Dissimilarity functions for rank-based hierarchical clustering of continuous variables

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Abstract

We present a theoretical framework for a (copula-based) notion of dissimilarity between subsets of continuous random variables and study its main properties. Special attention is paid to those properties that are prone to the hierarchical agglomerative methods, such as reducibility. We hence provide insights for the use of such a measure in clustering algorithms, which allows us to cluster random variables according to the association/dependence among them, and present a simulation study. Real case studies illustrate the whole methodology.

Keywords: Copula, Cluster analysis, Dissimilarity, Stochastic dependence, Rank statistics

1 Introduction

Concepts of stochastic dependence and association among random variables have been extensively studied and applied in many fields. Various indices and measures have been introduced in order to study the many facets of relationships among random variables, from classical linear correlation coefficients to indices for detecting concordance, tail dependence, radial symmetry, etc. In this respect, the contribution of copula methods to describe relationships among (mainly, continuous) random variables has been largely recognized (see, e.g., [20, 39, 45, 49, 57] and references therein).

In the high-dimensional setting, in order to visualize stochastic association and guide the process of model building and selection, a powerful way consists in performing cluster algorithms to identify sub-groups of random variables that have a common behaviour. For instance, cluster algorithms have been used in [31] for the identification of a nested Archimedean structure, and in [9, 16] for the determination of a vine copula model. Moreover, a procedure is illustrated in [6] for selecting the tree structure of a risk aggregation model by combining hierarchical clustering techniques with a distance metric based on Kendall’s tau.

In multivariate time series analysis, moreover, clustering methods have been used to detect similarities in financial time series based on (Pearson) correlation coefficient and some of its variants (see, for instance, [3, 22]), with possible applications in portfolio selection and diversification measurements [12, 14, 17]. Related clustering methods are also based on other measures of association/concordance such as Kendall’s and Spearman’s correlation (see, e.g., [14]), mutual information

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as well as various measures of tail dependence as done, for instance, in \cite{10, 18}. Other clustering techniques grounded on copula concepts have been largely applied also to expression levels of genes and expression profiles of biological tissue samples, and they have been successfully used to identify expression patterns of functionally related/co-regulated genes as well as samples with similar biological characteristics (see, e.g., \cite{15, 42, 43}).

In order to describe association in high–dimensional random vectors most of the current approaches are of (agglomerative) hierarchical type, since they can also provide an intuitive graphical representation in terms of a dendrogram. However, to the best of our knowledge, little attention has been devoted to investigate how the way one measures the “distance” between subvectors satisfies some desirable theoretical properties (for example, reducibility and comonotonic invariance) and how it can ease the interpretation of some dependence concepts.

Motivated by these previous investigations, here the goal is to introduce and formalize a rank-based notion of dissimilarity between two subsets of random variables. In essence, the dissimilarity measure will be of probabilistic nature, i.e. it will depend on the joint probability distribution function of the involved variables, and will be related to the degree of comonotonicity among the variables (see, e.g., \cite{13, 40, 53}). Specifically, first, we define the general framework where our dissimilarity concept is build up (Section 2) and, in particular, we introduce possible desirable properties that a dissimilarity may satisfy with particular emphasis on those properties that are prone to the hierarchical agglomerative methods. In Section 3 we consider and compare to each other various examples of dissimilarity mappings. Moreover, in Section 4 we show how the dissimilarity can be used to detect various kinds of stochastic dependence of a random vector. From the computational side, we hence provide a simulation study in order to show how algorithms based on linkage and pairwise dissimilarities work in a finite sample and discuss their advantages and disadvantages (Section 4.1). Real case studies illustrate the whole methodology (Section 5), while section 6 summarizes the main findings.

2 The framework

We consider a (finite) set \( \mathcal{X} = \{X_1, \ldots, X_m\} \) of continuous random variables defined on a same probability space (with possibly additional properties like existence of second-order moments). Any subset of \( \mathcal{X} \) will be denoted by upper-case black-board letters, e.g. \( X \). Given a subset \( \mathcal{X} \subset \mathcal{X} \) composed of \( k \) random variables the corresponding random vector will be denoted by \( \vec{X} \).

Here, we aim at quantifying how two non-empty subsets of \( \mathcal{X} \) are similar or, analogously, how we can define a suitable dissimilarity degree between them.

Formally, the dissimilarity degree can be defined as a mapping \( \tilde{d}: \mathcal{P}_0(\mathcal{X}) \times \mathcal{P}_0(\mathcal{X}) \rightarrow [0, +\infty] \), where \( \mathcal{P}_0(\mathcal{X}) \) is the set of all non–empty subsets of \( \mathcal{X} \), with the following properties:

\begin{align*}
(A1) \quad & \tilde{d}(X, Y) = 0 \text{ for every } X, Y \in \mathcal{X} \text{ such that } X = Y \text{ almost everywhere}; \\
(A2) \quad & \tilde{d}(\mathcal{X}, \mathcal{Y}) = \tilde{d}(\mathcal{Y}, \mathcal{X}) \text{ for every } \mathcal{X}, \mathcal{Y} \in \mathcal{P}_0(\mathcal{X}).
\end{align*}

Conditions \( \tilde{A1} \) and \( \tilde{A2} \) express the fact that \( \tilde{d} \) is symmetric and assigns its minimal value to a pair of elements that are equal each other (almost everywhere).

As it is well known, the chosen form of \( \tilde{d} \) should correspond to the subject matter meaning of “similarity”. As a particular feature of our methodology, the dissimilarity is characterized by the following additional assumptions:
Assumption 1 (Distributional invariance)

The dissimilarity degree between two classes $X$ and $Y$ only depends on the probability distribution function of the random vector $(\vec{X}, \vec{Y})$.

Assumption 2 (Rank invariance)

The dissimilarity degree between two classes $X$ and $Y$ is invariant under strictly monotonic transformations of the components of the random vector $(\vec{X}, \vec{Y})$.

Assumption 1 states that the dissimilarity is law-invariant, as the various notions of association for random vectors considered in the literature. Assumption 2 states that the dissimilarity degree is rank-invariant. In particular, together with property (A1), it implies that two random variables have dissimilarity degree equal to 0 whenever one is a strictly increasing function of the other one (almost everywhere). This latter aspect obviously is related to the notion of comonotonicity (see, e.g., [13, 53]). In a sense, for a pair $(X, Y)$ of random variables with fixed marginals, a dissimilarity degree quantifies the closeness of the joint distribution of $(X, Y)$ to the upper extreme of the related Fréchet class (see, also, [5, 19] for an historical overview).

Thanks to Sklar’s theorem (see, e.g., [20]) and Assumption 1, it follows that the dissimilarity degree is only related to the copula of the involved random variables, regardless the respective marginal behaviour. For instance, any pair of independent (respectively, comonotonic, antitonic) random variables has the same degree of dissimilarity. Since, in our setting, a dissimilarity mapping only depends on copulas, which are the distribution functions associated with a vector of random variables that are uniformly distributed on $\mathbb{I} := [0, 1]$, along this manuscript we can hence assume without loss of generality that the involved variables are uniformly distributed on $\mathbb{I}$.

Thus, in view of the previous considerations and assumptions, we are hence able to give the following definition. Let $m \geq 2$ be an integer which will be kept fixed throughout this paper, and denote by $L^0(I^m)$ the space of all $m$–dimensional vectors of random variables that are uniformly distributed on $\mathbb{I}$.

Definition 2.1. For every $m_1, m_2 \in \mathbb{N}$ with $2 \leq m_1 + m_2 \leq m$,

$$d^{m_1, m_2} : L^0(I^{m_1}) \times L^0(I^{m_2}) \to [0, +\infty[$$

is called a $(m_1, m_2)$–dissimilarity function if it satisfies the following properties:

(A1) For every $(\vec{X}, \vec{Y}) \in L^0(I^{m_1}) \times L^0(I^{m_2})$, $d^{m_1, m_2}(\vec{X}, \vec{Y}) = 0$ when the copula of $(\vec{X}, \vec{Y})$ is equal to the comonotonicity copula $\hat{M}$.

(A2) For every $(\vec{X}, \vec{Y}) \in L^0(I^{m_1}) \times L^0(I^{m_2})$,

$$d^{m_1, m_2}(\vec{X}, \vec{Y}) = d^{m_1, m_2}(\sigma_1(\vec{X}), \sigma_2(\vec{Y}))$$

holds for every permutation $\sigma_1$ and $\sigma_2$.

Property (A1) extends the general property (A1) from the bivariate to the multivariate case; moreover, it also takes in account the rank invariance of the dissimilarity measure. As it is well known from copula theory (see, e.g., [20]), it is equivalent to the fact that $d^{m_1, m_2}(\vec{X}, \vec{Y}) = 0$ when there exists a random variable $Z$ such that each component of the vector $(\vec{X}, \vec{Y})$ is a monotonic increasing function of $Z$ (almost everywhere). For sake of completeness, we recall that the comonotonicity copula $M$ is defined by $M(u_1, \ldots, u_m) = \min\{u_1, \ldots, u_m\}$ for every $u_1, \ldots, u_m$ in $\mathbb{I}$.

Property (A2) is, again, an extension of (A2). Here, it should be also stressed that the dissimilarity between two vectors does not change when the components of each vector are permuted.

All the dissimilarity functions can be glued together into the following concept.
Definition 2.2. An extended dissimilarity function (of degree $m$) is a map

$$d : \bigcup_{2 \leq m_1 + m_2 \leq m} L^0(\mathbb{R}^{m_1}) \times L^0(\mathbb{R}^{m_2}) \to \mathbb{R}_+$$

whose restriction $d^{m_1, m_2} := d|_{L^0(\mathbb{R}^{m_1}) \times L^0(\mathbb{R}^{m_2})}$ to $L^0(\mathbb{R}^{m_1}) \times L^0(\mathbb{R}^{m_2})$ is a $(m_1, m_2)$-dissimilarity function for any $m_1, m_2 \in \mathbb{N}$ with $2 \leq m_1 + m_2 \leq m$, such that, for every $(\vec{x}, \vec{y}) \in L^0(\mathbb{R}^{m_1}) \times L^0(\mathbb{R}^{m_2})$,

$$d^{m_1, m_2}(\vec{x}, \vec{y}) = d^{m_2, m_1}(\vec{y}, \vec{x})$$

holds.

Roughly speaking, an extended dissimilarity function allows to assign a degree of dissimilarity to any pair of subsets of random variables, regardless of the respective dimension. The condition given by (2.1) simply ensures that the dissimilarity has some natural symmetry.

Before introducing basic examples of such functions, we present here some additional desirable properties they may satisfy. First, we present some local properties, i.e. properties that are satisfied by the restriction $d^{m_1, m_2}$ of the extended dissimilarity function $d$ for any possible choice of $m_1, m_2$ with $2 \leq m_1 + m_2 \leq m$.

(L1) Monotonicity with respect to lower orthant order

For every $2 \leq m_1 + m_2 \leq m$ and every $(\vec{x}, \vec{y}), (\vec{x'}, \vec{y'}) \in L^0(\mathbb{R}^{m_1}) \times L^0(\mathbb{R}^{m_2})$, $(\vec{x}, \vec{y}) \preceq_{lo} (\vec{x'}, \vec{y'})$ in the lower orthant order implies $d^{m_1, m_2}(\vec{x}, \vec{y}) \leq d^{m_1, m_2}(\vec{x'}, \vec{y'})$.

(L1c) Monotonicity with respect to concordance order

For every $2 \leq m_1 + m_2 \leq m$ and every $(\vec{x}, \vec{y}), (\vec{x'}, \vec{y'}) \in L^0(\mathbb{R}^{m_1}) \times L^0(\mathbb{R}^{m_2})$, $(\vec{x}, \vec{y}) \preceq_C (\vec{x'}, \vec{y'})$ in the concordance order implies $d^{m_1, m_2}(\vec{x}, \vec{y}) \leq d^{m_1, m_2}(\vec{x'}, \vec{y'})$.

(L2) Rotation invariance

For every $2 \leq m_1 + m_2 \leq m$ and every $(\vec{x}, \vec{y}) \in L^0(\mathbb{R}^{m_1}) \times L^0(\mathbb{R}^{m_2})$, we have $d^{m_1, m_2}(\vec{x}, \vec{y}) = d^{m_1, m_2}(\vec{x} - \vec{1}, \vec{y} - \vec{1})$, where $\vec{1}$ is a vector with all components equal to 1.

