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On certain transformations of Archimedean copulas: Application to the non-parametric estimation of their generators

Elena Di Bernardino∗, Didier Rullière†

Abstract

We study the impact of certain transformations within the class of Archimedean copulas. We give some admissibility conditions for these transformations, and define some equivalence classes for both transformations and generators of Archimedean copulas. We extend the $r$-fold composition of the diagonal section of a copula, from $r \in \mathbb{N}$ to $r \in \mathbb{R}$. This extension, coupled with results on equivalence classes, gives us new expressions of transformations and generators. Estimators deriving directly from these expressions are proposed and their convergence is investigated. We provide confidence bands for the estimated generators. Numerical illustrations show the empirical performance of these estimators.

Keywords: Transformations of Archimedean copulas, self-nested diagonal, non-parametric estimation, tail dependence.

1 Introduction

1.1 Basic notions and preliminaries

Assume that we have a $d$-dimensional nonnegative real-valued random vector $X = (X_1,\ldots,X_d)$. Denote its multivariate distribution function by $F : \mathbb{R}^d \to [0,1]$ with continuous univariate margins $F_i(x_i) = P(X_i \leq x_i)$, for $i = 1,\ldots,d$. Sklar’s Theorem (1959) is a well-known result which states that for any random vector $X$, its multivariate distribution function has the representation

$$F(x_1,\ldots,x_d) = C(F_1(x_1),\ldots,F_d(x_d)),$$

where $C$ is called the copula. Effectively, it is a distribution function on the $d$-cube $[0,1]^d$ with uniform margins and it links the univariate margins to their full multivariate distribution. In the case where we have a continuous random vector, we know that $U_i = F_i(X_i)$ is an uniform random variable so that we can write

$$C(u_1,\ldots,u_d) = F(F_1^{-1}(u_1),\ldots,F_d^{-1}(u_d)),$$

to be the unique copula associated with $X$, with quantile functions $F_i^{-1}$ defined by:

$$F_i^{-1}(p) = \inf\{x \in \mathbb{R} : F_i(x) \geq p\}, \quad \text{for } p \in (0,1).$$

In this paper, we mainly consider Archimedean copulas, which are copulas that can be written

$$C_\phi(u_1,\ldots,u_d) = \phi(\phi^{-1}(u_1) + \ldots + \phi^{-1}(u_d)),$$

where the function $\phi$ is called the generator of the Archimedean copula $C_\phi$. The generator is a continuous and decreasing function, with $\phi(0) = 1$, satisfying some supplementary assumptions that will be discussed hereafter. In this paper, generators are assumed to be strict generators, such that $\phi(t) > 0$, $\forall t \geq 0$ and $\lim_{t \to +\infty} \phi(t) = 0$. In this case the generalized inverse $\phi^-$ of the generator coincides with the inverse $\phi^{-1}$

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Archimedean copulas are symmetrical copulas, that is \( C_\varphi(u_1, \ldots, u_d) = C_\varphi(u_{\sigma(1)}, \ldots, u_{\sigma(d)}) \) for any permutation \( \sigma \) of the set \( \{1, \ldots, d\} \). Such copulas play a central role in the understanding of dependencies of multivariate random vectors. A good introduction to copulas in general is given in Nelsen (1999). For a focus on Archimedean copulas in particular the reader is referred to McNeil and Nešlehová (2009).

Transformations of copulas are a simple way to generate new copulas from initial ones. Many types of transformations of copulas have been considered in the literature, see for example Valdez and Xiao (2011) or Michiels and De Schepper (2012) for a review of some existing transforms. Transformations of bivariate copula, semicopulas and quasi-copulas are studied in Durante and Sempi (2005). Klement et al. (2005a) and Klement et al. (2005b) focused on transformations of bivariate Archimax copulas.

A particular class of transformation, based on mixtures, is also considered in Morillas (2005). Applications to transformations of copulas to pricing credit derivatives are given in Crane and van der Hoek (2008).

We consider here a particular transformation of a copula, using a function \( T \) and leading to the definition of a transformed copula \( \tilde{C} \) of an initial copula \( C_0 \),

\[
\tilde{C}(u_1, \ldots, u_d) = T \circ C_0(T^{-1}(u_1), \ldots, T^{-1}(u_d)), \quad \text{for } u_1, \ldots, u_d \in [0, 1].
\]

The function \( T : [0, 1] \to [0, 1] \) is a continuous and increasing function on the interval \([0, 1]\), with \( T(0) = 0 \), \( T(1) = 1 \), with supplementary assumptions that will be chosen to guarantee that \( \tilde{C} \) is also a copula, detailed hereafter. In the following, we will restrict ourselves to the case where \( C_0 \) is an Archimedean copula. In this case, we will see that (under supplementary assumptions on the transformation \( T \)) the transformed copula \( \tilde{C} \) will be Archimedean, so that these transformations are essentially transforms of a given Archimedean copula into another Archimedean copula (then the obtained transformed copula is still symmetric, for example).

