

## Sampling from hierarchical Kendall copulas

**Titre:** Génération d'échantillons pseudo-aléatoires à partir de copules de Kendall hiérarchiques

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**Abstract:** As copulas are frequently used to model dependence in statistical models, it is of central importance to be able to accurately and efficiently sample from them. In the case of hierarchical Kendall copulas, a top-down sampling strategy involves simulation of a random vector given that it lies in a particular level set. While explicit solutions are available when hierarchical Kendall copulas are built from Archimedean copulas, this paper presents new results for the Plackett copula and for Archimax copulas, which also include the class of extreme-value copulas. Additionally, new approximate sampling procedures for hierarchical Kendall copulas are proposed and evaluated in a simulation study.

**Résumé :** Les copules étant fréquemment utilisées pour modéliser la dépendance, il est crucial de disposer d'algorithmes efficaces permettant de générer des échantillons pseudo-aléatoires à partir de ces distributions. Dans le cas des copules de Kendall hiérarchiques, une stratégie d'échantillonnage descendante repose sur la simulation d'un vecteur aléatoire sachant qu'il prend ses valeurs dans un ensemble de niveau de la copule. Après avoir rappelé les solutions explicites dans le cas où la construction repose sur les copules Archimédiennes, cet article présente de nouveaux résultats pour la copule de Plackett et pour les copules Archimax contenant la classe des copules de valeurs extrêmes. En complément, de nouveaux algorithmes approchés de génération d'échantillons pseudo-aléatoires pour les copules de Kendall hiérarchiques sont proposés et évalués par le biais de simulations.

**Keywords:** sampling copulas, hierarchical copulas, Kendall distribution function, copula level set, sample reordering

**Mots-clés :** génération d'échantillons pseudo-aléatoires, copules hiérarchiques, fonction de distribution de Kendall, ensembles de niveau d'une copule

**AMS 2000 subject classifications:** 62D05, 62H99

### 1. Introduction

Developing accurate and efficient sampling methods for dependence models is a major challenge. Copulas arise as a fundamental tool to model statistical dependence in Sklar's Theorem [Sklar, 1959]. It states that the  $d$ -dimensional distribution function  $F$  of a random vector  $\mathbf{X} = (X_1, \dots, X_d)'$  equals a copula  $C$  evaluated at the values of the univariate marginal distribution functions  $F_1, \dots, F_d$ :

$$F(\mathbf{x}) = C(F_1(x_1), \dots, F_d(x_d)) \quad \forall \mathbf{x} = (x_1, \dots, x_d)' \in [-\infty, \infty]^d. \quad (1)$$

Furthermore, the copula  $C$  is unique if  $F_1, \dots, F_d$  are continuous. It follows that a copula is just a multivariate distribution function with uniform margins. Comprehensive references on copulas are [Joe, 1997] and [Nelsen, 2006], while applications in finance and environmental sciences can be found in, e.g., [Cherubini et al., 2004] and [Salvadori et al., 2007].

Sampling from different classes of copulas has been a major subject of the copula literature of the last years. For instance, Archimedean and nested Archimedean copulas have been treated

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in [Whelan, 2004], [McNeil, 2008], [Hofert, 2008] and [Hofert, 2011], while solutions for pair-copula constructions have been discussed in [Kurowicka and Cooke, 2006], [Aas et al., 2009] and [Dißmann et al., 2013]. For an overview, we refer to [Mai and Scherer, 2012].

Recently, hierarchical Kendall copulas were proposed in [Brechmann, 2012] as a new dependence model. By grouping variables at different hierarchical levels, this model lends itself to analyses of high dimensional data that arise from applications in areas like finance and insurance. To facilitate statistical inference, groups of variables, whose dependence is described by a specific copula, are aggregated at each hierarchical level through the Kendall distribution function. This Kendall distribution function is derived from the copula of the variables and can be interpreted as the multivariate analog of the univariate probability transform. The construction therefore naturally mimics Sklar's Theorem (1) for multivariate margins.

Properties and statistical inference of hierarchical Kendall copulas are discussed in [Brechmann, 2012]. In particular, a top-down sampling procedure is proposed, which is based on the distribution of a random vector given that it lies in a particular level set. More specifically, let  $\mathbf{U} := (U_1, \dots, U_d)' \sim C$  and  $z \in (0, 1)$ . Then, the procedure involves the  $(d - 1)$ -dimensional distribution of  $\mathbf{U} | C(\mathbf{U}) = z$ . While a closed-form solution for Archimedean copulas is derived in [Brechmann, 2012], such explicit solutions are generally hard to find.

In this paper, we fill the gaps and present new top-down sampling procedures for the Plackett copula [Plackett, 1965] as well as the class of Archimax copulas [Capéraà et al., 2000], which includes the popular extreme-value copulas. In addition, we propose three approximate sampling methods that are not restricted to any particular copula class: top-down rejection-like sampling, bottom-up sample reordering, and bottom-up density resampling. The sampling accuracy of these approaches is evaluated in a simulation study.

The remainder of the paper is organized as follows. The concept of hierarchical Kendall copulas is defined and motivated in Section 2. Section 3 treats closed-form top-down sampling procedures of Plackett and Archimax copulas and reviews the method for Archimedean copulas. As an approximate solution, rejection-like sampling is proposed. Subsequently, Section 4 discusses approximate bottom-up simulation algorithms. These are evaluated and compared in Section 5.

## 2. Hierarchical Kendall copulas

Hierarchical Kendall copulas are dependence models built up from different hierarchical levels. In order to stay tractable for inference, information is aggregated at each level using Kendall distribution functions. Kendall distribution functions are multivariate analogs of the univariate probability integral transform and were first studied in [Genest and Rivest, 1993] and [Barbe et al., 1996]. For a random vector  $\mathbf{U} := (U_1, \dots, U_d)' \sim C$ , where  $C$  is a  $d$ -dimensional copula, the Kendall distribution function is defined as  $K(t) = P(C(\mathbf{U}) \leq t)$  for  $t \in (0, 1)$ . Hence, it is the distribution of the level sets of a copula,

$$L(z) = \{\mathbf{u} \in [0, 1]^d : C(\mathbf{u}) = z\}, \quad z \in (0, 1). \quad (2)$$

Here and in the following, it is assumed that copulas are absolutely continuous with continuous Kendall distribution functions. The Kendall distribution function  $K$  is then such that  $K(C(\mathbf{U})) \sim U(0, 1)$ . As such, it is a natural choice to aggregate information of a random vector within a

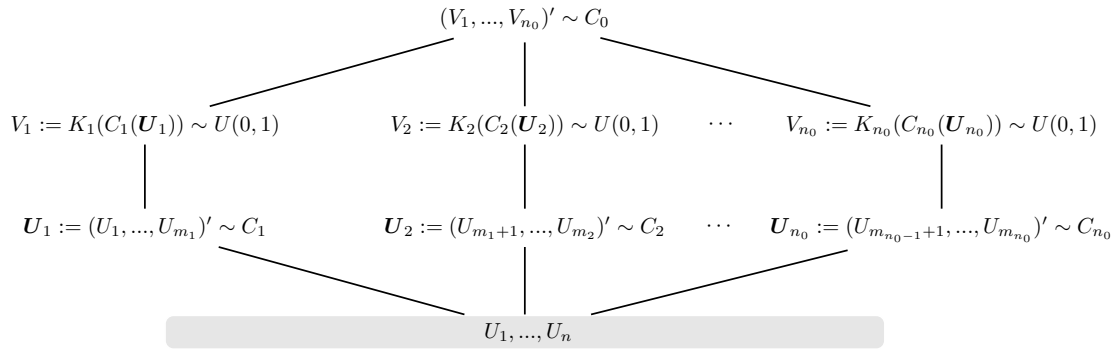


FIGURE 1. Illustration of Definition 1.

hierarchical dependence model. The following definition for the case of two hierarchical levels is given in [Brechmann, 2012].

