the Gumbel (G) and Clayton (C) copulas. Together, these pair copulas define the set of candidate families  $\mathbf{B}$ . The transformations of the copulas’ natural parameters to their Kendall’s  $\tau$ ’s is provided in Tables 1 and 2 of Brechmann and Schepsmeier (2013).

Suppose a pair copula has a density function  $c_0(u_1, u_2)$  and strength of dependence parameter Kendall’s  $\tau = \tau_0$ . The  $90^\circ$  rotation of a pair copula is defined by the density  $c_{90}(u_1, u_2) = c_0(1 - u_1, u_2)$ , the  $180^\circ$  rotation by  $c_{180}(u, v) = c_0(1 - u_1, 1 - u_2)$  and the  $270^\circ$  rotation by  $c_{270}(u, v) = c_0(u_1, 1 - u_2)$ . The  $90^\circ$  and  $270^\circ$  rotations have Kendall’s  $\tau$ ’s  $\tau_{90} = \tau_{270} = -\tau_0$ , while the Kendall’s  $\tau$  of the  $180^\circ$  rotation stays at  $\tau_{180} = \tau_0$ .

To shorten the notation in figures and tables, we will abbreviate the pair copula families as above, possibly followed by the degrees of the copulas’ rotation and the values of their parameters in parentheses. For example, C270(−0.8) will indicate the  $270^\circ$  rotation of a Clayton copula with strength of association parameter Kendall’s  $\tau = -0.8$ .

## 3 Bayesian Estimation of Regular Vine Copulas Using Reversible Jump MCMC

Bayesian selection of regular vine copulas aims at estimating the joint posterior distribution of the regular vine  $\mathcal{V}$ , pair copula families  $\mathcal{B}_{\mathcal{V}}$  and parameters  $\boldsymbol{\theta}_{\mathcal{V}}$ .

The multi-layered composition of a regular vine copula and its density function makes analytical inference infeasible. Instead, we use reversible jump MCMC (Green

Dimension $d$	Vine Search Space		Vine Copula Search Space	
	Joint Selection	Stepwise Selection	Joint Selection	Stepwise Selection
2	1	1	7	7
3	3	3	1,029	154
4	24	< 20	2,823,576	< 5,642
5	480	< 145	1.3559e+11	< 305,767
6	23,040	< 1,441	1.0938e+17	< 22,087,639
7	2,580,480	< 18,248	1.4413e+24	< 1.9994e+9
8	660,602,880	< 280,392	3.0387e+32	< 2.1789e+11
9	3.8051e+11	< 5,063,361	1.0090e+42	< 2.7791e+13
10	4.8705e+14	< 105,063,361	5.2118e+52	< 4.0632e+15

Table 1: Size of the search space for vines  $\mathcal{V}$  and vine copulas  $(\mathcal{V}, \mathcal{B}_{\mathcal{V}})$  with seven candidate families, i.e.,  $|\mathbf{B}| = 7$ , by dimension  $d$ .

(1995)), which is an extension the Metropolis–Hastings algorithm (Metropolis et al. (1953); Hastings (1970)) to include the selection of models with different numbers of parameters in the scope of inference, as a simulation-based approach to estimate the posterior distribution. Convergence of the sampling chain to the target distribution, here to the posterior distribution, is theoretically established under regularity conditions.

### 3.1 General Tree-by-Tree Model Selection

Our tree-by-tree model selection strategy first estimates the first level of the regular vine copula, which consists of tree  $T_1 = (N_1, E_1)$  and the pair copula families  $\mathcal{B}_1$  with parameters  $\theta_1$ . For each higher level  $k = 2, \dots, d - 1$ , the density factorization  $T_k = (N_k, E_k)$  and pair copula families  $\mathcal{B}_k$  with parameters  $\theta_k$  are selected conditionally on the estimates of the lower levels  $(T_1, \mathcal{B}_1, \theta_1)$  to  $(T_{k-1}, \mathcal{B}_{k-1}, \theta_{k-1})$ , which remain unchanged from the previous steps.

**Motivation of Tree-by-Tree Estimation** In the context of model selection for regular vine copulas, sequential approaches exhibit distinct strengths that make them more tractable than joint approaches.

Sequential approaches are much faster than joint approaches, as they break the overall problem into a sequence of smaller problems that can be solved more quickly. Table 1 shows the enormous reduction of the regular vine search space, if a sequential procedure is followed. The entries of Table 1 follow Morales-Napoles (2011)’s calculation of the number of vines and use the sum of the number of spanning trees with  $k$  nodes,  $\sum_{k=2}^d k^{k-2}$ , as an upper bound of the size of the sequential search space. Here the number of spanning trees is calculated using Cayley (1889)’s formula. Furthermore, the reduced number of model alternatives improves the convergence behavior of MCMC samplers as it allows for a quicker exploration of the search space.

Furthermore, a tree-by-tree approach avoids a regular vine copula-specific model identification issue. Different regular vine copulas can be representatives of the same multivariate copula, the most prominent example of which is the multivariate Gaussian copula (Kurowicka and Cooke (2006)). The tree-by-tree approach is characterized by leaving previously selected trees unchanged and modifying only one tree at a time. Under the tree-by-tree paradigm, there is only one scenario in which the copula of the current state and proposed state are the same with a non-zero probability: all pair copulas—those on all previously selected trees and those on the current tree—are either Gaussian or independent. These states can be easily detected and collapsed into one state.

**Priors** Following our tree-by-tree estimation approach, the priors are specified for each level  $k = 1, \dots, d - 1$ . Given that the proximity condition restricts which trees  $T_k$  are allowed for a level  $k > 1$ , these priors are inherently conditional on the selection on the previous trees  $T_1, \dots, T_{k-1}$ .

We choose a noninformative yet proper prior over the set  $\mathbf{STP}_k$  of all spanning trees that satisfy the proximity condition for level  $k$  for tree  $T_k$ , a sparsity-enforcing prior for the pair copula families  $\mathcal{B}_k$  and proper noninformative priors for the parameters  $\theta_k$ . We combine flat  $(-1, 1)$ -priors for the Kendall's  $\tau$  parameters with flat  $(0, \log(30))$ -priors for the logarithm of the degrees of freedom  $\nu$  of Student's t pair copulas:

$$\begin{aligned} \pi(T_k) &\propto \text{discrete Uniform}(\mathbf{STP}_k), \\ \pi(\mathcal{B}_k | T_k) &= \frac{\exp(-\lambda d_k)}{\sum_{i=1}^{|E_k|} \sum_{d=0}^2 \exp(-\lambda d)} \propto \exp(-\lambda d_k), \\ \pi(\theta_e | T_k, \mathcal{B}_e) &\propto \begin{cases} \text{Uniform}_{(-1,1)}(\tau_e) & \text{if } \mathcal{B}_e \text{ is a single parameter copula,} \\ \text{Uniform}_{(-1,1)}(\tau_e) \cdot \frac{1_{(1,30)}(\nu_e) \cdot \log(\nu_e)}{\int_1^{30} \log(x) dx} & \text{if } \mathcal{B}_e \text{ is the Student's t copula,} \end{cases} \end{aligned}$$

where  $d_k$  denotes the dimension of the parameter vector  $\theta_k = (\theta_{e;\mathcal{B}_e} | e \in E_k)$  of the pair copula families  $\mathcal{B}_k$  of level  $k$ . Analogously,  $d_e$  denotes the dimension of the parameter vector of the pair copula family  $\mathcal{B}_e$  of edge  $e \in E_k$  and it holds that  $d_k = \sum_{e \in E_k} d_e$ . Our prior on the pair copula families  $\mathcal{B}_k$  depends solely on the size  $d_k$  of their parameter vectors  $\theta_k$ ; if  $\mathcal{B}_e$  is the independence copula, it holds that  $d_e = 0$ .

The prior density  $\pi$  of state  $(T_k = (N_k, E_k), \mathcal{B}_k, \theta_k)$  results as

$$\pi(T_k, \mathcal{B}_k, \theta_k) \propto \prod_{e \in E_k} \exp(-\lambda d_e) \pi(\theta_e | T_k, \mathcal{B}_e). \tag{4}$$

This prior gives the posterior distribution the following form:

$$\begin{aligned} p(T_k, \mathcal{B}_k, \theta_k | \mathbf{U}) &\propto \pi(\theta_k | T_k, \mathcal{B}_k) \cdot \exp(\ell(T_k, \mathcal{B}_k, \theta_k | \mathbf{U}) - \lambda d_k) \\ &\propto \exp(\ell(T_k, \mathcal{B}_k, \theta_k | \mathbf{U}) - \lambda d_k), \end{aligned}$$

where  $\ell$  denotes the log-likelihood function and  $\propto$  means ‘‘approximately proportional.’’ At  $\lambda = 0$ , no shrinkage occurs and the posterior mode estimate of level  $k$  will approximate that level's maximum likelihood estimate, while at  $\lambda = 1$ , the posterior mode estimate of level  $k$  will approximately minimize the Akaike Information Criterion (AIC).

**Posterior Distribution** The posterior distribution of level  $k$  given observed data  $\mathbf{U}$  factorizes into the likelihood  $L$  and prior density  $\pi$ :

$$p(T_k, \mathcal{B}_k, \boldsymbol{\theta}_k \mid \mathbf{U}) \propto L(T_k, \mathcal{B}_k, \boldsymbol{\theta}_k \mid \mathbf{U}) \cdot \pi(T_k, \mathcal{B}_k, \boldsymbol{\theta}_k).$$

The tree-by-tree procedure requires the Bayesian posterior sample of each tree to be collapsed into a single model estimate. We choose the empirical mode of the sampled models  $(T_k, \mathcal{B}_k)$  as the model estimate, given that we chose our priors for their effects on the posterior mode. The parameters are set to the means of the MCMC posterior iterates of the selected model. Other centrality estimates may be used as well.

**Implementation** At each iteration  $r = 1, \dots, R$ , the sampling mechanism performs a within-model move and a between-models move. The within-model move updates all parameters  $\boldsymbol{\theta}_{1:k}$  of the regular vine copula, but leaves the pair copula families  $\mathcal{B}_{1:k}$  and tree structure  $T_{1:k}$  unchanged. The between-models move operates only on level  $k$  and updates the tree structure  $T_k$ , pair copula families  $\mathcal{B}_k$  along with the parameters  $\boldsymbol{\theta}_k$ .

