On mixtures of extremal copulas and attainability of concordance signatures

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Summary. The concordance signature of a random vector or its distribution is defined to be the set of concordance probabilities for margins of all orders. It is proved that the concordance signature of a copula is always equal to the concordance signature of some unique mixture of the extremal copulas. Applications of the result include a characterization of the set of Kendall rank correlation matrices as the cut polytope as well as a method for determining whether sets of concordance probabilities are attainable. The elliptical copulas are shown to yield a strict subset of the attainable concordance signatures as well as a strict subset of the attainable Kendall rank correlation matrices; the Student $t$ copula is shown to converge to a mixture of extremal copulas sharing its concordance signature with all elliptical distributions that have the same correlation matrix. A method of estimating an attainable concordance signature from data is derived and shown to correspond to using standard estimates of bivariate and multivariate Kendall’s tau in the absence of ties†.

Keywords: attainable correlations; concordance; copulas; cut polytope; elliptical distributions; extremal distributions; Kendall’s rank correlation; multivariate Bernoulli distributions.

1. Introduction

For a random vector $X = (X_1, \ldots, X_d)$ the probability of concordance corresponding to a subset $I \subseteq \{1, \ldots, d\}$ of the indices of the vector with cardinality $|I| \geq 2$ is given by

$$\kappa_I = \kappa(X_I) = 2 \mathbb{P}(X_I < X^*_I) = \mathbb{P}(\{X_I < X^*_I\} \cup \{X^*_I < X_I\}),$$

(1)

where $X^*$ denotes an independent random vector with the same distribution as $X$ and $\{X_I < X^*_I\} = \{X_i < X^*_i, i \in I\}$. In this paper we assume throughout that the marginal distributions of $X$ are continuous.

Continuity of the margins implies that the probabilities $\kappa_I$ are determined by the unique copula of $X$, in other words the distribution function (df) $C$ of the random vector $U = (F_1(X_1), \ldots, F_d(X_d))$, where $F_1, \ldots, F_d$ denote the marginal distribution functions. We can write $\kappa_I = \kappa(C_I) = \kappa(U_I)$ where $C_I$ denotes the marginal copula for subset $I$. The bivariate probabilities $\kappa_{\{i,j\}}$ are related to the Kendall’s tau rank correlation values $\tau_{\{i,j\}}$ by $2\kappa_{\{i,j\}} - 1 = \tau_{\{i,j\}}$ and higher-dimensional concordance probabilities are related to a higher-dimensional generalization of Kendall’s tau proposed by Joe (1990) and investigated by Genest et al. (2011).

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By the concordance signature of a copula \( C \), we refer to the set of all probabilities of concordance corresponding to all subsets \( I \). It is convenient to write this in terms of the power set \( \mathcal{P}(D) \) of the index set \( D = \{1, \ldots, d\} \) where trivially \( \kappa_{\{i\}} = 1 \) for a singleton and we adopt the convention \( \kappa_{\emptyset} = 1 \). The concordance signature of \( C \) is then
\[
\mathcal{K}_C = \{ \kappa_I : I \in \mathcal{P}(D) \}.
\] (2)

In fact we will show that all the probabilities corresponding to sets \( I \) of odd cardinality can be expressed in terms of probabilities of lower dimensional sets of even cardinality so that a signature may be fully described by taking the even elements of the power set.

We prove that the concordance signature \( \mathcal{K}_C \) of a copula \( C \) in dimension \( d \) is always equal to the concordance signature of some unique mixture of the extremal copulas in dimension \( d \). The extremal copulas are the distributions of the \( 2^{d-1} \) possible random vectors \( U^{(k)} \) with uniform margins and extremal correlation matrices, that is, random vectors satisfying the requirement that every pair of components has correlation (Pearson, Kendall or Spearman) equal to 1 or \(-1\) \cite{Tiih1996}.

This result has a number of attractive applications. First, it allows us to characterize the set of all possible Kendall’s tau rank correlation matrices as the set of convex combinations of the extremal correlation matrices, a set known as the cut polytope \cite{LaurentPoljak1995}, and thus to prove a conjecture of Hofert and Koike \cite{HofertKoike2019}. Our approach makes explicit the links between mixtures of extremal distributions and multivariate Bernoulli distributions and explains why the set of attainable Kendall correlation matrices is identical to the set of attainable correlation matrices for multivariate Bernoulli random vectors with symmetric margins as derived by Huber and Marić \cite{HuberMaric2015, HuberMaric2019}, Hofert and Koike \cite{HofertKoike2019} have also shown that this is the set of Blomqvist’s beta matrices.

Going beyond pairwise dependencies, the result allows us to investigate compatibility and attainability problems for concordance probabilities, that is, to work out whether a particular set of putative concordance probabilities forms a subset of the concordance signature of a copula and, if it does, to determine possible values for the remainder of the signature. The solution involves the application of standard techniques from linear optimization and convex analysis.

Study of the compatibility problem for concordance probabilities sheds light on the difficult problem of compatibility of lower-dimensional margins of higher-dimensional copulas, as considered by Joe \cite{Joe1996, Joe1997}: the compatibility of the concordance probabilities implied by the lower-dimensional margins provides a necessary condition if they are to form the margins of a higher-dimensional copula.

We look in detail at the concordance signature of elliptical copulas. Fang and Fang \cite{FangFang2002} and Lindskog et al. \cite{Lindskog2003} have shown that the Kendall correlation matrix of an elliptical distribution with correlation matrix \( P \) is given by the componentwise transformation \( P = 2\pi^{-1} \arcsin(P) \) regardless of the exact type of the elliptical distribution \( \‡ \). Genest et al. \cite{Genest2011} have shown that this invariance property carries over to multivariate Kendall’s tau values and hence to concordance signatures. Our work shows that the concordance signatures of the family of elliptical copulas form a strict subset of the set of all possible attainable concordance signatures. A surprising consequence is the existence of Kendall correlation matrices that do not correspond to elliptically distributed random vectors; this behaviour provides a contrast with Pearson correlation matrices, which are always the correlation matrices of elliptical distributions.

Moreover, we show that the \( d \)-dimensional \( t \) copula \( C_{\nu,P}^t \) with correlation matrix \( P \in \mathbb{R}^{d \times d} \) and degree-of-freedom parameter \( \nu > 0 \) converges weakly to a mixture of extremal

\‡This is subject to the technical condition that we omit distributions with an atom of probability at their location parameter.
copulas as $\nu \to 0$ and we determine the weights in the limiting mixture. Figure 1 shows a scatterplot of the copula $C^t_{\nu,P}$ when $\nu = 0.03$ and $P = (\rho_{ij})$ is the $3 \times 3$ matrix with elements $\rho_{12} = 0.2$, $\rho_{13} = 0.5$ and $\rho_{23} = 0.8$. Clearly the points are distributed very close to the four diagonals of the unit cube. The extremal copulas in three dimensions are the four copulas with probability mass concentrated on these diagonals and the methods of this paper show that the limiting weights attached to each diagonal are as given in Table 1. Thus the $t$ copulas with $\nu < 1$ provide a class of absolutely continuous distributions that can model behaviour that is close to that of a subclass of the mixture of extremal copulas, namely the subclass sharing its concordance signature with the elliptical copulas.

Finally, we show how to estimate a consistent concordance signature from data; in the absence of ties, the resulting estimate is equivalent to using standard estimators of bivariate and multivariate Kendall’s tau. This potentially offers a powerful technique in Monte Carlo simulation studies or risk analyses. It allows us to generate data from a model with identical concordance signature to that estimated from the data but with a very extreme form of tail dependence in which extreme values (of large or small size) are always coincident in each margin.

The paper is organized as follows. In Section 2 we define extremal copulas and mixtures of extremal copulas and establish a notation to allow the enumeration of the former. The link

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### Table 1. Probabilities associated with diagonals of unit cube for copula in Figure 1.

| Diagonal                  | Probability |
|---------------------------|-------------|
| $(0,0,0) \leftrightarrow (1,1,1)$ | 51.3%       |
| $(0,0,1) \leftrightarrow (1,1,0)$ | 5.1%        |
| $(0,1,0) \leftrightarrow (1,0,1)$ | 15.4%       |
| $(0,1,1) \leftrightarrow (1,0,0)$ | 28.2%       |
between mixtures of extremal copulas and multivariate Bernoulli distributions is explored in Section 3. In Section 4 we calculate concordance probabilities for mixtures of extremal copulas and prove the main result linking concordance signatures of general copulas to those of extremal mixtures. The question of attainability of concordance signatures given incomplete knowledge of the concordance probabilities of a random vector is analysed in Section 5 while concordance signatures of elliptical copulas are investigated in Section 6. Finally, in Section 7 we treat the problem of estimating consistent concordance signatures.

2. Mixtures of extremal copulas

In dimension $d \geq 2$ there are $2^{d-1}$ extremal copulas and we enumerate them in the following way. For $k \in \{1, \ldots, 2^{d-1}\}$ let $s_k = (s_{k,1}, \ldots, s_{k,d})$ be the vector consisting of the digits of $k - 1$ when represented as a $d$-digit binary number. For example, when $d = 4$ we have exactly eight extremal copulas corresponding to the vectors

$$s_1 = (0, 0, 0, 0), \quad s_2 = (0, 0, 0, 1), \quad s_3 = (0, 0, 1, 0), \quad s_4 = (0, 0, 1, 1),$$

$$s_5 = (0, 1, 0, 0), \quad s_6 = (0, 1, 0, 1), \quad s_7 = (0, 1, 1, 0), \quad s_8 = (0, 1, 1, 1).$$

The extremal copulas concentrate their probability mass on the diagonals between the points given by the vectors $s_k = (s_{k,1}, \ldots, s_{k,d})$ and the vectors $1 - s_k = (1 - s_{k,1}, \ldots, 1 - s_{k,d})$. These are the main diagonals of the unit hypercube and there are $2^{d-1}$ such diagonals.

For the vector $s_k$ we define the index set $J_k \subseteq \mathcal{D} = \{1, \ldots, d\}$ to be the set of indices corresponding to zeros and $J_k^c$ to be the set of indices corresponding to ones; in other words, $j \in J_k$ if $s_{k,j} = 0$ and $j \in J_k^c$ if $s_{k,j} = 1$. For the 4-dimensional example above we have $J_1 = \{1, 2, 3, 4\}$, $J_2^c = \emptyset$, $J_3 = \{1, 2, 3\}$, $J_4^c = \{4\}$ and so on. The $k$th extremal copula in dimension $d$ can then be written as

$$C^{(k)}(u) = C^{(k)}(u_1, \ldots, u_d) = \left( \min_{j \in J_k} u_j + \min_{j \in J_k^c} u_j - 1 \right)^+,$$  \hspace{1cm} (3)

where for any $x \in \mathbb{R}$, $x^+ = \max(x, 0)$ denotes the positive part of $x$. A random vector $U^{(k)} = (U_1^{(k)}, \ldots, U_d^{(k)})$ with distribution function $C^{(k)}$ satisfies

$$U_j^{(k)} \equiv \begin{cases} U & \text{if } j \in J_k, \\ 1 - U & \text{if } j \in J_k^c, \end{cases}$$

where $U$ is a uniform random variable. Moreover it has correlation matrix $P^{(k)}$ consisting exclusively of $1$’s and $-1$’s, known as an extremal correlation matrix. This correlation matrix is simultaneously the matrix of pairwise Pearson, Spearman and Kendall correlations of $U^{(k)}$. It can be represented as the outer product $P^{(k)} = (2s_k - 1)(2s_k - 1)^T$.