(L3) Continuity

For every $2 \leq m_1 + m_2 \leq m$, any sequence $\{\vec{z}_k = (\vec{x}_k, \vec{y}_k)\}_{k \in \mathbb{N}} \subseteq L^0(\mathbb{R}^{m_1}) \times L^0(\mathbb{R}^{m_2})$ and any vector $\vec{z} = (\vec{x}, \vec{y}) \in L^0(\mathbb{R}^{m_1}) \times L^0(\mathbb{R}^{m_2})$, if $\vec{z}_k$ weakly converges to $\vec{z}$ (as $k$ tends to $+\infty$), then $\lim_{k \to +\infty} d^{m_1, m_2}(\vec{x}_k, \vec{y}_k) = d^{m_1, m_2}(\vec{x}, \vec{y})$.

Property (L1) (respectively, (L1c)) implies that the dissimilarity degree is decreasing with respect to lower orthant (also called PLOD) order (respectively, concordance order). For the definitions of these orderings see, for instance, [49, 47]. Since the upper bound of a random vector in the lower orthant (respectively, concordance) order is given by the comonotonic case, this property simply means that the dissimilarity degree tends to vanish as soon as one is approaching the comonotonic case. Notice that, in the bivariate case, lower orthant and concordance order coincide, while in higher dimensions concordance order implies lower orthant order, but not vice versa (see, e.g., [38, 46]).

Property (L2) expresses the invariance of the dissimilarity degree with respect to the total reflection of the involved random vectors. The practical aspect of this property is that a change of sign in all the random variables does not influence the clustering output.
Property (L3) ensures that the dissimilarity degree is continuous with respect to weak convergence. This latter property is usually required, for instance, for various measures of concordance (see, e.g., [26, 58, 60]).

Now, we provide some global properties of an extended dissimilarity function \( d \) that connect the values of the degree of dissimilarity at a given dimension, say \( m_1 + m_2 \), with the values that it assumes at lower (respectively, higher) dimensions:

(G1) Reducibility

For every \( 3 \leq m_1 + m_2 + m_3 \leq m \) and for every \( (\vec{x}', \vec{x}'', \vec{y}) \in L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \times L^0(\mathbb{I}^{m_3}) \) such that \( \vec{x}', \vec{x}'', \) and \( \vec{y} \) are pairwise disjoint, if

\[
d^{m_1,m_2}(\vec{x}', \vec{x}'') \leq \min \{d^{m_1,m_3}(\vec{x}', \vec{y}), d^{m_2,m_3}(\vec{x}'', \vec{y})\},
\]

then the inequality

\[
\min \{d^{m_1,m_3}(\vec{x}', \vec{y}), d^{m_2,m_3}(\vec{x}'', \vec{y})\} \leq d^{m_1+m_2,m_3}(\vec{x}, \vec{y})
\]

holds, where \( \vec{x} := \vec{x}' \cup \vec{x}'' \).

(G1s) Strict reducibility

(G1) holds with \( (\vec{x}', \vec{x}'', \vec{y}) \) being strict for some \( 3 \leq m_1 + m_2 + m_3 \leq m \) and at least one \( (\vec{x}', \vec{x}'', \vec{y}) \in L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \times L^0(\mathbb{I}^{m_3}) \), where \( \vec{x} := \vec{x}' \cup \vec{x}'' \) and \( \vec{x}', \vec{x}'' \) and \( \vec{y} \) are pairwise disjoint.

(G2) Comonotonic invariance

For every \( 3 \leq m_1 + m_2 \leq m \) with \( 2 \leq m_1 \), the identity

\[
d^{m_1,m_2}(\vec{x}, \vec{y}) = d^{m_1-1,m_2}(\vec{x}, \vec{y})
\]

holds whenever \( \vec{x}' \in L^0(\mathbb{I}^{m_1-1}) \) and \( (\vec{x}, \vec{y}) \in L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \) are random vectors such that \( \vec{x}' \cup \{X\} = \vec{x} \), where \( X \in \vec{x} \) is comonotonic with at least one element of \( \vec{x}' \).

All these properties have an intuitive stochastic interpretation. Property (G1) is usually referred to as reducibility property (see, e.g., [42]). It guarantees that the dissimilarity degree between two vectors \( \vec{x} \) and \( \vec{y} \) is larger than the dissimilarity degree between \( \vec{y} \) and (at least) a subvector of \( \vec{x} \). Roughly speaking, increasing the diversity inside each group decreases the similarity between the groups.

**Example 2.1.** Given three random variables \( X_1, X_2, Y \), property (G1) ensures that, if \( (\vec{x}, \vec{y}) \) holds, i.e. \( X' \) and \( X'' \) is the most similar pair among \( (X', X''), (X', Y) \) and \( (X'', Y) \), then

\[
d^{2,1}((X', X''), Y) \geq d(X', X'').
\]

The related property (G1s) says, furthermore, that there exist specific dependence structures such that the dissimilarity degree between two vectors \( \vec{x} \) and \( \vec{y} \) is strictly larger than the dissimilarity degree between \( \vec{y} \) and a subvector of \( \vec{x} \). Clearly, property (G1s) implies property (G1), although the converse implication is not true (see Theorem 3.2).

On the other side, property (G2) ensures that the dissimilarity degree between \( \vec{x} \) and \( \vec{y} \) does not change if we add to \( \vec{x}' \) another random variable that is comonotone with at least one element of \( \vec{x}' \). Property (G2) is similar to the point proportion admissible property considered for data points.
in [23] that states that “if after we duplicate one or more points any number of times and reapply the procedure the boundaries of the clusters are not changed at any stage.”. Here, in fact, we should remark that two comonotonic random variables are equal up to increasing transformations (see, e.g., [20]).

Obviously, because of the symmetry of the dissimilarity function, properties (G1), (G1s) and (G2) can be also reformulated for the second argument of the involved dissimilarity functions.

### 3 Extended dissimilarity functions: properties and examples

In the following section, we provide various examples of dissimilarity functions and we study whether they satisfy some of the previously introduced properties. Notice that, in view of Assumptions 1 and 2, any \((m_1, m_2)\)-dissimilarity function aiming at quantifying the proximity degree of two random vectors \(X\) and \(Y\) of dimension \(m_1\) and \(m_2\), respectively, only depends on the \((m_1 + m_2)\)-dimensional copula of the random vector \((\overline{X}, \overline{Y})\). Thus, in some cases, it could be also convenient to define the dissimilarity functions directly on the space of copulas.

Moreover, for the sake of a concise use of copulas and their margins, for \(L \subseteq \{1, \ldots, m\}\), we define the map \(\eta_L : \mathbb{I}^m \times \mathbb{I}^m \to \mathbb{I}^m\) given coordinatewise by

\[
(\eta_L(u, v))_\ell := \begin{cases} u_\ell & \ell \in \{1, \ldots, m\} \setminus L \\ v_\ell & \ell \in L \end{cases}
\]

and, for \(l \in \{1, \ldots, m\}\), we put \(\eta_l := \eta_{\{l\}}\). We denote by \(0\) the vector with all entries equal to 0, by \(1\) the vector with all entries equal to 1 and by \(\mathcal{G}^k\) the collection of all \(k\)-dimensional copulas, \(2 \leq k \leq m\). For any subset \(L = \{l_1, \ldots, l|L|\} \subseteq \{1, \ldots, m\}\) with \(2 \leq |L| \leq m\) such that \(l_i < l_j\) for all \(i, j \in \{1, \ldots, |L|\}\) with \(i < j\), we further define by \(T_L(C)\) the lower dimensional margin of the copula \(C\) related to the indices of the components of \(C\) belonging to \(L\).

**Example 3.1.**

- The identity \(T_L(M) = M\) holds for all \(L \subseteq \{1, \ldots, m\}\) with \(2 \leq |L| \leq m\).
- The identity \(T_L(\Pi) = \Pi\) holds for all \(L \subseteq \{1, \ldots, m\}\) with \(2 \leq |L| \leq m\). Here, \(\Pi\) is the independence copula given, for every \(u_1, \ldots, u_m\) in \(\mathbb{I}\), by \(\Pi(u_1, \ldots, u_m) = \prod_{i=1}^m u_i\).
- For every \(3 \leq m_1 + m_2 + m_3 \leq m\) and every random vector \((\overline{X}, \overline{X}', \overline{Y}) \in L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \times L^0(\mathbb{I}^{m_3})\) with copula \(C_{(\overline{X}, \overline{X}', \overline{Y})} \in \mathcal{G}^{m_1+m_2+m_3}\), the copulas \(C_{(\overline{X}, \overline{Y})} \in \mathcal{G}^{m_1+m_3}\) and \(C_{(\overline{X}' , \overline{Y})} \in \mathcal{G}^{m_2+m_3}\) satisfy \(C_{(\overline{X}, \overline{Y})} = T_{\{1,\ldots,m_1+m_2+m_3\}\setminus\{m_1+1,\ldots,m_1+m_2+m_3\}}(C_{(\overline{X}, \overline{Y})})\) and \(C_{(\overline{X}', \overline{Y})} = T_{\{m_1+1,\ldots,m_1+m_2+m_3\}}(C_{(\overline{X}', \overline{Y})})\).

For every \(k\) such that \(2 \leq k \leq m\), we further define the map \([\cdot, \cdot] : \mathcal{G}^k \times \mathcal{G}^k \to \mathbb{R}\) introduced, e.g., in [25] and given by

\[
[C, D] := \int_{\mathcal{G}^k} C(u) \, dQ^D(u)
\]

where \(Q^D\) denotes the probability measure associated with the copula \(D\). The map \([\cdot, \cdot]\) is linear with respect to convex combinations in both arguments and is therefore called a biconvex form. Moreover, the map \([\cdot, \cdot]\) satisfies \([M, M] = 1/2\) and \([\Pi, \Pi] = 1/2^m\).

The following technical result will be needed in the following and it is reported here.
Lemma 3.1. Consider $2 \leq k \leq m$ and $C \in \mathcal{C}^k$ satisfying $T_{i,j}(C) = M$ for some $i, j \in \{1, \ldots, k\}$ with $i \neq j$.

(i) Then $Q^C \left[ \{u \in \mathbb{I}^k \mid u_i = u_j\} \right] = 1$.

(ii) The identity $\int_{\mathbb{I}^k} f(u) \, dQ^C(u) = \int_{\mathbb{I}^k} f(\eta_i(u, u_j e_i)) \, dQ^C(u)$ holds for every measurable function $f : \mathbb{I}^k \to \mathbb{R}$.

(iii) The identity $C(u 1) = C(\eta_i(u 1, 1))$ holds for all $u \in \mathbb{I}$.

(iv) Then $[C, C] = [T_{\{1, \ldots, k\}\backslash\{i\}}(C), T_{\{1, \ldots, k\}\backslash\{i\}}(C)]$.

(v) The identity $T_{i,l}(C) = T_{j,l}(C)$ holds for all $l \in \{1, \ldots, k\} \backslash \{i, j\}$.