This kind of transformations has been considered for example in Durrleman et al. (2000), in Valdez and Xiao (2011) (Definitions 3.6, in dimension \( d = 2 \)), in Hofert (2011) (see Section 3.3, with \( T = \psi_0 \circ (−\log) \) for an Archimedean generator \( \psi_0 \)). If we focus on the two-dimensional setting, the transformation considered in this paper corresponds to the Right Composition (RC, see Lemma 5 in Michiels and De Schepper (2012)), initially defined in Genest et al. (1998).

Among advantages of such transformations, we may cite the possible improvement of the fit of an initial copula, the easy development of iterative transformation schemes, and some properties that may ease the estimation of the transformed copula (for further details see for instance Di Bernardino and Rullière (2013)).

### 1.2 Some problematic points

Among problems generated by transformations of Archimedean copulas, one can point out, in particular

i) The problem of uniqueness: transformations of a given initial copula leading to a given target copula are not unique. This raises some problems for the analysis of the convergence of estimators of the transformation. This also causes problems to compare transformations and to understand their impact on the dependence structure. A further analysis shows that also a generator of an Archimedean copula is not unique, causing the same kind of problems.

ii) The estimation problem: we aim here at finding non-parametric estimators of the transformation \( T \) in Equation (2) and non-parametric estimators of the generator of a transformed Archimedean copula, when no parametric shape is assumed for this generator. This kind of non-parametric estimation of transformed copulas has been treated by using level curves properties and an iterative algorithm in Di Bernardino and Rullière (2013). However, the convergence of this algorithm is not yet demonstrated, and properties of the obtained estimator are not easy to get. Concerning tail dependence estimation, Embrechts and Hofert (2011) show that some non-parametric estimators of...
the generator fail to properly model tail dependence. As detailed further, this problem will remain with estimators that will be proposed in this paper.

iii) The tail problem: the impact on the tail of transformed copulas are only partially known (see for instance Durante et al. (2010)). In practice this impact has to be investigated. In particular the relationship between the asymptote of some class of parametric transformations \( T \) (see Example 1) and the regular variation of the transformed tails represents an open interesting point. A good understanding of the tail behavior is indeed required to estimate the shape of the transformation near 0 and 1, in extreme quantiles where there is a lack of data.

We try to provide, in the following, some answers to these problems in the case of Archimedean families of copulas.

The determination of sufficient and necessary conditions in order to obtain admissible transformations \( T \) is fundamental to propose tractable transformations in operational problems. Some elements on equivalence classes of generators of Archimedean copulas have been given, e.g. in Nelsen et al. (2009). The definition of equivalence classes for both transformations and generators is necessary to select some standardized forms for practical use, for the comparison and the interpretation of obtained distribution functions.

Transformed copulas permit to introduce, in a more flexible way, families of copulas exhibiting different behaviour in the tails. The tail behavior of a transformed copula can be assessed by determining the tail coefficients of transformed copulas, or by transforming some existing models like the one of Ledford and Tawn (1996). Much of the recent literature focuses on how the tail dependence properties are modified under transformations (see e.g. Durante et al. (2010)). Results about the tail dependence coefficients of an Archimedean copulas are given by Juri and Wüthrich (2002), Juri and Wüthrich (2003) and Charpentier and Segers (2007) in terms of regularly varying properties of the additive generator. Furthermore some results about tail dependence coefficients of certain transforms of Archimedean copulas are given by Hofert (2011). However, these interesting perspectives about the transformed tails are beyond the scope of the present paper.

At last, the construction of non-parametric estimators of an Archimedean copula or its generator are of great interest for practical studies. There is a huge literature concerning the estimation of copula structures, see for example Genest and Rivest (1993), Joe (2005), Autin et al. (2010), Hernández-Lobato and Suárez (2011).

A comparison of different parametric and non-parametric methods for estimating a copula is given, for example, in Kim et al. (2007). Due to the complicated theoretical results, Kim et al. (2007) have mainly investigated the bivariate case \( (d = 2) \). A particular focus on the dimensionality problem \( (d > 2) \) was developed in Embrechts and Hofert (2013). Non-parametric rank-based estimator for the generator of Archimedean copula has been recently proposed by Genest et al. (2011). However this estimator is constructed using successive numerical resolutions of root.

Conversely with the cited literature, our goal in this paper is to easily obtain a non-parametric estimator for the generator of an Archimedean copula, and estimators of the transformation \( T \) in Equation (2).