For $k = 1, \ldots, 2^{d-1}$, let $X^{(k)} = (X_1^{(k)}, \ldots, X_d^{(k)})$ be a random vector with continuous margins and copula $C^{(k)}$. Then the sets $\{X_j^{(k)} : j \in J_k\}$ and $\{X_j^{(k)} : j \in J_k^c\}$ are sets of comonotonic random variables, while any pair $(X_i^{(k)}, X_j^{(k)})$ such that $i \in J_k$ and $j \in J_k^c$, or vice versa, is a pair of countermonotonic random variables. In particular $X^{(1)}$ has copula $C^{(1)}(u) = M(u) = \min(u_1, \ldots, u_d)$, the $d$-dimensional comonotonicity or Fréchet–Hoeffding upper bound copula. For $I \subseteq \mathcal{D}$ we introduce the notation

$$a_{I,k} = \begin{cases} 1 & \text{if } I \subseteq J_k \text{ or } I \subseteq J_k^c, \\ 0 & \text{otherwise}. \end{cases}$$  \hspace{1cm} (4)
For sets with $|I| > 1$ the value $a_{I,k}$ indicates whether the components of $X^{(k)}$ with indices in $I$ are comonotonic variables or not. However, the values $a_{I,k}$ are also defined for sets $I$ which are singletons and for the empty set; in these cases we have $a_{\{i\},k} = 1$ and $a_{\emptyset,k} = 1$ for all $k$ and $i$.

We now define an extremal mixture copula, which is a central concept in this paper.

**Definition 1.** An extremal mixture copula is a copula of the form $C^* = \sum_{k=1}^{2^{d-1}} w_k C^{(k)}$, where the weights satisfy $w_k \geq 0$ for all $k \in \{1, \ldots, 2^{d-1}\}$ and $\sum_{k=1}^{2^{d-1}} w_k = 1$.

For $k \in \{1, \ldots, 2^{d-1}\}$, let $U^{(k)}$ be a random vector with df $C^{(k)}$ in $[0,1)^d$. If $N$ is a multinomial random variable taking values in $\{1, \ldots, 2^{d-1}\}$ and independent of $U^{(1)}, \ldots, U^{(2^{d-1})}$, then it is easily seen that the distribution function of the random vector $U^{(N)}$ has the property that $U^{(N)} = U^{(k)}$ if $N = k$ is an extremal mixture copula. Indeed, we can calculate that $U^{(N)}$ has distribution function $\sum_{k=1}^{2^{d-1}} \Pr(N = k) C^{(k)}$.

### 3. Multivariate Bernoulli representations

Multivariate Bernoulli distributions play an important role in the study of extremal mixtures. To see this, we first consider a standard uniform variable $U$ and a random vector $B = (B_1, \ldots, B_d)$ of Bernoulli variables with $\Pr(B_j = 1) = p_j$. Suppose that for any $j \in \{1, \ldots, d\}$, $U$ is independent of $B_j$. Then the distribution function of

$$UB + (1-U)(1-B)$$

is a copula, because its margins are standard uniform, as is easily verified by direct calculation. By the independence of $U$ and $B_j$,

$$\Pr\left(B_j U + (1-B_j)(1-U) \leq u\right) = p_j \Pr(U \leq u) + (1-p_j) \Pr(1-U \leq u) = u.$$ 

When $U$ and $B$ are independent, we have the following result.

**Proposition 1.** Let $U$ be a standard uniform random variable and $B$ a multivariate Bernoulli vector independent of $U$. Then the distribution function of the vector in (5) is an extremal mixture with weights given, for each $k \in \{1, \ldots, 2^{d-1}\}$, by

$$w_k = \Pr(B = s_k) + \Pr(B = 1 - s_k),$$

where $s_k$ is as defined in Section 2. Conversely, any extremal mixture copula $C^* = \sum_{k=1}^{2^{d-1}} w_k C^{(k)}$ is the distribution function of a random vector of the form (5), where $U$ is independent of $B$ and (6) holds for all $k \in \{1, \ldots, 2^{d-1}\}$.

**Proof.** Let $U$ be of the form (5) where $U$ and $B$ are independent. For any $u \in (0,1]$,

$$\Pr(U \leq u) = \sum_{b \in \{0,1\}^d} \Pr\left(\max_{j: b_j = 0} (1-v_j) \leq U \leq \min_{j: b_j = 1} v_j | B = b\right) \Pr(B = b)$$

$$= \sum_{b \in \{0,1\}^d} \left(\min_{j: b_j = 1} v_j + \min_{j: b_j = 0} v_j - 1\right)^+ \Pr(B = b)$$

$$= \sum_{k=1}^{2^{d-1}} \left(\min_{j \in J_k} v_j + \min_{j \notin J_k} v_j - 1\right)^+ \left(\Pr(B = s_k) + \Pr(B = 1 - s_k)\right).$$
From (5), one can see that the distribution function of $U$ is indeed an extremal mixture with weights as given in (6).

Conversely, given an extremal mixture copula of the form $C^* = \sum_{k=1}^{2^{d-1}} w_k C^{(k)}$, it suffices to consider any Bernoulli vector $B$ independent of $U$ with the property that $w_k = \mathbb{P}(B = s_k) + \mathbb{P}(B = 1 - s_k)$; this is possible because the events $\{B = s_k\}$ and $\{B = 1 - s_k\}$ are disjoint and their union forms a partition of $\{0, 1\}^d$. We can then retrace the steps of the argument in reverse to establish the representation (5).

Proposition 1 establishes that extremal mixture copulas have a stochastic representation (5). However, the class of Bernoulli distributions satisfying (6) is infinite since the mass $w_k$ can be split between the events $\{B = s_k\}$ and $\{B = 1 - s_k\}$ in an arbitrary way. It is convenient to single out a representative and we present two different ways of doing this.

### 3.1. Type 1 representation

One option is to set $B = (1, Z_1, \ldots, Z_{d-1})$ so that for each $k \in \{1, \ldots, 2^{d-1}\}$, $\mathbb{P}(B = s_k) = 0$ while $\mathbb{P}(B = 1 - s_k) = w_k$. A random vector $U$ distributed according to the extremal mixture copula $C^* = \sum_{k=1}^{2^{d-1}} w_k C^{(k)}$ then has stochastic representation

$$U \overset{d}{=} U \begin{pmatrix} 1 \\ Z_1 \\ \vdots \\ Z_{d-1} \end{pmatrix} + (1 - U) \begin{pmatrix} 0 \\ 1 - Z_1 \\ \vdots \\ 1 - Z_{d-1} \end{pmatrix},$$

(7)

where $Z = (Z_1, \ldots, Z_{d-1})$ is a multivariate Bernoulli vector, independent of $U$. Since there are $2^{d-1}$ distinct outcomes for the vector $Z$, this means that there is a bijective mapping between the extremal mixture copulas and the multivariate Bernoulli distributions in dimension $d - 1$. The set of mixture weights $\{w_1, \ldots, w_{2^{d-1}}\}$ of the extremal mixture copula is exactly the set of probabilities that parameterizes the multivariate Bernoulli distribution of $Z = (Z_1, \ldots, Z_{d-1})$, viz.

$$\mathbb{P}(Z_1 = 1 - s_{k,2}, \ldots, Z_{d-1} = 1 - s_{k,d}) = w_k$$

for any $k \in \{1, \ldots, 2^{d-1}\}$. Note that the independence between $U$ and $Z$ is an important assumption. Without it, the distribution function of the vector in (7) may not be an extremal mixture. A counter-example is provided below.

**Example 1.** Suppose that $Z_1$ and $Z_2$ are Bernoulli variables with success probability 0.5 and such that for each $u \in [0, 1],$

$$\mathbb{P}(U \leq u, Z_1 = 0, Z_2 = 0) = \frac{1}{4} u + \frac{\theta}{16} u(1 - u),$$

where $\theta \in [-1, 1]$. This means that a copula of $(U, Z_1, Z_2)$ is the multivariate generalization of the Farlie–Gumbel–Morgenstern copula given, for all $u_1, u_1, u_3 \in [0, 1],$ by

$$C_{\theta}(u_1, u_2, u_3) = (u_1 u_2 u_3) \left( 1 + \theta (1 - u_1)(1 - u_2)(1 - u_3) \right).$$

Because all bivariate margins of $C_1$ are independence copulas, $U$, $Z_1$, and $Z_2$ are pairwise independent, but not jointly independent. In particular, $U$ is not independent of $(Z_1, Z_2)$.
By direct calculation, we can easily derive that for all $u \in [0, 1]$,

\[
\begin{align*}
\mathbb{P}(U \leq u | Z_1 = 0, Z_2 = 0) &= u + \theta \frac{1}{4} u (1 - u), \\
\mathbb{P}(U \leq u | Z_1 = 1, Z_2 = 0) &= u - \theta \frac{1}{4} u (1 - u), \\
\mathbb{P}(U \leq u | Z_1 = 0, Z_2 = 1) &= u - \frac{\theta}{4} u (1 - u), \\
\mathbb{P}(U \leq u | Z_1 = 1, Z_2 = 1) &= u + \frac{\theta}{4} u (1 - u).
\end{align*}
\]

The distribution function of the random vector on the right-hand side of (7) is a copula, say $C$, which is given, for each $u_1, u_2, u_3 \in [0, 1]$, by

\[
4C(u_1, u_2, u_3) = \min(u_1, u_2, u_3) + \frac{\theta}{4} \min(u_1, u_2, u_3) \max(1 - u_1, 1 - u_2, 1 - u_3)
\]

\[+ I_{\{\min(u_1, u_2) + u_3 - 1 \geq 0\}} \left( \min(u_1, u_2) - \frac{\theta}{4} \min(u_1, u_2) \max(1 - u_1, 1 - u_2) 
\right.
\]

\[\left. - 1 + u_3 + \frac{\theta}{4} u_3 (1 - u_3) \right) 
\]

\[+ I_{\{\min(u_1, u_3) + u_2 - 1 \geq 0\}} \left( \min(u_1, u_3) - \frac{\theta}{4} \min(u_1, u_3) \max(1 - u_1, 1 - u_3) 
\right. 
\]

\[\left. - 1 + u_2 + \frac{\theta}{4} u_2 (1 - u_2) \right) 
\]

\[+ I_{\{\min(u_2, u_3) + u_1 - 1 \geq 0\}} \left( \min(u_2, u_3) - \frac{\theta}{4} \min(u_2, u_3) \max(1 - u_2, 1 - u_3) 
\right. 
\]

\[\left. - 1 + u_1 + \frac{\theta}{4} u_1 (1 - u_1) \right),
\]

where we use the notation $I_S$ for the indicator function of a set $S$. Unless $\theta = 0$, $C$ is not of the form (3) and hence not an extremal mixture copula. Interestingly, all its bivariate margins are. Indeed, because $C$ is symmetric with respect to any permutation of its arguments, it suffices to set $u_3 = 1$ to verify that each bivariate margin of $C$ equals $0.5M + 0.5W$ where $M(u_1, u_2) = \min(u_1, u_2)$ and $W(u_1, u_2) = (u_1 + u_2 - 1)^+$ are the two bivariate extremal copulas.

