A framework for measuring dependence between random vectors

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2018-01-12

Abstract

A framework for quantifying dependence between random vectors is introduced. With the notion of a collapsing function, random vectors are summarized by single random variables, called collapsed random variables in the framework. Using this framework, a general graphical assessment of independence between groups of random variables for arbitrary collapsing functions is provided. Measures of association computed from the collapsed random variables are then used to measure the dependence between random vectors. To this end, suitable collapsing functions are presented. Furthermore, the notion of a collapsed distribution function and collapsed copula are introduced and investigated for certain collapsing functions. This investigation yields a multivariate extension of the Kendall distribution and its corresponding Kendall copula for which some properties and examples are provided. In addition, non-parametric estimators for the collapsed measures of dependence are provided along with their corresponding asymptotic properties. Finally, data applications to bioinformatics and finance are presented.

Keywords
Dependence between random vectors, hierarchical models, collapsing functions, collapsed random variables, multivariate Kendall distribution and Kendall copula, graphical test of independence.

MSC2010
62H99, 65C60, 62-09
1 Introduction

While there are numerous well established methods to measure dependence between random variables, the extension to random vectors (for example, for modeling groups of random variables) poses a significant challenge. This challenge arises from the lack of a unique axiomatic framework that outlines desirable properties a measure of dependence between random vectors should exhibit. Moreover, there is no unique extension of bivariate measures of association to arbitrary dimensions and the multivariate measures of association available do not naturally capture dependence between more than one random vector as is of interest in applications such as bioinformatics, finance, insurance or risk management.

Proposed solutions to this problem are rather difficult to find in the literature. A classical methodology to summarize (linear) dependence between random vectors is the well known canonical correlation coefficient; see Hotelling (1936). A non-linear extension of canonical correlation has been suggested through the use of kernel functions in Bach and Jordan (2002) and Ghoraie et al. (2015a). A faster version of the kernel canonical correlation method has been developed by adopting the idea of randomized kernels; see Lopez-Paz et al. (2013). Székely et al. (2007) proposed a novel distance covariance coefficient, defined as a weighted $L^2$-norm between the joint characteristic function and product of marginal characteristic functions of the random vectors under consideration. In the context of copula modeling, Grothe et al. (2014) recently derived versions of Spearman’s rho and Kendall’s tau between random vectors and corresponding estimation procedures. Our framework will generalize their approach. This generalization will also allow us to derive a couple of interesting results as by-products of our framework.

Note that there is neither an inherently correct nor a canonical way of measuring dependence between random vectors. As a result, one can think of multiple variations of quantifying such dependence. Approaches are primarily motivated by the purpose, for example, detection or ranking of dependencies and the salient features of the dataset under investigation. In this paper, we subsume several such approaches under a general framework which allows us to detect, quantify, visualize and check dependence between random vectors.

The paper is organized as follows. In Section 2 we present the said framework for measuring dependence between random vectors and utilize it to develop a visual assessment of independence between random vectors. Section 3 develops the notion of a collapsed distribution function and collapsed copula with explicit characterizations for some choices of collapsing functions (to be detailed later). In Section 4 we discuss non-parametric estimators for the dependence measures introduced in Section 2 and their corresponding asymptotic properties. Empirical examples from the realm of bioinformatics and finance are covered in Section 5. Section 6 concludes.
2 The framework

For introducing a framework for measuring dependence between random vectors, it suffices to consider the case of two, a $p$-dimensional random vector $\mathbf{X} = (X_1, \ldots, X_p)$ (with continuous marginal distribution functions $F_{X_1}, \ldots, F_{X_p}$) and a $q$-dimensional random vector $\mathbf{Y} = (Y_1, \ldots, Y_q)$ (with continuous marginal distribution functions $F_{Y_1}, \ldots, F_{Y_q}$), defined on some probability space with probability measure $\mathbb{P}$. Our target is to measure dependence between $\mathbf{X}$ and $\mathbf{Y}$ with a measure of association $\chi = \chi(\mathbf{X}, \mathbf{Y})$ mapping to $[-1, 1]$; note the missing “the” before “dependence”, depending on the context, various notions of dependence are possible. As mentioned before, this is different from multivariate extensions of measures of association which aim to summarize dependence of a single random vector (say, just $\mathbf{X}$); see Schmid et al. (2010) and the references therein for a comprehensive treatment.

A natural first step is to establish properties $\chi$ should satisfy. For bivariate measures of association, that is, measures of association between two random variables $X$ and $Y$, such properties were listed in Rényi (1959) and with minor revisions later in Schweizer and Wolff (1981). Scarsini (1984) introduced the notion of concordance measures by adding the property that measures should respect a pointwise partial ordering on the set of copulas also known as concordance ordering; see Embrechts et al. (2002) for more on concordance (or rank-correlation) measures and their motivation due to pitfalls of (linear) correlation. Prominent examples are Kendall’s tau and Spearman’s rho. Another type of bivariate measure of association, focusing on the (extremal) dependence in the joint tails of a bivariate distribution, is the (lower or upper) coefficient of tail dependence.

Note that, more recently, Reshef et al. (2011) described an ideal measure of association in the bivariate case as so-called equitable dependence measures. The notion of an equitable dependence measure extends the invariance property of concordance measures to include invariance under non-monotone marginal transforms. However, the maximal information coefficient (MIC) introduced in Reshef et al. (2011), which supposedly satisfies this equitability condition, is purely data-driven and heuristic. As a result, the MIC measure does not naturally fit into our probabilistic framework. Various versions of this equitability condition have since been proposed including more mathematically formal definitions; see, for example, Kinney and Atwal (2014). Hence, there is some consensus of an “ideal” bivariate measure of association but our problem demands generalizations of these properties to vector-based measures of association, which is non-trivial.

Grothe et al. (2014) recently approached this problem and listed properties of a concordance measure which easily carry over from random variables $X, Y$ to random vectors $\mathbf{X}, \mathbf{Y}$. These include:

1) $\chi(\mathbf{X}, \mathbf{Y}) \in [-1, 1]$;

2) $\chi(\mathbf{X}, \mathbf{Y})$ is invariant to permutations of the components of the random vectors $\mathbf{X}$ and $\mathbf{Y}$;
3) independence of $X$ and $Y$ implies $\chi(X, Y) = 0$.

The translation of more non-trivial properties such as the invariance to (some sort of) increasing transformations of $X$ and $Y$ and the concordance ordering to the vector case is less transparent. One such generalization of these properties proposed in Grothe et al. (2014) is as follows.

1) Invariance property. $\chi(X, Y)$ is invariant to increasing transformations of the components of the random vectors $X$ and $Y$;

2) Concordance ordering property. Suppose one has two distribution functions with margins $F_{X_1}, \ldots, F_{X_p}, F_{Y_1}, \ldots, F_{Y_q}$ and copulas $C_1$ and $C_2$, respectively, such that $C_1 \succeq C_2$, that is, $C_1(u) \leq C_2(u)$ for all $u \in [0, 1]^{p+q}$. Then $\chi_{C_1}(X, Y) \leq \chi_{C_2}(X, Y)$, where $\chi_{C_1}$ and $\chi_{C_2}$ denote the measures of association expressed as functions of only the copula $C_1$ and $C_2$, respectively.

The difficulty lies in hypothesizing invariance and concordance properties when the marginal distributions $F_{X_1}, \ldots, F_{X_p}, F_{Y_1}, \ldots, F_{Y_q}$ and the copula $C_X, C_Y$ of $X, Y$, respectively, all can vary; generalizing the concept of equitable dependence faces similar difficulties.

2.1 The collapsed random variables

The framework we suggest consists of collapsing or summarizing the two random vectors $X$ and $Y$ to single random variables $S(X)$ and $S(Y)$ referred to as collapsed random variables. The function $S$ maps random vectors to random variables and is referred to as a collapsing (or summary) function. Note that in the most general setup, we could use separate collapsing functions, $S_X(X)$ and $S_Y(Y)$. Different collapsing functions could be particularly useful when $X$ and $Y$ lie in different domains, that is, continuous vs discrete. However, in what follows, we will for the sake of simplicity restrict ourselves to using the same collapsing function $S$ to collapse $X$ and $Y$, and remain in the continuous domain to facilitate development of theoretical results. The (bivariate) distribution function of $(S(X), S(Y))$ is called the collapsed distribution function in our framework and its copula (if unique) is termed collapsed copula; see Section 3 for more details.

Collapsing functions for different random vectors typically are of similar functional form; see Section 2.4 for several examples. However, they can differ, for example, due to the different dimensions of $X$ and $Y$. Furthermore, as we will see in Section 2.4 a collapsing function for $X$ does not necessarily have to be a $p$-variate function, it can also be a $2p$-variate function (denoted as $S(X, X')$, where $X'$ is an independent copies of $X$), for example.

As such, the notion of a collapsing function is quite general, the only requirement being that a random vector is mapped to a single random variable. For simplicity, we denote all collapsing functions by $S$ and speak of the collapsing function as being applied to $X$ or to $Y$. Options for $S$ are provided in Section 2.4 and estimation is addressed in Section 4; concrete choices of $S$ are also provided and discussed, for example, in the applications in Section 5. We start by presenting a general graphical assessment (can be converted to a statistical test if needed) of independence between groups of random variables.
2 The framework

2.2 A graphical assessment of independence between random vectors

As mentioned in the introduction, Székely et al. (2007) suggest a formal test of independence between \(X\) and \(Y\) based on the distance between the characteristic function of \((X, Y)\) and the product of the characteristic functions of \(X\) and \(Y\). Furthermore, they derived that this distance can equivalently be expressed as a function of the correlation coefficient of Euclidean distances. Using this formal test as motivation, Wang (2013) introduced a graphical test of independence between random variables with Euclidean distance and rank transform. We further extend this work to a graphical assessment of independence between groups of random variables with various different transforms (that is, collapsing functions).

The method we suggest is based on the Grouping Lemma, see Resnick (2014, Lemma 4.4.1), which states that measurable functions of independent random variables are independent; see also Durrett (2004, Theorem 2.1.6). This result can be conveniently used to construct a test of independence between two or more groups of random variables by testing independence of the collapsed random variables in our framework; note that the corresponding hypothesis \(H_{0,c}\) tested (namely the collapsed random variables to be independent) is only a subset of the hypothesis \(H_0\) that all random variables are independent.

In principle, all known statistical tests of independence between two or more random variables can be applied for testing \(H_{0,c}\). What we suggest here is a graphical assessment for \(H_{0,c}\). As is typically of interest in practice, see also our example in Section 5.2, we consider \(G \geq 2\) random vectors here.

Algorithm 2.1 (Graphical assessment of independence of groups of variables)

Let \(X_{i1}, \ldots, X_{iG}, i \in \{1, \ldots, n\}\), be a random sample from \(G\) groups of random variables \(X_1, \ldots, X_G\) of dimensions \(p_1, \ldots, p_G\). To visually check independence of the groups of random variables \(X_1, \ldots, X_G\) based on the sample \(X_{i1}, \ldots, X_{iG}, i \in \{1, \ldots, n\}\), do:

1) For each group \(g \in \{1, \ldots, G\}\) of variables, compute the collapsed variables \(S_{ig} = S(X_{ig}), i \in \{1, \ldots, k\}\), where \(k = n\) for \(p\)-variate functions and \(k = \binom{n}{2}\) for \(2p\)-variate functions.
2) Compute the pseudo-observations

\[
U_{k,ig} = \frac{R_{ig}}{k+1}, \quad i \in \{1, \ldots, k\}, \quad g \in \{1, \ldots, G\},
\]

where, for each \(g \in \{1, \ldots, G\}\), \(R_{ig}\) denotes the rank of \(S_{ig}\) among \(S_{1g}, \ldots, S_{kg}\).
3) Visualize all pairs of pseudo-observations \((U_{k,ig}, U_{k,ih}), i \in \{1, \ldots, k\}, g, h \in \{1, \ldots, G\}: g < h\). This can be done in a scatter-plot matrix (for small to moderate \(G\)) or with a zenplot (for large \(G\)); see Hofert and Oldford (2017) and Section 5 for the latter. The less the visualized samples resemble realizations from \(U(0, 1)^2\) the greater the evidence against \(H_{0,c}\) and thus \(H_0\).