Proof. For $p, q \in \{1, \ldots, k\}$ with $p \neq q$, we define the projection $\pi_{\{p,q\}} : \mathbb{I}^k \to \mathbb{I}^2$, $\pi_{\{p,q\}}(u) := (u_p, u_q)$. Then $(Q^C)_{\pi_{\{p,q\}}}(0, v_1) \times [0, v_2] = C(\eta_{\{p,q\}}(1, v_1 e_p + v_2 e_q)) = (T_{\{p,q\}}(C))(v_1, v_2) = M(v_1, v_2)$ for all $v \in \mathbb{I}^2$ and hence $(Q^C)_{\pi_{\{p,q\}}} = Q^{T_{\{p,q\}}(C)} = Q^M$ which implies

$$Q^C \left[ \{u \in \mathbb{I}^k \mid u_i < u_j\} \right] = (Q^C)_{\pi_{\{i,j\}}} \left[ \{v \in \mathbb{I}^2 \mid v_1 < v_2\} \right] = Q^M \left[ \{v \in \mathbb{I}^2 \mid v_1 < v_2\} \right] = 0$$

Thus, $Q^C \left[ \{u \in \mathbb{I}^k \mid u_i = u_j\} \right] = 1$ which proves (i) and, immediately, implies (ii). Now, consider $u \in \mathbb{I}$. Then, (ii) yields

$$C(u 1) = \int_{\mathbb{I}^k} \chi_{[0,u 1]}(v) \, dQ^C(v) = \int_{\mathbb{I}^k} \chi_{[0,u 1]}(\eta_i(v, v_j e_i)) \, dQ^C(v) = \int_{\mathbb{I}^k} \prod_{l=1, l \neq i}^k \chi_{[0,u_l]}(v_l) \, dQ^C(v) = C(\eta_i(u 1, 1))$$

where $\chi_B$ denotes the indicator function with respect to the set $B$. This proves (iii). Moreover, (ii) together with [24, Theorem 5.3.1] yields

$$[C, C] = \int_{\mathbb{I}^k} C(u) \, dQ^C(u) = \int_{\mathbb{I}^k} C(\eta_i(u, u_j e_i)) \, dQ^C(u) = \int_{\mathbb{I}^k} \int_{\mathbb{I}^k} \chi_{[0,n_i(u,u_j e_i)]}(v) \, dQ^C(v) dQ^C(u) = \int_{\mathbb{I}^k} \int_{\mathbb{I}^k} \chi_{[0,n_i(u,u_j e_i)]}(\eta_i(v, v_j e_i)) \, dQ^C(v) dQ^C(u) = \int_{\mathbb{I}^k} \int_{\mathbb{I}^k} \prod_{l=1, l \neq i}^k \chi_{[0,u_l]}(v_l) \, dQ^C(v) dQ^C(u) = \int_{\mathbb{I}^k} \int_{\mathbb{I}^k} \chi_{[0,n_i(u, 1 e_i)]}(v) \, dQ^C(v) dQ^C(u) = \int_{\mathbb{I}^k} C(\eta_i(u, 1 e_i)) \, dQ^C(u) = [T_{\{1, \ldots, k\}\backslash\{i\}}(C), T_{\{1, \ldots, k\}\backslash\{i\}}(C)]$$

This proves (iv). Finally, consider $l \in \{1, \ldots, k\} \backslash \{i, j\}$. Applying (ii) we obtain

$$(T_{i,l}(C))(v_1, v_2) = \int_{\mathbb{I}^2} \chi_{[0,v_1] \times [0,v_2]}(w_1, w_2) \, dQ^{T_{i,l}(C)}(w_1, w_2)$$
The function $d$ satisfy some desirable properties; the next result is straightforward.

It is straightforward to show that, for every single, average and complete linkage) hierarchical clustering algorithms.

First, we introduce dissimilarity functions that are defined in a similar way as in the classical (i.e., single, average and complete linkage) hierarchical clustering algorithms.

3.1 Extended dissimilarity functions based on linkage methods and a pairwise dissimilarity function

Consider a $(1, 1)$–dissimilarity function $d^{1,1}$ and $m_1, m_2 \in \mathbb{N}$ with $2 \leq m_1 + m_2 \leq m$. We define the maps $d^{m_1,m_2}_{\min}, d^{m_1,m_2}_{\ave}, d^{m_1,m_2}_{\max} : L^0(I^{m_1}) \times L^0(I^{m_2}) \to \mathbb{R}_+$ by letting

$$d^{m_1,m_2}_{\min}(X, Y) := \min \{d^{1,1}(X, Y) \mid X \in X, Y \in Y\}$$

$$d^{m_1,m_2}_{\ave}(X, Y) := \frac{1}{m_1 m_2} \sum_{X \in X} \sum_{Y \in Y} d^{1,1}(X, Y)$$

$$d^{m_1,m_2}_{\max}(X, Y) := \max \{d^{1,1}(X, Y) \mid X \in X, Y \in Y\}$$

It is straightforward to show that, for every $2 \leq m_1 + m_2 \leq m$, $d^{m_1,m_2}_{\min}, d^{m_1,m_2}_{\ave}, d^{m_1,m_2}_{\max}$ are $(m_1, m_2)$–dissimilarity functions. Thus, they can be extended as mappings from $\bigcup_{2 \leq m_1 + m_2 \leq m} L^0(I^{m_1}) \times L^0(I^{m_2})$ to $\mathbb{R}_+$ denoted, respectively, by $d_{\min}, d_{\ave}, d_{\max}$. The mappings $d_{\min}, d_{\ave}$ and $d_{\max}$ are called, respectively, the single, average and complete extended dissimilarity functions induced by $d^{1,1}$.

In the sequel, we focus on the extended dissimilarity function based on the following $(1, 1)$–dissimilarity functions (see Section 3.2)

$$d^{1,1}_{\beta}(X, Y) := \frac{1}{2} - C_{(X,Y)}(\frac{1}{2}, \frac{1}{2})$$  \hspace{1cm} (3.1)

$$d^{1,1}_{\phi}(X, Y) := \frac{1}{2} - [C_{(X,Y)}, M]$$  \hspace{1cm} (3.2)

$$d^{1,1}_{r}(X, Y) := \frac{1}{2} - [C_{(X,Y)}, C_{(X,Y)}]$$  \hspace{1cm} (3.3)

$$d^{1,1}_{\rho}(X, Y) := \frac{1}{3} - [C_{(X,Y)}, \Pi]$$  \hspace{1cm} (3.4)

The function $d^{1,1}_{\beta}$ is related to the pairwise version of medial correlation coefficient (also known as Blomqvist’s beta), $d^{1,1}_{\phi}$ is related to the pairwise version of Spearman’s footrule, and the functions $d^{1,1}_{r}$ and $d^{1,1}_{\rho}$ are related to pairwise Kendall’s tau and pairwise Spearman’s rho. In Section 3.2 we list some properties of these $(1, 1)$–dissimilarity functions.

In the following we study whether single, average and complete extended dissimilarity functions satisfy some desirable properties; the next result is straightforward.
**Theorem 3.1.** Let $d_{\min}$, $d_{\text{ave}}$ and $d_{\max}$ be the extended dissimilarity functions induced by $d^{1,1}$. Then:

(i) $d_{\min}$, $d_{\text{ave}}$ and $d_{\max}$ satisfy (L1) whenever $d^{1,1}$ is increasingly monotone with respect to lower orthant order;

(ii) $d_{\min}$, $d_{\text{ave}}$ and $d_{\max}$ satisfy (L1c) whenever $d^{1,1}$ is increasingly monotone with respect to concordance order;

(iii) $d_{\min}$, $d_{\text{ave}}$ and $d_{\max}$ satisfy (L2) whenever $d^{1,1}(X,Y) = d^{1,1}(1-X,1-Y)$ for every $X, Y \in L^0(\mathbb{I})$;

(iv) $d_{\min}$, $d_{\text{ave}}$ and $d_{\max}$ satisfy (L3) whenever $d^{1,1}$ is continuous with respect to weak convergence.

In the following theorem we show that the single, the average and the complete extended dissimilarity functions satisfy the global properties introduced above.

**Theorem 3.2.** Let $d_{\min}$, $d_{\text{ave}}$ and $d_{\max}$ be the extended dissimilarity functions induced by $d^{1,1}$. Then:

(i) $d_{\min}$ satisfies (G1) and (G2), but fails to satisfy (G1s);

(ii) $d_{\text{ave}}$ satisfies (G1);

(iii) $d_{\max}$ satisfies (G1) and (G2).

**Proof.** We first prove (G1). To this end, consider $3 \leq m_1 + m_2 + m_3 \leq m$, the random vector $(\tilde{X}', \tilde{X}'', \tilde{Y}) \in L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \times L^0(\mathbb{I}^{m_3})$ satisfying $d_{m_1,m_2}(\tilde{X}', \tilde{X}'') \leq \min \{d_{m_1,m_3}(\tilde{X}', \tilde{Y}), d_{m_2,m_3}(\tilde{X}'', \tilde{Y})\}$ such that $\tilde{X}'$, $\tilde{X}''$ and $\tilde{Y}$ are pairwise disjoint and put $\tilde{X} := \tilde{X}' \cup \tilde{X}''$. Then

$$\min \left\{ d_{m_1,m_3}^{m_1}(\tilde{X}', \tilde{Y}), d_{m_2,m_3}^{m_2}(\tilde{X}'', \tilde{Y}) \right\} = \min \left\{ \min \left\{ d^{1,1}(X,Y) \mid X \in \tilde{X}', Y \in \tilde{Y} \right\}, \min \left\{ d^{1,1}(X,Y) \mid X \in \tilde{X}'', Y \in \tilde{Y} \right\} \right\} = \min \left\{ d^{1,1}(X,Y) \mid X \in \tilde{X}', Y \in \tilde{Y} \right\} = d^{m_1,m_2,m_3}(\tilde{X}, \tilde{Y}).$$

Thus, $d_{\min}$ satisfies (G1), but cannot satisfy (G1s). Moreover,

$$\min \left\{ d_{\text{ave}}^{m_1,m_3}(\tilde{X}', \tilde{Y}), d_{\text{ave}}^{m_2,m_3}(\tilde{X}'', \tilde{Y}) \right\} = \min \left\{ \frac{1}{m_1 m_3} \sum_{X \in \tilde{X}'} \sum_{Y \in \tilde{Y}} d^{1,1}(X,Y), \frac{1}{m_2 m_3} \sum_{X \in \tilde{X}''} \sum_{Y \in \tilde{Y}} d^{1,1}(X,Y) \right\} \leq \frac{m_1}{m_1 + m_2} \frac{1}{m_1 m_3} \sum_{X \in \tilde{X}'} \sum_{Y \in \tilde{Y}} d^{1,1}(X,Y) + \frac{m_2}{m_1 + m_2} \frac{1}{m_2 m_3} \sum_{X \in \tilde{X}''} \sum_{Y \in \tilde{Y}} d^{1,1}(X,Y) = \frac{1}{(m_1 + m_2) m_3} \sum_{X \in \tilde{X}} \sum_{Y \in \tilde{Y}} d^{1,1}(X,Y) = d_{\text{ave}}^{m_1,m_2,m_3}(\tilde{X}, \tilde{Y}).$$
Thus, the single and complete extended dissimilarity functions satisfy (G2).

Proof. Then order, i.e. Corollary 3.1. Assume that \( d^{1,1}(X,Y) \) is comonotonic with some element \( X' \in X \). Then, by Lemma 3.1 and Assumptions 1 and 2, the identity \( d^{1,1}(X',Y) = d^{1,1}(X'',Y) \) holds for all \( Y \in Y \), and we obtain

\[
\begin{align*}
\min \{ d_{\text{max}}^{m_1,m_2}(\vec{X}, \vec{Y}), d_{\text{max}}^{m_2,m_3}(\vec{X}', \vec{Y}) \} &= \min \left\{ \max \left\{ d^{1,1}(X,Y) \mid X \in X', Y \in Y \right\}, \max \left\{ d^{1,1}(X,Y) \mid X \in X'', Y \in Y \right\} \right\} \\
&\leq \max \left\{ \max \left\{ d^{1,1}(X,Y) \mid X \in X', Y \in Y \right\}, \max \left\{ d^{1,1}(X,Y) \mid X \in X'', Y \in Y \right\} \right\} \\
&= \max \left\{ d^{1,1}(X,Y) \mid X \in X, Y \in Y \right\} \\
&= d_{\text{max}}^{m_1+m_2,m_3}(\vec{X}, \vec{Y}) .
\end{align*}
\]

Thus, the average and complete extended dissimilarity functions satisfy (G1).

Now, we prove property (G2). To this end, consider \( 3 \leq m_1 + m_2 \leq m \) with \( 2 \leq m_1 \), \( \vec{X}' \in L^0(\mathbb{I}^{m_1-1}) \) and \( (\vec{X}, \vec{Y}) \in L^0(\mathbb{I}^{m_1}) \) such that \( X' \cup \{ X'' \} = X \), where \( X'' \in X \) is comonotonic with some element \( X' \in X \). Then, by Corollary 3.1 and Assumptions 1 and 2, the identity \( d^{1,1}(X',Y) = d^{1,1}(X'',Y) \) holds for all \( Y \in Y \), and we obtain

\[
\begin{align*}
d_{\text{min}}^{m_1,m_2}(\vec{X}, \vec{Y}) &= \min \left\{ d^{1,1}(X,Y) \mid X \in X, Y \in Y \right\} \\
&= \min \left\{ d^{1,1}(X,Y) \mid X \in X', Y \in Y \right\} \\
&= d_{\text{min}}^{m_1-1,m_2}(\vec{X}', \vec{Y}) \\
d_{\text{max}}^{m_1,m_2}(\vec{X}, \vec{Y}) &= \max \left\{ d^{1,1}(X,Y) \mid X \in X, Y \in Y \right\} \\
&= \max \left\{ d^{1,1}(X,Y) \mid X \in X', Y \in Y \right\} \\
&= d_{\text{max}}^{m_1-1,m_2}(\vec{X}', \vec{Y}) .
\end{align*}
\]

Thus, the single and complete extended dissimilarity functions satisfy (G2).