The between-models move is implemented as a 50:50 mixture of two mutually exclusive, collectively exhaustive (MECE) sub-routines: with a 50% probability, a local between-models move updates only the pair copula families  $\mathcal{B}_k$  but leaves the tree structure  $T_k$  unchanged (Algorithm 2). With the remaining 50% probability, a global between-models move updates the tree structure  $T_k$  along with the pair copula families  $\mathcal{B}_k$  (Algorithm 3). Algorithm 2 guarantees that the proposal state differs in at least one pair copula family from the current state; Algorithm 3 guarantees that the proposal state differs in at least one edge of tree  $T_k$  from the current state. This makes the proposals of the two sub-routines mutually exclusive and gives the acceptance probability a tractable analytical form that can be easily evaluated.

The between-models move is into two sub-routines because this allows an intuitive interpretation of a local search (Algorithm 2) and a global search (Algorithm 3) as well as optimizes the computational cost of these updates by containing between-models moves that leave the tree structure unchanged to a dedicated sub-routine.

**Algorithm 1** (Tree-by-Tree Bayesian Model Selection).

- 1: **for each** level  $k = 1, \dots, d - 1$  **do**
- 2:   Choose starting values: set tree  $T_k = (N_k, E_k)$  to an arbitrary tree that fulfills the proximity condition for level  $k$ ; set all pair copula families  $\mathcal{B}_k$  of level  $k$  to the independence copula, i.e.,  $c_e(\cdot, \cdot) = 1$  for  $e \in E_k$  and set the parameter vector  $\boldsymbol{\theta}_k$  of level  $k$  to an empty vector.
- 3:   **for each** MCMC iteration  $r = 1, \dots, R$  **do**
- 4:     Perform a within-model move: update all parameters  $\boldsymbol{\theta}_{1:k}$ . Obtain  $\boldsymbol{\theta}_{1:k}^{r,NEW}$  through a Metropolis–Hastings step with random walk proposals:

$$(T_k^r, \mathcal{B}_k^r, \boldsymbol{\theta}_{1:k}^r) = (T_k^{r-1}, \mathcal{B}_k^{r-1}, \boldsymbol{\theta}_{1:k}^{r,NEW}).$$

- 5:     Perform a between-models move: update the tree structure  $T_k$  along with, or only, the pair copula families  $\mathcal{B}_k$  and parameters  $\boldsymbol{\theta}_k$  (Algorithms 2, 3):

$$(T_k^r, \mathcal{B}_k^r, \boldsymbol{\theta}_k^r) = (T_k^{r,NEW}, \mathcal{B}_k^{r,NEW}, \boldsymbol{\theta}_k^{r,NEW}).$$



- 6: **end for**
- 7: Set the level  $k$ -estimate  $(\hat{T}_k, \hat{\mathcal{B}}_k, \hat{\boldsymbol{\theta}}_k)$  to the empirical mode of the posterior sample  $((T_k^r, \mathcal{B}_k^r, \boldsymbol{\theta}_k^r), r = 1, \dots, R)$ :
  - Set  $\hat{T}_k$  and  $\hat{\mathcal{B}}_k$  to the most frequently sampled combination of  $T_k$  and  $\mathcal{B}_k$  in  $((T_k^r, \mathcal{B}_k^r), r = 1, \dots, R)$ .
  - Set  $\hat{\boldsymbol{\theta}}_k$  to the sample mean of  $(\boldsymbol{\theta}_k^r, r \in \{1, \dots, R\})$  with  $T_k^r = \hat{T}_k$  and  $\mathcal{B}_k^r = \hat{\mathcal{B}}_k$ .
- 8: For all levels  $l = 1, \dots, k - 1$ , update  $\hat{\boldsymbol{\theta}}_l$  and set it to the sample mean of  $(\boldsymbol{\theta}_l^r, r \in \{1, \dots, R\})$  with  $T_k^r = \hat{T}_k$  and  $\mathcal{B}_k^r = \hat{\mathcal{B}}_k$ .
- 9: **end for**
- 10: **return** the stepwise Bayesian model estimate  $(\hat{\mathcal{V}}, \hat{\mathcal{B}}_{\mathcal{V}}, \hat{\boldsymbol{\theta}}_{\mathcal{V}})$ , where  $\hat{\mathcal{V}} = (\hat{T}_1, \dots, \hat{T}_{d-1})$ ,  $\hat{\mathcal{B}}_{\mathcal{V}} = (\hat{\mathcal{B}}_1, \dots, \hat{\mathcal{B}}_{d-1})$ , and  $\hat{\boldsymbol{\theta}}_{\mathcal{V}} = (\hat{\boldsymbol{\theta}}_1, \dots, \hat{\boldsymbol{\theta}}_{d-1})$ .

### 3.2 Update of the Pair Copulas of Level $k$

This section describes a sub-routine of Algorithm 1 to update the pair copula families  $\mathcal{B}_k$  and parameters  $\boldsymbol{\theta}_k$  of level  $k$  of a regular vine copula. This updating step leaves the density factorization  $\mathcal{V}$  unchanged.

This sub-routine first selects how many pair copulas will be updated (Line 1 of Algorithm 2) and then randomly selects which pair copulas will be updated—denoted by  $E \subseteq E_k$  in the remainder (Line 2). Next, it generates a proposal that updates the selected pair copulas (Lines 3–9), and, lastly, accepts or rejects the proposal based on a Metropolis–Hastings updating rules (Line 10).

The proposal step (Lines 3–9) iterates through all selected pair copulas  $e \in E$ . It first estimates the parameters  $\boldsymbol{\theta}_{e; \mathcal{B}_e^*}$  of each candidate pair copula family  $\mathcal{B}_e^* \in \mathbf{B} \setminus \mathcal{B}_e^r$ , where the estimates are denoted by  $\hat{\boldsymbol{\theta}}_{e; \mathcal{B}_e^*}$ . The likelihoods of the different candidate copulas,  $L(\mathcal{B}_e^*, \hat{\boldsymbol{\theta}}_{e; \mathcal{B}_e^*} \mid \mathbf{U})$ , are then used as the proposal probability weights of the respective copula families:  $q_{\mathcal{B}}(\mathcal{B}_e^r \rightarrow \mathcal{B}_e^*) \propto L(\mathcal{B}_e^*, \hat{\boldsymbol{\theta}}_{e; \mathcal{B}_e^*} \mid \mathbf{U})$ . After selecting a pair copula family, the proposal parameters  $\boldsymbol{\theta}_e^*$  are drawn from a normal distribution centered at the parameter estimate  $\hat{\boldsymbol{\theta}}_{e; \mathcal{B}_e^*}$ . The proposal distribution  $q_N$  from which  $N$  is drawn (Line 1), the parameter estimation procedure (Line 4) and the covariance matrix  $\Sigma$  of the parameters’ proposal distribution (Line 6) are MCMC tuning parameters.

Pair copula families that can model only positive or negative Kendall’s  $\tau$ ’s such as the Clayton copula or Gumbel copula are extended to cover the entire range  $[-1, 1]$ . This is implemented by replacing the first argument  $u_1$  of the copula density function  $c(u_1, u_2)$  by  $1 - u_1$  whenever the dependence parameter  $\tau$  changes signs.

As this sub-routine and the one from Section 3.3 produce non-overlapping proposals, the acceptance probability follows as

$$\alpha = \frac{L(T_k^r, \mathcal{B}_k^*, \boldsymbol{\theta}_k^* \mid \mathbf{U})}{L(T_k^r, \mathcal{B}_k^r, \boldsymbol{\theta}_k^r \mid \mathbf{U})} \cdot \frac{\pi(T_k^r, \mathcal{B}_k^*, \boldsymbol{\theta}_k^*)}{\pi(T_k^r, \mathcal{B}_k^r, \boldsymbol{\theta}_k^r)} \cdot \prod_{e \in E} \frac{q_{\mathcal{B}}(\mathcal{B}_e^* \rightarrow \mathcal{B}_e^r) \cdot \phi_{(\hat{\boldsymbol{\theta}}_{e; \mathcal{B}_e^*}, \Sigma)}(\boldsymbol{\theta}_e^r)}{q_{\mathcal{B}}(\mathcal{B}_e^r \rightarrow \mathcal{B}_e^*) \cdot \phi_{(\hat{\boldsymbol{\theta}}_{e; \mathcal{B}_e^*}, \Sigma)}(\boldsymbol{\theta}_e^*)}, \quad (5)$$

where  $\phi_{\boldsymbol{\mu}, \Sigma}(\cdot)$  denotes the density function of the truncated multivariate normal distribution with mean  $\boldsymbol{\mu}$  and covariance matrix  $\Sigma$ ; the truncation is assumed at the bounds of the respective parameters. Both the numerator and denominator of the acceptance probability contain  $q_N(N)$  as a factor that cancels out and does not appear in (5), given that the return move of any update must change the same number  $N$  of pair copulas as the outbound move.

**Algorithm 2** (Between-Models Move to Update the Pair Copula Families  $\mathcal{B}_k$  and Parameters  $\boldsymbol{\theta}_k$ ). *This is for the  $r$ th iteration of line 5 of Algorithm 1.*

- 1: Select how many pair copulas are updated:  $N \sim q_N(\cdot)$ ;  $N \in \{1, \dots, |E_k|\}$ .
- 2: Select which pair copulas are updated:  $E \subseteq E_k$  with  $|E| = N$ .
- 3: **for each** selected pair copula  $e \in E$  **do**
- 4: For each candidate pair copula family  $\mathcal{B}_e \in \mathbf{B} \setminus \mathcal{B}_e^r$  estimate the copula parameter  $\boldsymbol{\theta}_{e; \mathcal{B}_e}$  given the transformed data  $(\mathbf{u}_{i(e)|D(e)}^{t=1:T}, \mathbf{u}_{j(e)|D(e)}^{t=1:T})$  and denote the parameter estimate by  $\hat{\boldsymbol{\theta}}_{e; \mathcal{B}_e}$ .
- 5: Draw a new copula family  $\mathcal{B}_e^* \in \mathbf{B} \setminus \mathcal{B}_e^r$  from the proposal distribution

$$q_{\mathcal{B}}(\mathcal{B}_e^r \rightarrow \mathcal{B}_e^*) \propto L(\mathcal{B}_e^*, \hat{\boldsymbol{\theta}}_{e; \mathcal{B}_e^*} \mid \mathbf{U}). \tag{6}$$

- 6: Draw new parameters  $\boldsymbol{\theta}_e^* \sim \mathcal{N}(\hat{\boldsymbol{\theta}}_{e; \mathcal{B}_e^*}, \Sigma)$  from a normal distribution.
- 7: The proposal family for pair copula  $e \in E$  is  $\mathcal{B}_e^*$  and the proposal parameter is  $\boldsymbol{\theta}_e^*$ .
- 8: **end for**
- 9: The proposal families for level  $k$  are  $\mathcal{B}_k^*$  and the proposal parameters are  $\boldsymbol{\theta}_k^*$ , where

$$\begin{aligned} \mathcal{B}_k^* &= (\mathcal{B}_e^* \text{ for } e \in E \text{ and } \mathcal{B}_e^r \text{ for } e \in E_k \setminus E), \\ \boldsymbol{\theta}_k^* &= (\boldsymbol{\theta}_e^* \text{ for } e \in E \text{ and } \boldsymbol{\theta}_e^r \text{ for } e \in E_k \setminus E). \end{aligned}$$

- 10: Accept the proposal and set  $(T_k^{r, NEW}, \mathcal{B}_k^{r, NEW}, \boldsymbol{\theta}_k^{r, NEW}) = (T_k^r, \mathcal{B}_k^*, \boldsymbol{\theta}_k^*)$  with probability  $\alpha$  (5). If rejected, set  $(T_k^{r, NEW}, \mathcal{B}_k^{r, NEW}, \boldsymbol{\theta}_k^{r, NEW}) = (T_k^r, \mathcal{B}_k^r, \boldsymbol{\theta}_k^r)$ .