Note that we can turn this graphical assessment into a statistical test of independence by adopting the line up test proposed in Buja et al. (2009). That is, if in addition to the visualized samples, we also displayed groups of independent realizations from \(U(0, 1)^2\), then actual significance levels could be determined.
2 The framework

An interesting question is whether our visual assessment of independence is independent of the marginal distributions of any of the \( d = p_1 + \cdots + p_G \) components of \((X_1, \ldots, X_G)\). This certainly depends on the collapsing function. In general, it does not matter for an assessment of independence, but for better interpretability (of the visualized pseudo-observations) one could of course build pseudo-observations of the given data from \((X_1, \ldots, X_G)\) before applying Algorithm 2.1; note that in this case, one would apply pseudo-observations at two levels, to the original variables and the collapsed variables.

The distance correlation test developed in Székely et al. (2007) is a notable statistical test of independence between random vectors. In particular, the distance correlation (population) test statistic possesses the desirable property that it is zero if and only if \( X \) and \( Y \) are independent, thus making it particularly useful for testing independence. With an appropriately chosen collapsing function (see Table 1 for examples), our framework could yield a more powerful (graphical) test of independence. The main advantages when compared with distance correlation are that we are working with pseudo-observations and that there are many different types of departures from independence that can be observed in comparison to a single numerical test statistic.

2.3 Collapsed measures of association and dependence

After \( X \) and \( Y \) have been collapsed to \( S(X) \) and \( S(Y) \), respectively, the latter two random variables can be used to detect, quantify and check dependence between \( X \) and \( Y \) using a classical and well understood bivariate measure of association referred to as collapsed measure of association in our framework. Although there are various choices of collapsed measures of association (including, for example, tail dependence; see also later), we will mainly focus on Pearson’s correlation coefficient \( \rho \) and thus consider

\[
\chi(X, Y) = \rho(S(X), S(Y))
\]

as a measure of association between \( X \) and \( Y \). The choice of Pearson’s correlation coefficient seems careless given the known deficiencies of correlation for quantifying monotone dependence or concordance (as opposed to “just” linear dependence); see, for example, Embrechts et al. (2002). However, Spearman’s rho and Kendall’s tau both appear as a special case of (1) when choosing appropriate collapsing functions \( S \). This is obvious in the case of Spearman’s rho \( \rho_S \) which is simply Pearson’s correlation \( \rho \) of the (univariate) probability integral transformed random variables. In other words, if \( F_{S(X)} \) denotes the distribution function of the collapsed random variable \( S(X) \), we can use the collapsing functions \( \tilde{S}(x) = F_{S(X)}(S(x)) \) and \( \tilde{S}(y) = F_{S(Y)}(S(y)) \) to obtain

\[
\chi(X, Y) = \rho(\tilde{S}(X), \tilde{S}(Y)) = \rho_S(S(X), S(Y)).
\]

The following lemma shows that also Kendall’s tau appears as a special case of (1); note that the collapsing function is an example of a 2p-variate collapsing function as mentioned before.
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Lemma 2.2 (Kendall’s tau as a special case of \([1]\))

Let \(X\) and \(Y\) be continuously distributed random vectors and let \(X’\) and \(Y’\) be independent copies of \(X\) and \(Y\), respectively. Under our framework, the collapsing function \(\tilde{S}(X, X') = 1\{S(X) \leq S(X')\}\) leads to

\[
\chi(X, Y) = \rho(\tilde{S}(X, X'), \tilde{S}(Y, Y')) = \tau(S(X), S(Y)).
\]

Proof. Let \(S_1, S_2\) be continuously distributed random variables and let \(S'_1, S'_2\) be independent copies of \(S_1, S_2\), respectively. Then

\[
\tau(S_1, S_2) = \mathbb{P}((S_2 - S'_2)(S_1 - S'_1) > 0) - \mathbb{P}((S_2 - S'_2)(S_1 - S'_1) < 0)
\]

\[
= 2\mathbb{P}((S_2 - S'_2)(S_1 - S'_1) > 0) - 1 = 4\mathbb{P}(S_1 \leq S'_1, S_2 \leq S'_2) - 1
\]

\[
= \frac{\mathbb{E}(1_{\{S_1 \leq S'_1\}} 1_{\{S_2 \leq S'_2\}}) - \frac{1}{2} \cdot \frac{1}{2}}{\sqrt{\mathbb{E}(1_{\{S_1 \leq S'_1\}})^2} \sqrt{\mathbb{E}(1_{\{S_2 \leq S'_2\}})^2}}
\]

\[
= \rho(1_{\{S_1 \leq S'_1\}}, 1_{\{S_2 \leq S'_2\}}),
\]

that is, Kendall’s tau equals the correlation coefficient of the indicators \(1_{\{S_1 \leq S'_1\}}\) and \(1_{\{S_2 \leq S'_2\}}\). With the collapsing function \(\tilde{S}\) as claimed (and \(S_1 = S(X), S'_1 = S(X'), S_2 = S(Y), S'_2 = S(Y')\)), we thus obtain that

\[
\chi(X, Y) = \rho(\tilde{S}(X, X'), \tilde{S}(Y, Y')) = \rho(1_{\{S(X) \leq S(X')\}}, 1_{\{S(Y) \leq S(Y')\}}) = \tau(S(X), S(Y)).
\]

Finally let us briefly address the notion of tail dependence; see, for example, Joe (1997, Section 2.1.10) or Nelsen (2006, Section 5.4). Although there are multivariate notions of tail dependence, see Jaworski et al. (2010, Chapter 10) for an overview, there is, to the best of our knowledge, no notion of tail dependence between two random vectors \(X, Y\). An intuitive choice in our framework is simply

\[
\chi(X, Y) = \lambda(S(X), S(Y))
\]

where \(\lambda\) denotes the lower or upper coefficient of tail dependence as implied by the collapsed copula. This concept can be extended to more than two random vectors by considering matrices; see Embrechts et al. (2010).

Let us now go back to the case where the collapsed measure of association is Pearson’s correlation coefficient.

2.4 Choosing the collapsing function \(S\)

The choice of the collapsing function \(S\) for measuring dependence between random vectors is fairly open ended. We start by introducing various options for \(S\), summarized in Table \([1]\).
2 The framework

| Type of $S$                          | Collapsing function $S$                                                                 |
|-------------------------------------|----------------------------------------------------------------------------------------|
| Weighted average                    | $S(X) = w^\top X$ for $w = (w_1, \ldots, w_p)$, $\sum_{j=1}^p w_j = 1$                |
| Maximum (or minimum)                | $S(X) = \max_{1 \leq j \leq p} \{X_j\}$ (or $S(X) = \min_{1 \leq j \leq p} \{X_j\}$) |
| Distance                            | $S(X, X') = D(X, X')$                                                                   |
| Kernel similarity                   | $S(X, X') = K(X, X')$                                                                   |
| Multivariate rank                   | $S(X, X') = \mathbb{1}\{X \leq X'\}$                                                  |
| Probability integral transform      | $S(X) = F_X(X)$                                                                         |

Table 1 Examples of collapsing functions $S$ of a random vector $X$ (with independent copy $X'$); note that the inequality $X \leq X'$ in the multivariate rank collapsing function is understood componentwise.

As before, $X'$ is used to denote an independent copy of the random vector $X$. Note that if $F_{X_1}, \ldots, F_{X_p}$ are continuous, the multivariate rank transform satisfies

$$S((X_1, \ldots, X_p), (X'_1, \ldots, X'_p)) = \mathbb{1}\{X_1 \leq X'_1, \ldots, X_p \leq X'_p\}$$

$$= \mathbb{1}\{F_{X_1}(X_1) \leq F_{X'_1}(X'_1), \ldots, F_{X_p}(X_p) \leq F_{X'_p}(X'_p)\}$$

$$= S((F_{X_1}(X_1), \ldots, F_{X_p}(X_p)), (F_{X'_1}(X'_1), \ldots, F_{X'_p}(X'_p)))$$

and thus does not depend on the specific marginal distributions $F_{X_1}, \ldots, F_{X_p}$ involved; furthermore, $F_{X_j}(X_j) \sim U(0, 1)$, $j \in \{1, \ldots, p\}$. Similarly for the probability integral transform (PIT), by Sklar’s Theorem, see Sklar (1959),

$$S(X_1, \ldots, X_p) = F_{(X_1, \ldots, X_p)}(X_1, \ldots, X_p) = C_X(F_{X_1}(X_1), \ldots, F_{X_p}(X_p))$$

$$= S(F_{X_1}(X_1), \ldots, F_{X_p}(X_p)),$$

Therefore, the PIT as collapsing function also does not depend on the specific marginal distributions involved.

For collapsing functions which are not invariant under the marginal distributions (such as weighted average, maximum, minimum, distance and kernel similarity), one can easily introduce such property by replacing $(X_1, \ldots, X_p)$ by $(F_{X_1}(X_1), \ldots, F_{X_p}(X_p))$ in $S$. This is often useful for getting a (rank-based) picture of dependence independently of the margins which can be of interest for visualization or estimation purposes (empirically, this means computing pseudo-observations).

The following sections consider each of the collapsing functions listed in Table 1 in more detail.

2.4.1 The weighted average collapsing function

The weighted average function is a classical choice of collapsing function. Here are a few ways how the weights $w_1, \ldots, w_p$ can be chosen:
1) **Equal weights.** For equal weights \( w_j = \frac{1}{p}, j \in \{1, \ldots, p\} \), we obtain the simple average as collapsing function.

2) **Application-specific weights.** One can choose weights \( w_j \) which are tailor-made for a specific application in mind. See Section 5 for examples.

3) **Dimension reduction weights.** Typically by adopting any dimension reduction technique, one could use some normalized version of the measure (usually singular values of a specific matrix depending on the technique) used to order the dimensions as weights in our framework.

4) **Optimal weights.** One can choose optimal weights with respect to some objective function. For example, analogously to the notion of canonical correlation, one could empirically choose the weights for every pair of random vectors such that the resulting measure of association \( \chi \) is maximized. For example, if \( X, Y \) are elliptical, one could consider

\[
\chi(X, Y) = \sup_{w_1 \in \mathbb{R}^p, w_2 \in \mathbb{R}^q} \rho(w_1^\top X, w_2^\top Y)
\]

5) **Extreme weights.** One can consider the \( m \)-largest (or \( m \)-smallest) weighted average, that is, the average over the \( m \) largest (or \( m \) smallest) order statistics per group of random variables. This could be of interest in the context of financial risk management, where one needs to keep track of the \( m \) largest (or \( m \) smallest) losses in two or more portfolios or asset classes.

### 2.4.2 The maximum collapsing function

The componentwise maximum (or minimum) is a special case of the aforementioned extreme weighted case, with 1-largest (or 1-smallest) weighted average as collapsing function, that is,

\[
S(X) = \max\{X_1, \ldots, X_p\} \quad \text{(or } S(X) = \min\{X_1, \ldots, X_p\})
\]

This requires all dimensions of the random vector \( X \) to have a comparable interpretation and makes sense, for example, for quantifying dependence between market return data grouped into sectors. In this case we would be measuring dependence between different market sectors through the best (or worst) performer in each sector.

### 2.4.3 The pairwise distance collapsing function

The population version of the pairwise distance collapsing function requires invoking an independent copy of the random vector. For the sample version based on sample size \( n \), this implies that distances are computed between the \( \binom{n}{2} \) distinct pairs of the \( n \) samples.