Example 1 reveals an interesting contrast between the extremal copulas and the mixtures of extremal copulas. While a necessary and sufficient condition for a vector $U$ to be distributed according to an extremal copula is that its bivariate margins should be extremal copulas, the analogous statement does not hold for extremal mixture copulas. Although it is necessary that the bivariate margins of an extremal mixture copula are extremal mixture copulas, the counter-example shows that this is not sufficient.

**Theorem 1.** The distribution of a random vector $U = (U_1, \ldots, U_d)$ is a mixture of extremal copulas if and only if its bivariate marginal distributions are mixtures of extremal copulas and for all $u \in [0, 1]$,

\[
\mathbb{P}(U_1 \leq u | I_{\{U_j = U_{i^*}\}}, j \neq 1) = u.
\]

**Proof.** If $U$ follows an extremal mixture copula then, by Proposition 1 it has the representation (5) for some Bernoulli random vector $B$ and it is clear that all the bivariate
Note that the vectors $U$ representation and the independence of $U$ margins have the same structure. Now $U$ also has the representation $U$ and from this representation and the independence of $U$ and $Z = (Z_1, \ldots, Z_{d-1})$ we obtain

$$\mathbb{P}(U_1 \leq u \mid I_{\{U_j = U_{1j}\}}, j \neq 1) = \mathbb{P}(U \leq u \mid Z_1, \ldots, Z_{d-1}) = \mathbb{P}(U \leq u) = u.$$

Conversely, let us suppose that all the bivariate margins of $U$ are mixtures of extremal copulas. This implies that almost surely, $U$ takes values in the set

$$\bigcap_{i \neq j} \{u \in [0, 1]^d : u_j = u_i \text{ or } u_j = 1 - u_i\},$$

which simplifies to the union $E$ of the $2^{d-1}$ main diagonals of the unit hypercube, viz.

$$E = \bigcup_{k=1}^{2^{d-1}} \{u \in [0, 1]^d : u_j = u_1^{(1-s_{k,j})}(1-u_1)^{s_{k,j}}, j \neq 1\}.$$

Let $E_k = \{U_j = U_1^{(1-s_{k,j})}(1-U_1)^{s_{k,j}}, j \neq 1\}$ represent the event that $U$ lies on the $k$th diagonal and set $w_k = \mathbb{P}(E_k)$. By the law of total probability, we get

$$C(u) = \sum_{k=1}^{2^{d-1}} w_k \mathbb{P}(U_1 \leq u_1, \ldots, U_d \leq u_d \mid E_k) = \sum_{k=1}^{2^{d-1}} w_k \mathbb{P}(U_1 \in [\max(1-u_j), \min u_j] \mid E_k).$$

On the diagonals of the hypercube, $\{U \in E \cap \{I_{U_j = U_{1j}} = 1 - s_{k,j}, j \neq 1\} = E_k, \text{ so that } w_k = \mathbb{P}\{I_{U_j = U_{1j}} = 1 - s_{k,j}, j \neq 1\} \text{ and conditioning on the event } E_k \text{ is identical to conditioning on the event } \{I_{U_j = U_{1j}} = 1 - s_{k,j}, j \neq 1\}. \text{ We thus obtain that}$

$$C(u) = \sum_{k=1}^{2^{d-1}} w_k \mathbb{P}(U_1 \in [\max u_j, \min u_j] \mid I_{U_j = U_{1j}} = 1 - s_{k,j}, j \neq 1) = \sum_{k=1}^{2^{d-1}} w_k C^{(k)}(u)$$

where the last equality follows from (8) and (3). This shows that $C$ is indeed a mixture of extremal copulas as claimed.

### 3.2. Type 2 representation

Another option for uniquely defining $B$ in Proposition 1 is to set $B = Y$, where $Y$ is radially symmetric about $0.5$, that is, such that $Y \sim \text{b}^{-d}, Y \text{ is palindromic (Marchetti and Wermuth, 2016). Proceeding this way, we have that for each } k \in \{1, \ldots, 2^{d-1}\},$

$$\mathbb{P}(Y = s_k) = \mathbb{P}(Y = 1 - s_k) = 0.5 w_k. \quad \text{(9)}$$

Note that the vectors $Y$ and $Z$ mutually determine each other’s distribution. Starting with $Y$, $Z \stackrel{d}{=} Y_1(Y_2, \ldots, Y_d)$. Starting with $Z$, $Y \stackrel{d}{=} (Y_1, Y_1Z + (1 - Y_1)(1 - Z))$, where $Y_1$ is a Bernoulli variable independent of $U$ and $Z$ such that $\mathbb{P}(Y_1 = 1) = 0.5$.

A number of constraints apply to radially symmetric Bernoulli random vectors: they must have marginal probabilities $\mathbb{P}(Y_i = 1) = 0.5$ for all $i$; moreover, all probabilities of the form $p_{I} = \mathbb{P}(Y_{I} = 1)$ for sets $I$ with odd cardinality are fully determined by the equivalent probabilities for lower-dimensional sets of even cardinality. This follows from the fact that

$$p_{I} = \mathbb{E}\left(\prod_{i \in I} Y_i\right) = \mathbb{E}\left(\prod_{i \in I} (1 - Y_i)\right) = 1 + \sum_{A \subseteq I, |A| \geq 1} (-1)^{|A|} \mathbb{E}\left(\prod_{i \in A} Y_i\right).$$
When $I$ is odd, we then have

$$2p_I = 1 + \sum_{A \subseteq I, 1 \leq |A| < |I|} (-1)^{|A|}p_A = 1 - \frac{1}{2}|I| + \sum_{A \subseteq I, 2 \leq |A| < |I|} (-1)^{|A|}p_A, \quad (10)$$

where the last equality follows from the fact that $p_A = 0.5$ whenever $|A| = 1$. For example,

$$p_{\{1,2,3\}} = \mathbb{E}\left((1 - Y_1)(1 - Y_2)(1 - Y_3)\right) = 1 - p_{\{1\}} - p_{\{2\}} - p_{\{3\}} + p_{\{1,2\}} + p_{\{1,3\}} + p_{\{2,3\}} - p_{\{1,2,3\}} = \frac{1}{2} (p_{\{1,2\}} + p_{\{1,3\}} + p_{\{2,3\}}) - \frac{1}{4}.

Since the set of joint event probabilities $\{p_I : I \subseteq \mathcal{D}\}$ uniquely specifies the distribution of a Bernoulli random vector, this leads to the following insight.

**Proposition 2.** The radially symmetric Bernoulli distribution of a vector $Y$ in dimension $d$ is characterized by the set of probabilities $\{p_I = \mathbb{P}(Y_I = 1) : I \subseteq \mathcal{D}, |I| \text{ even}\}$.

It may be noted from Proposition 2 that the number of probabilities $p_I$ specifying the law of $Y$ is equal to

$$\sum_{j=1}^{\lfloor d/2 \rfloor} \binom{d}{2j} = 2^{d-1} - 1.$$

Since radially symmetric multivariate Bernoulli distributions in dimension $d$ are fully determined by multivariate Bernoulli distributions in dimension $d-1$, they must have the same number of free parameters, namely $2^{d-1} - 1$ (one less than the number of distinct outcomes for $d-1$ Bernoulli random variables).

### 4. Concordance signatures of copulas

Let $U$ and $U^*$ be independent random vectors with distribution given by the copula $C$. The concordance probabilities (11) corresponding to subsets $I \subseteq \mathcal{D}$ with $|I| \geq 2$ can be written in the form

$$\kappa_I = \kappa(C_I) = 2\mathbb{P}(U_I \leq U^*_I) = 2\int_{[0,1]^{|I|}} C_I(u)\,dC_I(u), \quad (11)$$

where, as before, $U_I$ and $C_I$ denote sub-vectors and marginal copulas of $U$ and $C$ respectively. The concordance probabilities are related to the multivariate Kendall’s tau coefficients $\tau(U_I)$ analysed in Genest et al. (2011) by the formula

$$(2^{|I|-1} - 1)\tau(U_I) = 2^{|I|-1}\kappa(U_I) - 1. \quad (12)$$

The probabilities of concordance for the $d$-dimensional extremal copulas are given by

$$\kappa(C^{(k)}) = \begin{cases} 1 & \text{if } k = 1, \\ 0 & \text{otherwise,} \end{cases}$$

and in general for the marginal copulas of $d$-dimensional extremal copulas we can write $\kappa(C^{(k)}_I) = a_{I,k}$ with $a_{I,k}$ as defined in (4). For mixtures of extremal copulas we have the following result.
Proposition 3. If $C$ is an extremal mixture copula of the form $\sum_{k=1}^{2^{d-1}} w_k C^{(k)}$, then for any $I \subseteq D$
\[ \kappa(C_I) = \sum_{k=1}^{2^{d-1}} w_k \kappa(C^{(k)}_I) = \sum_{k=1}^{2^{d-1}} w_k a_{I,k} \]  
with $a_{I,k}$ as defined in (4).

Proof. Note first that (13) holds trivially for sets $I$ which are singletons or the empty set. For sets such that $|I| \geq 2$ we can use (11) to write
\[ \kappa(C) = 2 \int_{[0,1]^d} C(u) dC(u) = 2 \sum_{j=1}^{2^{d-1}} \sum_{k=1}^{2^{d-1}} w_j w_k \int_{[0,1]^d} C^{(j)}(u) dC^{(k)}(u). \]
Introducing independent random vectors $U^{(j)} \sim C^{(j)}$ and $\tilde{U}^{(k)} \sim C^{(k)}$ for $j \in \{1, \ldots, 2^{d-1}\}$ and $k \in \{1, \ldots, 2^{d-1}\}$ we calculate that
\[ \int_{[0,1]^d} C^{(j)}(u) dC^{(k)}(u) = \mathbb{P}(U^{(j)} \leq \tilde{U}^{(k)}) = \begin{cases} \frac{1}{2} & \text{if } j = k = 1, \\ \frac{1}{4} & \text{if } j = 1 \text{ or } k = 1 \text{ but } j \neq k, \\ 0 & \text{if } j \neq 1 \text{ and } k \neq 1. \end{cases} \]
Hence we can verify that
\[ \kappa(C) = 2 w_1^2 + 4 w_1 \left( \frac{w_2}{4} + \cdots + \frac{w_{2^{d-1}}}{4} \right) = w_1^2 + w_1 (1 - w_1) = w_1, \]
which is the weight on $C^{(1)} = M$, the $d$-dimensional comonotonicity copula. If $U$ is distributed according to $C$ then the vector $U_I$ is distributed according to a mixture of extremal copulas in dimension $|I|$ and it follows that $\kappa(U_I) = \kappa(C_I) = \tilde{w}_1$ where $\tilde{w}_1$ is the weight attached to the case where $U_I$ is a comonotonic random vector. This is given by
\[ \tilde{w}_1 = \sum_{k=1}^{2^{d-1}} w_k a_{I,k} = \sum_{k=1}^{2^{d-1}} w_k \kappa(C^{(k)}_I). \]

A simple consequence of Proposition 3 is a formula for the multivariate Kendall’s tau coefficient for mixtures of extremal distributions.