**Definition 1** (Hierarchical Kendall copula). Let  $U_1, \dots, U_n \sim U(0, 1)$  and let  $C_0, C_1, \dots, C_{n_0}$  be copulas of dimensions  $n_0, n_1, \dots, n_{n_0}$ , respectively, where  $n_i \geq 1, i = 1, \dots, n_0$ , and  $n = \sum_{i=1}^{n_0} n_i$ . Further, let  $K_1, \dots, K_{n_0}$  denote the Kendall distribution functions corresponding to  $C_1, \dots, C_{n_0}$ . We define  $m_i = \sum_{j=1}^i n_j, i = 1, \dots, n_0$ , and  $m_0 = 0$  as well as  $\mathbf{U}_i := (U_{m_{i-1}+1}, \dots, U_{m_i})'$  and  $V_i := K_i(C_i(\mathbf{U}_i))$  for  $i = 1, \dots, n_0$ . Under the assumptions that

- $\mathcal{A}_1$ :  $\mathbf{U}_1, \dots, \mathbf{U}_{n_0}$  are mutually independent conditionally on  $(V_1, \dots, V_{n_0})'$ , and
- $\mathcal{A}_2$ : the conditional distribution of  $\mathbf{U}_i | (V_1, \dots, V_{n_0})'$  is the same as the conditional distribution of  $\mathbf{U}_i | V_i$  for all  $i = 1, \dots, n_0$ ,

the random vector  $(U_1, \dots, U_n)'$  is said to be distributed according to the hierarchical Kendall copula  $C_{\mathbb{K}}$  with nesting copula  $C_0$  and cluster copulas  $C_1, \dots, C_{n_0}$  if

1.  $\mathbf{U}_i \sim C_i \forall i \in \{1, \dots, n_0\}$ ,
2.  $(V_1, \dots, V_{n_0})' \sim C_0$ .

The construction is illustrated in Figure 1. Note that the cluster and nesting copulas can all be chosen from arbitrary copula families to build flexible models. According to [Brechmann, 2012], the density  $c_{\mathbb{K}}$  of a 2-level hierarchical Kendall copula  $C_{\mathbb{K}}$  is given as

$$c_{\mathbb{K}}(\mathbf{u}) = c_0(K_1(C_1(\mathbf{u}_1)), \dots, K_{n_0}(C_{n_0}(\mathbf{u}_{n_0}))) \prod_{i=1}^{n_0} c_i(\mathbf{u}_i), \tag{3}$$

where  $\mathbf{u} := (u_1, \dots, u_n)'$  and  $\mathbf{u}_i := (u_{m_{i-1}+1}, \dots, u_{m_i})'$  for  $i = 1, \dots, n_0$ .

The construction in Definition 1 can easily be extended to  $k > 2$  levels. In this way, it is even possible to construct higher-dimensional dependence models solely in terms of bivariate copulas. It is however sufficient to treat only the 2-level case here, since all sampling algorithms naturally extend to the general  $k$ -level case.

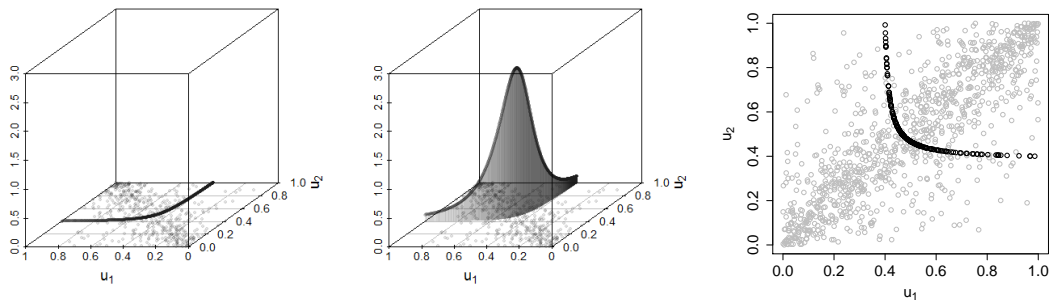


FIGURE 2. Distribution of  $\mathbf{U}|C(\mathbf{U}) = z$  for the Plackett copula. The left panel shows the level set  $L(z)$  for  $z = 0.4$  and the middle panel illustrates the probability density in  $L(z)$ . A sample in  $L(z)$  is shown in the right panel. The parameter of the Plackett copula is  $\alpha = 25$ , which corresponds to a Kendall's  $\tau$  of 0.62.

### 3. Top-down sampling

We first discuss top-down sampling procedures as proposed in [Brechmann, 2012]. The general idea of top-down simulation of hierarchical Kendall copulas is as follows.

**Algorithm 1** (Top-down sampling of hierarchical Kendall copulas). Let  $C_{\mathbb{K}}$  be a hierarchical Kendall copula with nesting copula  $C_0$  and cluster copulas  $C_1, \dots, C_{n_0}$ .

1. Sample  $\mathbf{v} = (v_1, \dots, v_{n_0})'$  from  $C_0$ .
2. Set  $z_i = K_i^{-1}(v_i) \forall i \in \{1, \dots, n_0\}$ .
3. Sample  $\mathbf{u}_i$  from  $\mathbf{U}_i|C_i(\mathbf{U}_i) = z_i$  for  $i = 1, \dots, n_0$ .
4. Return  $\mathbf{u} = (u_1, \dots, u_n)'$ .

In other words, top-down sampling proceeds by first sampling the level set (see Equation (2)) of each cluster (top of Figure 1) and then generating observations from each cluster given that level set (bottom of Figure 1). While Step 1 is fairly standard for most known copulas (see, e.g., [Mai and Scherer, 2012]), Step 3 is more challenging: Let  $\mathbf{U} \sim C$ , where  $C$  is a  $d$ -dimensional copula, then we need to sample from the distribution of  $\mathbf{U}|C(\mathbf{U}) = z$  as illustrated in Figure 2 for the Plackett copula (see Section 3.2). A common approach to this issue is using the conditional inverse method. It proceeds by iteratively sampling  $u_j$  from the conditional distribution of  $U_j|(U_1 = u_1, \dots, U_{j-1} = u_{j-1}, C(\mathbf{U}) = z)$  for  $j = 1, \dots, d - 1$ . Finally,  $u_d$  is given by solving  $C(\mathbf{u}) = z$  for  $u_d$ . Solutions for common classes of copulas are discussed in the following. Alternatively, rejection-like sampling may be used.