One can choose virtually any type of distance \( D \). For example, some of the standard distance functions we experimented with in Section 5 are Euclidean, Manhattan, Canberra, and Minkowski. Some distance functions for non-continuous measurements include cosine
distance (suitable for text data), hamming distance (datasets in information theory), and Jaccard distance.

Ideally one should have a data- or application-specific reason to choose distances other than Euclidean distance (but numerical experiments have shown that it can sometimes be advantageous to choose the Canberra distances to avoid issues due to large distances).

### 2.4.4 The pairwise kernel collapsing function

Similar to the distance transform, the kernel collapsing function $K$ results in $\binom{n}{2}$ samples in the transformed space. As for the choice of $K$, one can choose any kernel function, some of which are listed in Table 2. By default one can choose the Gaussian kernel unless the peculiarities of a dataset or application context suggest a potential alternative like the von Mises kernel which was used in Section 5.1 for the protein dataset.

| Type of $K$            | Kernel function $K(\cdot, \cdot) : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$ |
|-----------------------|-----------------------------------------------------------------------------------|
| Linear (trivial)      | $K(x_i, x_k) = x_i^\top x_k$                                                      |
| Polynomial (of order $d$) | $K(x_i, x_k) = (1 + x_i^\top x_k)^d$                                             |
| Gaussian              | $K(x_i, x_k) = \exp\left(-\left(\|x_i - x_k\|^2/(2\sigma^2)\right)\right)$        |
| von Mises             | $K(x_i, x_k) = \prod_{t=1}^{p} \exp(\kappa_t \cos(x_{it} - x_{kt}))$             |

Table 2 Examples of kernel functions.

### 2.4.5 The multivariate rank collapsing function

Utilizing the multivariate rank collapsing function $S(X, X’) = 1_{X \leq X’}$ to summarize multidimensional random vectors to a single dimension yields a rank-based measure of association $\chi$; as usual, the inequality $X \leq X’$, is understood componentwise. The resulting association measure was first introduced in Grothe et al. (2014) as one possible multivariate extension of Kendall’s tau. As is evident, this particular multivariate Kendall’s tau naturally fits into our framework with the aforementioned choice of collapsing function. Rank-based measures of association possess certain attractive properties, including the invariance property and the concordance ordering property as outlined at the onset of this section. Furthermore, as argued in Grothe et al. (2014), this particular dependence measure $\chi$ can effectively detect negative association between random vectors.

### 2.4.6 The probability integral transform collapsing function

The probability integral transform collapsing function bears some resemblance to the multivariate extension of Spearman’s rho discussed in Grothe et al. (2014). However, the definition according to our framework of the population version of $\chi$ and hence the estimation procedure differs. The PIT-transformed collapsed random variable $F_X(X)$ has
distribution function \( K_X(t) = P(F_X(X) \leq t), t \in [0, 1] \), known as Kendall distribution. Since \( F_X(X) = C_X(F_{X_1}(X_1), \ldots, F_{X_p}(X_p)) = C_X(U_1, \ldots, U_p) \) for \( U = (U_1, \ldots, U_p) \sim C_X \), \( K_X \) only depends on the copula \( C_X \) of \( X \) and can thus be viewed as a summary of the dependence among the components of \( X \) in the form of a \( p \)-variate function. Unfortunately, \( K_X \) itself is rarely analytically tractable for dimensions of \( X \) larger than two, an exception being Archimedean copulas \( C_X \) with generators \( \psi \) for which a calculation based on the stochastic representation and a connection with the Poisson distribution function can be used conveniently to show that

\[
K_X(t) = \sum_{k=0}^{p-1} \frac{\psi^{(k)}(\psi^{-1}(t))}{k!} (-\psi^{-1}(t))^k, \quad t \in [0, 1]; \tag{3}
\]

see the proof of Proposition 3.4 below for this approach or Barbe et al. (1996) for the first appearance of this result. Working with the multivariate PIT collapsing function and corresponding Kendall distribution naturally motivates a multivariate extension of the latter. Various properties and examples associated with such joint Kendall distributions, viewed as an example of a collapsed distribution function, are presented in 3.2.

3 Collapsed distribution functions and copulas

While we can always compute and visualize realizations from the empirical collapsed copula (see Algorithm 2.1), deriving an explicit characterization of the collapsed distribution function or copula in terms of the joint distribution of \( Z = (X, Y) \) is challenging. To this end, we present some results for the maximum and PIT collapsing functions. Most notably, characterizing the collapsed distribution function of the PIT collapsed random variables, yields a multivariate extension of the Kendall distribution.

3.1 Maximum collapsing function

**Proposition 3.1 (The collapsed distribution and its copula for the maximum collapsing function)**

Let \( X_1, \ldots, X_p, Y_1, \ldots, Y_q \) be continuously distributed random variables with distribution functions \( F_{X_1}, \ldots, F_{X_p}, F_{Y_1}, \ldots, F_{Y_q} \), respectively. Furthermore, let \( F_{X,Y} \) denote the distribution function of \( (X, Y) \) and consider the maximum collapsing function \( S \). Then the collapsed distribution function \( F_{S(X),S(Y)}(x,y) = F_{X,Y}(x,\ldots,x,y,\ldots,y) \) with corresponding collapsed copula

\[
C_{S(X),S(Y)}(u,v) = F_{X,Y}(F_{S(X)}^{-}(u),\ldots,F_{S(X)}^{-}(u),F_{S(Y)}^{-}(v),\ldots,F_{S(Y)}^{-}(v)), \quad u,v \in [0, 1],
\]

where \( F_{S(X)}^{-}(u) \) and \( F_{S(Y)}^{-}(v) \) denote the quantile functions of the distribution functions \( F_{S(X)}(x) = F_{X,Y}(x,\ldots,x,\infty,\ldots,\infty) \) and \( F_{S(Y)}(y) = F_{X,Y}(\infty,\ldots,\infty,y,\ldots,y) \), respectively.
Proof. Since \( F_{(S(X),S(Y))}(x,y) = P(\max\{X_1, \ldots, X_p\} \leq x, \max\{Y_1, \ldots, Y_q\} \leq y) = P(X_1 \leq x, \ldots, X_p \leq x, Y_1 \leq y, \ldots, Y_q \leq y) = F_{X,Y}(x, \ldots, y) \) with margins \( F_{S(X)}(x) = F_{X,Y}(x, \ldots, x) \) and \( F_{S(Y)}(y) = F_{X,Y}(\infty, \ldots, y) \), Sklar's Theorem implies that the collapsed copula \( C_{S(X),S(Y)} \) is given as stated. \( \Box \)

Using this setup, we can derive some properties of the collapsed copula to demonstrate that the maximum collapsing function can intuitively capture dependence between random vectors. To this end, we call \( X \) and \( Y \) comonotone (countermonotone) if \( X = (F_{X_1}^{-1}(U), \ldots, F_{X_p}^{-1}(U)) \) and \( Y = (F_{Y_1}^{-1}(U), \ldots, F_{Y_q}^{-1}(U)) \) for \( U \sim U(0,1) \); see also Proposition 3.5 where this concept is used.

**Proposition 3.2 (Basic properties of maximum collapsed copulas)**

Let \( X \sim F_X \) be a \( p \)-dimensional and \( Y \sim F_Y \) be a \( q \)-dimensional random vector, both with continuously distributed margins (denoted as before).

1) If \( X \) and \( Y \) are independent, then \( C_{S(X),S(Y)}(u,v) = uv \) for \( u,v \in [0,1] \).

2) If \( X \) and \( Y \) are comonotone and each have equal margins, then \( C_{S(X),S(Y)}(u,v) = \min\{u,v\} \) and thus the collapsed copula in this case is the upper Fréchet–Hoeffding bound.

3) If \( X \) and \( Y \) are countermonotone and each have equal margins, then \( C_{S(X),S(Y)}(u,v) = \max\{u+v-1,0\} \) and thus the collapsed copula in this case is the lower Fréchet–Hoeffding bound.

**Proof.** 1) Let \( F_{X,Y} \) denote the distribution function of \((X,Y)\). Independence and Proposition 3.1 imply that

\[
C_{S(X),S(Y)}(u,v) = F_{X,Y}(F_{S(X)}^{-1}(u), \ldots, F_{S(Y)}^{-1}(v), \ldots, F_{S(Y)}^{-1}(v)) = F_{X,Y}(F_{S(X)}^{-1}(u), \ldots, F_{S(X)}^{-1}(u)) F_{Y}(F_{S(Y)}^{-1}(v), \ldots, F_{S(Y)}^{-1}(v)) = F_{X,Y}(\infty, \ldots, \infty, F_{S(Y)}^{-1}(v), \ldots, F_{S(Y)}^{-1}(v)) = F_{S(X)}(F_{S(X)}^{-1}(u))F_{S(Y)}(F_{S(Y)}^{-1}(v)) = uv.
\]

2) \( F_{S(X)}(x) = \min_{1 \leq j \leq p}\{F_{X_j}(x)\} = F_X(x) \) so that \( F_{S(X)}^{-1}(u) = \max_{1 \leq j \leq p}\{F_{X_j}^{-1}(u)\} = F_X^{-1}(u) \) (similarly, \( F_{S(Y)}^{-1}(v) = F_Y^{-1}(v) \)). Therefore,

\[
C_{S(X),S(Y)}(u,v) = F_{X,Y}(F_{S(X)}^{-1}(u), \ldots, F_{S(X)}^{-1}(u), F_{S(Y)}^{-1}(v), \ldots, F_{S(Y)}^{-1}(v)) = F_{X,Y}(F_X^{-1}(u), \ldots, F_X^{-1}(u), F_Y^{-1}(v), \ldots, F_Y^{-1}(v)) = P(F_X(U) \leq F_X^{-1}(u), \ldots, F_X(U) \leq F_X^{-1}(u), F_Y(U) \leq F_Y^{-1}(v), \ldots, F_Y(U) \leq F_Y^{-1}(v)) = P(U \leq u, U \leq v) = P(U \leq \min\{u,v\}) = \min\{u,v\}.
\]
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3) Similarly as in Part 2.

Deriving the collapsed copula in special cases can provide a concrete understanding of how and to what extent the maximum collapsing function summarizes dependence between \(X\) and \(Y\) which we pre-specify. Here is an example.