We now present some sufficient condition on \( d^{1,1} \) such that both the average and complete extended dissimilarity functions satisfy (G1s).

Corollary 3.1. Assume that \( d^{1,1} \) is strictly monotonically decreasing with respect to the lower orthant order, i.e. \( (X,Y) \prec_{lo} (X',Y') \) in the lower orthant order implies \( d^{1,1}(X',Y') < d^{1,1}(X,Y) \). Then \( d_{\text{ave}} \) and \( d_{\text{max}} \) satisfy (G1s).

Proof. Consider \( n \geq 3 \), \( m_1 = m_2 = m_3 = 1 \) and the copula \( C : \mathbb{I}^n \to \mathbb{R} \) given by

\[
C(u) := \Pi(u) - \frac{1}{3} \left( (1-u_1)(1-u_2)+(1-u_1)(1-u_3)+(1-u_2)(1-u_3) \right) \prod_{i=1}^{3} u_i - \prod_{i=4}^{n} u_i. \quad (3.5)
\]

(To check that this function is actually a copula it is enough to compute its density). Then, for every random vector \( (X',X'',Y) \in L^1(\mathbb{I}) \times L^1(\mathbb{I}) \times L^1(\mathbb{I}) \) having copula \( T_{\{1,2,3\}}(C) \), we have

\[
(X'',Y) \prec_{lo} (X',Y) \prec_{lo} (X',X'')
\]

and hence \( d^{1,1}(X',X'') < \min \{ d^{1,1}(X',Y), d^{1,1}(X'',Y) \} \) as well as

\[
\begin{align*}
\min \{ d^{1,1}(X',Y), d^{1,1}(X'',Y) \} &< \frac{1}{2} d^{1,1}(X',Y) + \frac{1}{2} d^{1,1}(X'',Y) = d_{\text{ave}}^{1+1,1}(\vec{X}, \vec{Y}) \\
\min \{ d^{1,1}(X',Y), d^{1,1}(X'',Y) \} &< \max \{ d^{1,1}(X',Y), d^{1,1}(X'',Y) \} = d_{\text{max}}^{1+1,1}(\vec{X}, \vec{Y})
\end{align*}
\]

where \( X = X' \cup X'' \). Therefore, \( d_{\text{ave}} \) and \( d_{\text{max}} \) satisfy (G1s). □
where we have $d$ for specific choices of monotone decreasing with respect to the lower orthant order, satisfy (G1s).

**Example 3.3.** Consider copula $C$ given by (3.1). Applying the above copula, it is straightforward to check that also the average and complete extended dissimilarity functions induced by $d$, are strictly monotone decreasing with respect to the lower orthant order (see, e.g., [2]).

The following example shows that the condition stated in Corollary [3] is sufficient, but not necessary.

**Example 3.2.** Consider the map $d^{1,1}_β$ given by (3.1), $m ≥ 3$, $m_1 = m_2 = m_3 = 1$ and the copula $C$ given by (3.5). Further, note that $d^{1,1}_β$ fails to be strictly monotone decreasing with respect to the lower orthant order: to verify this, it is enough to consider two copulas with the same value in the point $(0.5, 0.5)$, like ordinal sums of two copulas with respect to the partition $([0, 0.5], [0.5, 1])$. Then, for every random vector $(X', X'', Y) ∈ L^0(I) × L^0(I) × L^0(I)$ having copula $T_{(1,2,3)}(C)$, we have

$$d^{1,1}_β(X', X'') ≤ \min \{d^{1,1}_β(X', Y), d^{1,1}_β(X'', Y)\} < d^{1+1,1}_α(\bar{X}, Y)$$

$$d^{1,1}_β(X', X'') \leq \min \{d^{1,1}_β(X', Y), d^{1,1}_β(X'', Y)\} < d^{1+1,1}_α(\bar{X}, Y)$$

where $\bar{X} = X' ∪ X''$. Indeed, we have

$$d^{1,1}_β(X', X'') = \frac{1}{4} + \frac{1}{3} \frac{1}{2^3}$$

$$\min \{d^{1,1}_β(X', Y), d^{1,1}_β(X'', Y)\} = \frac{1}{4} + \frac{1}{3} \frac{2}{2^3}$$

$$d^{1+1,1}_α(\bar{X}, Y) = \frac{1}{4} + \frac{1}{3} \frac{3}{2^3}$$

$$d^{1+1,1}_α(\bar{X}, Y) = \frac{1}{4} + \frac{1}{3} \frac{4}{2^3}$$

Thus, the average and complete extended dissimilarity functions induced by $d^{1,1}_β$ satisfy (G1s). By applying the above copula, it is straightforward to check that also the average and complete extended dissimilarity functions induced by $d^{1,1}_β$ and $d^{1,1}_τ$ given by (3.2) and (3.3), that both fail to be strictly monotone decreasing with respect to the lower orthant order, satisfy (G1s).

The next example shows that the average extended dissimilarity function may fail to satisfy (G2) for specific choices of $d^{1,1}$.

**Example 3.3.** Consider $d^{1,1}_β$ given by (3.1). Further, consider $m ≥ 4$, $m_1 = 3$, $m_2 = 1$ and the copula $C : \mathbb{I}^m → \mathbb{R}$ given by

$$C(u) := \min \{u_1, u_2\} \left(\prod_{i=3}^{m} u_i - \frac{1}{2} (1 - u_3)(1 - u_4) \prod_{i=3}^{m} u_i\right)$$

which is the copula of a random vector with two independent sub-vectors (see e.g. [20]). Then, for every random variable $X ≈ (X_1, X_2, X_3) ∈ L^0(\mathbb{I}^3)$ and every random variable $Y ∈ L^0(\mathbb{I})$ such that $(\bar{X}, Y)$ has copula $T_{(1,2,3)}(C)$ and hence $X_1$ and $X_2$ are comonotonic, the average extended dissimilarity function induced by $d^{1,1}$ satisfies

$$d^{1,1}_{ave}(\bar{X}, Y) ≠ \frac{d^{1,1}_{ave}((X_1, X_3), Y)}$$
Indeed, we obtain \( d_{\text{ave}}^{5,1}(\vec{X}, Y) = \frac{1}{4} + \frac{1}{2} \cdot \frac{1}{2^2} \neq \frac{1}{4} + \frac{1}{2} \cdot \frac{1}{2^3} = d_{\text{ave}}^{2,1}(X_1, X_3, Y) \). Thus, the average extended dissimilarity function based on \( d_{\beta}^{1,1} \) fails to satisfy (G2). By applying the above copula, it is straightforward to check that also the average extended dissimilarity functions induced by \( d_{\phi}^{1,1}, d_{\tau}^{1,1} \) and \( d_{\rho}^{1,1} \), given, respectively, by (3.2), (3.3) and (3.4) fail to satisfy (G2).

We conclude by noticing that the extended dissimilarity functions based on single, average and complete linkage share the same structural drawback: They take into account solely information about the pairwise dependence structure. Therefore, for each of these extended dissimilarity functions, the value of an \((m_1, m_2)\)-dissimilarity function of a random vector depends on its bivariate margins only. The next result is hence evident.

**Corollary 3.2.** Consider a \((1,1)\)-dissimilarity function \( d^{1,1} \), some constant \( c \in \mathbb{R}_+, 2 \leq m_1 + m_2 \leq m \) and let \((\vec{X}, \vec{Y}) \in L^0(\mathbb{P}^{m_1}) \times L^0(\mathbb{P}^{m_2})\) be a random vector satisfying \( d^{1,1}(X, Y) = c \) for all \( X \in \mathbb{X} \) and all \( Y \in \mathbb{Y} \). Then \( d_{\text{min}}^{m_1, m_2}(\vec{X}, \vec{Y}) = d_{\text{ave}}^{m_1, m_2}(\vec{X}, \vec{Y}) = d_{\text{max}}^{m_1, m_2}(\vec{X}, \vec{Y}) = c \).

**Example 3.4.** Consider \( 2 \leq m_1 + m_2 \leq m \) and the copula \( C : \mathbb{P}^m \to \mathbb{R} \) given by

\[
C(u) := \Pi(u) + \prod_{i=1}^n u_i(1 - u_i)
\]

Then \( C \neq \Pi \) and \( T_L(C) = \Pi \) for all \( L \subseteq \{1, \ldots, m\} \) with \(|L| = 2\), and the identities

\[
\begin{align*}
d_{\text{min}}^{m_1, m_2}(\vec{X}, \vec{Y}) &= d_{\text{min}}^{m_1, m_2}(\vec{X}', \vec{Y}') \\
d_{\text{ave}}^{m_1, m_2}(\vec{X}, \vec{Y}) &= d_{\text{ave}}^{m_1, m_2}(\vec{X}', \vec{Y}') \\
d_{\text{max}}^{m_1, m_2}(\vec{X}, \vec{Y}) &= d_{\text{max}}^{m_1, m_2}(\vec{X}', \vec{Y}')
\end{align*}
\]

hold for every random vector \((\vec{X}, \vec{Y}) \in L^0(\mathbb{P}^{m_1}) \times L^0(\mathbb{P}^{m_2})\) with copula \( C \) and every random vector \((\vec{X}', \vec{Y}') \in L^0(\mathbb{P}^{m_1}) \times L^0(\mathbb{P}^{m_2})\) with copula \( \Pi \). Thus, neither the single nor the average nor the complete extended dissimilarity function distinguishes between pairwise independence and global independence.

### 3.2 Extended dissimilarity functions based on measures of association

In this section we study extended dissimilarity functions which are derived from various measures of association (see, e.g., [49, 59]). Contrarily to the dissimilarity functions based on linkage methods, here we rely on global measures of association which do not only depend on the pairwise association. Thus, in principle, the derived dissimilarity functions could be able to detect high-dimensional features that are not apparent with the latter methods. To this end, for \( m_1, m_2 \in \mathbb{N} \) with \( 2 \leq m_1 + m_2 \leq m \), we define the maps \( d_{\beta}^{m_1, m_2}, d_{\phi}^{m_1, m_2}, d_{\tau}^{m_1, m_2}, d_{\rho}^{m_1, m_2} \) from \( L^0(\mathbb{P}^{m_1}) \times L^0(\mathbb{P}^{m_2}) \) to \( \mathbb{R}_+ \) by letting

\[
\begin{align*}
d_{\beta}^{m_1, m_2}(\vec{X}, \vec{Y}) &:= \frac{1}{2} - C(\vec{X}, \vec{Y}) \left( \frac{1}{2} \right) = M \left( \frac{1}{2} \right) - C(\vec{X}, \vec{Y}) \left( \frac{1}{2} \right) \\
d_{\phi}^{m_1, m_2}(\vec{X}, \vec{Y}) &:= \frac{1}{2} - \left[ C(\vec{X}, \vec{Y}) \cdot M \right] = \int_u (M(u) - C(\vec{X}, \vec{Y})(u)) \, d\lambda(u) \\
d_{\tau}^{m_1, m_2}(\vec{X}, \vec{Y}) &:= \frac{1}{2} - \left[ C(\vec{X}, \vec{Y}) \cdot C(\vec{X}, \vec{Y}) \right] = [M, M] - [C(\vec{X}, \vec{Y}), C(\vec{X}, \vec{Y})] \\
d_{\rho}^{m_1, m_2}(\vec{X}, \vec{Y}) &:= \frac{1}{m_1 + m_2 + 1} - \left[ C(\vec{X}, \vec{Y}), \Pi \right] = \int_{m_1 + m_2} (M(u) - C(\vec{X}, \vec{Y})(u)) \, d\lambda(u)
\end{align*}
\]
The function $d_{\beta}^{m_1,m_2}$ is related to the multivariate version of medial correlation coefficient (also known as Blomqvist’s beta) that was introduced by [48] (see also [61]), whose $n$–dimensional version is given by $(2^n C\left(\frac{1}{2}\right) - 1)/(2^{n-1} - 1)$. The function $d_{\phi}^{m_1,m_2}$ is related to the multivariate version of Spearman’s footrule considered in [61]. The functions $d_{\tau}^{m_1,m_2}$ and $d_{\rho}^{m_1,m_2}$ are related to some multivariate versions of Kendall’s tau and Spearman’s rho (see, for instance, [39] [59] [60]).