#### 3.1. Archimedean copulas

A  $d$ -dimensional Archimedean copula with  $d$ -monotone generator  $\varphi$  (see [McNeil and Nešlehová, 2009]) is defined as  $C(u_1, \dots, u_d; \varphi) = \varphi^{-1}(\varphi(u_1) + \dots + \varphi(u_d))$  and possesses a closed-form expression of the Kendall distribution function in terms of its generator (see [Barbe et al., 1996])

and [McNeil and Nešlehová, 2009]),

$$K(t; \varphi) = t + \sum_{i=1}^{d-2} \frac{(-\varphi(t))^i}{i!} (\varphi^{-1})^{(i)}(\varphi(t)) + \frac{(-\varphi(t))^{d-1}}{(d-1)!} (\varphi^{-1})^{(d-1)}(\varphi(t)),$$

where  $(\varphi^{-1})^{(d-1)}_-$  denotes the left-hand derivative of  $\varphi^{-1}$  of order  $d-1$ . Two alternatives to conditionally sample from an Archimedean copula are presented in [Brechmann, 2012]. First, a closed-form conditional inverse sampling algorithm is derived solely in terms of the generator (see also [Wu et al., 2007]).

**Algorithm 2** (Conditional inverse method for Archimedean copulas). Let  $C(\cdot; \varphi)$  be a  $d$ -dimensional Archimedean copula with generator  $\varphi$  and  $z \in (0, 1)$ .

1. Sample  $w_1, \dots, w_{d-1}$  independently from the uniform distribution.
2. Set  $u_j = \varphi^{-1}((1 - w_j^{1/(d-j)})(\varphi(z) - \sum_{1 \leq i < j} \varphi(u_i)))$  for  $j = 1, \dots, d-1$ .
3. Set  $u_d = \varphi^{-1}(\varphi(z) - \sum_{1 \leq i < d} \varphi(u_i))$ .
4. Then  $\mathbf{u} = (u_1, \dots, u_d)'$  are observations from  $\mathbf{U}|C(\mathbf{U}; \varphi) = z$ .

Alternatively, a result of [McNeil and Nešlehová, 2009] may be exploited, which relates Archimedean copulas to  $\ell_1$ -norm symmetric distributions and allows to precisely characterize the  $(d-1)$ -dimensional space, on which the distribution of  $\mathbf{U}|C(\mathbf{U}; \varphi) = z$  is defined. In particular,

$$[\mathbf{U}|C(\mathbf{U}; \varphi) = z] \stackrel{d}{=} (\varphi^{-1}(S_1 \varphi(z)), \dots, \varphi^{-1}(S_d \varphi(z))),$$

where  $\mathbf{S} = (S_1, \dots, S_d)'$  is uniformly distributed on the unit simplex  $\{\mathbf{x} \geq \mathbf{0} : \sum_{j=1}^d x_j = 1\}$ .

This characterization as a distribution projected to a  $(d-1)$ -dimensional space allows to state the following alternative sampling algorithm for Archimedean copulas.

**Algorithm 3** (Projected distribution sampling for Archimedean copulas). Let  $C(\cdot; \varphi)$  be a  $d$ -dimensional Archimedean copula with generator  $\varphi$  and  $z \in (0, 1)$ .

1. Sample  $(s_1, \dots, s_d)'$  from  $\mathbf{S}$ .
2. Set  $u_j := \varphi^{-1}(s_j \varphi(z))$  for  $j = 1, \dots, d$ .
3. Then  $\mathbf{u} = (u_1, \dots, u_d)'$  are observations from  $\mathbf{U}|C(\mathbf{U}; \varphi) = z$ .

For copulas with similar characterization results for the distribution of  $\mathbf{U}|C(\mathbf{U}) = z$ , analogous sampling procedures could be used. However, generally the conditional inverse method and variants of it, as also employed in the following two sections, seem more promising.

### 3.2. Plackett copula

The Plackett copula [Plackett, 1965, Mardia, 1970] is a bivariate copula, which is derived through the constant cross-product ratio

$$\frac{C(u_1, u_2; \alpha)(1 - u_1 - u_2 + C(u_1, u_2; \alpha))}{(u_1 - C(u_1, u_2; \alpha))(u_2 - C(u_1, u_2; \alpha))} = \alpha + 1, \quad \alpha \in (-1, \infty) \setminus \{0\},$$

and is of the form

$$C(u_1, u_2; \alpha) = \frac{1}{2\alpha} \left( 1 + \alpha(u_1 + u_2) - \sqrt{(1 + \alpha(u_1 + u_2))^2 - 4\alpha(\alpha + 1)u_1u_2} \right). \quad (4)$$

It does not belong to either one of the popular classes of elliptical, Archimedean and extreme-value copulas. If  $\alpha \rightarrow -1$ ,  $C(\cdot, \cdot; \alpha)$  converges to the countermonotonic copula, while comonotonicity is obtained for  $\alpha \rightarrow \infty$ . Further, the independence copula is the limit as  $\alpha \rightarrow 0$ . The density of the Plackett copula is denoted by  $c(\cdot, \cdot; \alpha)$ .

Let  $(U_1, U_2)' \sim C(\cdot, \cdot; \alpha)$  and define  $Z := C(U_1, U_2; \alpha)$ . In [Brechmann, 2012] it is shown that the conditional distribution function  $F_{U_1|Z}$  can be determined for  $u \in (z, 1)$  as

$$F_{U_1|Z}(u; z, \alpha) = \frac{\int_z^u g(u_1; z, \alpha) du_1}{\int_z^1 g(u_1; z, \alpha) du_1},$$

where  $g(u_1; z, \alpha) = c(u_1, C^{-1}(z; u_1, \alpha); \alpha) \frac{\partial}{\partial z} C^{-1}(z; u_1, \alpha)$ , and  $C^{-1}(\cdot; u_1, \alpha)$  denotes the inverse of the copula  $C(\cdot, \cdot; \alpha)$  with respect to the second argument such that  $C(u_1, C^{-1}(z; u_1, \alpha); \alpha) = z$ . This inverse can be determined for the Plackett copula (4) as

$$C^{-1}(z; u, \alpha) = z \frac{1 + \alpha(u - z)}{z + (\alpha + 1)(u - z)}.$$

If  $D(z, \alpha) = 4\alpha z(\alpha(1 - z) + 1) - \alpha - 1 > 0$ , the following closed-form expression for the conditional distribution function could be conveniently derived with the help of a computer algebra system:

$$F_{U_1|Z}(u; z, \alpha) = \left( \frac{\alpha^2 z(1 + \alpha)(u - z) \left( (1 + \alpha)(2\alpha(uz + z - u) - u - 1) - 2\alpha^2 z^2 \right)}{u(1 + \alpha)(1 + \alpha(u - 2z)) + \alpha^2 z^2} + h(u; z, \alpha, \sigma, \beta) \right) / \left( 2\alpha^2 z(1 + \alpha)(z - 1) + h(1; z, \alpha, \sigma, \beta) \right),$$

where

$$h(w; z, \alpha, \sigma, \beta) := \sigma \beta (\arctan(\sigma) + \arctan(\sigma(2\alpha(z - w) - 1)))$$

with

$$\sigma = \sigma(z, \alpha) := \sqrt{\frac{1 + \alpha}{4\alpha z(1 + \alpha(1 - z)) - \alpha - 1}}$$

$$\beta = \beta(z, \alpha) := -(1 + \alpha(1 - 2z) + 2\alpha^2 z(z - 1))(1 + \alpha(1 - 2z)).$$

If  $D(z, \alpha) < 0$ , the arctangent function in  $h(\cdot; z, \alpha, \sigma, \beta)$  needs to be replaced by the inverse hyperbolic (co)tangent function for  $\alpha < 0$  ( $\alpha > 0$ ). In the case  $D(z, \alpha) = 0$ , the conditional distribution function  $F_{U_1|Z}(\cdot; z, \alpha)$  reduces to a rational function.