We aim at deriving direct analytical expressions for the desired estimators, which does not rely on any numerical resolution of root or optimization, in order to simplify both practical use and theoretical analysis. Our construction is mainly based on the diagonal section of a copula. We recall that parametric estimators based on the diagonal section have been suggested already in the literature, see, for example, Hofert et al. (2011). However, we will try to find non-parametric estimators of transformations and generators based on the diagonal section, which is a central tool for Archimedean copulas (see, e.g., Nelsen et al. (2008)). These estimators will be given in any dimension \( d \geq 2 \), and will exploit results on equivalence classes of transformations and generators. As it will be discussed, estimators based on the diagonal section only use partial information about the dependence and thus might not be efficient, in particular in the tail, in order to capture tail dependence (as was pointed out by Hofert et al. (2011)). Despite these problems, the tractable expression of the obtained estimator plays a central role both in the numerical implementation (on real and simulated data) and in the construction of confidence bands.
1.3 Organization of the paper

In Section 2, we give properties of both transformations and generators. In particular, we detail admissibility conditions for transformations and generators (Section 2.1). In Section 2.2 we characterize equivalence classes for these transformations and generators.

In Section 3, we define the notion of self-nested diagonals which are extensions of $k$–fold composition of diagonal sections of a copula when $k$ belongs to the whole real line (see Section 3.1). Easy expressions of self-nested diagonals are given in the Archimedean case. Then in Section 3.2 we present the main result of the present work, i.e. some expressions for the transformations of self-nested diagonals are given in the Archimedean case. Remark 1 (Generator of a transformed copula)

2.1 Admissibility conditions

Properties of transformations and generators

in the case of most popular Archimedean copula families, are postponed in the Annex.

Exact analytical formulas for standardized generators, their inverses and theoretical self-nested diagonals, illustrations (Section 4.3).

generators (Section 4.2). At last, we show the empirical behavior of these estimators through numerical formations and generators of Archimedean copula. We propose some convergence properties for the proposed estimators (Section 4.1). Confidence bands are given for self-nested diagonals and for estimated generators (Section 4.2). Exact analytical formulas for standardized generators, their inverses and theoretical self-nested diagonals, in the case of most popular Archimedean copula families, are postponed in the Annex.

2 Properties of transformations and generators

2.1 Admissibility conditions

Remark 1 (Generator of a transformed copula). Let $C_0$ the initial Archimedean copula with an associated generator $\phi$. If $\tilde{\phi} = T \circ \phi$ then $\tilde{C}(u_1, \ldots, u_d) = T \circ C_0(T^{-1}(u_1), \ldots, T^{-1}(u_d))$. In general, $\tilde{C}$ is not necessarily a copula. However in this section we investigate some supplementary assumptions to guarantee that $\tilde{C}$ is also a copula, at least in some particular cases. In this case $\tilde{\phi}$ will be the generator of the transformed copula $\tilde{C}$.

From Theorem 2.2 in McNeil and Nešlehová (2009) $C_\phi(u_1, \ldots, u_d) = \phi(\phi^{-1}(u_1) + \ldots + \phi^{-1}(u_d))$ is a $d$–dimensional copula if and only if its generator $\phi$ is $d$–monotone on $[0, \infty)$, where the $d$–monotony definition is recalled hereafter.

Definition 2.1 ($d$-monotone function). A real function $f$ is called $d$–monotone in $(a, b)$, where $a, b \in \mathbb{R}$ and $d \geq 2$, if it is differentiable there up to the order $d - 2$ and the derivatives satisfy

$$(-1)^k f^{(k)}(x) \geq 0, \quad k = 0, 1, \ldots, d - 2$$

for any $x \in (a, b)$ and further if $(-1)^{d-2} f^{(d-2)}$ is non-increasing and convex in $(a, b)$. For $d = 1$, $f$ is called 1–monotone in $(a, b)$ if it is nonnegative and non-increasing there.

If $f$ has derivatives of all orders in $(a, b)$ and if $(-1)^k f^{(k)}(x) \geq 0$, for any $x \in (a, b)$, then $f$ is called completely monotone.

It follows some admissibility conditions for a transformation $T$.

Definition 2.2 (Admissible transformations and transformed copula). Let $T : [0, 1] \rightarrow [0, 1]$ be a continuous and increasing function on the interval $[0, 1]$, with $T(0) = 0$, $T(1) = 1$. Let $C_0$ an initial copula. We say that $T$ is an admissible transformation if

$$\hat{C}_{T,C_0}(u_1, \ldots, u_d) = T \circ C_0(T^{-1}(u_1), \ldots, T^{-1}(u_d)) \quad (3)$$

is a also copula.

In the following result we provide a specific characterization for an admissible transformation $T$, starting from a $d$–variate initial independent copula $C_0$. 4
Remark 2 (Multiplicative generators). Let $T$ be a bijection such that $T : [0, 1] \to [0, 1]$. Let $C_0$ be the $d$–variate initial independent copula, i.e., $C_0(u_1, \ldots, u_d) = \prod_{i=1}^{d} u_i$, and $\tilde{C}$ the associated transformed dependence structure as in Equation (3). It is obvious that $\phi(t) = T(\exp(-t))$, so that

$$\tilde{\phi} \left( \tilde{\phi}^{-1}(u_1) + \ldots + \tilde{\phi}^{-1}(u_d) \right) = T \left( T^{-1}(u_1) \ldots T^{-1}(u_d) \right)$$

(4)

It is thus clear that there is a simple isomorphism between additive and multiplicative generators of Archimedean copulas, as it appears in the book by Alzina et al. (2006). In this book, the authors give conditions in dimension $d = 2$ such that $\tilde{C}_{T,C_0}$ is a t-norm (see Theorem 2.2.1 of this book) and conditions such that $\tilde{C}_{T,C_0}$ is a copula (see Theorem 1.4.5. of this book).