**Theorem 3.3.** For every $2 \leq m_1 + m_2 \leq m$, $d_{\beta}^{m_1,m_2}$, $d_{\phi}^{m_1,m_2}$, $d_{\tau}^{m_1,m_2}$ and $d_{\rho}^{m_1,m_2}$ are $(m_1, m_2)$–dissimilarity functions, and thus, the maps

$$d_{\beta}, d_{\phi}, d_{\tau}, d_{\rho} : \bigcup_{2 \leq m_1 + m_2 \leq m} L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \to \mathbb{R}_+$$

with $d_{\beta}|_{L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2})} := d_{\beta}^{m_1,m_2}$, $d_{\phi}|_{L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2})} := d_{\phi}^{m_1,m_2}$, $d_{\tau}|_{L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2})} := d_{\tau}^{m_1,m_2}$ and $d_{\rho}|_{L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2})} := d_{\rho}^{m_1,m_2}$ are extended dissimilarity functions. Moreover:

(i) $d_{\beta}$ satisfies (L1), (L1c), (L3), (G1), (G1s) and (G2).

(ii) $d_{\phi}$ satisfies (L1), (L1c), (L3), (G1), (G1s) and (G2).

(iii) $d_{\tau}$ satisfies (L1c), (L2), (L3), (G1), (G1s) and (G2).

(iv) $d_{\rho}$ satisfies (L1), (L1c), (L3), but fails to satisfy (G1), (G1s) and (G2).

**Proof.** We first prove the local properties and then, step by step, all the global properties. Since $C^\xi(\frac{1}{2}) = C(\frac{1}{2}), [C^\xi, M] = [C, M], [C^\xi, C^\xi] = [C, C]$ and $[C^\xi, \Pi] = [C, \Pi]$ for every $C \in \mathcal{C}^k$, every permutation $\xi$ of $\mathbb{I}^k$, where $C^\xi$ is the copula obtained from $C$ by permuting its arguments, and for every $2 \leq k \leq m$ (see [25] Theorem 5.2), it follows that $d_{\beta}, d_{\phi}, d_{\tau}$ and $d_{\rho}$ are extended dissimilarity functions. It is evident that $d_{\beta}$ satisfies (L1), (L1c) and (L3), and it is immediate from [25] Theorems 3.6, 4.3, 4.4 and 5.2] that $d_{\phi}$ and $d_{\rho}$ satisfy (L1), (L1c) and (L3) and that $d_{\tau}$ satisfies (L1c), (L2) and (L3).

Now, consider $3 \leq m_1 + m_2 + m_3 \leq m$, the random vector $(\tilde{X}', \tilde{X}'', \tilde{Y}) \in L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \times L^0(\mathbb{I}^{m_3})$ such that $X', X''$ and $Y$ are pairwise disjoint and (2.2) holds, and put $X := X' \cup X''$. Then

$$C_{(\tilde{X}', \tilde{Y})}(\frac{1}{2}) \leq C_{(\tilde{X}, \tilde{Y})}(\eta_{\{m_1+1,\ldots,m_1+m_2\}}(\frac{1}{2}, 1))$$

$$= (T_{\{1,\ldots,m_1+m_2+m_3\}\{m_1+1,\ldots,m_1+m_2\}}(C_{(\tilde{X}, \tilde{Y})}))(\frac{1}{2}) = C_{(\tilde{X}', \tilde{Y})}(\frac{1}{2})$$

and, by [24] Theorem 5.3.1] and Example [3.1] we obtain

$$[C_{(\tilde{X}', \tilde{Y})}, M] \leq \int_{\mathbb{I}^{m_1+m_2+m_3}} C_{(\tilde{X}', \tilde{Y})}(\eta_{\{m_1+1,\ldots,m_1+m_2\}}(\mathbf{u}, 1)) \ dQ^M(\mathbf{u})$$

$$= [T_{\{1,\ldots,m_1+m_2+m_3\}\{m_1+1,\ldots,m_1+m_2\}}(C_{(\tilde{X}, \tilde{Y})}), T_{\{1,\ldots,m_1+m_2+m_3\}\{m_1+1,\ldots,m_1+m_2\}}(M)]$$

$$= [C_{(\tilde{X}', \tilde{Y})}, M]$$

And by [24] Theorem 5.3.1] and Example [3.1] we obtain

$$[C_{(\tilde{X}', \tilde{Y})}, M] \leq \int_{\mathbb{I}^{m_1+m_2+m_3}} C_{(\tilde{X}', \tilde{Y})}(\eta_{\{m_1,\ldots,m_1\}}(\mathbf{u}, 1)) \ dQ^M(\mathbf{u})$$

$$= [T_{\{m_1+1,\ldots,m_1+m_2+m_3\}}(C_{(\tilde{X}', \tilde{Y})}), T_{\{m_1+1,\ldots,m_1+m_2+m_3\}}(M)]$$

$$= [C_{(\tilde{X}', \tilde{Y})}, M]$$

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as well as

\[ [C(\bar{x}, \bar{y}), C(\bar{x}, \bar{y})] \leq \int_{m_1+1+m_2} C(\bar{x}, \bar{y})(\eta_{m_1+1,...,m_1+m_2}(u, 1)) \, dQ^C(\bar{x}, \bar{y})(u) \]

\[ = [T_{m_1+1,...,m_1+m_2}(C(\bar{x}, \bar{y})), T_{m_1+1,...,m_1+m_2}(C(\bar{x}, \bar{y}))] \]

\[ = [C(\bar{x}, \bar{y}), C(\bar{x}, \bar{y})] \]

Thus,

\[ \min \{d_{\beta}^{m_1,m_2}(\bar{x}, \bar{y}), d_{\phi}^{m_1,m_2}(\bar{x}, \bar{y})\} \leq d_{\beta}^{m_1+m_2,m_3}(\bar{x}, \bar{y}) \]

\[ \min \{d_{\phi}^{m_1,m_2}(\bar{x}, \bar{y}), d_{\phi}^{m_1,m_2}(\bar{x}, \bar{y})\} \leq d_{\phi}^{m_1+m_2,m_3}(\bar{x}, \bar{y}) \]

\[ \min \{d_{\tau}^{m_1,m_2}(\bar{x}, \bar{y}), d_{\tau}^{m_1,m_2}(\bar{x}, \bar{y})\} \leq d_{\tau}^{m_1+m_2,m_3}(\bar{x}, \bar{y}) \]

which implies that $d_{\beta}, d_{\phi}$ and $d_{\tau}$ satisfy (G1). In Examples 3.5 and 3.6 we show that the extended dissimilarity functions $d_{\beta}, d_{\phi}$ and $d_{\tau}$ satisfy also (G1s), and that $d_{\rho}$ fails to satisfy (G1) and (G1s).

Finally, consider $3 \leq m_1 + m_2 \leq m$ with $2 \leq m_1, \bar{x}' \in L^0(\mathbb{I}^{m_1-1})$ and $(\bar{x}, \bar{y}) \in L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2})$ such that $\bar{x}' \cup \{X''\} = \bar{x}$, where $X'' \in X$ is comonotonic with some element $X' \in X'$. Without loss of generality, denote by $i$ the position of $X''$ within the vector $(\bar{x}, \bar{y})$. Then, Lemma 3.1 and Example 3.1 yield

\[ C(\bar{x}, \bar{y})(u, 1) = C(\bar{x}, \bar{y})(\eta_i(u, 1, 1)) = (T_{m_1+1,...,m_1+m_2}\{i\}(C(\bar{x}, \bar{y}))(u, 1) = C(\bar{x}, \bar{y})(u, 1) \]

for all $u \in \mathbb{I}$ and, hence,

\[ [C(\bar{x}, \bar{y}), M] = \int_{m_1+1+m_2} C(\bar{x}, \bar{y})(u) \, dQ^M(u) \]

\[ = \int_{\mathbb{I}} C(\bar{x}, \bar{y})(u, 1) \, d\lambda(u) = \int_{\mathbb{I}} C(\bar{x}, \bar{y})(u, 1) \, d\lambda(u) \]

\[ = \int_{m_1-1+m_2} C(\bar{x}, \bar{y})(u) \, dQ^M(u) = [C(\bar{x}, \bar{y}), M] \]

and Lemma 3.1 together with Example 3.1 implies

\[ [C(\bar{x}, \bar{y}), C(\bar{x}, \bar{y})] = [T_{m_1+1,...,m_1+m_2}\{i\}(C(\bar{x}, \bar{y})), T_{m_1+1,...,m_1+m_2}\{i\}(C(\bar{x}, \bar{y}))] = [C(\bar{x}, \bar{y}), C(\bar{x}, \bar{y})] \]

Thus,

\[ d_{\beta}^{m_1,m_2}(\bar{x}, \bar{y}) = d_{\beta}^{m_1-1,m_2}(\bar{x}', \bar{y}) \]

\[ d_{\phi}^{m_1,m_2}(\bar{x}, \bar{y}) = d_{\phi}^{m_1-1,m_2}(\bar{x}', \bar{y}) \]

\[ d_{\tau}^{m_1,m_2}(\bar{x}, \bar{y}) = d_{\tau}^{m_1-1,m_2}(\bar{x}', \bar{y}) \]

which implies that $d_{\beta}, d_{\phi}$ and $d_{\tau}$ satisfy (G2). In Example 3.7 we show that the extended dissimilarity function $d_{\rho}$ fails to satisfy (G2).
The following example shows that the extended dissimilarity functions $d_\beta$, $d_\phi$ and $d_r$ satisfy (G1s).

**Example 3.5.** Consider $n \geq 3$, $m_1 = m_2 = m_3 = 1$ and the product copula $\Pi$. Then, for every random vector $(X', X'', Y) \in L^0(\mathbb{I}) \times L^0(\mathbb{I}) \times L^0(\mathbb{I})$ having copula $T_{\{1,2,3\}}(\Pi)$, the extended dissimilarity functions $d_\beta$, $d_\phi$ and $d_r$ satisfy

$$d_\beta^{1,1}(X', X'') \leq \min \{d_\beta^{1,1}(X', Y), d_\gamma^{1,1}(X'', Y)\} < d_\beta^{1+1,1}(\bar{X}, Y)$$
$$d_\phi^{1,1}(X', X'') \leq \min \{d_\phi^{1,1}(X', Y), d_\phi^{1,1}(X'', Y)\} < d_\phi^{1+1,1}(\bar{X}, Y)$$
$$d_r^{1,1}(X', X'') \leq \min \{d_r^{1,1}(X', Y), d_r^{1,1}(X'', Y)\} < d_r^{1+1,1}(\bar{X}, Y)$$

where $\bar{X} = X' \cup X''$. Indeed, we have

$$d_\beta^{1,1}(X', X'') = \min \{d_\beta^{1,1}(X', Y), d_\beta^{1,1}(X'', Y)\} = 2/8 < 3/8 = d_\beta^{1+1,1}(\bar{X}, Y)$$
$$d_\phi^{1,1}(X', X'') = \min \{d_\phi^{1,1}(X', Y), d_\phi^{1,1}(X'', Y)\} = 2/12 < 3/12 = d_\phi^{1+1,1}(\bar{X}, Y)$$
$$d_r^{1,1}(X', X'') = \min \{d_r^{1,1}(X', Y), d_r^{1,1}(X'', Y)\} = 2/8 < 3/8 = d_r^{1+1,1}(\bar{X}, Y)$$

Thus, the extended dissimilarity functions $d_\beta$, $d_\phi$ and $d_r$ satisfy (G1s).

We conclude this section by showing that the extended dissimilarity function $d_\rho$ fails to satisfy (G1), (G1s) and (G2).