Therefore, we have the following conditional inverse sampling algorithm for Plackett copulas.

**Algorithm 4** (Conditional simulation of the Plackett copula). Let  $C(\cdot, \cdot; \alpha)$  be a Plackett copula with parameter  $\alpha \in (-1, \infty) \setminus \{0\}$  and  $z \in (0, 1)$ .

1. Sample  $w$  from the uniform distribution.
2. Set  $u_1 = F_{U_1|Z}^{-1}(w; z, \alpha)$  and  $u_2 = C^{-1}(z; u_1, \alpha)$ .
3. Then  $(u_1, u_2)'$  are observations from  $(U_1, U_2) | C(U_1, U_2; \alpha) = z$ .

An exemplary sample drawn according to this conditional simulation algorithm is shown in the right panel of Figure 2.

Another copula that does not belong to the above-mentioned three popular classes of copulas is the Farlie-Gumbel-Morgenstern (FGM) copula, which may be interpreted as first-order approximation of the Plackett copula [Nelsen, 2006, Exercise 3.39]. For the FGM copula, a similar derivation as the above is possible but does not lead to such a convenient closed-form expression. Also note that the range of dependence that can be modeled by an FGM copula is rather limited in contrast to the Plackett copula family [Nelsen, 2006, Example 5.2].

### 3.3. Archimax copulas

A further class of bivariate copulas, which encompasses both the classes of Archimedean and of extreme-value copulas, are Archimax copulas [Capéraà et al., 2000]. They are defined as

$$C(u_1, u_2; \varphi, A) = \varphi^{-1} \left( (\varphi(u_1) + \varphi(u_2)) A \left( \frac{\varphi(u_1)}{\varphi(u_1) + \varphi(u_2)} \right) \right), \quad (5)$$

where  $\varphi$  is a 2-monotone Archimedean generator (see [McNeil and Nešlehová, 2009]) and  $A : [0, 1] \rightarrow [1/2, 1]$  is a convex function satisfying  $\max(t, 1-t) \leq A(t) \leq 1$  for all  $t \in [0, 1]$ . The function  $A$  is typically called *dependence function* but should not be confounded with the copula itself. Note that if  $A(t) \equiv 1$ , then the Archimax copula (5) becomes a bivariate Archimedean copula with generator  $\varphi$ . Conversely, if  $\varphi(t) = -\log(t)$  (generator of the independence copula), it corresponds to an extreme-value copula with dependence function  $A$  (see [Pickands, 1981]). The Gumbel copula is known to be the only copula that belongs to both classes [Genest and Rivest, 1989].

Let  $(U_1, U_2)' \sim C(\cdot, \cdot; \varphi, A)$  and define  $V := \varphi(U_1) / (\varphi(U_1) + \varphi(U_2))$  and  $Z := C(U_1, U_2; \varphi, A)$ . Assuming that all required derivatives exist, it holds according to [Capéraà et al., 2000, Proposition 5.1] that

$$P(V \leq v, Z \leq z) = K_\varphi(z) \left( v + v(1-v) \frac{A'(v)}{A(v)} \right) + (z - K_\varphi(z)) \tau_A(v), \quad v, z \in [0, 1],$$

where  $K_\varphi(z) = z - \varphi(z) / \varphi'(z)$  is the Kendall distribution function of the bivariate Archimedean copula with generator function  $\varphi$  and

$$\tau_A(v) = \int_0^v \frac{t(1-t)}{A(t)} dA'(t),$$

which is the Kendall's  $\tau$  of the extreme-value copula with dependence function  $A$  if  $v = 1$  (see also [Ghoudi et al., 1998]). It follows that the Kendall distribution function of an Archimax copula is given by

$$K(z; \varphi, A) = P(Z \leq z) = K_\varphi(z) + (z - K_\varphi(z)) \tau_A(1),$$



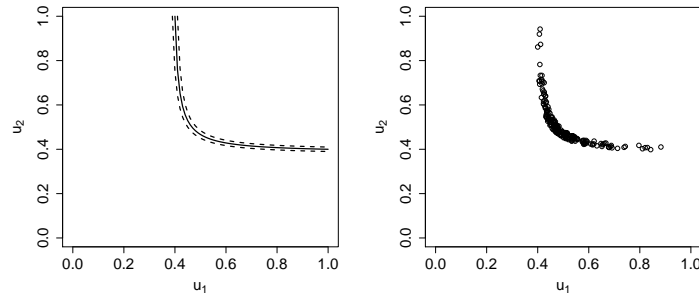


FIGURE 3. Left panel: level set  $L(z)$  at  $z = 0.4$  of the Plackett copula with parameter  $\alpha = 25$  (solid line). The dashed lines illustrate the non-rejection area  $(z - \varepsilon, z + \varepsilon)$  for  $\varepsilon = 0.01$ . Right panel: scatter plot of corresponding samples generated through rejection-like sampling.

and

$$F_{V|Z}(v; z, \varphi, A) := P(V \leq v | Z = z) = \frac{k_\varphi(z) \left( v + v(1-v) \frac{A'(v)}{A(v)} \right) + (1 - k_\varphi(z)) \tau_A(v)}{1 - (1 - \tau_A(1))(1 - k_\varphi(z))},$$

where  $k_\varphi(z) = K'_\varphi(z) = \varphi(z)\varphi''(z)/(\varphi'(z))^2$ .

This gives the following simulation algorithm for Archimax copulas, which is a variant of the standard conditional inverse method.

**Algorithm 5** (Conditional simulation of Archimax copulas). Let  $C(\cdot, \cdot; \varphi, A)$  be an Archimax copula with generator  $\varphi$  and dependence function  $A$ . Further, let  $z \in (0, 1)$ .

1. Sample  $w$  from the uniform distribution.
2. Set  $v = F_{V|Z}^{-1}(w; z, \varphi, A)$ .
3. Set  $u_1 = \varphi^{-1} \left( v \frac{\varphi(z)}{A(v)} \right)$  and  $u_2 = \varphi^{-1} \left( (1-v) \frac{\varphi(z)}{A(v)} \right)$ .
4. Then  $(u_1, u_2)'$  are observations from  $(U_1, U_2) | C(U_1, U_2; \varphi, A) = z$ .

Note that the values  $u_1$  and  $u_2$  are the solutions of the equations  $\varphi(u_1)/(\varphi(u_1) + \varphi(u_2)) = v$  and  $C(u_1, u_2; \varphi, A) = z$ .

### 3.4. Rejection-like sampling

For classes of copulas, for which no closed-form solutions are available, such as the elliptical copulas, approximate rejection-like sampling may be used to generate approximate observations from  $\mathbf{U} | C(\mathbf{U}) = z$ : Instead of sampling from  $\mathbf{U} | C(\mathbf{U}) = z$ , one chooses a small number  $\varepsilon > 0$  and samples from  $\mathbf{U} | (z - \varepsilon < C(\mathbf{U}) < z + \varepsilon)$ . This is illustrated in the left panel of Figure 3.

**Algorithm 6** (Rejection-like sampling). Let  $C$  be a  $d$ -dimensional copula,  $z \in (0, 1)$  and  $\varepsilon > 0$ .