Previous conditions do not require the differentiability of $T$. However, for some parametric forms of $T$, it may be useful to get supplementary conditions on the derivatives of $T$ when $T$ is differentiable, in the dimension $d > 2$. As an example, in Morillas (2005) (Theorem 4.7, see also Fischer and Kock (2012), Section 2.2), one can see that a sufficient condition for $T$ to be a copula if and only if the transformed dependence structure as in Equation (3) yields a copula if and only if $\tilde{C}$ is still an Archimedean copula, so that

$$C_0(u_1, \ldots, u_d) = \prod_{i=1}^{d} u_i$$

is a copula if and only if this transformed generator $\tilde{C}$ is still an Archimedean copula, so that

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is a t-norm (see Theorem 2.2.1 of this book) and conditions such that $\tilde{C}_{T,C_0}$ is a copula (see Theorem 1.4.5. of this book).

Proposition 2.1 (Admissibility conditions for the transformation). Let $T$ be a bijection such that $T : [0, 1] \to [0, 1]$. Let $C_0$ be the $d$–variate initial independent copula, i.e., $C_0(u_1, \ldots, u_d) = \prod_{i=1}^{d} u_i$, and $\tilde{C}$ the associated transformed dependence structure as in (3). If $T$ is $d$ times differentiable, then the formula (3) yields a copula if and only if

$$\sum_{r=1}^{n} \alpha^n_r x^{-r} T^{(r)}(x) \geq 0, \quad \forall n = 1, \ldots, d,$$

(5)

with $\alpha^n_1 = 1$, $\alpha^n_n = 1$ and $\alpha^n_r = r \alpha^n_{r-1} + \alpha^n_{r-1}$, for $2 \leq r \leq n - 1$.

Proof: We prove this proposition by induction. We first remark that the transformation of an Archimedean copula is still an Archimedean copula, so that $\tilde{C}$ is an Archimedean copula. From McNeil and Nešlehová (2009), $\tilde{C}$ is a copula if and only if this transformed generator $\tilde{\phi} = T \circ \phi$ is a $d$–monotone function. This condition implies a specific characterization for our admissible transformation $T$ in the case where $T$ is $d$ times differentiable. In this case, this means that $(-1)^k \tilde{\phi}^{(k)} \geq 0$ for $k = 0, 1, \ldots, d$. Firstly, we show that the statement of Proposition 2.1 holds for $d = 2$. In particular in the case of a bivariate independent copula, the transformed generator $T(e^{-t})$ has to be a $2$–monotone function. Since $T$ is increasing, this means $T^{(1)}(x) + x T^{(2)}(x) \geq 0$, for all $x \in [0, 1]$. This is exactly Equation (5) in the case $d = 2$. For $n \geq 2$, one can show that there exists coefficients $\alpha^n_r$, $r \in \{1, \ldots, n\}$ such that the derivative of order $n$ of $T(e^{-t})$ can be written

$$\tilde{\phi}^{(n)} = |T(e^{-t})|^{(n)} = (-1)^n \sum_{r=1}^{n} \alpha^n_r e^{-rt} T^{(r)}(e^{-t}) = (-1)^n \sum_{r=1}^{n} \alpha^n_r x^r T^{(r)}(x).$$

By differentiation, we get

$$\tilde{\phi}^{(n+1)} = (-1)^{n+1} \sum_{r=1}^{n+1} \alpha^n_{r+1} e^{-rt} T^{(r)}(e^{-t}) ,$$

so that for all $n \geq 2$, $\alpha^n_{r+1} = r \alpha^n_r + \alpha^n_{r-1}$ for $r \leq n$, $\alpha^n_{n+1} = \alpha^n_n = \ldots = \alpha^2_1 = 1$ and $\alpha^n_0 = 0$.

Remark that $(-1)^n \tilde{\phi}^{(n)} \geq 0$ if and only if $\sum_{r=1}^{n} \alpha^n_r x^r T^{(r)}(x) \geq 0$. Hence the result. Existence and alternative expressions of coefficients $\alpha^n_r$ can be obtained using a combinatoric approach derived by Faà di Bruno’s formula. The interested reader is referred for instance to Hardy (2006). The coefficients $\alpha^n_r$
can be written by using the number of branches of a given size in the tree-representation of the composed derivative (using theory of rooted trees, see for instance Chomette (2003)). □

A discussion on the class of reachable copulas by transforming an initial copula is available in Di Bernardino and Rullière (2013).