**Example 3.6.** Consider $n \geq 6$, $m_1 = m_2 = m_3 = 2$ and the product copula $\Pi$. Then, for every random vector $(\bar{X}', \bar{X}'', \bar{Y}) \in L^0(\mathbb{I}^2) \times L^0(\mathbb{I}^2) \times L^0(\mathbb{I}^2)$ having copula $T_{\{1,...,6\}}(\Pi)$, the extended dissimilarity function $d_\rho$ satisfies

$$d_\rho^{2,2}(\bar{X}', \bar{X}'') = \min \{d_\rho^{2,2}(\bar{X}', \bar{Y}), d_\rho^{2,2}(\bar{X}'', \bar{Y})\} > d_\rho^{2+2,2}(\bar{X}, \bar{Y})$$

where $\bar{X} = \bar{X}' \cup \bar{X}''$. Indeed, we have

$$d_\rho^{2,2}(\bar{X}', \bar{X}'') = \min \{d_\rho^{2,2}(\bar{X}', \bar{Y}), d_\rho^{2,2}(\bar{X}'', \bar{Y})\} = \frac{616}{4180} > \frac{570}{4180} = d_\rho^{2+2,2}(\bar{X}, \bar{Y})$$

Thus, the extended dissimilarity function $d_\rho$ fails to satisfy (G1) and also (G1s).

**Example 3.7.** Consider $n \geq 4$, $m_1 = 2$, $m_2 = n - 2$ and the copula $C : \mathbb{I}^2 \times \mathbb{I}^{n-2} \rightarrow \mathbb{R}$ given by

$$C(u, v) := M(u) \Pi(v)$$

(see e.g. [20]). Then, for every random vector $(\bar{X}, \bar{Y}) = (X_1, X_2)' \in L^0(\mathbb{I}^2)$ and every random vector $\bar{Y} \in L^0(\mathbb{I}^2)$ such that $(\bar{X}, \bar{Y})$ has copula $T_{\{1,2,3,4\}}(C)$ and hence $X_1$ and $X_2$ are comonotonic, the extended dissimilarity function $d_\rho$ satisfies

$$d_\rho^{2,2}(\bar{X}, \bar{Y}) \neq d_\rho^{1,2}(X_1, \bar{Y})$$

Indeed, we obtain $d_\rho^{2,2}(\bar{X}, \bar{Y}) = \frac{14}{120} \neq \frac{15}{120} = d_\rho^{1,2}(X_1, \bar{Y})$. Thus, the extended dissimilarity function $d_\rho$ fails to satisfy (G2).
Consider the measure of concordance Kendall’s tau (see, e.g., [29]) and, for \( m_1, m_2 \in \mathbb{N} \) with \( 2 \leq m_1 + m_2 \leq m \), define the map \( d_{\kappa}^{m_1,m_2} : L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \to \mathbb{R}_+ \) by letting

\[
d_{\kappa}^{m_1,m_2}(\vec{X}, \vec{Y}) := 1 - \kappa(\vec{X}, \vec{Y}) = \frac{[M,M] - [C(\vec{X}, \vec{Y}), C(\vec{X}, \vec{Y})]}{[M,M] - [\Pi, \Pi]} = \frac{d_r^{m_1,m_2}(\vec{X}, \vec{Y})}{[M,M] - [\Pi, \Pi]}
\]

Then (G1) is equivalent to the inequality \( \kappa(\vec{X}, \vec{Y}) \leq \max \{ \kappa(\vec{X}'', \vec{Y}), \kappa(\vec{X}', \vec{Y}) \} \) for every \( 3 \leq m_1 + m_2 + m_3 \leq m \) and every \( (\vec{X}', \vec{X}'', \vec{Y}) \in L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \times L^0(\mathbb{I}^{m_3}) \), where \( \vec{X} := \vec{X}' \cup \vec{X}'' \) and \( \vec{X}' \) and \( \vec{X}'' \) are pairwise disjoint. Now, consider \( n \geq 4 \) and the copula \( C : \mathbb{I}^n \to \mathbb{R} \) given by

\[
C(u) := \Pi(u) + \prod_{i=1}^{n} u_i \prod_{i=1}^{4} (1 - u_i)
\]

Then, for every random vector \( (X', X'', \vec{Y}) \in L^0(\mathbb{I}) \times L^0(\mathbb{I}) \times L^0(\mathbb{I}^2) \) having copula \( T_{(1,2,3,4)}(C) \), the above inequality reduces to \( \kappa(\vec{X}, \vec{Y}) \leq 0 \) where \( \vec{X} := X' \cup X'' \). However, straightforward calculation yields \( \kappa(\vec{X}, \vec{Y}) = \frac{2}{m^4} \) which contradicts (G1). Thus, although \( d_r^{m_1,m_2} \) satisfies (G1), \( d_{\kappa}^{m_1,m_2} \) fails to satisfy (G1).

### 3.3 Extended dissimilarity functions based on tail dependence

In this section we study an extended dissimilarity function based on a modified version of the classical lower tail dependence coefficient (see, e.g., [29]). This kind of dissimilarity concept is useful in order to detect different tail association in random vectors. In the literature, similar concepts have been considered for the analysis of financial time series. See, e.g., [10, 18, 37, 62].

For \( m_1, m_2 \in \mathbb{N} \) with \( 2 \leq m_1 + m_2 \leq m \), we define the function \( d_{\text{LTD}}^{m_1,m_2} : L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \to \mathbb{R}_+ \) by letting

\[
d_{\text{LTD}}^{m_1,m_2}(\vec{X}, \vec{Y}) := 1 - \lim_{u \to 0^+} \sup \frac{C(\vec{X}, \vec{Y}) (u1)}{u}
\]

Notice that, provided that the above limit superior coincides with the limit inferior, then \( d_1 = 1 - \lambda_L \), where \( \lambda_L \) is the lower tail dependence coefficient of \( (X, Y) \).

**Theorem 3.4.** For every \( 2 \leq m_1 + m_2 \leq m \), \( d_{\text{LTD}}^{m_1,m_2} \) is a \( (m_1, m_2) \)-dissimilarity function, and thus,

\[
d_{\text{LTD}} : \bigcup_{2 \leq m_1 + m_2 \leq m} L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \to \mathbb{R}_+
\]

with \( d_{\text{LTD}} |_{L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2})} := d_{\text{LTD}}^{m_1,m_2} \) is an extended dissimilarity function satisfying (L1), (L1c), (G1), (G1s) and (G2).

**Proof.** It is straightforward to show that \( d_{\text{LTD}} \) is an extended dissimilarity function satisfying (L1) and (L1c).

Now, consider \( 3 \leq m_1 + m_2 + m_3 \leq m \), the random vector \( (\vec{X}', \vec{X}'', \vec{Y}) \in L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \times L^0(\mathbb{I}^{m_3}) \) such that (2.2) holds, \( \vec{X}' \), \( \vec{X}'' \) and \( \vec{Y} \) are pairwise disjoint and put \( \vec{X} := \vec{X}' \cup \vec{X}'' \). Then

\[
C(\vec{X}, \vec{Y}) (u1) \leq C(\vec{X}, \vec{Y}) (\eta_{m_1+1, m_2+1, m_3+1}(u1, 1))
\]

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For each random variable, we have observed a sample of a given size. To determine a suitable partition of the (finite) set $X$, similarity functions can be implemented (see, for instance, [22, 30, 41]). To this end, we remind that we here, we summarize how a general agglomerative hierarchical algorithm based on extended dissimilarity functions can be implemented.

Remark 3.3. Without loss of generality, denote by $i$ the position of $X''$ within the vector $(X, Y)$. Then Lemma 3.1 yields $C_{(X,Y)}(u_1) = C_{(X,Y)}(u_1, 1) = (T_{1,...,m_1+m_2}(C_{(X,Y)}))(u_1)$ for all $u \in \Pi$ and hence $d_{LTD}^{m_1,m_2}(X, Y) = d_{LTD}^{m_1-1,m_2}(X', Y')$. This proves (G2) and, hence, the assertion.

Finally, consider $3 \leq m_1 + m_2 \leq m$ with $2 \leq m_1$, $X' \in L^0(\mathbb{I}^{m_1-1})$ and $(X', Y) \in L^0(\mathbb{T}^{m_1}) \times L^0(\mathbb{T}^{m_2})$ such that $X' \cup \{X''\} = X$, where $X'' \in X$ is comonotonic with some element $X' \in X'$. Without loss of generality, denote by $i$ the position of $X''$ within the vector $(X, Y)$. Then Lemma 3.1 yields $C_{(X,Y)}(u_1) = C_{(X,Y)}(u_1, 1) = (T_{1,...,m_1+m_2}(C_{(X,Y)}))(u_1) = C_{(X,Y)}(u_1)$ for all $u \in \Pi$ and hence $d_{LTD}^{m_1,m_2}(X, Y) = d_{LTD}^{m_1-1,m_2}(X', Y')$. This proves (G2) and, hence, the assertion.

The following example shows that the extended dissimilarity function $d_{LTD}$ satisfies (G1s).

Example 3.8. Consider $n \geq 3$, $m_1 = m_2 = m_3 = 1$, and the copula $C : \mathbb{I}^n \to \mathbb{R}$ given by

$$C(u) := \left( \sum_{i=1}^n u_i^{-1/2} - (n-1) \right)^{-2}$$

which is the Clayton copula with parameter 1/2. Then, for every random vector $(X', X'', Y) \in L^0(\mathbb{I}) \times L^0(\mathbb{I}) \times L^0(\mathbb{I})$ having copula $T_{1,2,3}(C)$, the extended dissimilarity function $d_{LTD}$ satisfies

$$d_{LTD}^{1,1}(X', X'') \leq \min \left\{ d_{LTD}^{1,1}(X', Y), d_{LTD}^{1,1}(X'', Y) \right\} < d_{LTD}^{1,1}(X, Y)$$

where $X = X' \cup X''$. Indeed, we have

$$d_{LTD}^{1,1}(X', X'') = \min \left\{ d_{LTD}^{1,1}(X', Y), d_{LTD}^{1,1}(X'', Y) \right\} = \frac{3}{4} < \frac{8}{9} = d_{LTD}^{1,1}(X, Y)$$

Thus, the extended dissimilarity function $d_{LTD}$ satisfies (G1s).

Remark 3.3. Notice that $d_{LTD}$ does not satisfy (L2), since lower and upper tail behaviour of a copula may be different, and (L3). In this latter case, consider, for instance, the bivariate copula $C_k$ that is an ordinal sum of $(M, \Pi)$ with respect to $([0,1/k], [1/k, 1])$ (see, e.g., [20]). Then $C_k$ tends to $\Pi$, as $k$ tends to $+\infty$ with $d_{LTD}^{1,1}(\Pi) = 1$, but $d_{LTD}^{1,1}(C_k) = 0$ for every $k \geq 2$.

4 The hierarchical clustering procedure

Here, we summarize how a general agglomerative hierarchical algorithm based on extended dissimilarity functions can be implemented (see, for instance, [22, 30, 41]). To this end, we remind that we aim at determining a suitable partition of the (finite) set $\mathcal{X} = \{X_1, \ldots, X_m\}$ of $m \geq 3$ continuous random variables defined on a same probability space into non-empty and non-overlapping classes. For each random variable, we have observed a sample of a given size.

Given an extended dissimilarity function

$$d : \bigcup_{2 \leq m_1 + m_2 \leq m} L^0(\mathbb{I}^{m_1}) \times L^0(\mathbb{I}^{m_2}) \to \mathbb{R}_+$$

the different steps of an agglomerative hierarchical clustering algorithm based on $d$ are given below:

...
1. Each object of $\mathcal{X}$ forms a class.

2. For each pair of classes $X$ and $Y$, one computes the dissimilarity degree $d(X, Y)$.

3. A pair of classes having the smallest dissimilarity degree, say $\{X_1, Y_1\}$, is identified, then the composite class $X_1 \cup Y_1$ is formed and the number of classes is decremented.

4. Steps 2, 3 and 4 are repeated until the number of classes is equal to 1.

The hierarchy of classes built by the clustering algorithm can be hence represented by means of a dendrogram, from which a suitable partition of $\mathcal{X}$ can be derived (see, for instance, [22]).