1. Sample  $\mathbf{u}$  from  $C$ .



2. If  $|C(\mathbf{u}) - z| < \varepsilon$ , return  $\mathbf{u}$ . Otherwise go back to Step 1.

The right panel of Figure 3 shows an exemplary sample from a Plackett copula with parameter  $\alpha = 25$  at level  $z = 0.4$ . The error  $\varepsilon$  is chosen as 0.01. Notice in particular the difference to the closed-form solution in Figure 2.

The accuracy of this approximate method can be controlled through the choice of  $\varepsilon > 0$ , which is an upper bound on the absolute sampling error  $|C(\mathbf{u}) - z|$ . The smaller  $\varepsilon$  is, the more accurate the results are, but, at the same time, the higher the computing time is. We will assess this trade-off in a simulation study in Section 5.

#### 4. Bottom-up sampling

In this section we propose two methods for bottom-up sampling of hierarchical Kendall copulas as alternatives to the top-down approach discussed above. Both methods have in common that they start by drawing a sample of multivariate independent observations. These observations are then appropriately reordered (first method) or resampled (second method) such that they represent an approximate sample of the hierarchical Kendall copula. This means that we essentially start at the bottom of Figure 1 and then adjust the sample according to the hierarchical dependence structure of the model.

Here, the nature of the approximation to the true distribution is different to rejection-like sampling, which allows for setting an explicit error bound. When using either one of the presented bottom-up sampling methods, convergence to the true distribution is only attained with increasing sample sizes. In other words, in small samples the exact underlying distribution is unknown, leading to potentially false conclusions. Such small-sample effects are therefore investigated in the simulation study in Section 5.

##### 4.1. Sample reordering

In the context of hierarchical dependence models, the use of sample reordering, which was originally described in [Iman and Conover, 1982], is proposed in [Arbenz et al., 2012]. The idea of sample reordering is to independently sample margins and the copula and then to reorder the independent margins according to the ranks of the dependent sample generated from the copula. For hierarchical copulas, this may be used to reorder aggregated samples from the different clusters according to a sample from the nesting copula. Bottom-up sampling using sample reordering proceeds as follows.

**Algorithm 7** (Sample reordering of hierarchical Kendall copulas). Let  $C_{\mathbb{K}}$  be a hierarchical Kendall copula with nesting copula  $C_0$  and cluster copulas  $C_1, \dots, C_d$ .

1. Generate a sample  $(\mathbf{u}_i^I)_{i=1, \dots, N}$  of size  $N$  from the  $n$ -dimensional independence copula.
2. Generate samples  $(u_{i, m_{k-1}+1}^0, \dots, u_{i, m_k}^0)_{i=1, \dots, N}$  of size  $N$  from the cluster copulas  $C_1, \dots, C_{n_0}$ .
3. Set  $p_j(i) = \sum_{\ell=1}^N \mathbf{1}_{\{u_{\ell j}^0 \leq u_{ij}^0\}}$ , the rank of  $u_{ij}^0$  among  $(u_{1j}^0, \dots, u_{Nj}^0)'$ , for  $j = 1, \dots, n$ .
4. Set  $u_{p_j(i), j}^C = u_{(i), j}^I$  for  $j = 1, \dots, n$ , where  $u_{(i), j}^I$  is the  $i$ th order statistic of  $(u_{1j}^I, \dots, u_{Nj}^I)'$  such that  $u_{(1), j}^I \leq u_{(2), j}^I \leq \dots \leq u_{(N), j}^I$ .

5. Set  $v_{ik}^I = K_k(C_k(u_{i,m_{k-1}+1}^C, \dots, u_{i,m_k}^C))$  for  $k = 1, \dots, n_0$ .
6. Generate a sample  $(v_i^0)_{i=1, \dots, N}$  of size  $N$  from the nesting copula  $C_0$ .
7. Set  $q_k(i) = \sum_{\ell=1}^N 1_{\{v_{ik}^0 \leq v_{i\ell}^0\}}$ , the rank of  $v_{ik}^0$  among  $(v_{1k}^0, \dots, v_{Nk}^0)'$ , and  $r_k(i) = \sum_{\ell=1}^N 1_{\{v_{ik}^I \leq v_{i\ell}^I\}}$ , the rank of  $v_{ik}^I$  among  $(v_{1k}^I, \dots, v_{Nk}^I)'$ , for  $k = 1, \dots, n_0$ .
8. Return the observations  $u_{q_{k(j)}(i), j} = u_{r_{k(j)}(i), j}^I$ ,  $i = 1, \dots, N$ , where  $k(j)$  is the cluster of variable  $j \in \{1, \dots, n\}$ .

In Steps 1-4 a sample from each cluster copula  $C_k$ ,  $k = 1, \dots, n_0$ , is generated using the method described in [Iman and Conover, 1982]. Clearly, Steps 1, 3 and 4 are redundant given Step 2, but we include them, since they show how other margins than uniform can be used instead. The final sample from the hierarchical Kendall copula is obtained by reordering the original independent sample according to the independent aggregated clusters in Step 5 and the dependent sample from the nesting copula  $C_0$  in Step 6. That is, the sample is reordered twice: first according to the cluster copulas, and second according to the nesting copula.

Strong uniform consistency of this method as  $N \rightarrow \infty$  was recently shown under certain regularity conditions stated in [Mainik, 2012], where also convergence rates are given. These conditions are satisfied by any componentwise non-decreasing aggregation function and by any copula with bounded density. Aggregation using the Kendall distribution function and the copula clearly is componentwise non-decreasing, since copulas are multivariate distribution functions and Kendall distribution functions are non-decreasing. However, most common copulas such as the Gaussian, the Student's t or the Clayton have unbounded density. In [Mainik, 2012] convergence is shown for the Gaussian and the Clayton copula but remains an open question for other families.

#### 4.2. Density resampling

In contrast to the bottom-up method presented in the previous section, this method does not modify the observations per variable but leaves them as they are. For copulas with available density, the density resampling approach has been proposed in [Kurowicka and Cooke, 2006, Section 6.4.3]. The idea is to resample from a large number of independent uniform observations according to probabilities proportional to the density evaluated at the observations (see also the sampling/importance resampling method described in [Rubin, 1987, Rubin, 1988]).

For hierarchical Kendall copulas with density given in Equation (3), this can be used as follows.

**Algorithm 8** (Density resampling of hierarchical Kendall copulas). Let  $C_{\mathbb{K}}$  be a hierarchical Kendall copula with density  $c_{\mathbb{K}}$ . To generate a sample of size  $N$ , let  $N' \gg N$ .

1. Generate a sample  $(\mathbf{w}_i)_{i=1, \dots, N'}$  of size  $N'$  from the  $n$ -dimensional independence copula.
2. Resample  $N$  times from  $(\mathbf{w}_i)_{i=1, \dots, N'}$  according to probabilities proportional to  $c_{\mathbb{K}}(\mathbf{w}_i)$ ,  $i = 1, \dots, N'$ . That is, draw a sample  $\Lambda$  of size  $N$  without replacement from  $\{1, \dots, N'\}$  according to probabilities  $p_i = c_{\mathbb{K}}(\mathbf{w}_i) / \sum_{i=1}^{N'} c_{\mathbb{K}}(\mathbf{w}_i)$ ,  $i = 1, \dots, N'$ .
3. Return the resulting sample  $(\mathbf{u}_i)_{i=1, \dots, N} := (\mathbf{w}_i)_{i \in \Lambda}$ .