2.2 Equivalent transformations and generators

We first remark that generators and transformations leading to a given copula are not unique, and thus define some equivalence classes, for the generator (see Definition 2.3) and for the transformations (see Definition 2.4).

Definition 2.3 (Invariant class for Archimedean generator). Let \( \phi \) be a generator of an Archimedean copula \( C_\phi \), i.e., \( C_\phi(u_1, \ldots, u_d) = \phi(\phi^{-1}(u_1) + \cdots + \phi^{-1}(u_d)) \). Then a generator \( \psi \) of a copula \( C_\psi \) is said to belong to the same invariance class of \( \phi \) if and only if \( C_\phi = C_\psi \). We denote this class \( I_\phi \) and we write \( \psi \in I_\phi \). A generator \( \psi \) belonging to \( I_\phi \) will be said to be equivalent to generator \( \phi \).

Definition 2.4 (Invariant class for transformations). Let \( \tilde{C}_{T_1,C_0} \) and \( \tilde{C}_{T_2,C_0} \) be two transformed copulas using transformations \( T_1 \) and \( T_2 \) respectively and with the same initial copula \( C_0 \) (see Equation (3)). Then the transformation \( T_2 \) is said to belong to the same invariance class of \( T_1 \) if and only if \( \tilde{C}_{T_1,C_0} = \tilde{C}_{T_2,C_0} \). We denote this class \( I_{T_1,C_0} \) and we write \( T_2 \in I_{T_1,C_0} \). A transformation \( T_2 \) belonging to \( I_{T_1,C_0} \) will be said to be equivalent to \( T_1 \) starting from the initial copula \( C_0 \).

We now provide some characterizations for the generators (see Lemma 2.1) and for the transformations (see Lemma 2.2) belonging to a same equivalence class. These characterizations will help us to select one expression for the generators and the transformations, within their equivalence class. They will be necessary to find some points of the functions of interest (the generator or some transformation functions), first step before proposing estimators of these quantities.

Lemma 2.1 (Equivalent generator, Nelsen (1999)). Let \( C_0 \) be an initial Archimedean copula with a strict generator \( \phi \). Consider the transformed function \( \tilde{\phi} \), then the transformed copula is unchanged with respect to \( C_0 \),
\[
\tilde{\phi} \in I_\phi \quad \text{if and only if} \quad \tilde{\phi} = \phi \circ L,
\]
where \( L \) is a linear function, i.e. \( L(x) = a x \), for some \( a \in \mathbb{R} \setminus \{0\} \). The function \( \tilde{\phi} \) in the case of \( a > 0 \) is a generator (in the sense of Lemma 4.1.2. in Nelsen (1999)). The generator \( \tilde{\phi} \) is thus equivalent to \( \phi \) since it leads to the same transformed copula.

Proof: The statement can be obtained from Theorem 4.1.5. c) in Nelsen (1999). Indeed using the Nelsen’s result we have that \( \tilde{\phi} \) is an equivalent generator with \( \tilde{\phi}^{-1}(x) = c \phi^{-1}(x) \), for \( c > 0 \). Hence the result. □

In Lemma 2.2 we characterize equivalence classes for the considered transformations of Archimedean copulas.

Lemma 2.2 (Equivalent transformations). Let \( C_0 \) be an initial Archimedean copula with associated strict generator \( \phi \). Let \( T_1 \) and \( T_2 \) be two transformations of this initial copula \( C_0 \), as in Definition 2.2. Then, starting from the initial copula \( C_0 \), the transformation \( T_2 \) is equivalent to the transformation \( T_1 \) as soon as it can be written \( T_2 = T_1 \circ \phi \circ L \circ \phi^{-1} \), where \( L \) is a linear function:
\[
T_2 \in I_{T_1,C_0} \quad \text{if and only if} \quad T_2 = T_1 \circ \phi \circ L \circ \phi^{-1}, \quad \text{with} \ L(x) = a x, \ x \in \mathbb{R}, \ a \in \mathbb{R} \setminus \{0\}.
\]
If furthermore \( T_2(x_0) = y_0 \), for any given point \( (x_0,y_0) \in (0,1)^2 \), then
\[
T_2 \in I_{T_1,C_0} \quad \text{if and only if} \quad T_2 = T_1 \circ \phi \circ L \circ \phi^{-1}, \quad \text{with} \ L(x) = a x, \ x \in \mathbb{R}, \ a = \frac{\phi^{-1}(T_1^{-1}(y_0))}{\phi^{-1}(x_0)}.
\]
The transformation \( T_2 \) is the unique equivalent transformation of \( T_1 \), starting from initial copula \( C_0 \), passing through the point \( (x_0,y_0) \).