**Example 3.3 (Meta nested Archimedean copula model and the maximum collapsing function)**

Let \(Z = (X, Y) \sim F_{X,Y}(x, y) = C_0(C_1(F_X(x)), C_2(F_Y(y)))\), where \(X_j \sim F_X, j \in \{1, \ldots, p\}\), and \(Y_k \sim F_Y, k \in \{1, \ldots, q\}\). Furthermore, interpret \(F_X(x)\) and \(F_Y(y)\) as \((F_X(x_1), \ldots, F_X(x_p))\) and \((F_Y(y_1), \ldots, F_Y(y_q))\), respectively. Let \(C_0, C_1, C_2\) be Archimedean copulas with generators \(\psi_0, \psi_1, \psi_2\), respectively, satisfying the sufficient nesting condition; see McNeil (2008) or Hofert (2012) for more details. Consider the maximum collapsing function \(S\). Since

\[
S(X) \sim F_S(X)(x) = C_1(F_X(x)) = \psi_1\left(\sum_{j=1}^p \psi_{-1}^{-1}(F_X(x_j))/p\right),
\]

\[
S(Y) \sim F_S(Y)(y) = C_2(F_Y(y)) = \psi_2\left(\sum_{k=1}^q \psi_{-1}^{-1}(F_Y(y_k))/q\right),
\]

with diagonals \(F_S(X)(x, \ldots, x) = \psi_1(p \psi_{-1}^{-1}(F_X(x)))\) and \(F_S(Y)(y, \ldots, y) = \psi_2(q \psi_{-1}^{-1}(F_Y(y)))\), the corresponding quantile functions are

\[
F_{S(X)}^-(u) = F_X^\psi_1^-\left(u\right) = F_X^\psi_1^-\left(\frac{\psi_{-1}^{-1}(u)}{p}\right),
\]

\[
F_{S(Y)}^-(v) = F_Y^\psi_2^-\left(v\right) = F_Y^\psi_2^-\left(\frac{\psi_{-1}^{-1}(v)}{q}\right),
\]

respectively. Proposition 3.1 implies that the collapsed copula equals

\[
C_{S(X),S(Y)}(u, v) = F_{X,Y}(F_{S(X)}^-(u), \ldots, F_{S(X)}^-(u), F_{S(Y)}^-(v), \ldots, F_{S(Y)}^-)(v),
\]

\[
= C_0\left(C_1\left(F_X(F_X^\psi_1^-(u)/p)\right), \ldots, F_X(F_X^\psi_1^-(u)/p))\right),
\]

\[
C_2\left(F_Y(F_Y^\psi_2^-(v)/q))\right), \ldots, F_Y(F_Y^\psi_2^-(v)/q))\right)
\]

\[
= C_0\left(C_1(\psi_1^-(u)/p), \ldots, \psi_1^-(u)/p)\right),
\]

\[
C_2(\psi_2^-(v)/q), \ldots, \psi_2^-(v)/q))
\]

\[
= C_0(u, v), \quad u, v \in [0, 1].
\]

This is an intuitive result, as any two random variables \((X_j, Y_k)\) have marginal copula \(C_0\) under this model and so do the group maxima (as long as the marginal distributions are equal per group). This implies that any collapsed measure of concordance is precisely the one corresponding to the copula \(C_0\) in this case.
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3.2 PIT collapsing function

For the PIT collapsing function, the collapsed distribution function and copula have notable terminology and notation following from the copula literature. In that spirit, we will present them as extensions of the Kendall distribution presented previously and as such adopt the same notation.

3.2.1 Definition

A natural extension of the univariate Kendall distribution $K_X(t) = P(F_X(X) \leq t)$, $t \in [0, 1]$, to the multivariate case is the multivariate (or joint) Kendall distribution, given by

$$K_{X,Y}(t_1, t_2) = P(F_X(X) \leq t_1, F_Y(Y) \leq t_2) = P(C_X(U) \leq t_1, C_Y(V) \leq t_2),$$

for all $t_1, t_2 \in [0, 1]$, where $U \sim C_X$ and $V \sim C_Y$ for the copulas $C_X$ and $C_Y$ of $X$ and $Y$, respectively; it is straightforward to define higher-dimensional Kendall distributions. By definition, multivariate Kendall distributions have univariate Kendall distributions as margins. The copula of $K_{X,Y}(t_1, t_2)$, if uniquely determined, follows from Sklar’s Theorem via

$$C_K(u_1, u_2) = K_{X,Y}(K_X^{-1}(u_1), K_Y^{-1}(u_2)), \quad u_1, u_2 \in [0, 1],$$

where $K_X^{-1}$ and $K_Y^{-1}$ denote the quantile functions of the marginal Kendall distributions $K_X$ and $K_Y$, respectively. We refer to $C_K$ as Kendall copula. Note that Kendall copulas have previously appeared in Brechmann (2014) as hierarchical Kendall copulas without explicitly investigating the notion of joint Kendall distributions; the latter naturally appear in our framework for measuring dependence between random vectors.

3.2.2 Properties

We now briefly discuss some basic properties of multivariate Kendall distributions and Kendall copulas. As before, we focus on the bivariate case.

As we have seen in (3), there is an analytical formula for (univariate) Kendall distributions for Archimedean copulas. As we will now see, there is also an explicit form for multivariate Kendall distributions in this case.

**Proposition 3.4 (Multivariate Kendall distributions in the Archimedean case)**

Let $(X, Y)$ be a $(p + q)$-dimensional random vector with Archimedean copula $C$ with completely monotone generator $\psi$. Then, for all $t_1, t_2 \in [0, 1]$,

$$K_{X,Y}(t_1, t_2) = \sum_{m=0}^{(p-1)(q-1)} \sum_{n=0}^{m} \frac{(\psi^{-1}(t_1))^n (\psi^{-1}(t_2))^{m-n}}{n! (m-n)!} (-1)^m \psi^{(m)}(\psi^{-1}(t_1) + \psi^{-1}(t_2)).$$

(5)
3Collapsed distribution functions and copulas

Proof. Let \( V \sim F_V \), where \( F_V \) is the Laplace–Stieltjes inverse of \( \psi \) and let \( E_{11}, \ldots, E_{1p}, E_{21}, \ldots, E_{2q} \) iid \( \sim \text{Exp}(1) \). Furthermore, let

\[
U = \left( \psi\left( \frac{E_{11}}{V} \right), \ldots, \psi\left( \frac{E_{1p}}{V} \right) \right), \quad V = \left( \psi\left( \frac{E_{21}}{V} \right), \ldots, \psi\left( \frac{E_{2q}}{V} \right) \right).
\]

Note that \((U, V) \sim C\) and that \( U \sim C_X \) and \( V \sim C_Y \), where \( C_X, C_Y \) are (also) Archimedean copulas with generator \( \psi \). Under our assumptions, \((X, Y)\) allows for the stochastic representation

\[
(X, Y) = (F_{X_1}(U_{11}), \ldots, F_{X_p}(U_{1p}), F_{Y_1}(U_{21}), \ldots, F_{Y_q}(U_{2q})),
\]

and thus

\[
K_{X,Y}(t_1, t_2) = \mathbb{P}(F_X(X) \leq t_1, F_Y(Y) \leq t_2) = \mathbb{P}(C_X(U) \leq t_1, C_Y(V) \leq t_2)
= \mathbb{P}(E_{11} + \cdots + E_{1p} > V\psi^{-1}(t_1), E_{21} + \cdots + E_{2q} > V\psi^{-1}(t_2))
= \int_0^\infty \mathbb{P}(E_{11} + \cdots + E_{1p} > v\psi^{-1}(t_1), E_{21} + \cdots + E_{2q} > v\psi^{-1}(t_2)) \, dF_V(v)
= \int_0^\infty \mathbb{P}(E_{11} + \cdots + E_{1p} > v\psi^{-1}(t_1)) \mathbb{P}(E_{21} + \cdots + E_{2q} > v\psi^{-1}(t_2)) \, dF_V(v)
= \int_0^\infty F_{\text{Poi}(v\psi^{-1}(t_1))}(p-1) F_{\text{Poi}(v\psi^{-1}(t_2))}(q-1) \, dF_V(v)
= \int_0^\infty \exp(-v\psi^{-1}(t_1)) \left( \sum_{k=0}^{p-1} \frac{(v\psi^{-1}(t_1))^k}{k!} \right) \exp(-v\psi^{-1}(t_2)) \left( \sum_{l=0}^{q-1} \frac{(v\psi^{-1}(t_2))^l}{l!} \right) \, dF_V(v)
= \int_0^\infty \exp(-v(\psi^{-1}(t_1) + \psi^{-1}(t_2))) \left( \sum_{m=0}^{(p-1)(q-1)} \left( \sum_{n=0}^m \frac{(\psi^{-1}(t_1))^m (\psi^{-1}(t_2))^{m-n}}{n! (m-n)!} \right) v^m \right) \, dF_V(v)
= \int_0^\infty \left( \sum_{m=0}^{(p-1)(q-1)} \left( \sum_{n=0}^m \frac{(\psi^{-1}(t_1))^m (\psi^{-1}(t_2))^{m-n}}{n! (m-n)!} \right) \psi^{(m)}(\psi^{-1}(t_1) + \psi^{-1}(t_2))(-1)^m \right) \, dF_V(v)
= \int_0^\infty \left( \sum_{m=0}^{(p-1)(q-1)} \left( \sum_{n=0}^m \frac{(\psi^{-1}(t_1))^m (\psi^{-1}(t_2))^{m-n}}{n! (m-n)!} \right) \psi^{(m)}(\psi^{-1}(t_1) + \psi^{-1}(t_2))(-1)^m \right) \, dF_V(v)

where we used the fact that the survival function of an Erlang distribution can be expressed as the distribution function \( F_{\text{Poi}} \) of a Poisson distribution. □

Note that (3) follows from (5) as a special case. Moreover, it is straightforward to extend (5) to higher dimensions. In this case, each random vector in the construction corresponds to one dimension of the multivariate Kendall distribution. As a special case, when each such random vector consists of only a single random variable, the multivariate Kendall distribution equals the copula of these random variables.

Figures 1 and 2 display scatter plots of \( n = 1000 \) independent observations of the bivariate Gumbel and Clayton Kendall copulas (with parameter of the underlying Gumbel and Clayton generator chosen such that Kendall’s tau equals 0.5), respectively. The different plots depict how varying dimensions \( p, q \) impact the dependence structure between the two.
random vectors. This difference manifests in the form of asymmetry (lower vs upper tails) and the strength of dependence (comparing the cases \( (p, q) = (2, 2) \) versus \( (p, q) = 50 \). Furthermore, note that there is asymmetry in the pull (that is, stronger towards the lower of \( p \) and \( q \) dimensions) of the realizations to the diagonal (perfect dependence).

The following proposition briefly addresses basic properties of Kendall copulas and shows that they can intuitively capture dependence between random vectors.

**Proposition 3.5 (Basic properties of Kendall copulas)**

Let \( X \sim F_X \) be a \( p \)-dimensional and \( Y \sim F_Y \) be a \( q \)-dimensional random vector, both with continuously distributed margins (denoted as before).

1) If \( X \) and \( Y \) are independent, then \( K_{X,Y}(t_1, t_2) = K_X(t_1)K_Y(t_2) \) and thus the Kendall copula is the independence copula.

2) If \( X \) and \( Y \) are comonotone, then \( K_{X,Y}(t_1, t_2) = \min\{t_1, t_2\} \) and thus the Kendall copula (which equals the multivariate Kendall distribution in this case) is the upper Fréchet–Hoeffding bound.

3) If \( X \) and \( Y \) are countermonotone, then \( K_{X,Y}(t_1, t_2) = \max\{t_1 + t_2 - 1, 0\} \) and thus the Kendall copula (which equals the multivariate Kendall distribution in this case) is the lower Fréchet–Hoeffding bound.

**Proof.** Let \( C_X, C_Y \) denote the copulas of \( X, Y \), respectively.

1) \( K_{X,Y}(t_1, t_2) = \mathbb{P}(F_X(X) \leq t_1, F_Y(Y) \leq t_2) \) ind. \( = \mathbb{P}(F_X(X) \leq t_1)\mathbb{P}(F_Y(Y) \leq t_2) = K_X(t_1)K_Y(t_2), \) \( t_1, t_2 \in [0, 1] \).

2) With \( X = (F_{X_1}(U), \ldots, F_{X_p}(U)) \) and \( Y = (F_{Y_1}(U), \ldots, F_{Y_q}(U)) \) for \( U \sim U(0, 1) \), Sklar’s Theorem implies that \( F_X(X) = C_X(U, \ldots, U) = \min\{U, \ldots, U\} = U \) and \( F_Y(Y) = C_Y(U, \ldots, U) = \min\{U, \ldots, U\} = U \). Therefore, \( K_{X,Y}(t_1, t_2) = \mathbb{P}(C_X(U, \ldots, U) \leq t_1, C_Y(U, \ldots, U) \leq t_2) = \mathbb{P}(U \leq t_1, U \leq t_2) = \min\{t_1, t_2\} \). Note that \( K_{X,Y}(t_1, t_2) \) has \( U(0, 1) \) margins in this case and thus equals its Kendall copula.

3) Similarly as in Part [2].