### 3.3 Joint Update of the Regular Vine and Pair Copulas of Level $k$

This section presents a sub-routine of Algorithm 1 to update the regular vine at level  $k$ —that is, tree  $T_k$ —and the pair copula families  $\mathcal{B}_k$  and parameters  $\boldsymbol{\theta}_k$  of that level. Definition 1 requires that the lower level trees  $T_1, \dots, T_{k-1}$  of the regular vine be specified before tree  $T_k$  is estimated.

Algorithm 3 describes our joint update procedure of tree  $T_k = (N_k, E_k)$  and the corresponding pair copula families  $\mathcal{B}_k$  and parameters  $\boldsymbol{\theta}_k$ . We denote the set of all spanning trees with node set  $N_k$  that satisfy the proximity condition by  $\mathbf{STP}_k$ . The cardinality of this set is computed using Kirchhoff’s matrix tree theorem (Kirchhoff (1847)) to obtain the normalizing constants of the proposal and prior distributions. In a first step, this sub-routine draws a new spanning tree  $T_k^* = (N_k, E_k^*) \in \mathbf{STP}_k \setminus T_k^r$  from the proposal distribution  $q_T(T_k^r \rightarrow T_k^*) \propto p^{|E_k^* \cap E_k^r|} \cdot (1-p)^{|E_k^* \setminus E_k^r|}$  (Line 1); this is just a random walk distribution on the set of allowable regular vine trees of level  $k$ ! Then, the

algorithm generates a proposal for the pair copula families  $\mathcal{B}_k^*$  and parameters  $\theta_k^*$  of this level as in Algorithm 2 (Lines 3–9 in Algorithm 2; Lines 2–8 in Algorithm 3). The only difference is that all pair copula families in  $\mathbf{B}$  are permissible candidates here and the edges  $e$  are different. We use the notation  $q_{\mathcal{B}}(\mathcal{B}_e^*)$  instead of  $q_{\mathcal{B}}(\mathcal{B}_e^r \rightarrow \mathcal{B}_e^*)$  to indicate the slightly different proposal distributions. The entire proposal for level  $k$  of the regular vine copula consists of a new tree  $T_k^*$ , pair copula families  $\mathcal{B}_k^*$  and parameters  $\theta_k^*$ , and is accepted or rejected based on Metropolis–Hastings updating rules (Line 9).

This sub-routine has three MCMC tuning parameters. The first is the parameter  $p$  of the proposal distribution for tree  $T_k$ : values  $p > 0.5$  make tree proposals  $T_k^*$  similar to the current tree  $T_k^r$  more likely than proposals that are less similar to the current state. The situation is reversed for values  $p < 0.5$ . The second tuning parameter is the choice of the estimation procedure for the pair copula parameter vectors (Line 3) and the last is the covariance matrix  $\Sigma$  of the proposal distribution of the parameters (Line 5).

The proposal mechanism of this update routine guarantees that the proposed regular vine tree  $T_k^*$  is different from the current state  $T_k$ . This ensures that the proposals of this sub-routine and the one of Section 3.2 are mutually exclusive. Furthermore, the proposal probability of the reverse move from tree  $T_k^*$  to  $T_k$  is the same as the proposal probability of the away move, given that the number of shared edges as well as differing edges is the same. As a result, the acceptance probability of a proposal of this algorithm can be easily obtained as

$$\alpha = \frac{L(T_k^*, \mathcal{B}_k^*, \theta_k^* \mid \mathbf{U})}{L(T_k^r, \mathcal{B}_k^r, \theta_k^r \mid \mathbf{U})} \cdot \frac{\pi(T_k^*, \mathcal{B}_k^*, \theta_k^*)}{\pi(T_k^r, \mathcal{B}_k^r, \theta_k^r)} \cdot \frac{\prod_{e \in E_k^r} q_{\mathcal{B}}(\mathcal{B}_e^r) \cdot \phi_{(\hat{\theta}_{e; \mathcal{B}_e^r}, \Sigma)}(\theta_e^r)}{\prod_{e \in E_k^*} q_{\mathcal{B}}(\mathcal{B}_e^*) \cdot \phi_{(\hat{\theta}_{e; \mathcal{B}_e^*}, \Sigma)}(\theta_e^*)}. \tag{7}$$

**Algorithm 3** (Between-Models Move for a Joint Update of Tree  $T_k = (N_k, E_k)$  and the Pair Copula Families  $\mathcal{B}_k$  and Parameters  $\theta_k$ ).

*This is for the  $r$ th iteration of line 5 of Algorithm 1.*

- 1: Draw a new spanning tree  $T_k^* = (N_k, E_k^*) \in \mathbf{STP}_k \setminus T_k^r$  that satisfies the proximity condition from the proposal distribution

$$q_T(T_k^r \rightarrow T_k^*) \propto p^{|E_k^* \cap E_k^r|} \cdot (1 - p)^{|E_k^* \setminus E_k^r|}. \tag{8}$$

- 2: **for** each pair copula  $e \in E_k^*$  **do**
- 3: For each candidate pair copula family  $\mathcal{B}_e \in \mathbf{B}$  estimate the copula parameter  $\theta_{e; \mathcal{B}_e}$  given the transformed data  $(\mathbf{u}_{i(e)|D(e)}^{t=1:T}, \mathbf{u}_{j(e)|D(e)}^{t=1:T})$  and denote the parameter estimate by  $\hat{\theta}_{e; \mathcal{B}_e}$ .
- 4: Draw a new copula family  $\mathcal{B}_e^* \in \mathbf{B}$  from the proposal distribution

$$q_{\mathcal{B}}(\mathcal{B}_e^*) \propto L(\mathcal{B}_e^*, \hat{\theta}_{e; \mathcal{B}_e^*} \mid \mathbf{U}). \tag{9}$$

- 5: Draw new parameters  $\theta_e^* \sim \mathcal{N}(\hat{\theta}_{e; \mathcal{B}_e^*}, \Sigma)$  from a normal distribution.
- 6: The proposal family for pair copula  $e \in E_k^*$  is  $\mathcal{B}_e^*$  and has proposal parameter  $\theta_e^*$ .
- 7: **end for**

8: The proposal state is  $(T_k^*, \mathcal{B}_k^*, \boldsymbol{\theta}_k^*)$ , where

$$\mathcal{B}_k^* = (\mathcal{B}_e^* \mid e \in E_k^*) \text{ and } \boldsymbol{\theta}_k^* = (\boldsymbol{\theta}_e^* \mid e \in E_k^*).$$

9: Accept the proposal and set  $(T_k^{r,NEW}, \mathcal{B}_k^{r,NEW}, \boldsymbol{\theta}_k^{r,NEW}) = (T_k^*, \mathcal{B}_k^*, \boldsymbol{\theta}_k^*)$  with probability  $\alpha$  (7). If rejected, set  $(T_k^{r,NEW}, \mathcal{B}_k^{r,NEW}, \boldsymbol{\theta}_k^{r,NEW}) = (T_k^r, \mathcal{B}_k^r, \boldsymbol{\theta}_k^r)$ .

### 3.4 Implementation in C++

The model selection algorithms presented in this section are implemented in a proprietary C++ software package. As the computational cost of evaluating the likelihood and calculating parameter estimates increases linearly with the number of observations in the data set, these tasks are parallelized onto multiple CPU cores using OpenMP to help reduce overall computing time. Furthermore, our software package relies heavily on the tools and functionality provided by the boost (Boost Community (2014)) and CppAD (COIN-OR Foundation (2014)) libraries: the boost library contains a function that generates random spanning trees from a product probability distribution based on edge weights, which we employ in our implementation of Algorithm 3; the CppAD library allows for automatic differentiation, which we use for parameter estimation.

## 4 Simulation Study

We present a simulation study that compare our sequentially Bayesian strategy with Dißmann et al. (2013)'s frequentist model selection algorithm, the independence model and the maximum likelihood estimate (MLE) of the multivariate Gaussian copula. The comparisons with the independence model and Gaussian copula illustrate that vine copulas are relevant dependence models that significantly improve model fit over simpler standard models, while the comparison with Dißmann's vine copula estimates highlights the improved model selection capabilities of our method.

Our simulation study uses copula data generated from four different six-dimensional vine copulas (Table 6 of Appendix A). These scenarios cover a wide range of dependence structures: the first two cover general cases of multivariate dependence, while the third and fourth scenario are special cases to investigate detailed characteristics of our model selection method. Scenario 3 consists of only one level, which means that all variables are conditionally independent. It also means that the true model lies in the search space of the first level of our selection procedure, so that this scenario can be used to validate our proposed scheme empirically. Scenario 4 is has only Gaussian pair copulas, which makes it a vine copula-representation of the multivariate Gaussian copula. As a result, this scenario allows for an isolated evaluation of the pair copula family selection aspect of our method, given that the multivariate Gaussian copula results from any vine density factorization  $\mathcal{V}$  as long as all pair copula families are Gaussian.

We generate 100 data sets consisting of 500 independent samples from the respective copula distribution of each scenario and allow the pair copula families listed in Section 2.3 as candidates.