Now, while these steps are common to any agglomerative algorithm, the use of the extended dissimilarity function may provide some important insights into the agglomerative hierarchical algorithm. In fact, the procedure can use: either (a) the information about the pairwise dependence, as in the dissimilarity function based on linkage methods; or (b) the information about their global (higher dimensional) copula. The latter method, in particular, will allow us to detect those dependencies that only appear in higher dimensions, a feature that can be quite appealing in applications.

**Example 4.1.** As an illustrative example, consider a random vector $Z$ formed by two independent components $X = (X_1, X_2, X_3)$ and $Y = (Y_1, Y_2)$, where $X$ is distributed according to the a hierarchical Frank copula (see [32][51]) of type $C_1(C_2(u_1, u_2), u_3)$, for some suitable bivariate Archimedean copulas $C_1$ and $C_2$, while $Y = (Y_1, Y_2)$ is distributed according to a Clayton copula $D$. Suppose that $\tau(C_2) > \tau(C_1) > \tau(D)$.

Consider the extended dissimilarity function based on Kendall’s tau as described in section 3.2. Then the corresponding dendrogram representation of $X$ is given in Figure 1 (left).

However, if we consider the extended dissimilarity function based on lower tail dependence coefficient as described in Section 3.3, then the corresponding dendrogram representation of $X$ is given in Figure 1 (right). In fact, it is known that Frank copula has zero lower tail dependence coefficient.

Apart from the case when the probability law of the $\mathcal{X} = \{X_1, \ldots, X_m\}$ ($m \geq 3$) is known (i.e. by some fitting procedures and/or expert opinion), the information about $\mathcal{X}$ is usually recovered from some available observations, which can be considered as random sample from $X_1, \ldots, X_m$, denoted by $(x_{ij})$ with $i = 1, \ldots, n$ and $j = 1, \ldots, m$. In such a case, depending on the dissimilarity functions, specific estimation procedures should be adopted.

**Example 4.2.** Consider the case when a dissimilarity function $d_{m_1,m_2}$ can be expressed as a smooth function of a given measure of association $\mu$ for $(m_1 + m_2)$-dimensional random vectors, say

$$d_{m_1,m_2} = f(\mu)$$

Then, in view of a suitable application of continuous mapping theorem, a (plug-in) estimator of $d_{m_1,m_2}$ is given by

$$\hat{d}_{m_1,m_2} = f(\hat{\mu})$$

where $\hat{\mu}$ is a convenient estimator of $\mu$. Such a procedure can be, for instance, applied to the dissimilarity functions considered in section 3.2.

**Remark 4.1.** In the case of multivariate time series, i.e. when, for a fixed $j$, $(x_{ij})$ presents a time-varying behaviour, it is common to apply the hierarchical algorithm not directly on the historical time series, but on the residual time series obtained after fitting each univariate time series with an appropriate time-varying model (like ARMA-GARCH specification). Such a general framework is described, for instance, in [52] (see also [1]) and applied, among others, in [10][17].
In general, every dissimilarity function has a strong impact on the clustering procedure, since each one can have a quite different interpretation. However, when extended dissimilarity functions based on different linkage methods are considered, it would be convenient to compare them since they are defined from the same bivariate dissimilarity function. Below, via a simulation study, we check whether the choice of the linkage method may have a relevant impact on the performance of the algorithm.

4.1 A simulation study about linkage methods

Here, we compare the performance of hierarchical clustering methods where the extended dissimilarity functions are based on average, single and complete linkage method, while the pairwise dissimilarities are obtained from $d_1^{1,1}, d_{\phi}^{1,1}, d_{\rho}^{1,1}$ and $d_{\tau}^{1,1}$. Notice that, since these pairwise dissimilarities are based on classical measures of association, their (non-parametric) estimation is grounded on the (classical) empirical versions of these measures, as described in [28, 59, 61] among others (see also Example 4.2).

First, we consider the following setup. A random vector $X$ of dimension $m = 15$ is constructed in the following way:

- the random vector is formed by three independent subvectors, say $(X_1, X_2, X_3)$;
- the dimension $m_i$ of each $X_i$ is randomly chosen from 2 to 11 to ensure that each group has 2 elements and $m_1 + m_2 + m_3 = m$;
- each $X_i$ is distributed according to a copula generated from four different copula models, namely Clayton, Frank, Gumbel and equicorrelated Gaussian (for the definition of these families, see, e.g., [20]), with pairwise Kendall’s tau equal to $\tau$.

For $B = 500$ replications, the simulation study is then performed simulating $N$ independent realizations ($N \in \{50, 100, 250\}$) from $X$ with $\tau \in \{0.1, 0.2, 0.3\}$. Hence, for each simulated scenario the Adjusted Rand Index [36] (ARI, hereafter) was calculated to measure the agreement between the obtained partition and the true one. Here, the partition is obtained by cutting the dendrogram so that three groups are derived.

The distribution of ARI for each scenario is shown in Figures 2, 3, 4 and 5. As the results for the four copula models were very similar, we only comment those obtained for the Clayton copula and shown in Fig. 2. We remind that a larger Adjusted Rand Index means a higher agreement between two partitions and the maximum value of the index is 1. As one could have expected, the lower the degree of dependence among the variables of a group, the harder it is for the hierarchical clustering algorithm to identify the true partition. Also, the larger the sample size, the better the results for a given dependence degree. As far as linkage methods are concerned, one can see that, remarkably differences appear only when the dependence level is really low, i.e. lower than 0.3. In these cases, irrespectively from the dissimilarity measures, the average linkage method appears to be more satisfactory than the complete and the single ones. As for the pairwise dissimilarity function, $d_1^{1,1}$ appears to be the worst choice in case of weak dependence among groups. Overall, the average linkage performed the best, which confirms its potential frequently proved in the literature [33, 21, 4, 44], especially when $d_{\phi}^{1,1}, d_{\rho}^{1,1}$ and $d_{\tau}^{1,1}$ are used.

Since the choice of the copula family was basically irrelevant in the previous simulation, we fix one specific family, namely Clayton class, and perform a similar simulation study in higher dimensions. Specifically, we consider a random vector $X$ of dimension $m \in \{60, 120\}$ such that:
• the random vector is formed by $K \in \{6, 10\}$ independent subvectors, say $X_i$;
• the dimension $m_i$ of each $X_i$ is $m/K$;
• each $X_i$ is distributed according to a Clayton copula with pairwise Kendall’s tau equal to $\tau$.

For $B = 500$ replications, the simulation study is then performed simulating $N$ independent realizations ($N \in \{100, 250\}$) from $X$ with $\tau \in \{0.1, 0.2, 0.3\}$.

The results can be seen from Figure 6 to Figure 9. Summarizing, both for $K = 6$ and $K = 10$, the average linkage performs better than the other two linkages, while the single linkage is the worst one. The complete linkage shows a performance similar to the average linkage when $\tau > 0.1$. There are no remarkable differences among dissimilarities by varying $m$ in $\{60, 120\}$ and the slight differences are remarkably reduced as when $\tau > 0.1$ and $N = 250$, cases where all the measures show an almost perfect performance (except for the single linkage and $d_{\rho}^{1,1}$).

5 Applications

In order to show the ability of our methodology in the statistical practice, we present some empirical analysis.

5.1 Analysis of gene expressions

First, we focus on the NCI60 data set which is available in the R package made4 [8] and contains 144 gene expression (log-ratio measurements) rows and 60 cell line columns. Gene expressions have been extracted by using the cDNA spotted microarray technology [56] and pre-processed as described by [7]. The study has been carried out by the National Cancer Institute’s (NCI) Developmental Therapeutics Program (DTP) and human tumour cell lines have been derived from patients with leukaemia (LEUK), melanoma (MELAN), non-small colon lung (NSCLC), colon (COLON), central nervous system (CNS), ovarian (OVAR), renal (RENAL), breast (BREAST) and prostate (PROSTATE) cancers. Here, we divided the human tumour cell lines in two groups according to the (bivariate) Kendall’s $\tau$ and using 0.3 as cut-off. Precisely, for each subset of human tumour cell lines, i.e. for each kind of tumour, the pairwise Kendall’s $\tau$ correlation matrix has been computed. If at least 60% (59.4% for the BREAST cancer group) of pairwise correlation coefficients is greater than or equal to 0.3, then that kind of tumour has been considered as ‘tumour with high dependence’, otherwise it has been classified as ‘tumour with low dependence’. The rationale is to show empirical results comparable with the scenarios simulated in the performed Monte Carlo studies. Hence, as for the tissues with low dependence ($\tau < 0.3$) we have 8 BREAST, 9 NSCLC, and 6 OVAR, while as for the tissues with high dependence ($\tau \geq 0.3$) we have 6 CNS, 7 COLON, 6 LEUK, 8 MELAN, 2 PROSTATE, and 8 RENAL.

Tables 1 and 2 show the obtained results. Coherently with the simulation results, when the dependence is low (see Tab. 1), any linkage method, irrespectively of the kind of extended dissimilarity function, is seldom able to recognize the true partition, whereas, when the dependence is mild or high (see Tab. 2), then $i$ the single linkage method appears to perform badly while the average and the complete are very good competitors, and $ii$ the kind of dissimilarity measure appears to have an impact on the goodness of the final partition only when the average linkage method is used, in this case $d_{\rho}$ appears to be the best dissimilarity measure.
The second example concerns the data set discussed in [50] containing the transcript of 7086 human mRNAs from 4 normal tissues and 4 adenoma tissues. By applying the hierarchical clustering we want to evaluate the capability of distinguishing the two tissue types. In this empirical case, all tissues have a quite high Kendall’s $\tau$ correlation ($> 0.607$) and high Spearman’s $\rho$ correlation ($> 0.766$). The resulting clusterings by varying dissimilarity measure and linkage method are shown in Tab. 3 and Fig. 10. Note that we are here using the Rand Index [55] instead of its adjusted version since the number and the size of groups are very small.

The dissimilarity measure $d_\beta$ and the complete linkage method is the only combination able to perfectly recognize the two tissue types, thus supporting the concept that genome-wide expression profiling may permit a classification of solid tumors. Again, the effect of the kind of dissimilarity measure appears to be irrelevant.

Here, it is interesting to note that the extended dissimilarity functions $d_\beta$, $d_\phi$ and $d_\tau$ based on measures of (global) dependence (see Section 3.2) perfectly group the tissues (Rand index equal to 1). For the extended dissimilarity function $d_\phi$, however, the obtained rand index equals 0.5714 since two adenoma tissues have been clustered with the normal ones. Thus, one may argue that the global properties and, particularly the reducibility property (G1), can play a role here.

Noteworthy, the dissimilarity $d_\tau$ in its multivariate version is the most computationally heavy measure.

Finally, for the sake of illustration, we discuss the steps of the clustering procedure by means of the extended dissimilarity function $d_\tau$ (see Section 3.2). Table 4 provides the merging steps together with the corresponding values of $d_\tau$ and multivariate Kendall’s tau (see, e.g., [29, 27]).

As can be seen from the values of Kendall’s tau there is a huge 4- and also 8-dimensional dependence between the tissues. Thus, it seems as if the multivariate versions of $d_\beta$, $d_\phi$ and $d_\tau$ perform entirely satisfactorily when the random variables are highly dependent and the sample size is large enough. Again, one may also conclude from the values of $d_\tau$ that the reducibility property is crucial.

5.2 Analysis of financial time series

Here, we provide an illustration of a copula-based clustering procedure based on financial time series. To this end, we consider the dataset formed by the end-day prices of the 505 constituents of the Standard & Poor 500 index (S&P hereafter) observed in the financial crisis of 2007-2008 which are analysed, by complementing the analysis performed in [14]. The dataset is available in the R package qrmdata [34], where the data are classified according to the Global Industry Classification Standard sector information. We consider 756 daily log-returns recorded from 2007-01-01 to 2009-12-31 on 461 constituents which have not missing data and belong to the following sectors (the number of companies in each sector is in parenthesis): Consumer discretionary (77), Consumer staples (33), Energy (36), Financials (84), Health care (51), Industrials (62), Information technology (59), Materials (25), Telecommunications services (5), and Utilities (29).

Following the copula-based approach for the analysis of time series (see, e.g., [52]), we fit a suitable marginal model to each of the 461 constituents to remove serial dependence. In particular, based on [14] we adopt the ARMA(1,1)-GARCH(1,1) model with innovations following a Student-t distribution. Once the corresponding residuals have been extracted, hierarchical clustering algorithms are applied by varying dissimilarity measures and linkage methods.