Clearly, this is rather inefficient, since  $N'$  should be chosen significantly larger than  $N$  to generate a reasonably good sample. Especially when the evaluation of the density  $c_{\mathbb{K}}$  is computationally

fast, it may however be considered as an alternative to rejection-like sampling (Section 3.4) and also to sample reordering (Section 4.1), which may also require a large number of observations to generate an accurate sample. The finite sample performance and the computing time of all three approximate sampling approaches are considered in a numerical study in the next section. In particular, two different choices of  $N'$  relative to  $N$  are compared.

## 5. Numerical comparison

Three of the methods discussed here are approximate: rejection-like sampling (Section 3.4), sample reordering (Section 4.1) and density resampling (Section 4.2). We therefore perform a simulation study in order to assess these approaches to sampling from hierarchical Kendall copulas. In particular, we investigate different choices of  $\varepsilon$  for rejection-like sampling (see Algorithm 6) and of  $N'$  for density resampling (see Algorithm 8); sample reordering does not require any choice of control parameters.

The sampling procedures are compared based on a four-dimensional hierarchical Kendall copula with bivariate Clayton and Joe cluster copulas and Gaussian nesting copula. The cluster copulas are tail-asymmetric with lower and upper tail dependence, respectively. The Gaussian nesting copula is tail independent. Parameters are chosen according to a Kendall's  $\tau$  of  $\tau_0 = 0.5$  for the Gaussian copula (medium dependence; copula parameter of  $\theta_0 = 0.71$ ) and  $\tau_1 = \tau_2 = 0.7$  for the cluster copulas (strong dependence; copula parameters of  $\theta_1 = 4.67$  for the Clayton and  $\theta_2 = 5.46$  for the Joe copula). In the case of sample reordering, convergence for the Clayton and the Gaussian copula is shown in [Mainik, 2012] but not for the Joe copula. We therefore verify the required regularity conditions (15) and (16) of [Mainik, 2012] along the lines of Proposition 4.2 in [Mainik, 2012]. The density of the Joe copula is given for  $\theta > 1$  as

$$c(u_1, u_2; \theta) = \left( (1-u_1)^\theta + (1-u_2)^\theta - (1-u_1)^\theta (1-u_2)^\theta \right)^{1/\theta-2} (1-u_1)^{\theta-1} (1-u_2)^{\theta-1} \quad (6)$$

$$\times \left( \theta - 1 + (1-u_1)^\theta + (1-u_2)^\theta - (1-u_1)^\theta (1-u_2)^\theta \right). \quad (7)$$

We observe that  $K(\varepsilon) = \text{esssup}\{c(u_1, u_2; \theta) : (u_1, u_2)' \in [\varepsilon, 1 - \varepsilon]^2\}$  is polynomial, since the term in (7) is bounded by  $\theta$ ,  $(1-u_i)^{\theta-1} \leq 1$  for  $i = 1, 2$ , and the first term in (6) can be rewritten as

$$\left( \left( \frac{1-u_1}{1-u_2} \right)^\theta + \left( \frac{1-u_2}{1-u_1} \right)^\theta - 1 \right)^{1/\theta-2} ((1-u_1)(1-u_2))^{1-2\theta} \leq ((1-u_1)(1-u_2))^{1-2\theta},$$

which is a polynomial. This proves condition (16) of [Mainik, 2012]. The proof of condition (15) is exactly as in [Mainik, 2012, Proposition 4.2], noting that for fixed  $u_2 \in (0, 1)$  the copula density  $c(\cdot, u_2; \theta)$  reaches its maximum at

$$u_1^* = u_1^*(u_2) = \max \left\{ 1 - \left( \frac{(1-u_2)^\theta (1 - (1-u_2)^\theta - \theta)}{((1-u_2)^\theta - 1)(\theta - (1-u_2)^\theta)} \right)^{1/\theta}, 0 \right\}.$$

This means that it is actually reasonable to use sample reordering here.

As benchmark for the approximate methods, we generate a large sample  $(\mathbf{u}_i^0)_{i=1, \dots, N^*}$  of size  $N^* = 1\,000\,000$  using closed-form conditional inverse sampling for Archimedean copulas (see

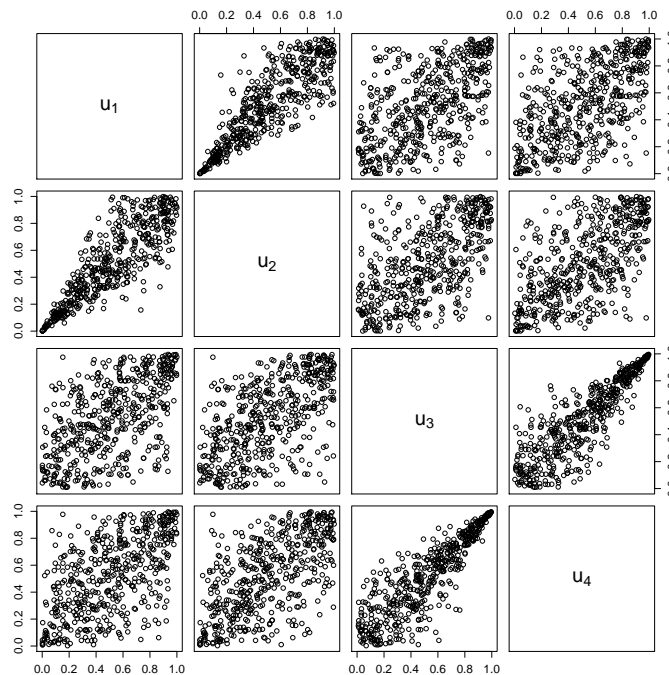


FIGURE 4. A sample of size 500 from the simulated benchmark data. Variables 1 and 2 form the first cluster with Clayton copula, variables 3 and 4 the second with Joe copula.

Algorithms 2, 3 and 5), since both the Clayton and the Joe copula families are Archimedean. As an illustration, a sample of size 500 of this benchmark data is shown in Figure 4.

To compare the different approaches, we generate samples  $(\mathbf{u}_i)_{i=1,\dots,N}$  of different sizes  $N \in \{100, 200, 500, 1000, 2000\}$  and compare different evaluation criteria. The following six criteria are considered based on  $R = 1000$  repetitions:

1. Mean squared difference of pairwise Kendall's  $\tau$  values:

$$\frac{1}{R} \sum_{r=1}^R \frac{1}{6} \sum_{1 \leq i < j \leq 4} \left( \widehat{\tau}_{ij}^{(r)} - \widehat{\tau}_{ij}^0 \right)^2,$$

where  $\widehat{\tau}_{ij}^{(r)}$  is the empirical Kendall's  $\tau$  of variables  $i$  and  $j$  in repetition  $r$  and  $\widehat{\tau}_{ij}^0$  that of the benchmark data.

2. Mean squared difference of pairwise lower-tail Kendall's  $\tau$  values:

$$\frac{1}{R} \sum_{r=1}^R \frac{1}{6} \sum_{1 \leq i < j \leq 4} \left( \widehat{\tau}_{ij,L}^{(r)} - \widehat{\tau}_{ij,L}^0 \right)^2,$$

where  $\widehat{\tau}_{ij,L}^{(r)}$  is the empirical 20% lower-tail Kendall's  $\tau$  of variables  $i$  and  $j$  in repetition  $r$  and  $\widehat{\tau}_{ij,L}^0$  that of the benchmark data. The 20% lower-tail Kendall's  $\tau$  is given for two

uniform random variables  $U_1$  and  $U_2$  as the Kendall's  $\tau$  of  $(U_1, U_2 | U_1 < 0.2, U_2 < 0.2)$ . It is a rank-based version of the exceedance correlation coefficient used in [Longin and Solnik, 2001] and serves as a measure of lower tail behavior.