## 4.1 Choice of the Benchmark Algorithm

The models selected by Dißmann et al. (2013)'s algorithm serve as a benchmark. This algorithm follows a stepwise frequentist approach that selects each tree  $T_k$ ,  $k = 1, \dots, 5$  as the maximum spanning tree using absolute values of Kendall's  $\tau$  of the variable pairs as edge weights. The pair copula families are selected to optimize the AIC copula-by-copula and the parameters are set to their individual maximum likelihood estimates.

Dißmann's algorithm and ours share their tree-by-tree selection strategy. However, there are two major differences between our approaches: firstly, Dißmann follows a heuristic scheme to select the tree structure  $\mathcal{V}$ , while we follow a proper Bayesian selection scheme on each level  $k$ ; secondly, Dißmann selects the pair copula families on an edge-by-edge basis, whereas we place priors on the distribution of the pair copula families across an entire level  $k$  to simultaneously select of all edges of that level.

## 4.2 Configuration of Our Reversible Jump MCMC Sampler

We use the shrinkage prior introduced in Section 3.1 with shrinkage parameter  $\lambda = 1$ . The posterior mode estimates of each level  $k$  will then be approximately AIC-optimal.

We use our reversible jump MCMC Algorithm 1 from Section 3 to generate  $R = 50,000$  posterior samples for each level  $k = 1, \dots, 5$  of the 6-dimensional regular vine copula. The MCMC tuning parameters are summarized in Table 5 of Appendix A. Furthermore, we apply a re-weighting on the proposal probabilities (see (6) and (9)) of the pair copula families in the sub-routines of Algorithms 2 and 3 to improve the mixing behavior of the sampling chain. This is achieved by ensuring that the ratio of smallest and biggest the proposal probabilities is bounded from below by 0.05,

$$\frac{\min_{\mathcal{B}^* \in \mathbf{B} \setminus \mathcal{B}^r} q_{\mathcal{B}}(\mathcal{B}^r \rightarrow \mathcal{B}^*)}{\max_{\mathcal{B}^* \in \mathbf{B} \setminus \mathcal{B}^r} q_{\mathcal{B}}(\mathcal{B}^r \rightarrow \mathcal{B}^*)} \geq 0.05 \quad \text{and} \quad \frac{\min_{\mathcal{B}^* \in \mathbf{B}} q_{\mathcal{B}}(\mathcal{B}^*)}{\max_{\mathcal{B}^* \in \mathbf{B}} q_{\mathcal{B}}(\mathcal{B}^*)} \geq 0.05, \text{ respectively.}$$

## 4.3 Evaluation of the Results

The results are based on 100 replications of the estimation procedures with independently generated data sets of size 500 from the four scenarios and are summarized in Table 2. The fitting capabilities of our algorithm and Dißmann et al. (2013)'s are measured by the log-likelihood of the estimated models. Knowing the underlying "true" models, we can also calculate the ratio of the estimated log-likelihoods and the true log-likelihoods to evaluate how well the selection methods perform in absolute terms. Figure 2 compares the performance of our Bayesian strategy with Dißmann's heuristic: markers above the diagonal line indicate replications in which our Bayesian model estimate has a higher likelihood than Dißmann's.

**Scenarios 1 and 2** The log-likelihoods of the models selected by our algorithm average 81% and 85% of the log-likelihoods of the true models, Dißmann's model estimates average 77% and 78% , and the multivariate Gaussian copula averages 64% and 68%,

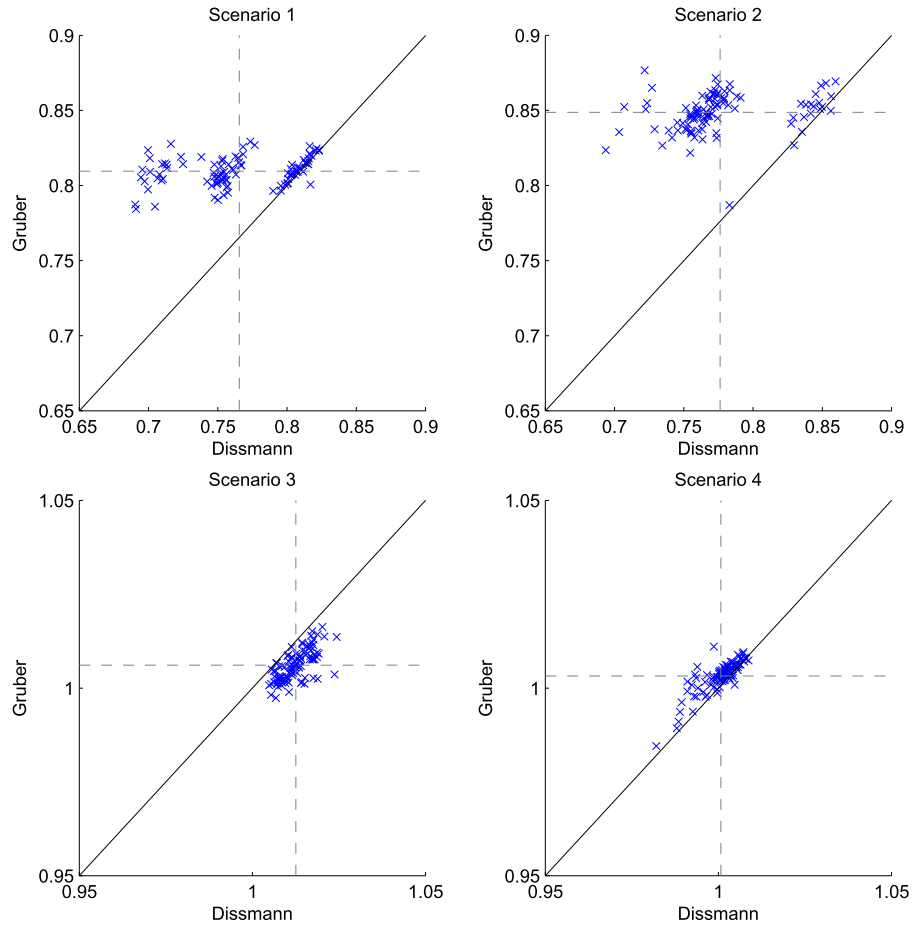


Figure 2: Comparison of relative log-likelihoods of our method and Dißmann's. The dashed lines indicate the respective averages across all 100 replications.

	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Gruber > Dißmann (out of 100)	97	98	0	86
Gruber rel. loglik (in %)	<b>81.0</b>	<b>84.9</b>	100.6	<b>100.3</b>
Dißmann rel. loglik (in %)	76.6	77.6	<b>101.3</b>	100.1
Gaussian MLE rel. loglik (in %)	64.0	67.6	84.7	100.1
Independence rel. loglik (in %)	0	0	0	0

Table 2: Number of replications in which our algorithm's estimate has a higher likelihood than Dißmann's; average percentage of the true log-likelihood of the estimated vine copulas, the multivariate Gaussian copula and the independence model.

respectively (Table 2). While neither Dißmann's method nor ours selects the correct tree  $T_1$  in any replication, these numbers still show that model fit is improved significantly by our approach, and that Dißmann's estimates are already more suitable models than the multivariate Gaussian copula.

Figure 2 shows that within each scenario, the relative log-likelihoods of our model selection procedure are distributed much more narrowly about the mean compared with Dißmann's. Furthermore, in 97 (Scenario 1) and 98 (Scenario 2) out of 100 replications, our method's estimates perform better than Dißmann's (Table 2). Together, this shows that our model selection strategy is more robust and performs consistently better.

**Scenario 3** The regular vine copula of Scenario 3 is truncated to the first level. As a result, the true model lies in the search space of the first step of our tree-by-tree model selection procedure, which makes this a test case to validate our implementation.

Our shrinkage prior effectively avoids over-fitting, given that, on average, only 0.8 of the 10 pair copulas on levels  $k = 2:5$  are selected as non-independence copulas, and in 43 out of 100 replications, all pair copulas on levels  $k = 2:5$  are selected as independence copulas. Furthermore, in all 100 replications, the posterior mode estimate has the true model's tree structure  $T_1$ . Dißmann's procedure is more prone to over-fitting with, on average, 3.3 out of the 10 pair copulas on levels  $k = 2:5$  being non-independence copulas and only 2 out of 100 replications selecting all pair copulas as independence copulas.

The log-likelihoods of the estimated models by our algorithm average 101% as do the log-likelihoods from Dißmann's models. This is an excellent result that confirms the validity of our model selection scheme and shows that it is implemented correctly. The consistently slightly higher log-likelihoods of Dißmann's model estimates are based on over-fitting. This scenario confirms our method as superior to Dißmann's, as it is important for an effective selection method to identify sparse patterns. The multivariate Gaussian copula lags behind with an average relative log-likelihood of 85% even though it is the model that has the most parameters.

*Detailed Analysis of the MCMC Output of Level 1 of Replication 1.* After discarding the first 2,500 iterations as burn-in, the posterior mode model has a posterior probability of 58% (Model 29; Table 3) and all posterior samples, after burn-in, have the correct tree structure  $T_1$ . The selected pair copula families agree with the correct pair copula families, except for the family of edge 3, 6: Model 29 selects a Gaussian pair copula, Model 30 selects the 180 degree rotation of the Gumbel copula, and Model 31 selects the Student's t copula. The fact that the correct model, Model 31, has only 4% posterior probability can be attributed to our shrinkage prior, given that the log-likelihoods of these three models are nearly identical. Figure 5 of Appendix A illustrates the MCMC mixing behavior using the model index and log-likelihood trace plots.

**Scenario 4** Both model selection procedures select models that average about 100% of the log-likelihoods of the true model. This extraordinary performance can be explained by a peculiarity of vine copulas: if all pair copulas are Gaussian or independence copulas, the vine copula equals a multivariate Gaussian copula irrespective of the density

Posterior Model	29	30	31
Posterior probability (in %)	<b>58.4</b>	32.1	4.0
Average relative log-likelihood (in %)	<b>100.2</b>	100.1	100.4
Number of parameters	<b>5</b>	5	6
Correct tree $T_1$	<b>yes</b>	yes	yes

Table 3: Scenario 3, Replication 1. Histogram table of selected models with an empirical posterior probability of at least 1%. The posterior probabilities and relative log-likelihoods are quoted in percentage points.

factorization  $\mathcal{V}$ . As a result, the selection of the density factorization  $\mathcal{V}$  does not play a role in selecting suitable vine copula models here. Our sequential Bayesian procedure selects, on average, 13.8 out of the 15 pair copulas as either Gaussian or independence copulas, while Dißmann’s procedure comes in second at 12.7 out of 15. This result, together with the high relative log-likelihoods, suggests that both algorithms perform similarly well at selecting suitable pair copula families.