Corollary 1. If $C = \sum_{k=1}^{2^{d-1}} w_k C^{(k)}$ then for any $I \subseteq D$ with $|I| \geq 2$, the multivariate Kendall’s tau coefficient satisfies
\[ \tau(C_I) = \sum_{k=1}^{2^{d-1}} w_k \tau(C^{(k)}_I). \]  

Proof. This follows from (13) and (12).

We can now state the main result of this paper.

Theorem 2. Let $C$ be a $d$-dimensional copula and $\mathcal{K}_C = \{ \kappa_I : I \in \mathcal{P}(D) \}$ its concordance signature given in (2). Then there exists a unique extremal mixture copula with the same concordance signature. The weights are given by the solution of the linear equation system
\[ \kappa_I = \sum_{k=1}^{2^{d-1}} w_k a_{I,k} \]  
on the $2^{d-1}$-dimensional unit simplex.
Extremal mixture copulas and concordance signatures

PROOF. For a vector \( \mathbf{U} \sim C \) we can write for any \( I \in \mathcal{P}(\mathcal{D}) \) with \( |I| \geq 1 \)

\[
\kappa_I = \kappa(C_I) = 2\mathbb{P}(\mathbf{U}_I < \mathbf{U}_I^*) = 2\mathbb{P}\left(\text{sign}(\mathbf{U}_I^* - \mathbf{U}_I) = 1\right)
\]

where \( \mathbf{U}^* \) is an independent copy of \( \mathbf{U} \). If we define the random vectors

\[
\mathbf{V} = \text{sign}(\mathbf{U}^* - \mathbf{U}), \quad \mathbf{Y} = \frac{1}{2}(\mathbf{V} + 1)
\]

then, by symmetry, \( \mathbf{V} \overset{d}{=} -\mathbf{V} \) so it must be the case that \( 2\mathbf{Y} - 1 \overset{d}{=} 1 - 2\mathbf{Y} \) or equivalently \( \mathbf{Y} \overset{d}{=} 1 - \mathbf{Y} \) so that \( \mathbf{Y} \) is a radially symmetric Bernoulli vector. Using the radial symmetry of \( \mathbf{Y} \) and the fact that the union of all the disjoint events \( \{ \mathbf{Y} = s_k \} \) and \( \{ \mathbf{Y} = 1 - s_k \} \) forms a partition of \( \{0, 1\}^d \) we obtain

\[
\kappa_I = 2\mathbb{P}(\mathbf{V}_I = 1) = 2\mathbb{P}(\mathbf{Y}_I = 1)
= \mathbb{P}(\mathbf{Y}_I = 0) + \mathbb{P}(\mathbf{Y}_I = 1)
= \sum_{k=1}^{2d-1} \left( \mathbb{P}(\mathbf{Y} = s_k) + \mathbb{P}(\mathbf{Y} = 1 - s_k) \right) I_{I \subseteq J_k \text{ or } I \subseteq \bar{J}_k} = \sum_{k=1}^{2d-1} w_k a_{I,k},
\]

where we have used (4) and (9) in the final step. Thus the weights \( w_k \) are the probabilities that specify the law of the radially symmetric Bernoulli vector \( \mathbf{Y} \). This is identical to the expression in (13) when \( w_k \) are the weights that specify the extremal mixture copula. The extremal mixture copula is unique since the set of probabilities \( \{ p_I = 0.5\kappa(C_I) : I \in \mathcal{P}(\mathcal{D}), |I| \text{ even} \} \) uniquely specify the law of \( \mathbf{Y} \) by Proposition 2.

Given a concordance signature \( K_C \) simple linear algebra allows us to determine the vector \( \mathbf{w} = (w_1, \ldots, w_{2d-1}) \). We only need the concordance probabilities for subsets of even cardinality. Let \( \mathcal{E}(\mathcal{D}) \) denote the subset of the power set of \( \mathcal{D} \) consisting of the subsets of even cardinality. We refer to the set \( K_C^+ = \{ \kappa_I : I \in \mathcal{E}(\mathcal{D}) \} \) as the minimal complete concordance signature of the copula \( C \). In this set we include the value \( \kappa_0 = 1 \) corresponding to the empty set.

Suppose we fix an ordering of the even power set; for \( d = 4 \) we might take

\[
\mathcal{E}(\mathcal{D}) = \emptyset, \{1, 2\}, \{1, 3\}, \{1, 4\}, \{2, 3\}, \{2, 4\}, \{3, 4\}, \{1, 2, 3, 4\}
\]

and this choice is illustrated below. Let \( \kappa \) be the corresponding vector of concordance probabilities. Let \( A_d \) be the \( 2d-1 \times 2d-1 \)-matrix such that the rows are given by \( \mathbf{a}_I = (a_{I,1}, \ldots, a_{I,2d-1}) \) and are ordered according to the ordering of the even power set \( \mathcal{E}(\mathcal{D}) \); the row corresponding to \( \emptyset \) is \( \mathbf{a}_\emptyset = (1, \ldots, 1) \) corresponding to the sum condition on the weights. We then obtain the linear equation

\[
\kappa = A_d \mathbf{w}
\]

and this can be solved to give \( \mathbf{w} = A_d^{-1} \kappa \). For example, when \( d = 4 \) we would have

\[
\begin{pmatrix}
1 \\
\kappa_{\{1,2\}} \\
\kappa_{\{1,3\}} \\
\kappa_{\{1,4\}} \\
\kappa_{\{2,3\}} \\
\kappa_{\{2,4\}} \\
\kappa_{\{3,4\}} \\
\kappa_{\{1,2,3,4\}}
\end{pmatrix}
= 
\begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\
1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\
1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
w_1 \\
w_2 \\
w_3 \\
w_4 \\
w_5 \\
w_6 \\
w_7 \\
w_8
\end{pmatrix}
\]
The existence of a unique solution to (15) means that the matrices $A_d$ must be invertible matrices of full rank. In fact, Theorem 2 has the following interesting corollary, the first part of which was proved in Genest et al. (2011).

**Corollary 2.**

(a) When $I$ is a set of odd cardinality

$$2\kappa_I = 2 - |I| + \sum_{I' \subset I, 2 \leq |I'| < |I|} (-1)^{|I'|} \kappa_{I'}.$$

(b) When $I$ is a set of even cardinality there is no linear formula relating $\kappa_I$ to concordance probabilities of order $|I'| \leq |I|$.

**Proof.** In the proof of Theorem 2 it is shown that $\kappa_I = 2p_I$ where the probabilities $p_i = P(Y_i = 1)$ specify the law of the Bernoulli random vector $Y$ describing the extremal mixture. Hence Part 1 is an immediate consequence of (10). If Part 2 were not true, the rows of the matrix $A_d$ would be linearly dependent, contradicting the assertion that $A_d$ is of full rank.

**Remark 1.** The implications of Corollary 2 can be extended. In view of (12) an analogous result could be stated for the multivariate Kendall’s tau coefficients: when $|I|$ is odd, a linear formula relating $\tau_I$ to the values for lower-dimensional subsets exists (see Proposition 1 in Genest et al. (2011)) but no such formula exists when $|I|$ is even. Moreover, as we will discuss in Section 6, the concordance probabilities of elliptical copulas are equal to twice the orthant probabilities of Gaussian distributions centred at the origin: thus if $Z \sim N_d(0, \Sigma)$ is a Gaussian random vector, recursive linear formulas exist for the probabilities $P(Z_I \geq 0)$ when $|I|$ is odd but not when $|I|$ is even.

5. Attainability of concordance signatures

Let $S \subseteq \mathcal{E}(D)$ be a subset of the even power set. Suppose we want to test whether a set of concordance probabilities $K = \{\kappa_I : I \in S\}$ could correspond to the concordance signature of some copula $C$. Theorem 2 shows that we can restrict attention to mixtures of extremal copulas. The set $K$ is is said to be attainable if there exists an extremal mixture copula which matches all the concordance probabilities $\kappa_I \in K$.

A particular special case of interest is when $K$ is the set of all pairwise concordance probabilities and, in view of (12), this is equivalent to determining whether a particular matrix of Kendall’s tau rank correlation coefficients is attainable. For a uniform random vector $U$ with distribution function given by the copula $C$, let us denote the Kendall’s tau matrix by $\rho_T(U)$. Note that Kendall’s tau matrices must be correlation matrices, i.e. positive semi-definite matrices with ones on the diagonal and all elements in $[-1, 1]$. This follows from the fact that we can write

$$\rho_T(U) = \rho\left(\text{sign}(U - U^*)\right),$$

in other words, as the linear correlation matrix of the sign vector of the difference between $U$ and an independent copy $U^*$.

In Theorem 3 below we provide an answer to the question of when is a correlation matrix also a Kendall’s tau matrix. The proof is a simple consequence of Theorem 2 and the following useful lemma.
Lemma 1. Let $U$ be distributed according to the mixture of extremal copulas given by $C^* = \sum_{k=1}^{2^d-1} w_k C^{(k)}$. Then

$$\rho_\tau(U) = \rho(U) = \sum_{k=1}^{2^d-1} w_k P^{(k)}.$$ (17)

Proof. The equality $\rho_\tau(U) = \sum_{k=1}^{2^d-1} w_k \rho_\tau(U^{(k)})$ follows from (14) while the equality $\rho(U) = \sum_{k=1}^{2^d-1} w_k \rho(U^{(k)})$ was proved by Tii (1996). Hence (17) follows from the equality of linear and Kendall correlations for extremal copulas.

Theorem 3. The $d \times d$ correlation matrix $P$ is a Kendall’s tau rank correlation matrix if and only if $P$ can be represented as a convex combination of the extremal correlation matrices in dimension $d$, that is,

$$P = \sum_{k=1}^{2^d-1} w_k P^{(k)}.$$ (18)

Proof. If $P$ is of the form (18) then Lemma 1 shows that it is the Kendall’s tau matrix of the extremal mixture copula $C^* = \sum_{k=1}^{2^d-1} w_k C^{(k)}$. Conversely if $P$ is the Kendall’s $\tau$ matrix of an arbitrary copula $C$ then, by Theorem 2, it is also the Kendall’s tau matrix of the extremal mixture copula with the same concordance signature and must take the form (17) by Lemma 1.