Nonparametric estimators of univariate Kendall distributions based on a random sample \( (X_i, Y_i), i \in \{1, \ldots, n\} \), can be constructed as follows. Let

\[
W_i = (W_{i1}, W_{i2}) = \left( \frac{1}{n-1} \sum_{k=1}^{n} \mathbb{1}_{\{X_k \leq X_i\}}, \frac{1}{n-1} \sum_{k=1 \atop k \neq i}^{n} \mathbb{1}_{\{Y_k \leq Y_i\}} \right),
\]

where, as usual, the inequalities are understood componentwise. Analogously to Genest and Rivest (1993) and Barbe et al. (1996) in the univariate case, one can use the multivariate empirical distribution function

\[
K_n(t) = K_n(t_1, t_2) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{W_i \leq t\}} = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{W_{i1} \leq t_1, W_{i2} \leq t_2\}}, \quad t = (t_1, t_2) \in [0, 1]^2,
\]

as a nonparametric estimator of \( K_{X,Y}(t_1, t_2) \).
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Figure 1 $n = 1000$ independent observations from different Gumbel Kendall copulas (with Gumbel parameter chosen such that Kendall’s tau of the underlying generator equals 0.5) corresponding to the joint Kendall distribution function as specified in \( [5] \). Note the dimensions of the two sectors are varied from $p \in \{2, 10, 50\}$ and $q \in \{2, 10, 50\}$ thus leading to nine different variations.
Figure 2 $n = 1000$ independent observations from different Clayton Kendall copulas (with Clayton parameter chosen such that Kendall’s tau of the underlying generator equals 0.5) corresponding to the joint Kendall distribution function as specified in \( \text{[5]} \). Note the dimensions of the two sectors are varied from $p \in \{2, 10, 50\}$ and $q \in \{2, 10, 50\}$ thus leading to nine different variations.
3.2.3 Dependence measures related to the multivariate Kendall distribution

We now turn to a link between multivariate Kendall distributions and dependence measures of the form $\chi(X, Y)$. Below are a few examples starting with the dependence measure resulting from the PIT collapsing function.

**Example 3.6 (Correlation via the joint Kendall distribution)**

Since $K_X(t_1)$ and $K_Y(t_2)$ are the distribution functions of $F_X(X)$ and $F_Y(Y)$, respectively, and $K_{X,Y}(t_1, t_2)$ is the joint distribution function of $(F_X(X), F_Y(Y))$, Hoeffding’s Identity implies that

$$
\chi(X, Y) = \rho(F_X(X), F_Y(Y)) = \frac{\text{Cov}(F_X(X), F_Y(Y))}{\sqrt{\text{Var}(F_X(X)) \text{Var}(F_Y(Y))}} = \frac{\int_{[0,1]^2} K_{X,Y}(t_1, t_2) - K_X(t_1)K_Y(t_2) \, dt_1 \, dt_2}{\sqrt{\int_{[0,1]} K_X(t_1) - K^2_X(t_1) \, dt_1 \int_{[0,1]} K_Y(t_2) - K^2_Y(t_2) \, dt_2}}.
$$

Note that the numerator is the (integrated) difference between the joint Kendall distribution of $X$ and $Y$ and the joint Kendall distribution under independence of $X$ and $Y$; $\chi(X, Y)$ thus represents in some sense how far on average the random vectors $X$ and $Y$ are from independence, thus mimicking the construction of standard bivariate dependence measures.

**Example 3.7 (Spearman’s rho via the joint Kendall distribution)**

One drawback of the measure presented in Example 3.6 is that it depends on the marginal distributions of the collapsed random variables. To rectify this, we can apply the marginal Kendall distributions $K_X$ and $K_Y$ to the collapsed random variables $F_X(X)$ and $F_Y(Y)$, respectively. The measure will then be a natural multivariate extension of Spearman’s rho as it only depends on the Kendall copula. To this end, let $U = K_X(F_X(X))$ and $V = K_Y(F_Y(Y))$. Then,

$$
\chi(X, Y) = \rho(K_X(F_X(X)), K_Y(F_Y(Y))) = \rho(U, V) = \frac{\mathbb{E}[UV] - 1/4}{1/12} = 12\mathbb{E}[UV] - 3 = 12 \int_{[0,1]^2} uv \, dC_K(u, v) - 3 = \rho_S(F_X(X), F_Y(Y)),
$$

where $C_K(u, v)$ denotes the Kendall copula introduced in [4]. Thus, $\chi(X, Y)$ equals Spearman’s rho of $F_X(X)$ and $F_Y(Y)$.

**Example 3.8 (Kendall’s tau via the joint Kendall distribution)**

Similarly, with $U$ and $V$ as defined in Example 3.7 for Kendall’s tau we have

$$
\chi(X, Y) = \rho(\mathbb{1}_{F_X(X) \leq F_X(X')} \mathbb{1}_{F_Y(Y) \leq F_Y(Y')}), \tau(F_X(X), F_Y(Y)) = 4 \int_{[0,1]^2} C_K(u, v) \, dC_K(u, v) - 1,
$$

where $C_K(u, v)$ denotes the Kendall copula as before. The first equality follows from Lemma 2.2 and the last equality follows by definition of Kendall’s tau of the collapsed random
variables in the bivariate case. This measure forms a multivariate extension of Kendall’s tau which only depends on the Kendall copula. An alternative albeit very similar extension was formed via the multivariate rank collapsing function presented in Section 2.4.5.

**Example 3.9 (Tail dependence via Kendall copulas)**

In light of using (2) for measuring tail dependence between the collapsed random variables, it is easy to see that when using the PIT collapsing function, (2) as measure of association corresponds to computing (classical) coefficients of tail dependence of the underlying Kendall copula $C_K$. For example, if $X \sim F_X, Y \sim F_Y$ with Kendall distributions $K_X, K_Y$, respectively, and if $U = K_X (F_X(X)), V = K_Y (F_Y(Y))$ (note that $(U,V) \sim C_K$ in this case), then the coefficient of upper tail dependence can be expressed as

$$\lambda_U (F_X(X), F_Y(Y)) = \lim_{u \uparrow 1} P (F_Y(Y) > K_Y^{-1}(u) \mid F_X(X) > K_X^{-1}(u))$$

$$= \lim_{u \uparrow 1} P (V > u \mid U > u) = \lim_{u \uparrow 1} \frac{1 - 2u + C_K(u,u)}{1 - u}.$$  

4 Estimation and properties

In this section, we study sample estimators of Equation (1), and derive asymptotic results which can be used to compute their standard errors.

4.1 Estimation for general collapsing functions $S$

Assume we have a random sample $(X_1, Y_1), \ldots, (X_n, Y_n)$ from $F_{X,Y}$. An estimator $\chi_n$ of $\chi(X,Y) = \rho(S(X), S(Y))$ can be constructed by replacing $\rho$ by the sample correlation coefficient. The following section investigates some properties of this estimator for general $S$ (but not the PIT collapsing function which, due to its nature, is treated in the section thereafter).

4.2 Asymptotic result for general $S$

In this section we closely follow Grothe et al. (2014) in order to construct $\chi_n$ through the lens of U-statistics for deriving its asymptotic distribution. To this end we have the following proposition.

**Proposition 4.1 (Asymptotic distribution of $\chi_n$)**

Suppose $\chi_n(X,Y)$ is defined as above. Then, as $n \to \infty$,

$$\sqrt{n}(\chi_n - \chi) \overset{d}{\longrightarrow} N(0, \sigma_\chi^2),$$

where

$$\sigma_\chi^2 = \begin{cases} 
(\nabla f_{5 \times 1|\mu})' \Sigma_1 (\nabla f_{5 \times 1|\mu}), & \text{if } S \text{ is a } p\text{-variate function}, \\
4(\nabla f_{5 \times 1|\mu})' \Sigma_2 (\nabla f_{5 \times 1|\mu}), & \text{if } S \text{ is a } 2p\text{-variate function}.
\end{cases}$$
4 Estimation and properties

Here, $\nabla f_{5 \times 1} | \mu$ denotes the gradient vector of the function

$$f(a, b, c, d, e) = \frac{e - ab}{\sqrt{c - a^2d - b^2}},$$

evaluated at the population mean $\mu = (\mu_x, \mu_y, \mu_{xx}, \mu_{yy}, \mu_{xy})$, where $\mu_x = \mathbb{E}[S(X)]$, $\mu_y = \mathbb{E}[S(Y)]$, $\mu_{xx} = \mathbb{E}[S(X)^2]$, $\mu_{yy} = \mathbb{E}[S(Y)^2]$, $\mu_{xy} = \mathbb{E}[S(X)S(Y)]$. Furthermore, $\Sigma_1$ denotes the covariance matrix of $(S(X), S(Y), S(X)^2, S(Y)^2, S(X)S(Y))$ and $\Sigma_2$ denotes the covariance matrix of $(\mathbb{E}_X[S(X, X')], \mathbb{E}_Y[S(Y, Y')], \mathbb{E}_X[S(X, Y')], \mathbb{E}_Y[S(Y, Y')])$.

**Proof.** Refer to Appendix [A.2] for the details. \hfill \Box

**Remark 4.2 (Estimation of $\sigma^2_X$)**

To estimate the asymptotic variance $\sigma^2_X$ we adopt a plug-in approach as was suggested by Grothe et al. [2014]. This procedure has two key ingredients as summarized below and it will slightly differ between the two cases given in the proof of Proposition 4.1. Further, note that the notation below is also explained in the proof of Proposition 4.1 in Appendix [A.1].

The two cases referred to below correspond to when $S$ is a $p$-variate (Case 1) or a $2p$-variate (Case 2) function.

1) In a first step, evaluate the gradient vector $\nabla f_{5 \times 1}$ at $m(k) = (m_x(k), m_y(k), m_{xx}(k), m_{yy}(k), m_{xy}(k))$, $k \in \{1, 2\}$ corresponding to the sample quantities in Case $k$. The analytical form of the gradient vector evaluated at the appropriate values is given in Appendix [A.2].

2) Now distinguish the two cases: In Case 1, estimate $\Sigma_1$ by the sample covariance matrix $\Sigma_{n,1}$ of $(S(X_i), S(Y_i), S(X_i)^2, S(Y_i)^2, S(X_i)S(Y_i))$, $i \in \{1, \ldots, n\}$. In Case 2, estimate $\Sigma_2$ by the sample covariance matrix $\Sigma_{n,2}$ of $(g_x(X_i), g_y(Y_i), g_{xx}(X_i), g_{yy}(Y_i), g_{xy}(X_i, Y_i))$, $i \in \{1, \ldots, n\}$, where

$$g_x(X_i) = \frac{1}{n - 1} \sum_{j=1}^{n} S(X_i, X_j), \quad g_y(Y_i) = \frac{1}{n - 1} \sum_{j=1, j \neq i}^{n} S(Y_i, Y_j),$$

$$g_{xx}(X_i) = \frac{1}{n - 1} \sum_{j=1}^{n} S(X_i, X_j)^2, \quad g_{yy}(Y_i) = \frac{1}{n - 1} \sum_{j=1, j \neq i}^{n} S(Y_i, Y_j)^2,$$

$$g_{xy}(X_i, Y_i) = \frac{1}{n - 1} \sum_{j=1, j \neq i}^{n} S(X_i, X_j)S(Y_i, Y_j).$$

The quantities $g_x, g_y, g_{xx}, g_{yy}, g_{xy}$ estimate the conditional expectations, $(\mathbb{E}_X[S(X, X')], \mathbb{E}_Y[S(Y, Y')], \mathbb{E}_X[S(X, X')], \mathbb{E}_Y[S(Y, Y')], \mathbb{E}_X[S(X', Y')|S(X, X')S(Y, Y')])$, and can be motivated from a jackknife methodology as Grothe et al. [2014] identified.