**Conclusion** Both algorithms perform equally well in fitting a vine copula to Gaussian data. Our tree-level Bayesian approach improves model selection of general regular vine copulas, which are not independent of the selected tree structure  $\mathcal{V}$ . The large performance gap between Scenarios 1, 2 and the special cases of Scenarios 3, 4 shows the limits of our tree-by-tree approach towards the selection of the tree structure  $\mathcal{V}$ . We acknowledge that our model selection scheme does not yet represent the definitive answer to the model selection challenge. Nevertheless, our proposed selection scheme consistently selects better-fitting models than existing selection strategies and is better at detecting sparsity patterns for model reduction than Dißmann et al. (2013)’s frequentist method.

#### 4.4 Analysis of the Computational Complexity and Runtime

**Computational Complexity** The computation of a single model estimate by our algorithm using the set-up described in Section 4.2 consists of 50,000 MCMC updates for each level of the vine copula. These sum up to 250,000 MCMC updates for the five levels of a six-dimensional regular vine copula. Each MCMC update consists of a between-models move and a within-model move: the between-models move consists of estimating the parameters and calculating the likelihood of each pair copula and each candidate pair copula family, and an additional evaluation of the likelihood after drawing a proposal parameter; the within-model move brings another evaluation of the likelihood of each pair copula.

**Computing Facilities and Runtime** The simulation study was performed on a Linux cluster with AMD Opteron-based 32-way nodes using 2.6 GHz dual core CPUs for parallel processing. The Linux cluster is hosted by the Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften near Munich, Germany. It took approximately 10 hours to execute our stepwise Bayesian selection strategy for a six-dimensional data



set of size 500, while it took 5–6 seconds to execute Dißmann et al. (2013)'s heuristic and less than 0.1 seconds to estimate the correlation matrix of the multivariate Gaussian copula. It may be noted that the runtime of our procedure could be cut significantly by reducing the number of MCMC iterations. Our analyses suggest that convergence is achieved quickly so  $R \in [15,000, 30,000]$  will be adequate choices in practice.

**Recommendations for Researchers** In most studies, researchers have to strike a balance between getting quick, or getting more accurate results. With that in mind, we propose the following approach to decide which dependence model to use. In a quick first analysis, estimate a multivariate Gaussian copula and select a regular vine copula using Dißmann et al. (2013)'s heuristic, which can be completed within a few seconds. If the log-likelihoods of both models are similar, use the multivariate Gaussian copula as a “good enough” standard model (see Scenario 4). However, if the log-likelihood of the selected vine copula is substantially higher than the one of the Gaussian copula, perform a sequential Bayesian analysis using our method for more accurate and more robust results, and better sparsity detection (see Scenarios 1–3).

## 5 Example: Portfolio Asset Returns

We consider a diversified portfolio that invests in multiple asset classes using iShares exchange-traded funds (ETFs) and commodity trusts. The daily log-returns of each investment are modeled by a univariate time series. The joint multivariate characteristics are modeled by a regular vine copula and a multivariate Gaussian copula.

We learn the copulas using one year's worth of data and then use the selected copulas together with the marginal time series to obtain joint multivariate step-ahead forecasts for six months. The quality of the forecasts is measured by comparing the forecast accuracy of various portfolio metrics with the actual realizations.

### 5.1 Description of the Data

The data set contains adjusted daily closing prices of nine iShares ETFs,  $j = 1:9$ , and covers the time period from January 2013 through June 2014.<sup>1</sup> The training set consists of 252 observations from January through December 2013 ( $t = 1:252$ ); the test set consists of 124 observations from January through June 2014 ( $t = 253:376$ ). The nine ETFs form a well-diversified portfolio that invests in multiple asset classes and can be easily replicated by retail investors (Table 4). Three of the funds invest in U.S. equities ( $j = 1, 2, 3$ ), two funds in U.S. treasuries ( $j = 4, 5$ ), two funds in U.S. real estate through real estate investment trusts (REITs,  $j = 6, 7$ ), and two funds are commodity trusts investing in gold and silver ( $j = 8, 9$ ).<sup>2</sup>

---

<sup>1</sup>The data were downloaded from <http://finance.yahoo.com>.

<sup>2</sup>More details on the selected funds can be found on the iShares homepage at <http://www.ishares.com/us/index>.

$j$	Symbol	Name	Exposure
1	IVV	iShares Core S&P 500 ETF	Large-cap U.S. stocks
2	IJH	iShares Core S&P Mid-Cap ETF	Mid-cap U.S. stocks
3	IJR	iShares Core S&P Small-Cap ETF	Small-cap U.S. stocks
4	HYG	iShares iBoxx \$ High Yield Corporate Bond ETF	High yield corporate bonds
5	LQD	iShares iBoxx \$ Investment Grade Corporate Bond ETF	U.S. investment grade corporate bonds
6	RTL	iShares Retail Real Estate Capped ETF	U.S. retail property real estate stocks and REITs
7	REZ	iShares Residential REIT Capped ETF	U.S. residential real estate stocks and REITs
8	SLV	iShares Silver Trust	Silver
9	IAU	iShares Gold Trust	Gold

Table 4: Overview of the ETFs selected for the real data example. The exposure information is taken from the iShares homepage.

## 5.2 Marginal Time Series

We model the daily log-returns  $y_{j,t}$ ,  $t = 1, 2, \dots$  of each series  $j = 1:9$  using a variance discounting dynamic linear model (DLM; (West and Harrison, 1997, Chapter 10.8)). The DLM is a fully Bayesian time series model that has closed-form posterior and forecast distributions, and the parameters are learned on-line. The following updating equations are adapted from Table 10.4 of West and Harrison (1997).

**Model Formulation** The general DLM models each time series  $y_{j,t}$ ,  $j = 1:9$ , by

$$y_{j,t} = \mathbf{F}'_{j,t} \boldsymbol{\theta}_{j,t} + \nu_{j,t}, \quad \nu_{j,t} \sim N(0, \lambda_{j,t}^{-1}), \quad (10)$$

$$\boldsymbol{\theta}_{j,t} = \mathbf{G}_{j,t} \boldsymbol{\theta}_{j,t-1} + \boldsymbol{\omega}_{j,t}, \quad \boldsymbol{\omega}_{j,t} \sim N(\mathbf{0}, \mathbf{W}_{j,t}), \quad (11)$$

$$\lambda_{j,t} = \lambda_{j,t-1} \frac{\eta_{j,t}}{\beta_j}, \quad \eta_{j,t} \sim \text{Beta} \left( \frac{\beta_j n_{j,t-1}}{2}, \frac{(1 - \beta_j) n_{j,t-1}}{2} \right), \quad (12)$$

with observation equation (10). Equations (11) and (12) describe the evolutions of the states  $\boldsymbol{\theta}_{j,t}$ , a vector with  $p_j$  entries, and  $\lambda_{j,t}$ , a positive scalar, where the innovations  $\nu_{j,t}$ ,  $\boldsymbol{\omega}_{j,t}$  and  $\eta_{j,t}$  are assumed mutually independent and independent over time. The predictors  $\mathbf{F}_{j,t}$  are a vectors of size  $p_j$  and the state evolution matrices  $\mathbf{G}_{j,t}$  are of dimensions  $p_j \times p_j$ . The parameters  $\mathbf{W}_{j,t}$ ,  $n_{j,t-1}$  and  $\beta_j$  of the state evolutions (11)–(12) are explained in the next paragraph.

**Forward Filtering** The information set at time  $t$  is denoted by  $\mathcal{D}_t$ . Suppose that at time  $t - 1$ , a normal–gamma prior for  $(\boldsymbol{\theta}_{j,t}, \lambda_{j,t})$ , given information  $\mathcal{D}_{t-1}$  has density

$$\pi_{j,t}(\boldsymbol{\theta}_{j,t}, \lambda_{j,t}) := N(\boldsymbol{\theta}_{j,t} \mid \mathbf{a}_{j,t}, \mathbf{R}_{j,t} / (c_{j,t} \lambda_{j,t})) \cdot G(\lambda_{j,t} \mid r_{j,t}/2, r_{j,t} c_{j,t}/2), \quad (13)$$

and parameters  $\mathbf{a}_{j,t} \in \mathbb{R}^{p_j}$ ,  $\mathbf{R}_{j,t} \in \mathbb{R}^{p_j \times p_j}$ ,  $r_{j,t} > 0$  and  $c_{j,t} > 0$ ; at  $t = 0$ , the initial prior parameters are  $\mathbf{a}_{j,1}$ ,  $\mathbf{R}_{j,1}$ ,  $r_{j,1}$  and  $c_{j,1}$ . As  $y_{j,t}$  is observed at time  $t$ , the information set is updated to  $\mathcal{D}_t$  and the posterior distribution of  $(\boldsymbol{\theta}_{j,t}, \lambda_{j,t})$ , given information  $\mathcal{D}_t$  follows as a normal–gamma

$$p_{j,t}(\boldsymbol{\theta}_{j,t}, \lambda_{j,t}) := N(\boldsymbol{\theta}_{j,t} \mid \mathbf{m}_{j,t}, \mathbf{C}_{j,t}/(s_{j,t}\lambda_{j,t}))G(\lambda_{j,t} \mid n_{j,t}/2, n_{j,t}s_{j,t}/2) \quad (14)$$

with parameters  $\mathbf{m}_{j,t} = \mathbf{a}_{j,t} + \mathbf{A}_{j,t}e_{j,t} \in \mathbb{R}^{p_j}$ ,  $\mathbf{C}_{j,t} = (\mathbf{R}_{j,t} - \mathbf{A}_{j,t}\mathbf{A}'_{j,t}q_{j,t})z_{j,t} \in \mathbb{R}^{p_j \times p_j}$ ,  $n_{j,t} = r_{j,t} + 1 > 0$  and  $s_{j,t} = z_{j,t}c_{j,t} > 0$ , where  $e_{j,t} = y_{j,t} - \mathbf{F}'_{j,t}\mathbf{a}_{j,t} \in \mathbb{R}$  is the forecast error,  $q_{j,t} = c_{j,t} + \mathbf{F}'_{j,t}\mathbf{R}_{j,t}\mathbf{F}_{j,t} > 0$  is the forecast variance factor,  $\mathbf{A}_{j,t} = \mathbf{R}_{j,t}\mathbf{F}_{j,t}/q_{j,t} \in \mathbb{R}^{p_j}$  is the adaptive coefficient vector, and  $z_{j,t} = (r_{j,t} + e_{j,t}^2/q_{j,t})/n_{j,t} > 0$  is the volatility update factor (see Table 10.4 of West and Harrison (1997)). The step-ahead priors  $(\boldsymbol{\theta}_{j,t+1}, \lambda_{j,t+1} \mid \mathcal{D}_t)$  at time  $t$  follow from the system equations (11)–(12) as evolutions of the posterior states  $(\boldsymbol{\theta}_{j,t}, \lambda_{j,t} \mid \mathcal{D}_t)$ . The normal–gamma step-ahead prior density  $\pi_{j,t+1}$  is as in (13) with  $t$  evolved to  $t + 1$  and parameters  $r_{j,t+1} = \beta_j n_{j,t}$ ,  $c_{j,t+1} = s_{j,t}$ ,  $\mathbf{a}_{j,t+1} = \mathbf{G}_{j,t+1}\mathbf{m}_{j,t}$ ,  $\mathbf{R}_{j,t+1} = \mathbf{G}_{j,t+1}\mathbf{C}_{j,t}\mathbf{G}'_{j,t+1} + \mathbf{W}_{j,t+1}$  and  $\mathbf{W}_{j,t+1} = \frac{1-\delta_j}{\delta_j}\mathbf{G}_{j,t+1}\mathbf{C}_{j,t}\mathbf{G}'_{j,t+1}$ . The discount factors  $\beta_j, \delta_j \in (0, 1)$  inflate the prior variances in the state evolution steps and determine the model’s responsiveness to new observations.