The set of convex combinations of extremal correlation matrices is known as the cut polytope; an illustration for $d = 3$ is shown in Figure 2. Laurent and Poljak (1995) showed that this set is a strict subset of the so-called elliptope of correlation matrices in dimensions $d \geq 3$; see also Section 3.3 of Hofert and Koike (2019). For example, the positive-definite correlation matrix

$$\begin{pmatrix} 1/12 & -5 & -5 \\ -5 & 12 & -5 \\ -5 & -5 & 12 \end{pmatrix}$$

is in the elliptope but not the cut polytope and therefore cannot be a matrix of Kendall’s tau values. If $\tau = -5/12$ and we set $\kappa = (1 + \tau)/2$ and $\kappa = (1, \kappa, \kappa, \kappa)$, there is no solution to the equation $A_3 w = \kappa$ on the 4-dimensional unit simplex and a representation of the form (18) is impossible.

Huber and Maric (2019) have shown that the cut polytope is also the set of attainable linear correlation matrices for multivariate distributions with symmetric Bernoulli marginal distributions. This can be deduced from Theorem 2 and Proposition 1 using the following lemma.

Lemma 2. Let $U = UB + (1 - U)(1 - B)$ where $B$ is a Bernoulli vector with symmetric marginal distributions and $U$ is a uniform random variable independent of $B$. Then $\rho_\tau(U) = \rho(B)$.

Proof. First note that $\rho_\tau(U) = \rho(U)$ by Proposition 1 and Lemma 1. By writing

$$UU^\top = U^2 B B^\top + (1 - U)^2 (1 - B)(1 - B)^\top + U(1 - U) \left( B(1 - B)^\top + (1 - B)B^\top \right)$$

$$= \left( 2U - 1 \right)^2 B B^\top + (2U - 1)(1 - U) \left( B1^\top + 1B^\top \right) + (1 - U)^2 11^\top$$

we find

$$\rho_\tau(U) = \rho(U) = \rho(B).$$
and using the fact that $E(B_i) = 0.5$ for all $i \in \{1, \ldots, d\}$, we find that
\[
\text{cov}(U) = E \left( UU^\top \right) - E(U) E(U)^\top \\
= \frac{1}{3} \left( E(BB^\top) - \frac{1}{2} \left( E(B1^\top) + E(1B^\top) \right) + 11^\top \right) - \frac{1}{4} 11^\top = \frac{1}{3} E(BB^\top) - \frac{1}{12} 11^\top.
\]
Since $\text{var}(U_i) = 1/12$ and $\text{var}(B_i) = 1/4$ for all $i \in \{1, \ldots, d\}$ we conclude that
\[
\rho(U) = 4E(BB^\top) - 11^\top = \rho(B).
\]

**Proposition 4.** The set of Kendall's tau matrices of copulas is identical to the set of linear correlation matrices of Bernoulli random vectors with symmetric margins.

**Proof.** If $\rho_\tau(U)$ is a Kendall's tau matrix then, by Theorem 2, it is identical to the Kendall's tau matrix of a random vector $U^*$ with distribution given by the extremal mixture copula with the same concordance signature as $U$. It follows from Proposition 4 that $U^*$ has the stochastic representation $U^* \overset{d}{=} U(Y + (1 - U)(1 - Y))$ where, without loss of generality, $Y$ has a radially symmetric Bernoulli distribution (with symmetric margins). Lemma 2 gives $\rho_\tau(U) = \rho_\tau(U^*) = \rho(Y)$.

Conversely if $\rho(B)$ is the correlation matrix of a Bernoulli random vector $B$ with symmetric margins (not necessarily radially symmetric) then by Proposition 1 we can take an independent uniform random variable $U$ and construct a random vector $U^* = UB + (1 - U)(1 - B)$ with an extremal mixture copula. Lemma 2 gives $\rho(B) = \rho_\tau(U^*)$.

**Remark 2.** It is clear from the proof that the set of linear correlation matrices of Bernoulli random vectors with symmetric margins is equal to the set of linear correlation matrices of radially symmetric Bernoulli random vectors. This insight also appears in Theorem 1 of Huber and Maric (2019).

We now turn to the problem of determining the attainable higher order concordance probabilities when lower order probabilities are fixed. Consider the case where $d = 4$ and
the full linear system is as given in (16). Suppose that all the joint concordance probabilities \( \kappa_{i,j} \) are equal to the value \( \kappa \). In other words the Kendall’s tau correlation matrix of the parent copula is an equicorrelation matrix. Let \( \kappa_4 := \kappa_{1,2,3,4} \). We have the following result.

**Proposition 5.** Let \( C \) be a copula in dimension \( d = 4 \) such that \( \rho_r(C) \) is an equicorrelation matrix. Let \( \kappa \) and \( \kappa_4 \) denote the bivariate and fourth order concordance probabilities. Then the concordance signature of \( C \) is equal to the concordance signature of the mixture of extremal copulas with weight vector

\[
\mathbf{w} = (\kappa_4, w_1(\kappa, \kappa_4), w_1(\kappa, \kappa_4), w_1(\kappa, \kappa_4), w_2(\kappa, \kappa_4), w_2(\kappa, \kappa_4), w_2(\kappa, \kappa_4), w_1(\kappa, \kappa_4)),
\]

where \( w_1(\kappa, \kappa_4) = (3\kappa - 1)/2 - \kappa_4 \) and \( w_2(\kappa, \kappa_4) = 1 - 2\kappa + \kappa_4 \). The concordance probabilities must satisfy \( \kappa \in [1/3, 1] \) and \( \kappa_4 \in [\max(2\kappa - 1, 0), (3\kappa - 1)/2] \).

**Proof.** We simply invert the matrix \( A_4 \) in (16) and calculate \( \mathbf{w} = A_4^{-1}\mathbf{\kappa} \) where \( \mathbf{\kappa} = (1, \kappa, \kappa, \kappa, \kappa, \kappa, \kappa, \kappa) \). Since the weights must satisfy \( 0 \leq w_1(\kappa, \kappa_4) \leq 1 \), the attainable intervals follow.

In general, attainability problems can be solved by linear programming. Let \( S \subset \mathcal{E}(D) \) be a strict subset of the even power set in dimension \( d \) containing \( \emptyset \). Let \( K = \{ \kappa_I : I \in S \} \) be the corresponding partial concordance signature and let \( \mathbf{\kappa} \) be the vector of concordance probabilities formed from the elements of \( K \). Let \( A_d^{(1)} \) be the \( |S| \times 2^{d-1} \)-matrix consisting of the rows of \( A_d \) that correspond to \( S \); let \( A_d^{(2)} \) be the matrix formed of the remaining rows of \( A_d \). Then we can attempt to solve the optimization problem

\[
\min \| A_d^{(2)} \mathbf{w} \| : A_d^{(1)} \mathbf{w} = \mathbf{\kappa}, \mathbf{w} \geq 0
\]

which is a standard minimization problem with both equality and inequality constraints. The partial concordance signature is attainable if a solution exists and the solution itself will be the weight vector which gives the (collectively) smallest values for the missing concordance probabilities in the Euclidean norm. To get the (collectively) largest values we could solve

\[
\min \| A_d^{(2)} \mathbf{w} - \mathbf{1} \| : A_d^{(1)} \mathbf{w} = \mathbf{\kappa}, \mathbf{w} \geq 0.
\]

If a partial concordance signature is attainable then the set of weight vectors \( \{ \mathbf{w} : A_d^{(1)} \mathbf{w} = \mathbf{\kappa}, \mathbf{w} \geq 0 \} \) is not empty and forms a convex polytope, that is, a set of the form

\[
\left\{ \sum_{i=1}^{m} \lambda_i \mathbf{w}_i, \sum_{i=1}^{m} \lambda_i = 1, \lambda_i \geq 0, i = 1, \ldots, m \right\}.
\]

It is possible to use the method of Avis and Fukuda (1992) to find the vertices \( \mathbf{w}_1, \ldots, \mathbf{w}_m \) of the polytope. The attainable concordance signatures also form a convex polytope, with vertices \( \mathbf{\kappa}_i = A_d \mathbf{w}_i, i \in \{1, \ldots, m\} \), while the unspecified elements of the concordance signature form a convex polytope with vertices \( \kappa_i^{(2)} = A_d^{(2)} \mathbf{w}_i, i \in \{1, \ldots, m\} \).

**Example 2.** For \( d = 5 \) let a partial concordance signature be given by \( \kappa_{i,j} = 2/3 \) for all pairs of random variables and \( \kappa_{1,2,3,4} = \kappa_{1,2,3,5} = 0.4 \). To complete the concordance signature, 3 further concordance probabilities are required: \( \kappa_{1,2,4,5}, \kappa_{1,3,4,5} \) and \( \kappa_{2,3,4,5} \). The set of attainable values for the missing values forms a polytope in three dimensions and the method of Avis and Fukuda (1992) finds nine vertices. The polytope is shown in Figure 3.
6. Application to copulas of elliptical distributions

The concordance signature $K$ in (2) is identical for the copulas of all elliptical distributions with the same correlation matrix $P$. This follows because the individual probabilities of concordance are identical for all such copulas. This is proved in Genest et al. (2011, Section 2.1) in the context of an analysis of multivariate Kendall’s tau coefficients.

Let $X$ have an elliptical distribution centred at the origin with dispersion matrix equal to the correlation matrix $P$ and assume that $P(X = 0) = 0$. If $X^*$ is an independent copy of $X$, then the concordance probabilities (1) are given by $\kappa_I = 2P(X_I < X_I^*) = 2P(X_I - X_I^* < 0)$. The random vector $X_I - X_I^*$ also has an elliptical distribution centred at the origin. Using a standard stochastic representation for elliptical distributions (see Fang et al. (1990) or McNeil et al. (2015)) we can write $X_I - X_I^* \sim R_1 AS$ and $X \sim R_2 AS$ where $S$ is a random vector uniformly distributed on the unit sphere, $A$ is a matrix such that $AA^\top = P$ and $R_1$ and $R_2$ are positive scalar random variables that are both independent of $S$. It follows that

$$\kappa_I = 2P(X_I - X_I^* < 0) = 2P((R_1 AS)_I < 0) = 2P((R_2 AS)_I < 0) = 2P(X_I < 0). \quad (22)$$

From this calculation, we see that the positive scalar random variable $R_2$ plays no role, so that the concordance probabilities $\kappa_I$ are the same for any elliptical random vector with the same dispersion matrix $P = AA^\top$. Moreover, they are equal to twice the orthant probabilities for a centred elliptical distribution with dispersion matrix $P$. In practice it is easiest to calculate the orthant probabilities of a multivariate normal distribution $X \sim N_d(0, P)$ and this is the approach we take in our examples. The results for the $6 \times 6$
Table 2. Results for the correlation matrix $P$ in (23).