3. Mean squared difference of pairwise upper-tail Kendall's  $\tau$  values:

$$\frac{1}{R} \sum_{r=1}^R \frac{1}{6} \sum_{1 \leq i < j \leq 4} \left( \widehat{\tau}_{ij,U}^{(r)} - \widehat{\tau}_{ij,U}^0 \right)^2,$$

where  $\widehat{\tau}_{ij,L}^{(r)}$  is the empirical 20% upper-tail Kendall's  $\tau$  of variables  $i$  and  $j$  in repetition  $r$  and  $\widehat{\tau}_{ij,L}^0$  that of the benchmark data. The 20% upper-tail Kendall's  $\tau$  is defined in an analogous way as the lower-tail Kendall's  $\tau$  and measures upper tail behavior.

4. Mean squared difference of empirical copulas:

$$\frac{1}{R} \sum_{r=1}^R \frac{1}{|\Delta|^4} \sum_{\mathbf{v} \in \Delta^4} \left( \widehat{C}^{(r)}(\mathbf{v}) - \widehat{C}^0(\mathbf{v}) \right)^2,$$

where  $\widehat{C}^{(r)}$  is the empirical copula of the sample  $(\mathbf{u}_i^{(r)})_{i=1,\dots,N}$  in the  $r$ th repetition and  $\widehat{C}^0$  that of the benchmark data. Further,  $\Delta$  is an equispaced partition of  $[0, 1]$  of size  $|\Delta| = 25$ . That is, in each repetition the empirical copulas are evaluated at  $|\Delta|^4 = 25^4 = 390625$  points of  $[0, 1]^4$ .

5. Mean squared difference of log-likelihoods:

$$\frac{1}{R} \sum_{r=1}^R \left( \frac{1}{N} \sum_{i=1}^N \log c_{\mathbb{K}}(\mathbf{u}_i^{(r)}) - \frac{1}{N^*} \sum_{i=1}^{N^*} \log c_{\mathbb{K}}(\mathbf{u}_i^0) \right)^2,$$

where  $\mathbf{u}_i^{(r)}$  denotes the  $i$ th observations in the  $r$ th repetition and  $c_{\mathbb{K}}$  is the density of the hierarchical Kendall copula (see Equation (3)) evaluated at the true parameters. The log-likelihoods are standardized by the sample sizes to allow for comparison.

6. Mean squared difference of parameters:

$$\frac{1}{R} \sum_{r=1}^R \frac{1}{3} \sum_{i \in \{0,1,2\}} \left( \tau_i(\widehat{\theta}_i) - \tau_i \right)^2,$$

where  $\widehat{\theta}_i$  are maximum likelihood estimates of  $\theta_i$ ,  $i = 0, 1, 2$ , which are transformed to Kendall's  $\tau$  values using the respective relationships  $\tau_i(\cdot)$  implied by the copulas (see, e.g., [Brechmann and Schepsmeier, 2013]).

While the first three criteria focus on data characteristics, namely the level of general dependence as well as lower and upper tail behavior, the fourth criterion directly compares the empirical copulas and the last two criteria investigate the effects on estimation and model selection.

Based on these six criteria we evaluate and compare the three approximate procedures. For rejection-like sampling we choose  $\varepsilon \in \{10^{-2}, 10^{-3}, 10^{-4}\}$ , while for density resampling we choose  $N'$  as a multiple of  $N$ , namely  $N'/N \in \{100, 1000\}$ . Simulation results for all three

TABLE 1. Results of the simulation study: evaluation criteria per method and sample size  $N$ . For better readability, all numbers, except for the mean computing time, are multiplied by 1000.

$N$	Rejection ( $\varepsilon = 10^{-2}$ )	Rejection ( $\varepsilon = 10^{-3}$ )	Rejection ( $\varepsilon = 10^{-4}$ )	Reordering	Resampling ( $N' = 100N$ )	Resampling ( $N' = 1000N$ )
Mean squared difference of pairwise Kendall's $\tau$ values						
100	2.370	2.288	2.320	2.349	6.937	2.790
200	1.157	1.141	1.155	1.129	5.835	1.586
500	0.433	0.435	0.446	0.410	5.165	0.907
1000	0.214	0.211	0.215	0.227	4.870	0.694
2000	0.107	0.108	0.107	0.106	4.752	0.585
Mean squared difference of pairwise lower-tail Kendall's $\tau$ values						
100	59.918	55.171	59.534	58.778	114.189	69.979
200	22.160	21.929	21.746	22.188	45.796	27.472
500	7.728	7.839	7.792	7.483	20.606	11.178
1000	3.722	3.663	3.658	3.754	14.754	6.290
2000	1.751	1.817	1.796	1.788	11.942	4.731
Mean squared difference of pairwise upper-tail Kendall's $\tau$ values						
100	58.545	57.782	55.722	54.802	131.255	77.715
200	21.718	21.071	21.520	21.387	47.561	28.954
500	7.335	7.478	7.397	7.573	24.404	12.906
1000	3.678	3.611	3.609	3.693	17.016	7.993
2000	1.816	1.773	1.854	1.721	14.539	6.306
Mean squared difference of empirical copulas						
100	1.069	1.072	1.086	0.870	1.410	1.010
200	0.550	0.557	0.563	0.423	0.930	0.545
500	0.219	0.220	0.220	0.173	0.694	0.245
1000	0.101	0.103	0.103	0.083	0.574	0.155
2000	0.056	0.057	0.057	0.043	0.539	0.102
Mean squared difference of log-likelihoods						
100	36.936	38.659	36.622	538.005	188.034	55.476
200	17.295	18.048	18.821	193.092	178.572	39.643
500	7.137	7.038	7.081	42.874	177.134	31.608
1000	3.764	3.638	3.532	14.238	171.918	30.154
2000	1.762	1.838	1.810	4.735	172.114	28.672
Mean squared difference of parameters						
100	2.089	2.019	2.019	8.280	5.164	4.337
200	0.561	0.545	0.547	3.321	2.269	1.206
500	0.162	0.159	0.160	0.896	0.574	0.196
1000	0.081	0.077	0.078	0.348	0.345	0.112
2000	0.039	0.039	0.039	0.135	0.303	0.068
Mean computing time (in seconds)						
100	0.642	4.486	42.517	0.006	0.126	1.304
200	1.017	6.019	54.021	0.008	0.257	2.816
500	2.060	9.818	87.708	0.014	0.709	9.574
1000	4.042	15.227	128.706	0.025	1.623	25.079
2000	9.067	28.012	218.319	0.044	4.279	69.327