**Forecasting** The forecast distribution of  $y_{j,t+1}$  at time  $t$  and with information  $\mathcal{D}_t$  follows as a non-standardized Student’s  $t$  distribution  $T_{\text{non std}}(\nu, \mu, \sigma^2)$  with  $\nu = r_{j,t+1}$  degrees of freedom, mean  $\mu = \mathbf{F}'_{j,t+1}\mathbf{a}_{t+1}$  and variance  $\sigma^2 = \mathbf{F}'_{j,t+1}\mathbf{R}_{j,t+1}\mathbf{F}_{j,t+1} + c_{j,t+1}$  by integration of the observation equation (10) over the prior distributions of the states  $(\boldsymbol{\theta}_{j,t+1}, \lambda_{j,t+1})$ . The non-standardized  $t$  distribution is a location–scale transformation

$$T_{\text{non std}}(\nu, \mu, \sigma^2) = \mu + \sqrt{\sigma^2} \cdot T_\nu \quad (15)$$

of a  $t$  distribution  $T_\nu$  with  $\nu$  degrees of freedom. In the remainder, we will denote the forecast distribution of  $y_{j,t+1}$  at time  $t$  by  $T_{j,t+1}$ .

**Model Choice** We use a local-level DLM that assumes  $\mathbf{F}_{j,t} = 1$  and has random walk evolutions  $\mathbf{G}_{j,t} = 1$  for all  $j$  and  $t$ . The discount factors are set to  $\beta_j = 0.96$  and  $\delta_j = 0.975$  for all  $j$  to balance responsiveness to new observations with sufficient robustness for reliable forecasts. We start the analysis with the initial prior parameters of each series  $j = 1:9$  set to  $\mathbf{a}_{j,1} = 0$ ,  $\mathbf{R}_{j,1} = 10^{-6}$ ,  $r_{j,1} = 10$ ,  $c_{j,1} = 10^{-5}$ . Figure 3 shows the sequential step-ahead forecasts and realized daily log-returns as well as the 10% quantiles of the forecast distributions as the daily value at risk of each series  $j = 1:9$ .

### 5.3 Estimation of the Dependence Models

Copula modeling is a two-step process: first, marginal models remove within-series effects from the data  $y_{j,t}$  to obtain i.i.d.—within each series  $j$ —uniform noise  $u_{j,t} := T_{j,t}(y_{j,t})$ ; second, a copula is selected to describe across-series dependence effects of the multivariate transformed  $U(0, 1)$  data  $\mathbf{u}_t = (u_{1,t}, \dots, u_{9,t})'$ ,  $t = 1, 2, \dots$

**Sequential Bayesian Selection** We use our model selection scheme to estimate a 9-dimensional regular vine copula using the  $t = 1:252$  observations from 2013. We apply

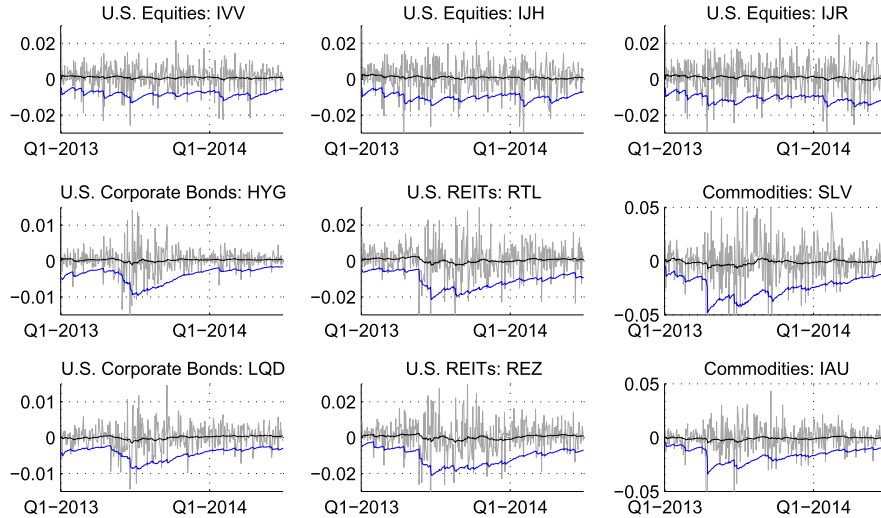


Figure 3: Realized returns (gray), forecast means (black) and 10% value at risk (blue).

the same priors and configuration of the sample as in Section 4. The selected model is shown in Table 7 of Appendix B: it has 10 Gaussian pair copulas, 0 Student's t copulas, 8 Gumbel copulas, 0 Clayton copulas, and 18 Independence copulas. The pair copulas of levels  $k \geq 5$  are selected as Independence copulas and omitted in Table 7.

**Dißmann's Frequentist Selection** We compare against our Bayesian tree-by-tree strategy to Dißmann et al. (2013)'s frequentist heuristic as we did in the simulation study of Section 4. Dißmann's vine copula is noticeably less parsimonious with only 13 Independence pair copulas and 5 Gaussian copulas, 7 Student's t copulas, 7 Gumbel copulas, and 4 Clayton copulas. The selected model is shown in Table 8 of Appendix B.

**Multivariate Gaussian Copula** For reference, we also included a maximum likelihood estimate of the multivariate Gaussian copula in our comparison. The estimated correlation matrix is shown in Table 9 of Appendix B.

## 5.4 Analysis of Portfolio Forecasts

**Sampling from the Joint Forecast Distribution** Samples  $\hat{\mathbf{y}}_t^{n=1:N} = (\hat{y}_{1,t}^n, \dots, \hat{y}_{9,t}^n)'$  from the joint forecast distribution are generated by transforming samples  $\mathbf{u}^n = (u_1^n, \dots, u_9^n)'$  from the copula to the observation scale through inverse cdfs of the marginal forecast distributions,  $\hat{y}_{j,t}^n := T_{j,t}^{-1}(u_j^n)$ .

**In-Sample Analysis** Consider a portfolio that invests equally in the ETFs from Table 4 and the weights  $\mathbf{w}_t := (w_{1,t}, \dots, w_{9,t})' = (\frac{1}{9}, \dots, \frac{1}{9})'$  are maintained throughout the time

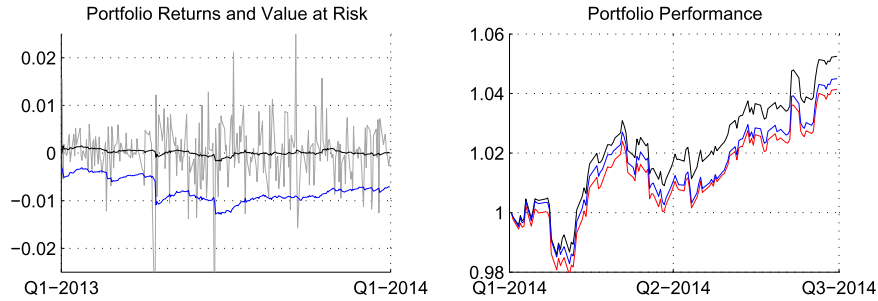


Figure 4: (Left) Realized portfolio returns (gray) vs. forecast means (black) and 10% value at risk (blue) from our sequential Bayesian vine copula model during the training date range  $t = 1:252$ . (Right) Portfolio performance of investment strategy (16) under our Bayesian vine copula model (black; highest line), Dißmann’s vine model (red; lowest line) and the Gaussian model (blue; middle line) during the test date range  $t = 253:376$ .

period  $t = 1:252$ . For each  $t$ , we draw  $N = 10,000$  samples  $\hat{\mathbf{y}}_t^{n=1:N}$  from the joint forecast distribution to simulate the portfolio returns  $\hat{r}_t^n := \mathbf{w}'_t \hat{\mathbf{y}}_t^n$ . We compute the 10% value at risk as the 10% sample quantile and the expected portfolio return as the sample mean of  $\hat{r}_t^{n=1:N}$ . This allows an evaluation of the adequacy of the joint multivariate model, which consists of the nine marginal DLMS and the selected copula.

Figure 4 (left) shows that the predicted quantities from our sequential Bayesian vine copula model are in line with the actual portfolio returns. The actual portfolio return is under the predicted 10% quantile of the simulated portfolio return distribution that uses our sequential Bayesian vine copula on 8.7%, or 22 out of 252 days; if Dißmann’s vine copula or the multivariate Gaussian copula are used in conjunction with the same marginal DLMS, the actual portfolio return is under the predicted 10% quantile on 8.3%, or 21 out of 252 days; if the independence copula is used, the 10% value at risk is exceeded 20%, or 50 out of 252 days.