3) Then, $\sigma^2_{n,1} = (\nabla f_{m(1)})' \Sigma_{n,1} (\nabla f_{m(1)})$ in Case 1 and $\sigma^2_{n,2} = 4(\nabla f_{m(2)})' \Sigma_{n,2} (\nabla f_{m(2)})$ in Case 2.
We now discuss the construction of an estimator for $\chi(X, Y) = \rho(F_X(X), F_Y(Y))$. In contrast to the asymptotic U-statistics framework developed earlier, we cannot directly express $\chi(X, Y)$ as a function of U-statistics in this case.

To begin with, let $W_1 = F_X(X)$ and $W_2 = F_Y(Y)$. As in Barbe et al. (1996), we consider the pseudo-observations

$$W_{i1} = \frac{1}{n-1} \sum_{k=1, k\neq i}^{n} 1\{X_k \leq X_i\}, \quad W_{i2} = \frac{1}{n-1} \sum_{k=1, k\neq i}^{n} 1\{Y_k \leq Y_i\}, \quad i \in \{1, \ldots, n\},$$

where the inequalities are understood componentwise. Similarly as before, an estimator for the dependence measure $\chi(X, Y)$ can simply be constructed via the sample correlation coefficient, that is, $\chi_n(X, Y) = \rho_n(W_{i1}, W_{i2})$. As this particular estimator does not fit in the U-statistics framework, it is harder to derive asymptotic normality with an expression for the asymptotic variance for this collapsing function. However, we can always construct bootstrap confidence intervals if required.

Based on the pseudo-observations defined above, one can also estimate $\chi(X, Y) = \rho_S(F_X(X), F_Y(Y))$ by $\chi_n(X, Y) = \rho_n(K_{n,X}(W_{i1}), K_{n,Y}(W_{i2}))$, where

$$K_{n,X}(t_1) = \frac{1}{n} \sum_{j=1}^{n} 1\{W_{i1} \leq t_1\}, \quad K_{n,Y}(t_2) = \frac{1}{n} \sum_{j=1}^{n} 1\{W_{i2} \leq t_2\}, \quad t_1, t_2 \in [0, 1].$$

## 5 Applications

We now present two applications, one in bioinformatics (see Section 5.1) and another in finance (see Section 5.2).

### 5.1 Protein data: An application from bioinformatics

#### 5.1.1 Introduction

Proteins are complex molecules composed of sequences of amino acid residues. There are 20 different types of amino acids. All of them have the same generic structure, R-CH(NH$_2$)-COOH, where the component labelled “R”, also known as a side chain, identifies the specific type of amino acid. In bioinformatics, scientists are interested in understanding how conformational changes at different side chains may be coupled together; see, for example, Ghorai et al. (2015a). For example, if two residues are far apart in the sequence but their side chains tend to change conformation together, it may be an indication that they are close in 3D. In turn, this may shed light on the all-important underlying protein folding process.

The conformation of a side chain can be characterized by a set of dihedral angles. To understand this, picture a side chain as a sequence of atoms spanning off the backbone of
the protein. The angle between planes formed by atoms 1–3 and atoms 2–4 in the sequence is referred to as the first dihedral angle, and so on. Typically, there are zero to four such dihedral angles depending on the size of the underlying amino acid.

Thus, let \( X = (X_1, \ldots, X_p), \) \( 0 \leq p \leq 4, \) and \( Y = (Y_1, \ldots, Y_q), \) \( 0 \leq q \leq 4, \) represent the dihedral angles of two side chains, respectively. We are then in need of a measure of dependence between the two random vectors \( X \) and \( Y. \) To quantify their dependence, Ghoraie et al. (2015b) applied the Graphical LASSO (GLASSO) developed by Friedman et al. (2008), while Ghoraie et al. (2015a) used “kernelized partial canonical correlation analysis” (KPCCA). Here, we apply our framework of collapsing functions.

5.1.2 Analysis

Below, we will report results using various collapsing functions – in particular, the weighted average, the pairwise distance, the pairwise kernel, and the PIT.

For the weighted average, we put more weight on the first few dihedral angles, starting with the extreme case of \( w = (1, 0, \ldots, 0), \) that is, full weight on the first dimension. This is because, biologically, the dihedral angles closer to the backbone of the protein are more meaningful than those further away.

For the pairwise distance, we include only the Euclidean distance because, after experimenting with other distance functions, there was little to no difference for this application.

For the pairwise kernel, we follow Ghoraie et al. (2015a) and use a multivariate von-Mises kernel,

\[
K(x_i, x_j) = \prod_{t=1}^{p} \exp(\kappa_t \cos(x_{it} - x_{jt})),
\]

where \( x_i, x_j \in \mathbb{R}^p \) are two different conformations of a given side chain. We simply use the same concentration parameters as those adopted and justified by Ghoraie et al. (2015a), so \( \kappa_1 = 8, \kappa_2 = 8, \kappa_3 = 4, \) and \( \kappa_4 = 2. \) These choices were because atoms farther away from the backbone have more freedom of motion.

Finally, the PIT is a general purpose choice of collapsing function that can capture both positive and negative association. However, for the purpose of ranking dependencies we are just interested in the strength (not the direction) of dependence, so we use \( |\chi(X, Y)| \) as the ranking criteria.

We use the same dataset as in Ghoraie et al. (2015a) which allows for a direct comparison of the results. Altogether, Ghoraie et al. (2015a) studied eight different types of proteins from three different families (Ras, Rho and Rab). Each protein has a varying number of residues approximately in the range of 160–190. Through a specific procedure explained in Ghoraie et al. (2015a), roughly 16,000–18,000 sample conformations for these proteins were generated.

Note that working with the pair-wise distance and kernel collapsing functions is computationally prohibitive. Since, for each protein, we have up to 18,000 sample conformations,
this would have resulted in \( \binom{18,000}{2} \) samples in the collapsed space. We thus consider ten random subsets of size 2500 (without replacement to avoid pair-wise distance or kernel similarity values of zero) from the original dataset and compute the relevant evaluation criteria as an average across the obtained subsets.

The objective here is to rank all pairs of residues in a protein according to various dependence measures, and to verify whether “known couplings” appear in the top-ranked pairs. Following Ghoraie et al. (2015a), “known couplings” were based on the Contact Rearrangement Network (CRN) method from Daily et al. (2008). The receiver-operating characteristic (ROC) curve – in particular, the area under the ROC curve (AUC) – is used as a summarizing evaluation criterion to determine how well the rankings produced by different dependence measures agree with the CRN method’s results.

5.1.3 Results and discussion

We compare the resulting AUC values from the chosen collapsing functions with results from KPCCA (see Ghoraie et al. (2015a)) and GLASSO (see Ghoraie et al. (2015b)). This comparison is summarized in Table 3.

| Protein | PDB ID | H-Ras | RhoA | Rap2A | Rheb | Sec4 | Cdc42 | Rac1 | Ypt7p |
|---------|--------|-------|------|-------|------|------|-------|------|-------|
| H-Ras   | 4Q21   | 80    | 75   | 69    | 70   | 68   | 68    | 67   | 72    |
| RhoA    | 1FTN   | 78    | 74   | 72    | 65   | 71   | 66    | 67   | 59    |
| Rap2A   | 1KAO   | 78    | 72   | 68    | 71   | 68   | 68    | 59   | 67    |
| Rheb    | 1XTQ   | 78    | 72   | 68    | 71   | 66   | 65    | 63   | 61    |
| Sec4    | 1G16   | 77    | 72   | 71    | 69   | 65   | 65    | 63   | 61    |
| Cdc42   | 1ANO   | 77    | 72   | 71    | 69   | 65   | 65    | 63   | 61    |
| Rac1    | 1HH4(A)| 74    | 68   | 70    | 71   | 68   | 61    | 59   | 57    |
| Ypt7p   | 1KY3   |       |      |       |      |      |       |      |       |

Table 3 AUC (values in percent) against CRN. The rows and columns are organized in decreasing order of row and column means. Note that the PDB ID is a unique identifier of the inactive state of the protein; see Berman et al. (2006).

Firstly, from all AUC values in Table 3, we see that dependence measures resulting from all collapsing functions often possessed significantly better allosteric coupling detection power than at random (when AUC is 50%). Furthermore, very simple yet meaningful collapsing functions, such as the weighted average (with \( w = (1, 0, ..., 0) \)), often yielded comparable (for 1G16 and 1KAO even better) results to KPCCA and GLASSO. This is an interesting observation, given that this particular collapsing function is considerably faster and easier to understand than the mathematically sophisticated KPCCA or GLASSO methods.
5.2 S&P 500: An application from finance

5.2.1 Introduction

There are numerous problems in finance and risk management that require to study the
dependence between random vectors or groups of random variables. In this section, we
explore such a problem in the setting of investigating dependence between S&P 500 business
sectors. Furthermore, as we are dealing with time series data, this problem can be viewed
both through the prism of static and dynamic dependence. Fixing a time period, we can
assess whether the business sectors are independent by visualizing the dependence between
them. Additionally, we can compute time-varying dependence measures to dynamically
capture dependence between business sectors.

5.2.2 S&P 500 constituent data

For the static case, we consider the 465 available constituent time series from the S&P 500
in the time period from 2007-01-01 to 2009-12-31 (756 trading days); see the R package
qrmda ta. For the dynamic case, we consider 461 (due to missing data) of these constituent
time series. We use the 10 Global Industry Classification Standard (GICS) sectors as
business sectors. Nine GICS sectors have Exchange Traded Funds (ETFs) which track the
performance of each business sector. These marketable securities are referred to as sector
SPDR ETFs. We use a bivariate measure of dependence between any two sector ETFs as a
market-determined benchmark for comparisons.

Turning to pre-processing of the dataset, we work with negative log-returns for each
constituent. Furthermore, we fit ARMA(1,1)-GARCH(1,1) models to each time series and
extract the corresponding standardized residuals to investigate dependence between the
component series; see Patton (2006) for this procedure. Note that we apply the same
pre-processing to the nine ETF time series.

5.2.3 A snapshot of S&P 500 sector dependence

Following Algorithm 2.1 we can perform an assessment of independence between business
sectors. In particular, we use (Euclidean) distance, weighted average (equal weights),
maximum, and PIT collapsing functions. We also visualize the dependence between all
36 ETF sector pairs (notice the Telecommunications sector does not have an ETF) for
comparison.

Figure 3 illustrates this graphical assessment of independence with four zenplots, one for
each choice of collapsing function. As can be clearly detected from any of these choices of
collapsing functions, the business sectors cannot be assumed to be independent. Furthermore
to facilitate the comparison of the collapsed variables with the benchmark, Figure 4 depicts
the pair-wise dependence structures between the nine sector ETFs.

The four plots in Figure 3 can be interpreted as (data) realizations from the underlying
(and unknown) collapsed copula. Clearly realizations from the (Euclidean) distance collapsed
Figure 3 Zenplots displaying all pairs of pseudo-observations for the 10 GICS sectors of the 465-dimensional S&P 500 data based on the (Euclidean) distance (top left), weighted average (top right), PIT (bottom left), and maximum (bottom right) collapsing functions.
5 Applications

Figure 4 Zenplot displaying all pairs of pseudo-observations for the nine GICS Sector ETFs.
copula is denser in comparison to realizations from the other three collapsing functions because it has \( \binom{756}{2} \) realizations as opposed to just 756. In particular, due to the nature of the distance function, it is difficult to interpret features (tail dependence, asymmetry, shape etc.) of the dependence structure between business sectors in the context of the original variables portrayed in the corresponding zenplot. As a result, for applications in finance, the distance collapsing function should mostly be used for (graphical) assessment of independence only.