The proof of Lemma 2.2 comes down trivially from Lemma 2.1. Lemma 2.2 will be useful in the proof of Lemma 3.3.
Corollary 2.1. Let $C_0$ be the independent copula. Let
\[
T_2(x) = T_1(x^a), \quad x \in [0,1], \quad \text{with} \quad a = \frac{\ln(T_1^{-1}(y_0))}{\ln(x_0)},
\]
then $T_2 \in I_{T_1,C_0}$ and $T_2(x_0) = y_0$, for any given point $(x_0,y_0) \in (0,1)^2$.

Lemma 2.2 and Corollary 2.1 can be useful in order to ensure the uniqueness of the transformation $T$ among the invariant class for transformations. In an iterative procedure of estimation the uniqueness of the transformation is essential in order to permit the convergence of the procedure. These results will be useful later in the estimation procedure of the transformation and generator functions (see Sections 3.2 and 4.1).

Example 1 (Transformations in the logit-scale). A particular class of transformation is constituted by transformations defined in Bienvenüe and Rullière (2011) with the form $T_f : [0,1] \to [0,1]$ such that
\[
T_f(u) = \begin{cases} 
0 & \text{if } u = 0, \\
\logit^{-1}(f(\logit(u))) & \text{if } 0 < u < 1, \\
1 & \text{if } u = 1,
\end{cases}
\]
(6)
where $f$ any bijective increasing function, $f : \mathbb{R} \to \mathbb{R}$. Function $f$ is said to be a conversion function. These transformations help working in the logit-scale, so that we only need to study composition of increasing functions from $\mathbb{R}$ to $\mathbb{R}$. The main advantage of $T_f$, with adequate conversion functions $f$, is to lead to simple analytic expressions for inverse transformations and for level curves of the associated multivariate distribution function. Developments using transformations in (6), with hyperbolic conversion function $f$, are given in Bienvenüe and Rullière (2011), Bienvenüe and Rullière (2012), Di Bernardino and Rullière (2013).

Let $C_0$ the initial Archimedean copula with associated generator $\phi$. Let $f_1$ and $f_2$ be two conversion functions respectively associated to transformations $T_{f_1}$ and $T_{f_2}$, i.e., $T_{f_1} = \logit^{-1} \circ f_1 \circ \logit(x)$ and $T_{f_2} = \logit^{-1} \circ f_2 \circ \logit(x)$, then
\[
C_{T_{f_1},C_0} = C_{T_{f_2},C_0}
\]
if and only if $f_2 = f_1 \circ \tau$, with $\tau = \logit \circ \phi \circ L \circ \phi^{-1} \circ \logit^{-1}$.

Then the conversion function $f_2$ is said to belong to the same invariance class of $f_1$, and we write $f_2 \in I_{f_1,C_0}$. The conversion function $f_2$ is said to be equivalent to conversion function $f_1$, starting from the initial copula $C_0$, since they lead to the same transformed copula. This result comes down easily from Lemma 2.2.

3 Self-nested diagonals

3.1 Definition and properties

In the following, we define the notion of self-nested diagonal. We have chosen this terminology in reference to the nested copulas (see e.g. Hofert and Pham (2013)), as detailed below. The self-nested diagonals introduced in the following will be essential for the non-parametric estimation proposed in Section 4. They will be build mainly from the diagonal section $\delta_1$ of a copula,
\[
\delta_1(u) = C(u,\ldots,u), \quad u \in [0,1].
\]
Remark that the diagonal section of a copula $C$ has several probabilistic interpretations; for instance, it is the restriction to $[0,1]$ of the distribution function of $\max(U_1,\ldots,U_n)$ whenever $(U_1,\ldots,U_n)$ is the random vector distributed as $C$. The interested reader is referred to Nelsen et al. (2008). Jaworski (2009) and Jaworski and Rychlik (2008) formulate the necessary and sufficient conditions for a function to be the diagonal section of a multivariate absolutely continuous copula. Different papers are devoted to copulas with a given diagonal sections (see, for instance Durante and Jaworski (2008)). Nelsen and Fredricks (1997) clearly distinguish the concept of a diagonal, diagonal section of a copula ($\delta_1$ above),
and a diagonal copula itself.

As it will be detailed, under some conditions, an Archimedean copula is uniquely determined by its diagonal section, and the existence conditions of a copula with a given diagonal section is presented in Erdely et al. (2013) (see Remark 3). Furthermore some properties of the diagonal of a copula, in the bivariate setting, are illustrated in Alsina et al. (2006), Section 3.8.

**Definition 3.1** (Discrete self-nested diagonal). Consider a d-dimensional copula C such that for all \( u \in [0,1] \), \( \delta_1(u) := C(u, \ldots, u) \) is a strictly increasing function of \( u \). The respective discrete self-nested diagonal of \( C \) of order \( k \) and \( -k \) are the functions \( \delta_k \) and \( \delta_{-k} \) such that for all \( u \in [0,1] \), for all \( k \in \mathbb{N} \),

\[
\begin{align*}
\delta_k(u) &= \delta_1 \circ \ldots \circ \delta_1(u), \quad (k \text{ times}) \\
\delta_{-k}(u) &= \delta_{-1} \circ \ldots \circ \delta_{-1}(u), \quad (k \text{ times}) \\
\delta_0(u) &= u.
\end{align*}
\]

where \( \delta_{-1} \) is the inverse function of \( \delta_1 \), so that \( \delta_1 \circ \delta_{-1} \) is the identity function.