**Out-of-Sample Analysis** During the out-of-sample period from January through June 2014,  $t = 253 : 376$ , we investigate the performance of a dynamic portfolio whose weights  $\mathbf{w}_t$  are updated daily to maximize the predicted Sharpe ratio (Sharpe (1966)):

$$\max_{\mathbf{w}_t} \widehat{SR}_t(\mathbf{w}_t) \text{ subject to } \sum_{j=1:9} w_{j,t} = 1 \text{ and } w_{j,t} \in (0.05, 0.25) \text{ for all } j = 1:9. \quad (16)$$

Here  $\widehat{SR}_t(\mathbf{w}_t)$  (see (17)) is the estimate of the annualized Sharpe ratio of a portfolio with investment weights  $\mathbf{w}_t$ , where  $\hat{\boldsymbol{\mu}}_t$  is the sample mean and  $\hat{\boldsymbol{\Sigma}}_t$  is the sample covariance matrix of the simulated joint forecasts  $\hat{\mathbf{y}}_t^{n=1:N}$ . Again,  $N = 10,000$  samples were used:

$$\widehat{SR}_t(\mathbf{w}_t) := \frac{252 \cdot \mathbf{w}'_t \hat{\boldsymbol{\mu}}_t}{\sqrt{252 \cdot \mathbf{w}'_t \hat{\boldsymbol{\Sigma}}_t \mathbf{w}_t}}. \quad (17)$$

Our calculation of the Sharpe ratio in (17) is under the assumption of a zero-return risk-free asset. The optimization constraints  $w_{j,t} \in (0.05, 0.25)$  in (16) refer to minimum and maximum weights of individual assets and are typical restrictions that aim at protecting investors from undue accumulation of risk.

When the regular vine copula selected by our sequential Bayesian procedure is used as the joint model's dependence model, the realized annualized Sharpe ratio of the investment strategy (16) during the out-of-sample period  $t = 253:376$  is  $SR = 1.95$ ; if the multivariate Gaussian copula is used to inform the investment decisions, the realized Sharpe ratio is  $SR = 1.67$ ; if Dißmann's frequentist vine model is used, the realized Sharpe ratio is  $SR = 1.53$ . In addition, the realized nominal return of the portfolio driven by our sequential Bayesian vine copula is higher than the returns of the portfolios using the Gaussian copula or Dißmann's copula (Figure 4 (right)). This example provides additional evidence of our sequential Bayesian vine model as the most reliable model for use in a real-life context.

## 5.5 Considerations on Use in Practice

The computing time of updating the univariate DLMS is a few milliseconds, which is negligible in the context of daily portfolio risk rebalancing. In contrast, the computational burden of estimating the regular vine copula is much higher—in our example, our Bayesian model selection could take as long as up to a day to complete.

We suggest that the dependence model be update in monthly, quarterly, or semi-annually intervals only. Under the assumption that the dependence structure of financial asset returns is only slowly changing, this is a prudent way to proceed. Even though the long computation time of our Bayesian strategy might be a deterrent to implementing our approach, the benefits of increasing a portfolio's performance in nominal as well as risk-adjusted terms will quickly pay for the investment in computing time.

The combination of univariate DLMS with a regular vine copula as the dependence model provides a robust framework for forecasting, yet is highly responsive to new observations. This can be seen, for example, in the way the value at risk changes instantly on the day of a large negative market move. Furthermore, it is a distinct strength of regular vine copulas to be able to model asymmetric dependence characteristics along with various tail dependence characteristics in one model. Our example shows that a regular vine copula-driven model can help in decision making to achieve superior investment performance as well as improved risk forecasts.

## 6 Concluding Remarks

We discussed a Bayesian approach to model selection of regular vine copulas and presented a reversible jump Markov chain Monte Carlo-based algorithm to facilitate posterior sampling. A key feature of our approach, sequential model selection in the levels  $k$  reduces the search space for candidate models to a fraction of the search space for joint selection to keep the computational run time at an acceptable level.

A simulation study (Section 4) demonstrated that our Bayesian model selection approach is superior to Dißmann et al. (2013)’s frequentist one. The better performance of our Bayesian selection scheme can be attributed to its simultaneous and prior-informed selection of the pair copula families  $\mathcal{B}_k$  of a given level  $k$ , while Dißmann’s algorithm selects them one-by-one. In addition to the simulation study, a real data example (Section 5) illustrated how regular vine copulas can be used to achieve superior portfolio risk forecasts and investment decisions.

Our estimation procedure extends previously available inference methods for regular vine copulas in two significant ways. Our Bayesian tree-by-tree strategy allows the selection of the pair copula families  $\mathcal{B}_\mathcal{V}$  from an arbitrary set of candidate families  $\mathbf{B}$ , which is a non-trivial extension of Smith et al. (2010)’s indicator-based approach that can only detect (conditional) pairwise independencies. Furthermore, we present the first Bayesian inference method for selecting the regular vine  $\mathcal{V}$  as the building plan of the pair copula construction jointly with the pair copula families  $\mathcal{B}_\mathcal{V}$ . A major selling point of our approach is that we demonstrated its superiority to existing procedures in a simulation study under controlled conditions (see Section 4) as well as in an application study using real data (see Section 5).

Sequential model selection schemes can fail to select the correct model. This is illustrated, e.g., in Section 4 by the failure of the selected models to have relative log-likelihoods close to 100% in Scenarios 1 and 2. Current research aims at developing a fully Bayesian model selection scheme to estimate all levels of a regular vine copula jointly as well as allowing for time-varying dependence effects.

## Appendix A: Supplements to the Simulation Study

Algorithm	Tuning Parameters
2	$q_N(N = k) = \frac{1}{3.5} \log \left( 1 - \frac{1 - e^{-3.5}}{ E_k e^{-3.5} + k(1 - e^{-3.5})} \right)$ , where $ E_k $ denotes the number of pair copulas of level $k$
2, 3	Parameter estimation is done by matching the Kendall’s $\tau$ parameter to the sample Kendall’s $\tau$ . The degrees of freedom $\nu$ of a Student’s t pair copula is maximum likelihood estimated on a discrete grid.
2, 3	$\Sigma = 0.0125^2$ for the Kendall’s $\tau$ of single-parameter copulas; $\Sigma = \begin{pmatrix} 0.0125^2 & 0 \\ 0 & 0.1^2 \end{pmatrix}$ for the $(\tau, \log \nu)$ parameter vector of the Student’s t copula
3	$p = 0.667$

Table 5: MCMC tuning parameters used in the simulation study and real data example.

Scenario 1	Scenario 2	Scenario 3	Scenario 4
$c_{1,2}$ N(0.59)	$c_{1,2}$ T(0.54, 5)	$c_{1,2}$ N(0.41)	$c_{1,2}$ N(0.41)
$c_{2,3}$ C(0.71)	$c_{1,3}$ C90(-0.67)	$c_{2,3}$ C(0.50)	$c_{2,3}$ N(0.49)
$c_{3,4}$ C180(0.80)	$c_{1,4}$ C180(0.64)	$c_{3,4}$ C180(0.50)	$c_{2,4}$ N(-0.33)
$c_{3,5}$ N(-0.71)	$c_{1,5}$ N(-0.59)	$c_{3,5}$ N(-0.33)	$c_{3,5}$ N(-0.26)
$c_{3,6}$ T(0.65, 3)	$c_{1,6}$ T(0.54, 6)	$c_{3,6}$ T(0.49, 5)	$c_{3,6}$ N(0.13)
$c_{1,3 2}$ G(0.75)	$c_{2,3 1}$ G(0.71)		$c_{1,3 2}$ N(0.59)
$c_{2,4 3}$ N(0.41)	$c_{2,4 1}$ G270(-0.71)		$c_{2,5 3}$ N(0.13)
$c_{2,5 3}$ C270(-0.60)	$c_{2,5 1}$ C270(-0.60)		$c_{3,4 2}$ N(0.41)
$c_{2,6 3}$ N(-0.37)	$c_{2,6 1}$ N(-0.45)		$c_{5,6 3}$ N(-0.33)
$c_{1,4 2,3}$ T(0.26, 5)	$c_{3,4 1,2}$ T(0.30, 8)		$c_{1,5 2,3}$ N(0.26)
$c_{1,5 2,3}$ N(-0.26)	$c_{3,5 1,2}$ N(-0.30)		$c_{2,6 3,5}$ N(-0.41)
$c_{1,6 2,3}$ C90(-0.56)	$c_{3,6 1,2}$ C90(-0.43)		$c_{4,5 2,3}$ N(0.19)
$c_{4,6 1,2,3}$ N(0.13)	$c_{4,5 1,2,3}$ N(0.19)		$c_{1,6 2,3,5}$ N(0.49)
$c_{5,6 1,2,3}$ C(0.20)	$c_{4,6 1,2,3}$ C(0.43)		$c_{4,6 2,3,5}$ N(0.41)
$c_{4,5 1,2,3,6}$ G180(0.52)	$c_{5,6 1,2,3,4}$ G180(0.50)		$c_{1,4 2,3,5,6}$ N(-0.33)
17 parameters	18 parameters	6 parameters	15 parameters

Table 6: The vine copulas used in the simulation study. The parameters shown are the Kendall’s  $\tau$  and the degrees of freedom  $\nu$ .

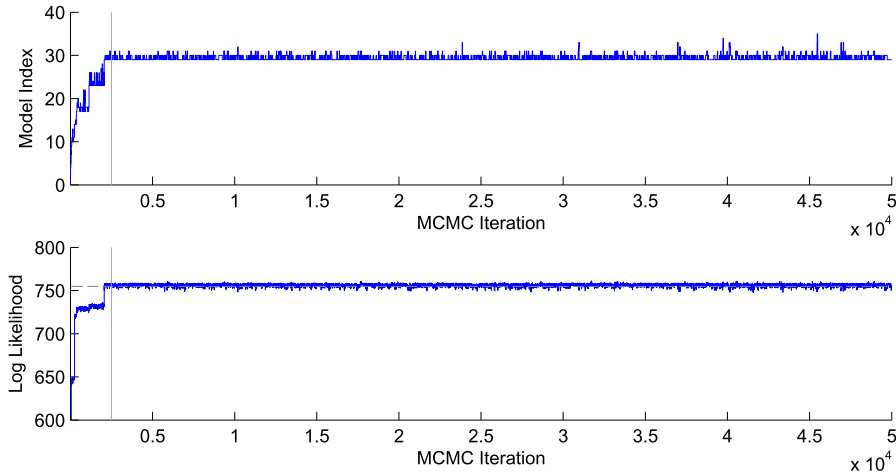


Figure 5: Model index and log-likelihood trace plot of Replication 1 of Scenario 3. The horizontal line in the lower plot indicates the true model’s log-likelihood; the vertical lines show the burn-in period.