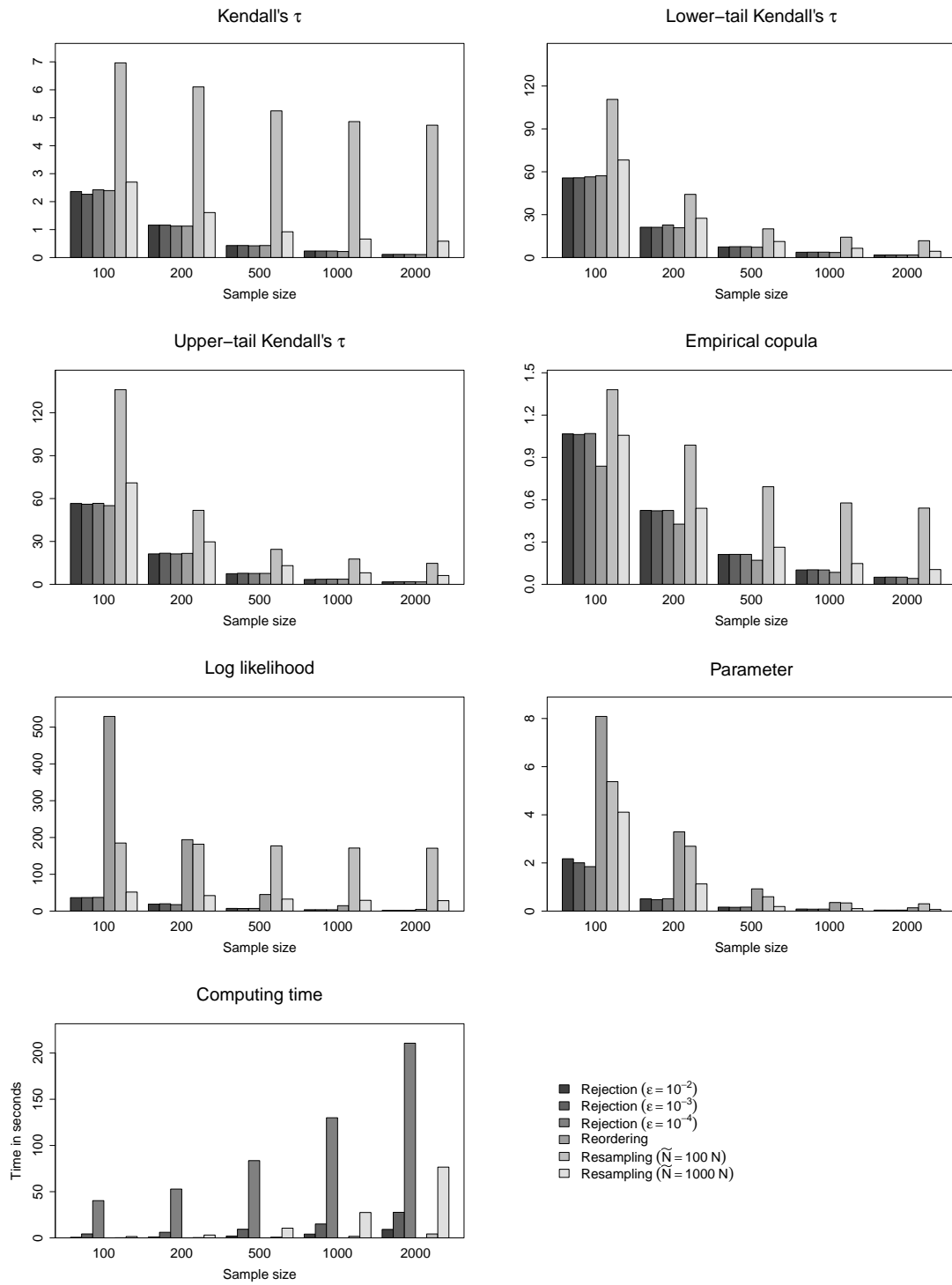


FIGURE 5. Illustration of the results of the simulation study reported in Table 1.



methods and all six criteria are shown in Table 1 and illustrated in Figure 5. In addition, we report the mean computing time in seconds (on a 2.6Ghz AMD Opteron).

With respect to the data characteristics of Kendall's  $\tau$  as well as lower- and upper-tail Kendall's  $\tau$ , rejection-like sampling and sample reordering give very similar results. Most interestingly, the choice of the error  $\varepsilon$  in rejection-like sampling has only little influence on the results. The choice of  $N'$  in relation to the sample size  $N$  for density resampling however strongly influences the performance. Only if  $N'/N = 1000$ , the results are similarly good as for the other two methods. In general, it should be noted that the general dependence in terms of Kendall's  $\tau$  is better approximated than tail behavior as measured by the lower- and upper-tail Kendall's  $\tau$ . For larger sample sizes, the differences are however quite small, so that we can conclude that simulation using rejection-like sampling, sample reordering and, to some extent, density resampling appropriately reproduces data characteristics.

Results are similar for the empirical copula. The criterion is minimized when sample reordering is used, but also rejection-like sampling and density resampling with  $N'/N = 1000$  work quite well. As before, this holds irrespective of the choice of  $\varepsilon$  in rejection-like sampling. Choosing  $N'/N = 100$  for density resampling is however clearly too small.

In terms of log-likelihoods and copula parameters, the results provide additional insights which allow to better discriminate among the methods. While rejection-like sampling does very well and shows little dependence on  $\varepsilon$  (notable difference between the choices of  $\varepsilon$  only for  $N = 100$  and the log-likelihood difference), sample reordering strongly suffers from small sample sizes (in particular  $N \leq 500$ ), where convergence of the method can clearly not be assumed. Density resampling also performs rather poorly in terms of the log-likelihood but does not suffer as heavily from small sample sizes as sample reordering. Once again, the results clearly show that  $N'/N = 100$  is not appropriate.

Finally, a look at the computing times reveals that rejection-like sampling with very small  $\varepsilon$  is inefficient and also density resampling with  $N'/N = 1000$  is quite time-consuming. Sample reordering, on the other hand, is computationally very efficient for any sample size. This is due to the fact that no spare samples need to be generated, from which the final sample is selected, as in the other two methods. Rejection-like sampling with  $\varepsilon = 10^{-2}$  also has reasonable computing times even for larger sample sizes.

In summary, rejection-like sampling appears to work best and already a choice of  $\varepsilon = 10^{-2}$  seems to lead to a very good approximation. As the computing time strongly depends on  $\varepsilon$ , these results are very beneficial for the method of rejection-like sampling; a choice of  $\varepsilon = 10^{-2}$  requires only little computing time. For density resampling we compared two choices of  $N'/N$ , which, of course, also determine the computing time, and only  $N'/N = 1000$  gave satisfactory results, yet indicating that choices of  $N'/N > 1000$  may be necessary. But this would require an excessive computing time, even when the density of the hierarchical Kendall copula is efficient to evaluate, as it is the case here. Overall, based on the results of this simulation study, we cannot recommend the use of density resampling for hierarchical Kendall copulas. Sample reordering however proved to be a valid alternative to rejection-like sampling if sample sizes are sufficiently large (at least  $N \geq 1000$ ), so that convergence of the method can be assumed. This is e.g. the case when risk capital figures need to be simulated in finance and insurance as discussed in [Arbenz et al., 2012]. The generation of such large samples using sample reordering is very time-efficient.

If a closed-form solution as for Archimedean (Section 3.1), Plackett (Section 3.2) or Archimax

copulas (Section 3.3) is not available for the simulation of a hierarchical Kendall copula, we therefore recommend to use either top-down rejection-like sampling (Section 3.4) or, for sufficiently large sample sizes, bottom-up sample reordering (Section 4.1).

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