| $k$ | $S_k$ | $w_k$ | $I$ | $\kappa_I$ |
|-----|-------|-------|-----|------------|
| 1   | {0, 0, 0, 0, 0} | 0.2627 | 0   | 1.0000     |
| 2   | {0, 0, 0, 0, 1} | 0.0009 | {1, 2} | 0.5199     |
| 3   | {0, 0, 0, 1, 0} | 0.0131 | {1, 3} | 0.5399     |
| 4   | {0, 0, 0, 1, 1} | 0.0037 | {1, 4} | 0.5600     |
| 5   | {0, 0, 1, 0, 0} | 0.0304 | {1, 5} | 0.5804     |
| 6   | {0, 0, 1, 0, 1} | 0.0037 | {1, 6} | 0.6012     |
| 7   | {0, 0, 1, 1, 0} | 0.0088 | {2, 3} | 0.6224     |
| 8   | {0, 0, 1, 1, 1} | 0.0179 | {2, 4} | 0.6441     |
| 9   | {0, 1, 0, 0, 0} | 0.0579 | {2, 5} | 0.6667     |
| 10  | {0, 1, 0, 0, 1} | 0.0029 | {2, 6} | 0.6902     |
| 11  | {0, 1, 0, 1, 0} | 0.0100 | {3, 4} | 0.7149     |
| 12  | {0, 1, 0, 1, 1} | 0.0108 | {3, 5} | 0.7413     |
| 13  | {0, 1, 1, 0, 0} | 0.0165 | {3, 6} | 0.7699     |
| 14  | {0, 1, 1, 0, 1} | 0.0085 | {4, 5} | 0.8019     |
| 15  | {0, 1, 1, 1, 0} | 0.0063 | {4, 6} | 0.8391     |
| 16  | {0, 1, 1, 1, 1} | 0.0659 | {5, 6} | 0.8869     |
| 17  | {0, 1, 0, 0, 0} | 0.1037 | {1, 2, 3, 4} | 0.2804 |
| 18  | {0, 1, 0, 0, 1} | 0.0029 | {1, 2, 3, 5} | 0.2977 |
| 19  | {0, 1, 0, 1, 0} | 0.0114 | {1, 2, 3, 6} | 0.3150 |
| 20  | {0, 1, 0, 1, 1} | 0.0091 | {1, 2, 4, 5} | 0.3244 |
| 21  | {0, 1, 1, 0, 0} | 0.0193 | {1, 2, 4, 6} | 0.3437 |
| 22  | {0, 1, 1, 0, 1} | 0.0073 | {1, 2, 5, 6} | 0.3675 |
| 23  | {0, 1, 1, 1, 0} | 0.0062 | {1, 3, 4, 5} | 0.3702 |
| 24  | {0, 1, 1, 1, 1} | 0.0390 | {1, 3, 4, 6} | 0.3909 |
| 25  | {0, 1, 0, 0, 0} | 0.0338 | {1, 3, 5, 6} | 0.4161 |
| 26  | {0, 1, 0, 0, 1} | 0.0064 | {1, 4, 5, 6} | 0.4581 |
| 27  | {0, 1, 0, 1, 0} | 0.0076 | {2, 3, 4, 5} | 0.4503 |
| 28  | {0, 1, 0, 1, 1} | 0.0232 | {2, 3, 4, 6} | 0.4725 |
| 29  | {0, 1, 1, 0, 0} | 0.0100 | {2, 3, 5, 6} | 0.4993 |
| 30  | {0, 1, 1, 0, 1} | 0.0136 | {2, 4, 5, 6} | 0.5427 |
| 31  | {0, 1, 1, 1, 0} | 0.0036 | {3, 4, 5, 6} | 0.6153 |
| 32  | {0, 1, 1, 1, 1} | 0.1831 | {1, 2, 3, 4, 5, 6} | 0.2627 |

correlation matrix

$$P = \frac{1}{16} \begin{pmatrix} 16 & 1 & 2 & 3 & 4 & 5 \\ 1 & 16 & 6 & 7 & 8 & 9 \\ 2 & 6 & 16 & 10 & 11 & 12 \\ 3 & 7 & 10 & 16 & 13 & 14 \\ 4 & 8 & 11 & 13 & 16 & 15 \\ 5 & 9 & 12 & 14 & 15 & 16 \end{pmatrix}$$ (23)

are given in Table 2.

Every linear correlation matrix can be the correlation matrix of a multivariate elliptical (or multivariate normal) distribution. We now show by means of a counterexample that an analogous statement is not true of Kendall’s tau rank correlation matrices.
Example 3. The positive-definite correlation matrix

\[ P_{\tau} = \begin{pmatrix} 1 & -0.19 & -0.29 & 0.49 \\ -0.19 & 1 & -0.34 & 0.30 \\ -0.29 & -0.34 & 1 & -0.79 \\ 0.49 & 0.30 & -0.79 & 1 \end{pmatrix} \]  

(24)

is a Kendall’s tau matrix but is not the Kendall’s tau matrix of an elliptical distribution. The elements of this matrix are attainable values for the Kendall’s tau correlations \( \tau_{ij} \) if the corresponding concordance probabilities \( \kappa_{ij} = (1 + \tau_{ij})/2 \) are attainable. Using the methods of the previous section we can verify that

\[ K = \{ \kappa_0, \kappa_{1, 2}, \kappa_{1, 3}, \kappa_{1, 4}, \kappa_{2, 3}, \kappa_{2, 4}, \kappa_{3, 4} \} \]

is an attainable set of concordance probabilities. Solving the linear programming problem (19) gives the weight vector

\[ w_1 = (0.04, 0.005, 0.36, 0, 0.0625, 0.2475, 0.2825, 0.0025) \]

corresponding to the minimum attainable fourth order concordance probability of 0.04. Solving the linear programming problem (20) gives the weight vector

\[ w_2 = (0.0425, 0.0025, 0.3575, 0.0025, 0.06, 0.25, 0.285, 0) \]

corresponding to the maximum attainable fourth order concordance probability of 0.04/25. In this case \( w_1 \) and \( w_2 \) are precisely the two vertices of the polytope of attainable weights given by the set (21), which takes the form of a line segment connecting \( w_1 \) and \( w_2 \). Any weight vector in this set will give the Kendall’s tau matrix \( P_{\tau} \).

Let us assume that \( P_{\tau} \) in (24) corresponds to an elliptical copula. Lindskog et al. (2003) and Fang and Fang (2002) have shown that the pairwise Kendall’s tau correlation matrix of an elliptical copula with correlation matrix \( P \) is given by the componentwise transformation \( \tau_{ij} = 2\pi^{-1} \arcsin(P_{ij}) \). It must be the case that \( P = \sin(\pi P_{\tau}/2) \) is the correlation matrix of the elliptical copula. However, by calculating the eigenvalues we find that \( P \) is not positive semi-definite, which is a contradiction.

We now turn to the copula of the multivariate Student \( t \) distribution \( C_{\nu, P}^{t} \) with degree of freedom parameter \( \nu \) and correlation matrix parameter \( P \). It is unusual to consider this copula for degrees of freedom \( \nu < 1 \), but we consider the limiting behaviour as \( \nu \to 0 \). The next result shows that \( C_{\nu, P}^{t} \) with \( \nu \) very small provides an absolutely continuous parametric model that can approximate the mixture of extremal copulas that shares its concordance signature with all elliptical distributions with correlation matrix \( P \). The proof relies on some limiting results for the univariate and multivariate \( t \) distribution which are collected in the Appendix.

Theorem 4. As \( \nu \to 0 \) the \( d \)-dimensional \( t \) copula \( C_{\nu, P}^{t} \) converges pointwise to the unique extremal mixture copula that shares its concordance signature.

Proof. Let the function \( h_{\nu}(w, s) \) be defined by

\[ h_{\nu}(w, s) = F_{\nu}\left(G_{d, \nu}^{-1}(w)As\right), \quad w \in (0, 1), \quad s = (s_1, \ldots, s_d), \quad s^\top s = 1, \]

where \( F_{\nu} \) is the cdf of a \( t \) distribution with \( \nu \) degrees of freedom, \( G_{d, \nu} \) is the cdf of the radial component of a \( d \)-dimensional multivariate \( t \) distribution with \( \nu \) degrees of freedom and \( A \)
is a $d \times d$ matrix such that $AA^\top = P$; such a matrix can be constructed for any positive semi-definite $P$. Let $S = (S_1, \ldots, S_d)$ be uniformly distributed on the unit sphere and let $W$ be an independent uniform random variable. Then $X = G_{U_0}(W)AS$ has a multivariate $t$ distribution and $U = h_0(W, S)$ has joint cdf $C_{\nu, P}^t$. We want to show that the joint cdf of $h_0(W, S)$ converges to the joint cdf of an extremal mixture as $\nu \to 0$.

We first argue that the random vector given by $AS$ satisfies $\mathbb{P}((AS)_j = 0) = 0$. Let $a_j$ denote the $j$th row of $A$. If $a_j = 0$ then the $j$th row and column of $P$ would consist of zeros implying that the $j$th margin of the multivariate $t$ distribution of $X$ was degenerate; this case can be discounted because the $t$ copula with such a matrix $P$ is not defined. Suppose therefore that $\mathbb{P}(a_j^\top S = 0) > 0$ for $a_j \neq 0$. If $R$ is the radial random variable corresponding to multivariate normal, then $\mathbb{P}(a_j^\top RS = 0) = \mathbb{P}(a_j^\top Z = 0) > 0$, where $Z$ is a vector of $d$ independent standard normal variables. However $a_j^\top Z$ is univariate normal with variance $a_j^\top a_j > 0$ and cannot have an atom of mass at zero.