### Appendix B: Supplements to the Data Example

Tree $T_1$	Tree $T_2$	Tree $T_3$	Tree $T_4$
$c_{1,2}$ N(0.74)	$c_{1,3;2}$ N(0.07)	$c_{1,9;5,7}$ I	$c_{1,8;6,7,9}$ G180(0.06)
$c_{1,4}$ N(0.46)	$c_{1,5;7}$ G270(-0.10)	$c_{2,6;1,7}$ G180(0.08)	$c_{2,9;1,6,7}$ I
$c_{1,7}$ N(0.39)	$c_{1,6;7}$ N(0.14)	$c_{3,7;1,2}$ I	$c_{3,6;1,2,7}$ I
$c_{2,3}$ N(0.79)	$c_{2,7;1}$ G(0.12)	$c_{4,5;1,7}$ N(0.27)	$c_{4,6;1,5,7}$ I
$c_{5,7}$ G(0.19)	$c_{4,7;1}$ G180(0.13)	$c_{5,6;1,7}$ N(0.12)	$c_{5,9;1,6,7}$ G(0.12)
$c_{6,7}$ N(0.51)	$c_{6,8;9}$ I	$c_{7,8;6,9}$ I	
$c_{6,8}$ G(0.09)	$c_{7,9;6}$ I		
$c_{8,9}$ N(0.71)			

Table 7: Sequential Bayesian estimate of the regular vine copula, given the training data  $t = 1:252$ . This tables shows the Kendall’s  $\tau$  parameters of the pair copulas.

Tree $T_1$	Tree $T_2$	Tree $T_3$
$c_{1,2}$ N(0.74)	$c_{1,5;4}$ T(-0.18, 12.8)	$c_{1,3;2,7}$ N(0.06)
$c_{1,4}$ N(0.46)	$c_{1,7;2}$ G180(0.08)	$c_{1,9;4,5}$ G180(0.03)
$c_{2,3}$ T(0.79, 8.67)	$c_{2,4;1}$ I	$c_{2,5;1,4}$ I
$c_{2,7}$ T(0.41, 8.58)	$c_{2,6;7}$ N(0.16)	$c_{3,6;2,7}$ I
$c_{4,5}$ T(0.39, 4.93)	$c_{3,7;2}$ G270(-0.05)	$c_{4,7;1,2}$ G180(0.13)
$c_{5,9}$ G(0.16)	$c_{4,9;5}$ C(0.05)	$c_{4,8;5,9}$ C180(0.05)
$c_{6,7}$ T(0.51, 14.5)	$c_{5,8;9}$ C270(-0.05)	
$c_{8,9}$ N(0.70)		

Tree $T_4$	Tree $T_5$	Tree $T_6$
$c_{1,6;2,3,7}$ I	$c_{2,8;1,4,5,9}$ T(-0.04, 16.7)	$c_{3,9;1,2,4,5,7}$ I
$c_{1,8;4,5,9}$ G(0.06)	$c_{2,5;1,2,4,7}$ I	$c_{5,6;1,2,3,4,7}$ T(0.10, 14.3)
$c_{2,9;1,4,5}$ C(0.04)	$c_{4,6;1,2,3,7}$ I	$c_{7,8;1,2,4,5,9}$ I
$c_{3,4;1,2,7}$ I	$c_{7,9;1,2,4,5}$ I	
$c_{5,7;1,2,4}$ G(0.17)		

Table 8: Regular vine copula selected by Dißmann’s heuristic, given the training data  $t = 1:252$ . This tables shows the Kendall’s  $\tau$  parameters of the pair copulas.

$$\Sigma = \begin{pmatrix} \mathbf{1} & 0.92 & 0.89 & 0.64 & 0.02 & 0.58 & 0.61 & 0.21 & 0.16 \\ 0.92 & \mathbf{1} & 0.95 & 0.61 & 0.03 & 0.59 & 0.61 & 0.21 & 0.17 \\ 0.89 & 0.95 & \mathbf{1} & 0.58 & 0.00 & 0.54 & 0.57 & 0.20 & 0.15 \\ 0.64 & 0.61 & 0.58 & \mathbf{1} & 0.37 & 0.53 & 0.57 & 0.23 & 0.23 \\ 0.02 & 0.03 & 0.00 & 0.37 & \mathbf{1} & 0.32 & 0.32 & 0.14 & 0.20 \\ 0.58 & 0.59 & 0.54 & 0.53 & 0.32 & \mathbf{1} & 0.74 & 0.20 & 0.18 \\ 0.61 & 0.61 & 0.57 & 0.57 & 0.32 & 0.74 & \mathbf{1} & 0.18 & 0.16 \\ 0.21 & 0.21 & 0.20 & 0.23 & 0.14 & 0.20 & 0.18 & \mathbf{1} & 0.90 \\ 0.16 & 0.17 & 0.15 & 0.23 & 0.20 & 0.18 & 0.16 & 0.90 & \mathbf{1} \end{pmatrix}$$

Table 9: Maximum likelihood estimate of the correlation matrix of the multivariate Gaussian copula, given the training data  $t = 1:252$ .

## References

- Bedford, T. and Cooke, R. M. (2001). “Probability Density Decomposition for Conditionally Dependent Random Variables Modeled by Vines.” *Annals of Mathematics and Artificial Intelligence*, 32: 245–268. MR1859866. doi: <http://dx.doi.org/10.1023/A:1016725902970>. 937, 939, 940
- Boost Community (2014). “Boost C++ Libraries.” <http://boost.org>. Accessed: 2014-03-20. 948
- Brechmann, E. C., Czado, C., and Aas, K. (2012). “Truncated regular vines in high dimensions with application to financial data.” *Canadian Journal of Statistics*, 40(1): 68–85. MR2896931. doi: <http://dx.doi.org/10.1002/cjs.10141>. 940
- Brechmann, E. C. and Schepsmeier, U. (2013). “Modeling Dependence with C- and D-Vine Copulas: The R Package CDVine.” *Journal of Statistical Software*, 52(3): 1–27. <http://www.jstatsoft.org/v52/i03>. 941
- Cayley, A. (1889). “A Theorem on Trees.” *The Quarterly Journal of Mathematics*, 23: 376–378. 942
- COIN-OR Foundation (2014). “A Package for Differentiation of C++ Algorithms.” <http://www.coin-or.org/CppAD/>. Accessed: 2014-03-20. 948
- Dißmann, J. F., Brechmann, E. C., Czado, C., and Kurowicka, D. (2013). “Selecting and estimating regular vine copulae and application to financial returns.” *Computational Statistics & Data Analysis*, 59(1): 52–69. MR3000041. doi: <http://dx.doi.org/10.1016/j.csda.2012.08.010>. 938, 948, 949, 952, 953, 956, 959
- Green, P. J. (1995). “Reversible jump Markov chain Monte Carlo computation and Bayesian model determination.” *Biometrika*, 82: 711–732. MR1380810. doi: <http://dx.doi.org/10.1093/biomet/82.4.711>. 938, 941
- Hastings, W. (1970). “Monte Carlo sampling methods using Markov chains and their applications.” *Biometrika*, 57: 97–109. doi: <http://dx.doi.org/10.1093/biomet/57.1.97>. 942
- Joe, H. (1996). “Families of  $m$ -variate distributions with given margins and  $m(m-1)/2$  bivariate dependence parameters.” *Lecture Notes–Monograph Series*, 28: 120–141. MR1485527. doi: <http://dx.doi.org/10.1214/lnms/1215452614>. 937, 939
- (2001). *Multivariate Models and Dependence Concepts*. Chapman & Hall. 937, 941
- Kirchhoff, G. (1847). “Über die Auflösung der Gleichungen, auf welche man bei der Untersuchung der linearen Verteilung galvanischer Ströme geführt wird.” *Annual Review of Physical Chemistry*, 72: 497–508. 946
- Kurowicka, D. and Cooke, R. M. (2006). *Uncertainty Analysis with High Dimensional Dependence Modelling*. John Wiley & Sons Ltd. MR2216540. doi: <http://dx.doi.org/10.1002/0470863072>. 937, 939, 943
- Kurowicka, D. and Joe, H. (eds.) (2010). *Dependence Modeling: Vine Copula Handbook*. World Scientific Publishing Co. Pte. Ltd. MR2849701. 937

- McNeil, A. J., Frey, R., and Embrechts, P. (2005). *Quantitative Risk Management: Concepts, Techniques, and Tools*. Princeton University Press. [MR2175089](#). 937
- Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., and Teller, E. (1953). “Equation of State Calculations by Fast Computing Machines.” *Journal of Chemical Physics*, 21: 1087–1092. doi: <http://dx.doi.org/10.1063/1.1699114>. 942
- Min, A. and Czado, C. (2010). “Bayesian Inference for Multivariate Copulas Using Pair-Copula Constructions.” *Journal of Financial Econometrics*, 8(4): 511–546. 938
- (2011). “Bayesian model selection for D-vine pair-copula constructions.” *Canadian Journal of Statistics*, 39: 239–258. [MR2839479](#). doi: <http://dx.doi.org/10.1002/cjs.10098>. 938
- Morales-Napoles, O. (2011). “Counting vines.” In: Kurowicka, D. and Joe, H. (eds.), *Dependence Modeling: Vine Copula Handbook*. World Scientific Publishing Co. [MR2849701](#). 938, 942
- Nelsen, R. B. (2006). *An Introduction to Copulas*. Springer. [MR2197664](#). 937
- Sharpe, W. F. (1966). “Mutual Fund Performance.” *The Journal of Business*, 39(1): 119–138. Part 2: Supplement on Security Prices. doi: <http://dx.doi.org/10.1086/294846>. 957
- Sklar, A. (1959). “Fonctions de répartition à n dimensions et leurs marges.” *Publications de l’Institut de Statistique de l’Université de Paris*, 8: 229–231. [MR0125600](#). 938
- Smith, M., Min, A., Almeida, C., and Czado, C. (2010). “Modeling Longitudinal Data Using a Pair-Copula Decomposition of Serial Dependence.” *Journal of the American Statistical Association*, 105(492): 1467–1479. [MR2796564](#). doi: <http://dx.doi.org/10.1198/jasa.2010.tm09572>. 938, 959
- Stöber, J., Joe, H., and Czado, C. (2013). “Simplified Pair Copula Constructions—Limitations and Extensions.” *Journal of Multivariate Analysis*, 119(0): 101–118. [MR3061418](#). doi: <http://dx.doi.org/10.1016/j.jmva.2013.04.014>. 940
- West, M. and Harrison, J. (1997). *Bayesian Forecasting & Dynamic Models*. Springer Verlag, 2nd edition. <http://www.stat.duke.edu/~mw/book.html> [MR1482232](#). 954, 955

### Acknowledgments

The numerical computations were performed on a Linux cluster supported by DFG grant INST 95/919-1 FUGG.

We thank the Editor, Associate Editor and three unnamed reviewers for constructive comments on our original manuscript.