Since the weighted average collapsing function is most natural for return data, the interpretations of tail dependence and asymmetry translate well from the bivariate case. We naturally see the similarity in the dependence structures between the weighted average collapsing function and the benchmark (ETFs) in Figure 4. Furthermore, since the PIT collapsing function leads to realizations from the Kendall copula, it also yields an attractive interpretation of the dependence structure depicted in its corresponding zenplot. For instance as noted in Example 3.9, the tail dependence coefficients in this case can be interpreted as natural multivariate extensions of bivariate tail dependence. Owing to the justification of these two collapsing functions and interpretability, one could potentially fit a copula model directly on the collapsed variables if needed to model a notion of dependence between groups of random variables, but this framework will in general not offer an analytically tractable link back to the original random variables.

The maximum collapsing function appears to capture a weaker form of dependence compared to the other collapsing functions and the benchmark. This is to be expected as this collapsing function depicts a notion of dependence between the worst performers only (in a plural sense in that the constituent chosen as the maximum can change daily in each business sector over the time period considered). One would use this collapsing function only if one is interested in such a notion of dependence between random vectors.

### 5.2.4 Dynamic S&P 500 sector dependence

Having garnered an understanding of the dependence structures between business sectors in a fixed time period, we will now dynamically capture the dependence between these sectors using a moving window setup. In particular, we investigate time varying dependence from 2006-01-01 to 2015-12-31. Due to our missing data handling, we will be working with a subset of 461 time series from the S&P 500 data.

Figure 5 depicts for four randomly chosen pairs of business sectors, the time-varying dependence as captured by the distance, average, maximum, and PIT collapsing functions. Also included (for a form of comparison with the benchmark) is the dependence measure between ETFs for each pair. Note that we used a 250-day moving window for the plots in Figure 5. The first takeaway from the four collapsed and ETF dependence series is that they seem to capture a very similar shape across time. While the dependence measures resulting from different collapsing functions lie on different scales, they all capture the same shifts in dependence not only with respect to each other but also with respect to the market-determined ETF dependence series. This indicates the suitability of any of these
collapsing function in the task of detecting dependence and the shifts in the strength of
dependence over time. Furthermore, note that ETFs are marketed as weighted average of
sector constituents, but are tradeable securities themselves and thus exposed to market
forces. Such a construction of the ETFs explains why the average collapsing function would
most closely track the dependence between ETFs (despite the use of equal weights in our
collapsing function and the influence that market forces might have on the dependence
between sector ETFs).

Figure 6 showcases the time-varying dependence as captured by the distance, average,
and maximum collapsing functions with their corresponding confidence intervals constructed
using Proposition A.1 and Remark 4.2. For the plots in this figure, we used a 150-day moving
window. Shown in the background are all pair-wise (bivariate) time-varying dependence
measures between individual constituents of the two sectors. This juxtaposition highlights
that the dependence measures between collapsed random variables capture fairly similar
shifts in strength of dependence over time compared with all the pair-wise (classical)
dependence measures between the sectors. Furthermore, one can see that the width of
confidence intervals for the various collapsed dependence measures is well-within the width
of the background band representing all the bivariate dependence series between individual
constituents from each sector. This further provides some intuitive corroboration that the
collapsing functions in some sense sufficiently capture time-varying dependence between
groups of random variables (that is, sufficient when compared to a series of matrices of
pair-wise dependence measures).

6 Conclusion and discussion

In this paper, we introduced a framework for quantifying dependence between random
vectors. With the notion of a collapsing function, random vectors were summarized by
collapsed random variables which were then used as a proxy for the purposes of studying
dependence between random vectors. Based on this framework, a graphical assessment of
independence between random vectors was proposed and its applicability demonstrated
with examples from finance. Furthermore, various measures of association and dependence
between random vectors were suggested as a natural by-product of this framework.

Additionally, we introduced and explored the notion of a collapsed distribution function
and collapsed copula for the maximum and PIT collapsing functions. As a result, we
were able to relate the dependence between collapsed random variables to the dependence
between the original random vectors. Particularly for both of these collapsing functions, we
derived analytical forms of the collapsed distribution or copula in the Archimedean case.
Moreover, for the PIT collapsing function, this lead to a multivariate extension of Kendall
distributions.

General asymptotic results for the dependence measures resulting from the framework
were derived through the lens of U-statistics with the exception of the PIT collapsing
function for which an estimator not amenable to the U-statistics theory was proposed.
Figure 5 Time-varying dependence measure for various collapsing functions and the ETFs between a few selected pairs of business sectors. The four pairs of sectors arbitrarily selected are as follows: Consumer Discretionary vs. Consumer Staples (top left), Energy vs. Industrials (Top right), Health Care vs. Industrials (bottom left), and Industrials vs Materials (bottom right).
Figure 6 Time-varying dependence measure for average (top plots), distance (middle plots), and maximum (bottom plots) collapsing functions with 95% confidence intervals against a backdrop of all pair-wise time-varying measures between assets in two business sectors. On the left panel we present the plots for Consumer Discretionary vs. Energy sectors and on the right panel we present the plots for Energy vs. Health Care sectors.
These asymptotic results then allowed us to construct confidence intervals for collapsed dependence measures constructed within our framework. Our results were showcased in Section 5.2 where we captured the evolution of dependence between business sectors over time. In addition, for this finance example we visualized dependence between sectors via realizations from various collapsed copulas. Beyond this example, we considered protein data from the realm of bioinformatics. The task involved to rank pairs of residues which were modeled by random vectors of varying dimensions. Dependence measures resulting from our framework were thus naturally used as a metric for this ranking task. We showed that for some collapsing functions, our measures were fairly comparable with prior tailor-made methods used in the literature while requiring a lesser computational burden.

We conclude that there is no notion of a “best” collapsing function. All reasonable collapsing functions we investigated tend to capture the dependence between random vectors in a similar fashion with subtle variations. However, there are some advantages for each collapsing function that are noteworthy. The maximum and PIT collapsing functions allow for a (more direct) link between the collapsed and the original (high-dimensional) distribution function or copula. Furthermore, the PIT and multivariate rank collapsing functions lead to multivariate extensions of Kendall’s tau and Spearman’s rho as highlighted in Grothe et al. (2014). The distance function is often a good choice of collapsing function for the graphical assessment of independence between random vectors. Furthermore, the distance and kernel collapsing functions, if carefully chosen, can naturally detect various non-linear (beyond monotone) dependencies between groups of random variables. The maximum and weighted average collapsing functions require the least computational time. Moreover, the weighted average collapsing function seems natural in the context of finance and yields very competitive results for the ranking task in the protein example.

An interesting and open challenge for our collapsing function framework lies in understanding the relationship between the collapsed copula and the inherent higher dimensional copula between the original random variables. Naturally, one loses information when compressing random vectors into single random variables. Having an explicit connection between the collapsed copula and the original copula helps in better understanding this loss of information. Some collapsing functions such as distance or kernel functions involve complicated non-linear transformations of the original random variables and hence render this task complicated. For the weighted average collapsing function, understanding the collapsed copulas remains a pertinent and open question.

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A Proofs and additional details for the asymptotic framework

A.1 Proof of Proposition 4.1

Proof. We begin by explicitly writing out the population version of our dependence measure. For a general collapsing function $S$,

$$
\chi(X, Y) = \rho(S(X), S(Y)) = \frac{\mu_{xy} - \mu_x \mu_y}{\sqrt{\mu_{xx} - \mu_x^2} \sqrt{\mu_{yy} - \mu_y^2}}.
$$
Case 1: $S$ is a $p$-variate function

Based on the $n$ independent random samples, define

$$
m_x^{(1)} = \frac{1}{n} \sum_{i=1}^{n} S(X_i), \quad m_y^{(1)} = \frac{1}{n} \sum_{i=1}^{n} S(Y_i), \quad m_{xx}^{(1)} = \frac{1}{n} \sum_{i=1}^{n} S(X_i)^2
$$

$$
m_{yy}^{(1)} = \frac{1}{n} \sum_{i=1}^{n} S(Y_i)^2, \quad m_{xy}^{(1)} = \frac{1}{n} \sum_{i=1}^{n} S(X_i)S(Y_i).
$$

By Hoeffding (1948), $m_x^{(1)}$, $m_y^{(1)}$, $m_{xx}^{(1)}$, $m_{yy}^{(1)}$, $m_{xy}^{(1)}$ are U-statistics for $\mu_x$, $\mu_y$, $\mu_{xx}$, $\mu_{yy}$, $\mu_{xy}$ respectively. Following from Hoeffding’s decomposition theorem, see Lee (1990, Chapter 3), we can conclude that, as $n \to \infty$,

$$
\sqrt{n}(m_x^{(1)} - \mu_x) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (S(X_i) - \mu_x) + o_p(1),
$$

$$
\sqrt{n}(m_y^{(1)} - \mu_y) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (S(Y_i) - \mu_y) + o_p(1),
$$

$$
\sqrt{n}(m_{xx}^{(1)} - \mu_{xx}) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (S(X_i)^2 - \mu_{xx}) + o_p(1),
$$

$$
\sqrt{n}(m_{yy}^{(1)} - \mu_{yy}) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (S(Y_i)^2 - \mu_{yy}) + o_p(1),
$$

$$
\sqrt{n}(m_{xy}^{(1)} - \mu_{xy}) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (S(X_i)S(Y_i) - \mu_{xy}) + o_p(1).
$$

Combining all the terms, it follows that, for $n \to \infty$,

$$
\sqrt{n} \begin{pmatrix}
m_x^{(1)} - \mu_x \\
m_y^{(1)} - \mu_y \\
m_{xx}^{(1)} - \mu_{xx} \\
m_{xy}^{(1)} - \mu_{xy} \\
\end{pmatrix}
\xrightarrow{d} N_5(0, \Sigma_1),
$$

where $\Sigma_1$ is the covariance matrix of the random vector

$$(S(X), S(Y), S(X)^2, S(Y)^2, S(X)S(Y)).$$

Then, we construct an estimator for the population dependence measure, $\chi(X, Y)$, as a function of the U-statistics.

$$
\chi_n(X, Y) = f(m_x^{(1)}, m_y^{(1)}, m_{xx}^{(1)}, m_{xy}^{(1)}, m_{yy}^{(1)}) = \frac{m_{xy}^{(1)} - m_x^{(1)} m_y^{(1)}}{\sqrt{m_{xx}^{(1)} - (m_x^{(1)})^2} \sqrt{m_{yy}^{(1)} - (m_y^{(1)})^2}}.
$$
where \( m_x^{(1)}, m_y^{(1)}, m_{xx}^{(1)}, m_{yy}^{(1)}, \) and \( m_{xy}^{(1)} \) are the sample quantities as previously defined. Then, by the delta method we have

\[
\sqrt{n}(\chi_n(X, Y) - \chi(X, Y)) \xrightarrow{d} N(0, \sigma_X^2), \quad (n \to \infty),
\]

where \( \sigma_X^2 = (\nabla f_{5 \times 1}|\mu)'\Sigma_1(\nabla f_{5 \times 1}|\mu) \). Note that the gradient vector is evaluated at \( \mu = (\mu_x, \mu_y, \mu_{xx}, \mu_{yy}, \mu_{xy}) \).