We can therefore define the set $A = \{s : s^\top s = 1, (As)_j \neq 0, j = 1, \ldots, d\}$ such that $\mathbb{P}(S \in A) = 1$. Given that $S = s \in A$, then

$$
\begin{align*}
\{U_j \leq u_j\} &= \left\{W \leq G_{d, \nu} \left( \frac{F_{\nu}^{-1}(u_j)}{(As)_j} \right) \right\} \quad \text{if } (As) > 0, \\
\{U_j \leq u_j\} &= \left\{W \geq G_{d, \nu} \left( \frac{F_{\nu}^{-1}(u_j)}{(As)_j} \right) \right\} \quad \text{if } (As) < 0,
\end{align*}
$$

and hence the conditional distribution function of $U$ given $S = s$ has the form

$$
\mathbb{P}(U_1 \leq u_1, \ldots, U_d \leq u_d | S = s) = \mathbb{P}\left(\max_{j \in I_{As}} \left\{G_{d, \nu} \left( \frac{F_{\nu}^{-1}(u_j)}{(As)_j} \right) \right\} \leq W \leq \min_{j \in I_{As}} \left\{G_{d, \nu} \left( \frac{F_{\nu}^{-1}(u_j)}{(As)_j} \right) \right\}\right),
$$

where $I_{As}$ is the set of indices $j$ for which $(As)_j > 0$. Writing, for any $u \in (0, 1)^d$,

$$
C_{\nu, P}(u) = \mathbb{P}(U_1 \leq u_1, \ldots, U_d \leq u_d) = \int \mathbb{P}(U_1 \leq u_1, \ldots, U_d \leq u_d | S = s) dF_S(s),
$$

we can use Proposition 9 in the Appendix and Lebesgue’s Dominated Convergence Theorem to conclude that $C_{\nu, P}(u)$ converges, as $\nu \to 0$, to

$$
C(u) = \int \left( \min_{j \in I_{As}} (2u_j - 1)^+ - \max_{j \notin I_{As}} (1 - 2u_j)^+ \right)^+ dF_S(s), \quad (25)
$$

We now show that this limit is a mixture of extremal copulas. To this end, consider the random vector $(\text{sign}(AS) + 1)/2$. This has the same distribution as the multivariate Bernoulli random vector $Y$ whose distribution is defined by the probabilities $p_I = \mathbb{P}(Y_I = 1) = \mathbb{P}((AS)_j > 0, j \in I)$ for $I \subseteq \mathcal{D}$; the random vectors $(\text{sign}(AS) + 1)/2$ and $Y$ differ only on the null set where components of $AS$ are zero. Moreover, the distribution of $Y$ is radially symmetric since the spherical symmetry of $S$ implies $AS \overset{d}{=} -AS$ which in turn implies $Y \overset{d}{=} 1 - Y$. The limiting distribution (25) may be written in the form

$$
C(u) = \sum_{y \in (0, 1)^d} \mathbb{P}(\text{sign}(AS) + 1)/2 \left( \min_{j:y_j=1} (2u_j - 1)^+ - \max_{j:y_j=0} (1 - 2u_j)^+ \right)^+ \mathbb{P}(Y = y).
$$
and using the index set notation defined in Section 2, this may also be written as

\[ C(u) = \sum_{k=1}^{2^d-1} \left( \min_{j \in J_k} (2u_j - 1)^+ - \max_{j \in J_k} (1 - 2u_j)^+ \right)^+ \mathbb{P}(Y = s_k) + \sum_{k=1}^{2^d-1} \left( \min_{j \in J_k}^c (2u_j - 1)^+ - \max_{j \in J_k} (1 - 2u_j)^+ \right)^+ \mathbb{P}(Y = 1 - s_k). \]

Setting \( \mathbb{P}(Y = s_k) = \mathbb{P}(Y = 1 - s_k) = 0.5w_k \) as in Section 3.2 we obtain \( C(u) = \sum_{k=1}^{2^d-1} w_k C_k(u) \), where

\[ 2C_k(u) = \left( \min_{j \in J_k} (2u_j - 1)^+ - \max_{j \in J_k} (1 - 2u_j)^+ \right)^+ + \left( \min_{j \in J_k^c} (2u_j - 1)^+ - \max_{j \in J_k} (1 - 2u_j)^+ \right)^+ \]

and we need to check that \( C_k \) is in fact the \( k \)th extremal copula \( C^{(k)} \) given by Eq. (3). To do so, we have to distinguish the four cases below:

(i) Suppose that there is at least one \( j \in J_k \) and at least one \( j \in J_k^c \) such that \( u_j \leq 0.5 \). Then \( C_k(u) = 0 = C^{(k)}(u) \).

(ii) Suppose that for all \( j \in J_k \), \( u_j > 0.5 \) and there exists at least one \( j \in J_k^c \) such that \( u_j \leq 0.5 \). Then

\[ 2C_k(u) = \left( \min_{j \in J_k} (2u_j - 1)^+ - \max_{j \in J_k^c} (1 - 2u_j)^+ \right)^+ = 2\left( \min_{j \in J_k} u_j + \min_{j \in J_k^c} u_j - 1 \right)^+ = 2C^{(k)}(u). \]

(iii) The case when for all \( j \in J_k^c \), \( u_j > 0.5 \) and there exists at least one \( j \in J_k \) such that \( u_j \leq 0.5 \) is analogous to case (ii) and is omitted.

(iv) Suppose that for all \( j \in D \), \( u_j > 0.5 \). Then

\[ 2C_k(u) = \min_{j \in J_k} (2u_j - 1) + \min_{j \in J_k^c} (2u_j - 1) = 2\left( \min_{j \in J_k} u_j + \min_{j \in J_k^c} u_j - 1 \right) = 2C^{(k)}(u). \]

Finally, we need to verify that the concordance signature of the limiting mixture of extremal copulas is the same as the concordance signature of \( C^{(k)}_{\nu,P} \) for any \( \nu > 0 \). If \( \kappa_I \) denotes a concordance probability for the \( t \) copula, we need to show that \( \kappa_I = \sum_{k=1}^{2^d-1} w_k a_{I,k} \), which is the corresponding concordance probability for the limit. Recall that the vector \( X = G_{d,\nu}^{-1}(W)AS \) has a multivariate \( t \) distribution. Equation (22) implies that

\[ \kappa_I = 2\mathbb{P}\left( G_{d,\nu}^{-1}(W)(AS)_I < 0 \right) = 2\mathbb{P}\left( (AS)_I < 0 \right) = 2\mathbb{P}(Y_I = 0) = 2\mathbb{P}(Y_I = 1) = \sum_{k=1}^{2^d-1} w_k a_{I,k}, \]

where the final step uses the reasoning employed in the proof of Theorem 2.

**Remark 3.** The steps of the above proof go through even when the matrix \( P \) is not of full rank. However, because in such cases the copula is distributed on a strict subspace of the unit hypercube \([0,1]^d\), the limiting extremal mixture copula has zero mass on certain diagonals of the hypercube. Suppose, for example, that rows \( i \) and \( j \) of the matrix \( A \) satisfying \( AA^\top = P \) are identical. Then the components \( Y_I \) and \( Y_J \) of the vector \( Y \) defined in the proof are identical, i.e. they are both 0 or both 1. For any vector \( s_k \) such that \( s_{k,i} \neq s_{k,j} \) it must be the case that \( w_k = \mathbb{P}(Y = s_k) + \mathbb{P}(Y = 1 - s_k) = 0 \) and so the \( k \)th diagonal would have zero mass.
7. Signature estimation

Consider a random sample \( X_1, \ldots, X_n \) from an unknown distribution with copula \( C \) and continuous marginals \( F_1, \ldots, F_d \). In this section, we explain how the concordance signature \( \kappa_C \) of \( C \) can be estimated intrinsically, i.e. in a way that the set of estimated concordance signatures is a concordance signature of a bona fide \( d \)-dimensional copula. We do this under the assumption that there are no ties in the data; this is not restrictive because the continuity of the margins ensures the absence of ties with probability 1.

For any index set \( I \) with \( |I| \geq 2 \), empirical estimators of \( \kappa_I \) can be derived from empirical estimators of \( \tau(U_I) \) using Eq. (12). When \( d = 2 \) and \( I = \{k, \ell\} \) for some \( k \neq \ell \in \{1, \ldots, d\} \), the classical estimator of \( \tau(U_I) \) going back to Hoeffding (1947) is

\[
\tau_{I,n} = -1 + \frac{4}{n(n-1)} \sum_{i \neq j} I\{X_{ik} \leq X_{jk}, X_{i\ell} \leq X_{j\ell}\}.
\]

It is a special case of the estimator of \( \tau(U_I) \) for \( |I| \geq 2 \) proposed and investigated by Genest et al. (2011), which is given by

\[
\tau_{I,n} = \frac{1}{2|I|-1} \left( -1 + \frac{2|I|}{n(n-1)} \prod_{k \in I} I\{X_{ik} \leq X_{j\ell}\} \right).
\]

Plugging in this estimator into (12) yields the empirical estimator of \( \kappa_I \), viz.

\[
\kappa_{I,n} = \frac{2}{n(n-1)} \prod_{i \neq j} I\{X_{ik} \leq X_{jk}\}.
\]

From the theory of U-statistics (Hoeffding, 1948), we know that the estimated concordance probabilities for all subsets \( I \) with \( |I| \geq 2 \), if ordered in a vector \( \kappa_n \), satisfy

\[
\sqrt{n}(\kappa_n - \kappa) \sim \mathcal{N}(0, \Sigma)
\]

as \( n \to \infty \), where \( \kappa \) denotes vector of the corresponding concordance probabilities of \( C \), \( \Sigma \) is the variance-covariance matrix of the random vector with components \( C_I(U_I) + \bar{C}_I(U_I) \) and \( \bar{C}_I \) is the survival function of \( C_I \). The surprising fact is the following result, which shows that the empirical concordance signature \( \{\kappa_{I,n}, I \subseteq \mathcal{P}(D)\} \) is in fact the concordance signature of a \( d \)-dimensional copula.

**Theorem 5.** Assuming that \( n \geq 2 \) and there are no ties in the sample, there exists a \( d \)-dimensional copula \( C_n \) such that \( \{\kappa_{I,n}, I \subseteq \mathcal{P}(D)\} \) is the concordance signature of \( C_n \).

**Proof.** Let \( Y_{ij} = (\text{sign}(X_i - X_j) + 1)/2 \) for \( i \neq j \) and set

\[
\hat{w}_k = \frac{2}{n(n-1)} \sum_{i \neq j} (I(Y_{ij} = s_k) + I(Y_{ij} = 1 - s_k)).
\]

These empirical weights are estimators of \( w_k = \mathbb{P}(Y = s_k) + \mathbb{P}(Y = 1 - s_k) \), the weights of the extremal mixture which has the same concordance signature as \( C \). Because the sample is assumed to have no ties, the weights \( \hat{w}_k \) are clearly positive and sum to 1. Thus they describe a mixture of extremal copulas, say \( C_n \). To establish the result, it suffices to show that for any \( I \in \mathcal{P}(D) \) with \( |I| \geq 2 \), \( \kappa_{I,n} = \kappa(C_n,I) \), where \( C_n,I \) is the margin of \( C_n \).
corresponding to the index set $I$. This can be seen as follows

\[
\kappa(C_{n,I}) = \sum_{k=1}^{2^{d-I}} \tilde{w}_k a_{I,k} = \sum_{k=1}^{2^{d-I}} \sum_{i<j} I_{\{Y_{ij}=s_k\}} + I_{\{Y_{ij}=1-s_k\}} a_{I,k} \\
= \frac{2}{n(n-1)} \sum_{i<j} \sum_{k=1}^{2^{d-I}} (I_{\{Y_{ij}=s_k\}} + I_{\{Y_{ij}=1-s_k\}}) I_{\{I \subseteq I_k \text{ or } I \subseteq I_k^c\}} \\
= \frac{2}{n(n-1)} \sum_{i<j} (I_{\{Y_{ij}=0\}} + I_{\{Y_{ij}=1\}}) \\
= \frac{2}{n(n-1)} \sum_{i<j} (I_{\{X_{i,j}<X_{i,i}\}} + I_{\{X_{i,j}>X_{i,i}\}}) \\
= \frac{2}{n(n-1)} \sum_{i<j} I_{\{X_{i,k}<X_{i,k}\}} = \frac{2}{n(n-1)} \sum_{i<j,k \in I} I_{\{X_{i,k}<X_{i,k}\}},
\]

where the last expression is $\kappa_{I,n}$ since there are no ties in the sample.