Table 5 shows the agreement between the sector classification given by S&P index and the group composition determined for each considered combination of a dissimilarity measure and a linkage method (here, ARI is used). As it can be seen, single linkage method shows the worst agreement.
irrespective from the dissimilarity measure. On the contrary, the performance of the average and the complete linkage method appear quite different from each other and, on this set of data, the complete linkage outperforms the average linkage. As expected, however, the benchmark group composition provided by sectors reflects poorly the comovements of financial time series, especially in crisis periods.

6 Conclusions

We have provided a theoretical foundation for the study of hierarchical clustering algorithms based on (rank-based) dissimilarity measures. The procedure aims at clustering continuous variables and it is based on the use of copulas. Novel properties of a dissimilarity have been considered (see Table 6) and various dissimilarity measures have been analysed with respect to their main features (see Table 7). The provided properties may provide computational and practical insights that may guide for the choice of the most appropriate dissimilarity function for the problem at hand.

Finally, we would like to remark that the simulations and the empirical analysis have been performed in [54], also by means of the package [35].

Acknowledgements

FD has been supported by the project “Stochastic Models for Complex Systems” by Italian MIUR (PRIN 2017, Project no. 2017JFFHSH). FMLDL has been supported by the project “The use of Copula for the Analysis of Complex and Extreme Energy and Climate data (CACEEC)” by the Free University of Bozen-Bolzano, Faculty of Economics and Management (Grant Nos. WW200S).

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Table 1: NCI60 data: ARI index of hierarchical clustering of low (< 0.3) dependent tissues by varying dissimilarity measure and linkage method.

|       | $d_\beta$ | $d_\phi$ | $d_\rho$ | $d_\tau$ |
|-------|-----------|-----------|-----------|-----------|
| Average | 0.056     | 0.056     | 0.043     | 0.039     |
| Single  | 0.056     | 0.056     | 0.056     | 0.056     |
| Complete| -0.024    | 0.005     | 0.039     | 0.039     |

Table 2: NCI60 data: ARI index of hierarchical clustering of high ($\geq 0.3$) dependent tissues by varying dissimilarity measure and linkage method.

|       | $d_\beta$ | $d_\phi$ | $d_\rho$ | $d_\tau$ |
|-------|-----------|-----------|-----------|-----------|
| Average | 0.547     | 0.743     | 0.820     | 0.574     |
| Single  | 0.116     | 0.076     | 0.076     | 0.298     |
| Complete| 0.752     | 0.752     | 0.691     | 0.773     |

Table 3: Notterman’s data: Rand index of hierarchical clustering results by varying dissimilarity measure and linkage method.

|       | $d_\beta$ | $d_\phi$ | $d_\rho$ | $d_\tau$ |
|-------|-----------|-----------|-----------|-----------|
| Average | 0.464     | 0.464     | 0.464     | 0.464     |
| Single  | 0.464     | 0.464     | 0.464     | 0.464     |
| Complete| 1.000     | 0.464     | 0.571     | 0.464     |

Table 4: Notterman’s data: Steps of the hierarchical clustering procedure via dissimilarity function based on multivariate Kendall’s tau.

| merging variables | $d_\tau$ | Kendall’s tau |
|-------------------|----------|---------------|
| 5 and 7           | 0.061    | 0.756         |
| 6 and 8           | 0.068    | 0.728         |
| 1 and 2           | 0.076    | 0.696         |
| 3 and 4           | 0.095    | 0.620         |
| (5, 7) and (6, 8) | 0.124    | 0.717         |
| (1, 2) and (3, 4) | 0.159    | 0.637         |
| (1, 2, 3, 4) and (5, 6, 7, 8) | 0.209 | 0.579 |

Table 5: S&P 500: ARI index between the S&P sector classification and the group composition provided by hierarchical clustering with different dissimilarity measures and linkage methods.

|       | $d_\beta$ | $d_\phi$ | $d_\rho$ | $d_\tau$ |
|-------|-----------|-----------|-----------|-----------|
| Average | 0.003     | 0.006     | 0.003     | 0.003     |
| Single  | 0.002     | 0.003     | 0.003     | 0.003     |
| Complete| 0.331     | 0.337     | 0.320     | 0.370     |
Table 6: Properties of dissimilarity functions.

|                        | (L1)                      | (L1c)                    | (L2)                      | (L3)                      | (G1)                      | (G1s)                     | (G2)                      |
|------------------------|---------------------------|--------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|
| Order preserving       | Order preserving property (lower orthant order) | Order preserving property (concordance order) | Radially symmetry | Continuity/Weakly convergence | Reducibility property | Strict reducibility property | Comonotonic invariance |

Table 7: Summary of the properties satisfied (symbol: √), not satisfied (symbol: ×), or satisfied under specific conditions on $d^{1,1}$ (symbol: *) by the extended dissimilarity functions.

|                        | (L1) | (L1c) | (L2) | (L3) | (G1) | (G1s) | (G3) |
|------------------------|------|-------|------|------|------|-------|------|
| single linkage         | *    | *     | *    | *    | √    | ×     | √    |
| average linkage        | *    | *     | *    | *    | √    | *     | √    |
| complete linkage       | *    | *     | *    | *    | √    | *     | √    |
| tail dependence        | √    | √     | ×    | ×    | √    | √     | √    |
| Blomqvist’s beta       | √    | √     | ×    | √    | √    | √     | √    |
| Spearman’s footrule    | √    | √     | ×    | √    | √    | √     | √    |
| Kendall’s tau          | ×    | √     | √    | √    | √    | √     | √    |
| Spearman’s rho         | √    | √     | ×    | √    | ×    | ×     | ×    |
Figure 1: Two illustrative examples of dendrogram representation of a random vector based on different extended dissimilarity functions. See Example 4.1.
Figure 2: Boxplots of ARI (y-axis) by varying i) pairwise dissimilarity measure among $d_{\beta}^{1,1}$, $d_{\phi}^{1,1}$, $d_{\rho}^{1,1}$ and $d_{\tau}^{1,1}$ and ii) linkage method among the average, single (minimum) and complete (maximum) one (x-axis starting with the average linkage and $d_{\beta}^{1,1}$, continuing with the single linkage and $d_{\phi}^{1,1}$ and ending with the complete linkage and $d_{\tau}^{1,1}$), iii) Kendall’s $\tau = (.1, .2, .3)$ (panels by cols), and iv) sample size $N = 50, 100, 250$ (panels by rows). Data simulated from independent groups with a Clayton copula within each group (see text).
Figure 3: Boxplots of ARI (y-axis) by varying i) pairwise dissimilarity measure among $d^{1,1}_\beta$, $d^{1,1}_\phi$, $d^{1,1}_\rho$ and $d^{1,1}_\tau$ and ii) linkage method among the average, single (minimum) and complete (maximum) one (x-axis starting with the average linkage and $d^{1,1}_\beta$, continuing with the single linkage and $d^{1,1}_\beta$ and ending with the complete linkage and $d^{1,1}_\tau$), iii) Kendall’s $\tau = (.1, .2, .3)$ (panels by cols), and iv) sample size $N = 50, 100, 250$ (panels by rows). Data simulated from independent groups with a Frank copula within each group (see text).
Figure 4: Boxplots of ARI (y-axis) by varying i) pairwise dissimilarity measure among $d_{\beta}^{1,1}$, $d_{\phi}^{1,1}$, $d_{p}^{1,1}$ and $d_{\tau}^{1,1}$ and ii) linkage method among the average, single (minimum) and complete (maximum) one (x-axis starting with the average linkage and $d_{\beta}^{1,1}$, continuing with the single linkage and $d_{p}^{1,1}$ and ending with the complete linkage and $d_{\tau}^{1,1}$), iii) Kendall’s $\tau = (.1, .2, .3)$ (panels by cols), and iv) sample size $N = 50, 100, 250$ (panels by rows). Data simulated from independent groups with a Gumbel copula within each group (see text).
Figure 5: Boxplots of ARI (y-axis) by varying i) pairwise dissimilarity measure among $d_{1,1}^{1,1}$, $d_{1,1}^{1,1}$, $d_{1,1}^{1,1}$ and $d_{1,1}^{1,1}$ and ii) linkage method among the average, single (minimum) and complete (maximum) one (x-axis starting with the average linkage and $d_{1,1}^{1,1}$, continuing with the single linkage and $d_{1,1}^{1,1}$ and ending with the complete linkage and $d_{1,1}^{1,1}$), iii) Kendall’s $\tau = (1, .2, .3)$ (panels by cols), and iv) sample size $N = 50, 100, 250$ (panels by rows). Data simulated from independent groups with a equicorrelated Gaussian copula within each group (see text).
Figure 6: Boxplots of ARI (y-axis) by varying i) pairwise dissimilarity measure among $d_{\beta}^{1,1}$, $d_{\phi}^{1,1}$, $d_{\tau}^{1,1}$ and $d_{\phi}^{1,1}$ and ii) linkage method among the average, single (minimum) and complete (maximum) one (x-axis starting with the average linkage and $d_{\beta}^{1,1}$, continuing with the single linkage and $d_{\beta}^{1,1}$ and ending with the complete linkage and $d_{\tau}^{1,1}$), iii) Kendall’s $\tau = (.1, .2, .3)$ (panels by cols), and iv) clustering size (total number of variables) $m = 60, 120$ (panels by rows). Sample size is equal to $N = 100$ and data are simulated from $K = 6$ independent Clayton copulas of dimension $m/K$. 

Figure 7: Boxplots of ARI (y-axis) by varying i) pairwise dissimilarity measure among $d_{\beta}^{1,1}$, $d_{\phi}^{1,1}$, $d_{\psi}^{1,1}$ and $d_{\lambda}^{1,1}$ and ii) linkage method among the average, single (minimum) and complete (maximum) one (x-axis starting with the average linkage and $d_{\beta}^{1,1}$, continuing with the single linkage and $d_{\phi}^{1,1}$ and ending with the complete linkage and $d_{\lambda}^{1,1}$), iii) Kendall’s $\tau = (.1, .2, .3)$ (panels by cols), and iv) clustering size (total number of variables) $m = 60, 120$ (panels by rows). Sample size is equal to $N = 250$ and data are simulated from $K = 6$ independent Clayton copulas of dimension $m/K$. 
Figure 8: Boxplots of ARI (y-axis) by varying i) pairwise dissimilarity measure among $d_{\beta}^{1,1}$, $d_{\phi}^{1,1}$, $d_{\tau}^{1,1}$ and $d_{\phi}^{1,1}$ and ii) linkage method among the average, single (minimum) and complete (maximum) one (x-axis starting with the average linkage and $d_{\beta}^{1,1}$, continuing with the single linkage and $d_{\phi}^{1,1}$ and ending with the complete linkage and $d_{\tau}^{1,1}$), iii) Kendall’s $\tau = (.1, .2, .3)$ (panels by cols), and iv) clustering size (total number of variables) $m = 60, 120$ (panels by rows). Sample size is equal to $N = 100$ and data are simulated from $K = 10$ independent Clayton copulas of dimension $m/K$. 
Figure 9: Boxplots of ARI (y-axis) by varying (i) pairwise dissimilarity measure among $d_{\beta}^{1,1}$, $d_{\phi}^{1,1}$, $d_{\phi}^{1,1}$ and $d_{\tau}^{1,1}$ and (ii) linkage method among the average, single (minimum) and complete (maximum) one (x-axis starting with the average linkage and $d_{\beta}^{1,1}$, continuing with the single linkage and $d_{\phi}^{1,1}$, and ending with the complete linkage and $d_{\tau}^{1,1}$), (iii) Kendall’s $\tau = (1, 2, 3)$ (panels by cols), and (iv) clustering size (total number of variables) $m = 60, 120$ (panels by rows). Sample size is equal to $N = 250$ and data are simulated from $K = 10$ independent Clayton copulas of dimension $m/K$. 
Figure 10: Dendrograms of the data set by [50] by varying $i$) dissimilarity measure among $d_{\beta}$, $d_{\phi}$, $1 - \rho$ and $1 - \tau$ by cols, and $ii$) linkage method among the average, single (minimum) and complete (maximum) one by row.