**Case 2: \( S \) is a 2p-variate function**

Consider

\[
m_x^{(2)} = \frac{1}{(n/2)} \sum_{i=1}^{n} \sum_{j \neq i} S(X_i, X_j), \quad m_y^{(2)} = \frac{1}{(n/2)} \sum_{i=1}^{n} \sum_{j \neq i} S(Y_i, Y_j), \quad m_{xx}^{(2)} = \frac{1}{(n/2)} \sum_{i=1}^{n} \sum_{j \neq i} S(X_i, X_j)^2
\]

\[
m_{yy}^{(2)} = \frac{1}{(n/2)} \sum_{i=1}^{n} \sum_{j \neq i} S(Y_i, Y_j)^2, \quad m_{xy}^{(2)} = \frac{1}{(n/2)} \sum_{i=1}^{n} \sum_{j \neq i} S(X_i, X_j)S(Y_i, Y_j).
\]

Similar to the setup presented in Case 1, these sample quantities are naturally U-statistics for their corresponding population quantities. Again following from Hoeffding’s decomposition theorem, we have that, as \( n \to \infty \),

\[
\sqrt{n}(m_x^{(2)} - \mu_x) = \frac{2}{\sqrt{n}} \sum_{i=1}^{n} (\mathbb{E}X' [S(X_i, X')] - \mu_x) + o_p(1),
\]

\[
\sqrt{n}(m_y^{(2)} - \mu_y) = \frac{2}{\sqrt{n}} \sum_{i=1}^{n} (\mathbb{E}Y' [S(Y_i, Y')] - \mu_y) + o_p(1),
\]

\[
\sqrt{n}(m_{xx}^{(2)} - \mu_{xx}) = \frac{2}{\sqrt{n}} \sum_{i=1}^{n} (\mathbb{E}X' [S(X_i, X')^2] - \mu_{xx}) + o_p(1),
\]

\[
\sqrt{n}(m_{yy}^{(2)} - \mu_{yy}) = \frac{2}{\sqrt{n}} \sum_{i=1}^{n} (\mathbb{E}Y' [S(Y_i, Y')^2] - \mu_{yy}) + o_p(1),
\]

\[
\sqrt{n}(m_{xy}^{(2)} - \mu_{xy}) = \frac{2}{\sqrt{n}} \sum_{i=1}^{n} (\mathbb{E}(X', Y') [S(X_i, X')S(Y_i, Y')] - \mu_{xy}) + o_p(1),
\]

where the conditional expectations in the expressions above represent the first order Hoeffding decomposition of the corresponding U-statistic. Combining all the terms, it follows that

\[
\sqrt{n} \begin{pmatrix} m_x^{(2)} - \mu_x \\ m_y^{(2)} - \mu_y \\ m_{xx}^{(2)} - \mu_{xx} \\ m_{yy}^{(2)} - \mu_{yy} \\ m_{xy}^{(2)} - \mu_{xy} \end{pmatrix} \xrightarrow{d} N_5(\mathbf{0}, 4\Sigma_2),
\]

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where \( \Sigma_2 \) is the covariance matrix of the random vector

\[
(\mathbb{E}_X[S(X, X')], \mathbb{E}_Y[S(Y, Y')], \mathbb{E}_X[S(X, X')^2], \mathbb{E}_Y[S(Y, Y')^2], \mathbb{E}_{(X, Y)}[S(X, X')S(Y, Y')]).
\]

We can then construct an estimator for the population dependence measure \( \chi(X, Y) \) exactly as we did in Case 1 but instead with the use of the sample quantities \( m_x^{(2)}, m_y^{(2)}, m_{xx}^{(2)}, m_{yy}^{(2)}, m_{xy}^{(2)} \). By the delta method we have that, as \( n \to \infty \),

\[
\sqrt{n}(\chi_n(X, Y) - \chi(X, Y)) \xrightarrow{d} N(0, \sigma^2_\chi),
\]

where \( \sigma^2_\chi = (\nabla f_{5 \times 1}|\mu)' \Sigma_2 (\nabla f_{5 \times 1}|\mu) \).

A.2 Additional details for estimation of \( \sigma^2_\chi \)

Analytical forms of the components of the gradient vector are given below; note that \( m = (m_x, m_y, m_{xx}, m_{yy}, m_{xy}) \) acts as a place holder for both \( m^{(1)} \) and \( m^{(2)} \) defined in Remark 4.2.

\[
\begin{align*}
\nabla f_1|_m &= \frac{m_x (m_{xy} - m_x m_y)}{(m_{xx} - m_x^2)^{3/2} \sqrt{m_{yy} - m_y^2}} - \frac{m_y}{\sqrt{m_{xx} - m_x^2} \sqrt{m_{yy} - m_y^2}}, \\
\nabla f_2|_m &= \frac{m_y (m_{xy} - m_x m_y)}{(m_{yy} - m_y^2)^{3/2} \sqrt{m_{xx} - m_x^2}} - \frac{m_x}{\sqrt{m_{xx} - m_x^2} \sqrt{m_{yy} - m_y^2}}, \\
\nabla f_3|_m &= -\frac{m_{xy} - m_x m_y}{2(m_{xx} - m_x^2)^{3/2} \sqrt{m_{yy} - m_y^2}}, \\
\nabla f_4|_m &= -\frac{m_{xy} - m_x m_y}{2(m_{yy} - m_y^2)^{3/2} \sqrt{m_{xx} - m_x^2}}, \\
\nabla f_5|_m &= \frac{1}{\sqrt{m_{xx} - m_x^2} \sqrt{m_{yy} - m_y^2}}.
\end{align*}
\]

A.3 Additional asymptotic results

An estimator \( \tau_n \) of \( \tau(S(X), S(Y)) = \rho(\mathbb{1}_{S(X) \leq S(X')}, \mathbb{1}_{S(Y) \leq S(Y')}) \) can be constructed through the U-statistics framework with the corresponding asymptotic results following as a consequence of Proposition 4.1.

**Corollary A.1 (Asymptotic distribution of \( \tau_n \))**

Assume \( X', X'', X''' \) are independent copies of \( X \). Suppose \( \tau_n(X, Y) \) is constructed as a function of U-statistics. Then, as \( n \to \infty \),

\[
\sqrt{n}(\tau_n(S(X), S(Y)) - \tau(S(X), S(Y))) \xrightarrow{d} N(0, \sigma^2_\tau),
\]

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where

\[ \sigma^2_{\tau} = \begin{cases} 
4(\nabla f_{3 \times 1}|_{\mu})'\Sigma_1(\nabla f_{3 \times 1}|_{\mu}), & \text{if } S \text{ is a } p\text{-variate function}, \\
16(\nabla f_{3 \times 1}|_{\mu})'\Sigma_2(\nabla f_{3 \times 1}|_{\mu}), & \text{if } S \text{ is a } 2p\text{-variate function}. 
\end{cases} \]

Here, \( \nabla f_{3 \times 1}|_{\mu} \) denotes the gradient vector of the function

\[ f(a, b, c) = \frac{c - ab}{\sqrt{a - a^2 \sqrt{b - b^2}}}, \]

evaluated at the population mean \( \mu = (\mu_x, \mu_y, \mu_{xy}) \), where \( \mu_x = P[S(X) \leq S(X')] \), \( \mu_y = P[S(Y) \leq S(Y')] \) and \( \mu_{xy} = P[S(X) \leq S(X'), S(Y) \leq S(Y')] \). Furthermore, \( \Sigma_1 \) denotes the covariance matrix of

\[ (P_{X'|X}[S(X) \leq S(X')], P_{Y'|Y}[S(Y) \leq S(Y')], P_{X',Y'|X,Y}[S(X) \leq S(X'), S(Y) \leq S(Y')]) \]

and \( \Sigma_2 \) denotes the covariance matrix of

\[ (P_{X',X'',X'''|X}[S(X, X') \leq S(X'', X''')], P_{Y',Y'',Y'''|Y}[S(Y, Y') \leq S(Y'', Y''')], P_{X',X'',X''',Y',Y''',Y'''|X,Y}[S(X, X') \leq S(X'', X'''), S(Y, Y') \leq S(Y'', Y''')]) \]

where \( P_{\cdot|\cdot} \) denotes a conditional probability.

Proof. We begin by explicitly writing out the population version of our dependence measure. For a general collapsing function \( S \),

\[ \tau(S(X), S(Y)) = \rho(1_{\{S(X) \leq S(X')\}}, 1_{\{S(Y) \leq S(Y')\}}) = \frac{\mu_{xy} - \mu_x \mu_y}{\sqrt{\mu_x - \mu_x^2} \sqrt{\mu_y - \mu_y^2}}. \]

Case 1: \( S \) is a \( p \)-variate function

Based on a random sample \( (X_1, Y_1), \ldots, (X_n, Y_n) \), estimators \( m_x^{(1)}, m_y^{(1)} \), and \( m_{xy}^{(1)} \) can be constructed using the setup of the proof of Case 2 of Proposition 4.1. The convergence result follows from a similar delta method argument.

Case 2: \( S \) is \( 2p \)-variate function

The sample quantities

\[ m_x^{(2)} = \frac{1}{(m)} \sum_{i<j<k<l} 1_{\{S(X_i, X_j) \leq S(X_k, X_l)\}}, \quad m_y^{(2)} = \frac{1}{(m)} \sum_{i<j<k<l} 1_{\{S(Y_i, Y_j) \leq S(Y_k, Y_l)\}}, \]

\[ m_{xy}^{(2)} = \frac{1}{(m)} \sum_{i<j<k<l} 1_{\{S(X_i, X_j) \leq S(X_k, X_l), S(Y_i, Y_j) \leq S(Y_k, Y_l)\}} \]
are naturally U-statistics for their corresponding population quantities. Then, following Hoeffding’s decomposition theorem, we have that, as $n \to \infty$,

$$
\sqrt{n}(m_{x}^{(2)} - \mu_x) = \frac{4}{\sqrt{n}} \sum_{i=1}^{n} (\mathbb{P}_{X^{i},X'^{i},X''^{i},X'''^{i}} | X(S(X_i, X') \leq S(X'', X'''^{i})) - \mu_x) + o_p(1),
$$

$$
\sqrt{n}(m_{y}^{(2)} - \mu_y) = \frac{4}{\sqrt{n}} \sum_{i=1}^{n} (\mathbb{P}_{Y^{i},Y'^{i},Y''^{i},Y'''^{i}} | Y(S(Y_i, Y') \leq S(Y'', Y'''^{i})) - \mu_y) + o_p(1),
$$

$$
\sqrt{n}(m_{xy}^{(2)} - \mu_{xy}) = \frac{4}{\sqrt{n}} \sum_{i=1}^{n} (\mathbb{P}_{X^{i},X'^{i},X''^{i},X'''} | X(Y(S(X_i, X') \leq S(X'', X''')}, Y(S(Y_i, Y') \leq S(Y'', Y'''^{i})) - \mu_{xy}) + o_p(1),
$$

where the conditional probabilities in the expressions above represent the first order Hoeffding decomposition of the corresponding U-statistic. Combining all the terms, it follows that

$$
\sqrt{n} \begin{pmatrix}
  m_{x}^{(2)} - \mu_x \\
  m_{y}^{(2)} - \mu_y \\
  m_{xy}^{(2)} - \mu_{xy}
\end{pmatrix} \overset{d}{\to} N_3(0, 16\Sigma_2),
$$

where $\Sigma_2$ denotes the covariance matrix of the random vector defined in (6). One can then construct an estimator using $\tau_n(S(X), S(Y)) = f(m_{x}^{(2)}, m_{y}^{(2)}, m_{xy}^{(2)})$ where $f$ is defined as in the claim Using the delta method, the convergence result follows. \qed

**Remark A.2**

In the U-statistics framework, one usually works with symmetric kernels as noted in Lee (1990, Chapter 1). For choices of collapsing functions which would yield non-symmetric kernels, note that one can easily replace the kernel with a symmetric variant. Suppose for example $\phi(X_1, \ldots, X_m)$ is a kernel of order $m$. Then, the symmetric variant can be constructed as

$$
\phi(X_1, \ldots, X_m) = \frac{1}{m!} \sum_{\alpha_1, \ldots, \alpha_m} \phi(X_{\alpha_1}, \ldots, X_{\alpha_m}),
$$

where the summation is taken over all permutations $(\alpha_1, \ldots, \alpha_m)$ of $(1, \ldots, m)$. By replacing any non-symmetric kernel with its symmetric variant, the rest of the derivation for the asymptotic distribution would then naturally follow.