We now explain the chosen terminology of self-nested diagonal. Indeed in Hofert and Pham (2013), for a vector \( u \in [0,1]^d \) and some specific vectors \( u_1, \ldots, u_d \), such that \( u = (u_1, \ldots, u_d)^T \), the authors state that a partially nested Archimedean copula \( C \) with two nesting levels and \( d_0 \) child copulas (or sectors or groups), is given by

\[
C(u) = C_0(C_1(u_1), \ldots, C_{d_0}(u_{d_0})).
\]

One can easily check that the self-nested diagonals deal with the particular case where \( C_0 = C_1 = \ldots = C_{d_0} = C \) and \( u_i = u = (u, \ldots, u) \) for all \( i \in \{1, \ldots, d_0\} \). From Definition 3.1 we get, for instance,

\[
\begin{align*}
\delta_1(u) &= C(u), \\
\delta_2(u) &= C(C(u), \ldots, C(u)) = \delta_1 \circ \delta_1(u), \\
\delta_3(u) &= C(C(C(u), \ldots, C(u)), \ldots, C(u)) = C(C(u, \ldots, C(u))), \\
&\quad \ldots
\end{align*}
\]

Another difference with classical nested copulas scheme is that here all child vectors are identical, \( u = u_1 = \ldots = u_{d_0} \), whereas in classical schemes \( u = (u_1, \ldots, u_{d_0})^T \).

Discrete self-nested diagonals presented in Definition 3.1, correspond to the \( k \)-fold composition of the diagonal section \( \delta_1 \) of the copula (see Wysocki (2012)). They are defined for \( k \in \mathbb{Z} \) (hence justifying the prefix discrete). They can be linked with what is defined as iterates of the diagonal of a t-norm, and with T-powers in Alsina et al. (2006) (see Lemma 1.3.5. of this book for example, in dimension \( d = 2 \)).

For a family of discrete self-nested diagonals \( \{\delta_k\}_{k \in \mathbb{Z}} \), one can easily check that for all \( j \in \mathbb{Z}, k \in \mathbb{Z} \), for all \( u \in [0,1] \),

\[
\delta_{j+k}(u) = \delta_j \circ \delta_k(u).
\]

A function of a family satisfying this proposition for all \( j, k \in \mathbb{R} \) will be called an extended self-nested diagonal, or simply a self-nested diagonal. The following definition aims at defining the \( r \)-fold composition of the diagonal section \( \delta_1 \) of the copula when \( r \in \mathbb{R} \) is not a relative integer.

**Definition 3.2** (Self-nested diagonals). Functions of a family \( \{\delta_r\}_{r \in \mathbb{R}} \) are called (extended) self-nested diagonals of a copula \( C \), if \( \delta_k(u) \) is the discrete self-nested diagonal of \( C \) of order \( k \) for all \( k \in \mathbb{Z} \), as in Definition 3.1, and if furthermore

\[
\delta_{r_1+r_2}(u) = \delta_{r_1} \circ \delta_{r_2}(u), \quad \forall r_1, r_2 \in \mathbb{R}, \forall u \in [0,1].
\]

The existence of (extended) self-nested diagonals of a copula \( C \) is automatically guaranteed when \( C \) is an Archimedean copula (see detailed discussion below and in particular Lemma 3.1).

The study of self-nested diagonals is thus relying on the study of a family of univariate functions. **Extended self-nested diagonals** can be seen as cumulative distribution functions of some indexed random variables \( X^{o_r} \), \( r \in \mathbb{R} \), distributed on \( [0,1] \), such that for all \( r_1, r_2 \in \mathbb{R} \), for all \( x \in [0,1] \),

\[
P[X^{o_{r_1+r_2}} \leq x] = P[X^{o_{r_1}} \leq P[X^{o_{r_2}} \leq x]],
\]

with \( P[X^{o_r} \leq x] = \delta_r(x) \), for \( r \in \mathbb{R} \), and in particular \( X^{o_0} \) uniformly distributed on \( [0,1] \).
Self-nested Archimedean diagonals

We first remark that the diagonal of an Archimedean copula, under some suitable conditions, is essential to describe the copula. So, in the following we recall important assumptions (which are fulfilled for many Archimedean copulas, including the independent copula) for the unique determination of an Archimedean copulas starting from the diagonal section (see, for instance, Erdely et al. (2013) and references therein). Some constructions of copulas starting from the diagonal section are given for example in Nelsen et al. (2008) and Wysocki (2012).