Remark 4. While the probability of ties in a sample from a distribution with continuous margins is zero, rounding effects may lead to occasional ties in practice. In this case it is possible that some of the vectors $Y_{ij}$ have components equal to 0.5. Let us suppose that $Y_{ij}$ has $k$ such values for $k \in \{1, \ldots, d\}$. A possible approach to incorporating this information in the estimator is to replace $Y_{ij}$ by the $2^k$ vectors that have zeros and one in the same positions as $Y_{ij}$, each weighted by $2^{-k}$, and to generalize \((26)\) to be a weighted sum of indicators. For example, the observation $Y_{ij} = (1, 0, 0, 0, 0.5)$ would be replaced by $(1, 0, 1, 1)$, $(1, 0, 1, 0)$, $(1, 0, 0, 1)$ and $(1, 0, 0, 0)$, each weighted by $1/4$. This would still deliver estimates $\tilde{w}_k$ that are positive and sum to one and thus yield a proper concordance signature.

Software

The methods and examples discussed in this paper are documented as vignettes in the \texttt{R} package \texttt{extremalCopula} at https://github.com/ajmcneil/extremalcopula.

Appendix: Some limiting properties of the univariate and multivariate $t$ distribution as $\nu \to 0$

Univariate $t$ distribution

Let $F_\nu$, $F^{-1}_\nu$ and $f_\nu$ denote the cdf, inverse cdf and density of a univariate $t$ distribution with $\nu$ degrees of freedom. The cdf satisfies

\[
F_\nu(x) - 0.5 = \frac{x \Gamma(\frac{\nu+1}{2})}{\sqrt{\pi \nu} \Gamma(\frac{\nu}{2})} 2F_1 \left( \frac{1}{2}, \frac{\nu+1}{2}; \frac{3}{2}; -\frac{x^2}{\nu} \right), \quad x \in \mathbb{R}, \ \nu > 0, \quad (27)
\]

where $2F_1$ denotes the hypergeometric function and $\Gamma$ the gamma function. We will show that, for fixed $u \neq 0.5$, the quantile function $F^{-1}_\nu(u)$ is unbounded as a function of $\nu$ as $\nu \to 0$. To that end we first prove the following lemma.

Lemma 3. $\lim_{\nu \to 0} F_\nu(x) = 0.5$ for all $x \in \mathbb{R}$.

Proof. The lemma is trivially true for $x = 0$ so we consider $x \neq 0$. Making the substitution $y = x/\sqrt{\nu}$ in \((27)\) gives

\[
\frac{2F_\nu(\sqrt{\nu} y) - 1}{\nu} = \frac{2y \Gamma(\frac{\nu+1}{2})}{\sqrt{\pi \nu} \Gamma(\frac{\nu}{2})} 2F_1 \left( \frac{1}{2}, \frac{\nu+1}{2}; \frac{3}{2}; -y^2 \right)
\]
and we can use the limits [Abramowitz and Stegun 1965]

\[
\lim_{\nu \to 0} y \frac{2F_1 \left( \frac{1}{2}, \frac{\nu + 1}{2}; -3; -y^2 \right)}{2F_1 \left( \frac{1}{2}, \frac{\nu + 1}{2}; -3; -y^2 \right)} = \ln \left( y + \sqrt{1 + y^2} \right)
\]

\[
\lim_{\nu \to 0} \frac{2F_1 \left( \frac{\nu + 1}{2}; \frac{1}{2}, -y^2 \right)}{\sqrt{\pi} \Gamma \left( \frac{3}{2} \right)} = \lim_{\nu \to 0} \frac{1}{\sqrt{\pi} \Gamma \left( \frac{\nu + 2}{2} \right)} = 1
\]

to conclude that

\[
\lim_{\nu \to 0} \frac{2F_\nu \left( \sqrt{\nu}y \right) - 1}{\nu} = \ln \left( y + \sqrt{1 + y^2} \right) = \text{sign}(y) \ln \left( |y| + \sqrt{1 + y^2} \right)
\]

Reversing the earlier substitution and setting \( x = \sqrt{\nu}y \) now gives

\[
\lim_{\nu \to 0} \frac{2F_\nu(x) - 1}{\nu \text{sign}(x) \left( \ln \left( |x| + \sqrt{\nu + x^2} \right) - \frac{1}{2} \ln(\nu) \right)} = 1.
\]

The result follows from the fact that the denominator tends to 0 as \( \nu \to 0 \).

**Lemma 4.**

\[
\lim_{\nu \to 0} F_\nu^{-1}(u) = \begin{cases} -\infty & \text{if } u < 0.5, \\ 0 & \text{if } u = 0.5, \\ \infty & \text{if } u > 0.5. \end{cases}
\]

**Proof.** The case \( u = 0 \) is obvious, since \( F_\nu^{-1}(0.5) = 0 \) for all \( \nu > 0 \). To show that \( \lim_{\nu \to 0} F_\nu^{-1}(u) = -\infty \) for \( u < 0.5 \), we need to show that, for all \( k < 0 \), there exists \( \delta \) such that \( \nu < \delta \Rightarrow F_\nu^{-1}(u) \leq k \). Suppose we fix an arbitrary \( k < 0 \). Since \( F_\nu(k) \to 0.5 \) as \( \nu \to 0 \), there exists \( \delta > 0 \) such that \( \nu < \delta \) implies that \( F_\nu(k) > u \), since \( u < 0.5 \). But then, for any \( \nu < \delta \), it follows that \( k \in \{ x : F_\nu(x) \geq u \} \) and hence \( F_\nu^{-1}(u) = \inf \{ x : F_\nu(x) \geq u \} \leq k \). Analogously, to show that \( \lim_{\nu \to 0} F_\nu^{-1}(u) = \infty \) for \( u > 0.5 \), we need to show that, for all \( k > 0 \), there exists \( \delta \) such that \( \nu < \delta \Rightarrow F_\nu^{-1}(u) \geq k \). Suppose we fix an arbitrary \( k > 0 \). Since \( F_\nu(k) \to 0.5 \) as \( \nu \to 0 \), there exists \( \delta > 0 \) such that \( \nu < \delta \) implies that \( F_\nu(k) < u \), since \( u > 0.5 \). But then, for any \( \nu < \delta \), it follows that \( k \in \{ x : F_\nu(x) \geq u \} \). Hence \( F_\nu^{-1}(u) = \inf \{ x : F_\nu(x) \geq u \} \geq k \).

**Multivariate t distribution**

If the random vector \( \mathbf{X} \) has a \( d \)-dimensional multivariate \( t \) distribution with \( \nu \) degrees of freedom, then it has the stochastic representation \( \mathbf{X} \overset{\text{d}}{=} \mathbf{\mu} + \mathbf{RAS} \) where \( \mathbf{S} \) is a uniform random vector on the \( d \)-dimensional uniform unit sphere, \( \mathbf{R} \) is an independent, positive, scalar random variable such that \( R^2/d \sim F(d, \nu) \) (a Fisher–Snedecor \( F \) distribution), \( \mathbf{\mu} \) is a location vector and \( \mathbf{A} \) is a matrix; see Section 6.3 in [McNeil et al. (2015)]. Let \( G_{d, \nu} \) denote the cdf of the radial random variable \( R \) and \( g_{d, \nu} \) the corresponding density; the latter is given by

\[
g_{d, \nu}(r) = \frac{2}{\nu} \left( 1 + \frac{r^2}{\nu} \right)^{-\frac{d}{2}} \left( 1 + \frac{r^2}{\nu} \right)^{-\frac{d}{2}} \frac{\Gamma \left( \frac{\nu + d}{2} \right)}{\Gamma \left( \frac{\nu}{2} \right) \Gamma \left( \frac{d}{2} \right)}.
\]
Proposition 6. For a constant \( \lambda \neq 0 \) and any \( u \in [0, 1] \),
\[
\lim_{\nu \to 0} G_{d,\nu} \left( \frac{F_{\nu}^{-1}(u)}{\lambda} \right) = \begin{cases} 
(2u - 1)^+ & \text{if } \lambda > 0, \\
(1 - 2u)^+ & \text{if } \lambda < 0.
\end{cases}
\] (29)

Proof. When \( \lambda > 0 \), \( F_{d,\nu}(u) = G_{d,\nu} \left( \lambda^{-1}F_{\nu}^{-1}(u) \right) \) is a distribution function supported on \([0,5,1]\). Similarly, when \( \lambda < 0 \), \( F_{d,\nu}(u) = 1 - G_{d,\nu} \left( \lambda^{-1}F_{\nu}^{-1}(u) \right) \) is a distribution function supported on \([0,0.5]\). The density of \( F_{d,\nu} \) is given by
\[
f_{d,\nu}(u) = g_{d,\nu} \left( \frac{|F_{\nu}^{-1}(u)|}{|\lambda|} \right) \frac{1}{|\lambda|} \frac{1}{f_\nu (F_{\nu}^{-1}(u))}
\]
where \( u \in [0.5, 1] \) when \( \lambda > 0 \) and \( u \in (0, 0.5] \) when \( \lambda < 0 \).

Note that, when \( u = 0.5 \), \( F_{\nu}^{-1}(u) = 0 \) for all \( \nu \) and (29) clearly holds; we thus restrict our analysis of the density to the case where \( u \neq 0.5 \). Using the notation \( x_{\nu,u} = F_{\nu}^{-1}(u) \) and the expression (28) we have that
\[
f_{d,\nu}(u) = g_{d,\nu} \left( \frac{|x_{\nu,u}|}{|\lambda|} \right) \frac{1}{|\lambda|} \frac{1}{f_\nu (x_{\nu,u})}
\]

The limit as \( \nu \to 0 \) of each of the five terms above is 1. For terms 1, 2, 4 and 5, this is obvious from the properties of the gamma function and the fact that \( |x_{\nu,u}| \to \infty \) for \( u \neq 0.5 \) (Lemma [4] above). For term 3 note that the term within the outer brackets converges to \( \lambda^2 \) and hence the assertion follows. The density in the limit thus satisfies
\[
\lim_{\nu \to 0} f_{d,\nu}(u) = \begin{cases} 
2 \times I_{\{0.5 \leq u < 1\}} & \lambda > 0, \\
2 \times I_{\{0 < u \leq 0.5\}} & \lambda < 0.
\end{cases}
\]

From Scheffé’s Theorem we conclude that the limiting distribution of \( F_{d,\nu} \) is uniform on either \([0, 0.5]\) or \([0.5, 1]\), depending on the sign of \( \lambda \). Hence if \( \lambda > 0 \), \( F_{d,\nu}(u) \to (2u - 1)^+ \) as \( \nu \to 0 \), and if \( \lambda < 0 \), \( F_{d,\nu}(u) \to 1 - (1 - 2u)^+ \) as \( \nu \to 0 \). In either case (29) holds.

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