Remark 3 (Identity of Archimedean copulas, Theorem 3.5 by Erdely et al. (2013)). Let $C$ a $d-$dimensional Archimedean copula whose diagonal section $\delta_C$ satisfies $\delta_C(1^-) = d$. Then $C$ is uniquely determined by its diagonal.

Note that if $|\phi'(0)| < +\infty$ then the condition on the diagonal in Remark 3 is automatically satisfied. Wysocki (2012) proves the same result asking that the strict generator of the $d-$dimensional Archimedean copula satisfies : $\phi(0) = -1$. Remark that, under the multiplicative scaling in the equivalence class (see Lemma 2.1), this condition is equivalent to $|\phi'(0)| < +\infty$ (see Lemma 1 in Wysocki (2012)). Condition in Remark 3 is referred to as Frank’s condition in Erdely et al. (2013) (see their Theorems 1.2 and 3.5). Then if $|\phi'(0)| < +\infty$, up to a multiplicative constant, the function $\phi$ can be reconstructed from the diagonal $\delta$ (see also Segers (2011)). As pointed out by Embrechts and Hofert (2011) a possible limitation is that if $\phi$ has finite right-hand derivative at zero, the Archimedean copula generated by $\phi$ has upper tail independence (for further details see also Section 4.3.1 about “Upper tail dependence”).

In Alsina et al. (2006), Section 3.8, a counterexample is given, in order to show that if $d = 2$ and $\phi$ is generator for an Archimedean copula $C$ such that $\phi(0) = -\infty$, or equivalently $\delta_C(1^-) < 2$, then the diagonal does not characterize uniquely the generator $\phi$. To show that the situation of many Archimedean copulas having the same diagonal is far from exceptional, a recipe to construct further examples is given in Segers (2011). Furthermore, it should be remarked that conditions satisfied by a diagonal section are given in Erdely et al. (2013), Section 1, and existence of a copula with given diagonal section is recalled in their Theorem A. These considerations will be also useful in Section 4.3.1 about “Upper tail dependence”.

Let now $C_0, C_1, \ldots, C_d$, be Archimedean copulas with the same generator $\phi$. Then, using the model in Equation (8) we simply obtain an Archimedean copula of the corresponding dimension. Furthermore, if we assume equal arguments, i.e. $u_i = u = (u, \ldots, u)$ for all $i \in \{1, \ldots, d\}$, with $d_0 = d$, then we get the diagonal of this Archimedean copula. Using these two (trivial) considerations we introduce below the notion of self-nested diagonal of an Archimedean copula.

Lemma 3.1 (Self-nested diagonal of an Archimedean copula). If $C$ is an Archimedean copula associated with a generator $\phi$, then a family of self-nested diagonal of $C$ is defined at each order $r \in \mathbb{R}$ by

$$\delta_r(x) = \phi(d^r \cdot \phi^{-1}(x)), \quad \text{for } x \in (0, 1), r \in \mathbb{R}. \quad \square$$

Proof: We notice that $\delta_1(u) = \phi(d \cdot \phi^{-1}(u))$, so that $\delta_2(u) = \delta_1 \circ \delta_1(u) = \phi(d^2 \cdot \phi^{-1}(u))$, and we can show by induction that $\delta_k(u) = \phi(d^k \cdot \phi^{-1}(u))$ for all $k \in \mathbb{Z}$. For any $r \in \mathbb{R}$, we can easily check that setting $\delta_r(x) = \phi(d^r \cdot \phi^{-1}(x))$ is a discrete self-nested diagonal for any $r \in \mathbb{Z}$, and that $\delta_{r_1+r_2} = \delta_{r_1} \circ \delta_{r_2}$ for any $r_1, r_2 \in \mathbb{R}$. \quad \square

One can remark that the previous equation can be written $\phi^{-1} \circ \delta_r(x) = d^r \cdot \phi^{-1}(x)$ and corresponds to the Schröder’s equation. The set of all $\delta_n(x)$, for positive integers $n$, is also referred as the splinter or Picard sequence of $\delta_1(x)$ (see, e.g., Curtright and Zachos (2009)).

Consider an Archimedean copula with generator $\phi$ and diagonal $\delta_1$. Denote by $\delta_r$ the corresponding self-nested diagonals, for $r \in \mathbb{R}$. Under particular conditions, self-nested diagonals $\delta_r$ can be seen as diagonal sections of Archimedean copulas. Firstly, one can remark that, for $k \in \mathbb{N} \setminus \{0\}$, the self-nested diagonals $\delta_k$ can obviously be seen as diagonal sections of some Archimedean copulas with dimension $d^k$. In the case where $r > 0$, one can easily check that if $\phi(t) = \phi(t')$ is a valid generator in the dimension $d$, the function $\delta_r$ is the diagonal section of the Archimedean copula of generator $\phi$, in the dimension $d$. In particular, for $r \in (0, 1]$, $\phi(t) = \phi(t')$ is a generator of the outer (or exterior) power copula family (see Theorem 4.5.1.
in Nelsen (1999) in the bivariate case, and Theorem 8 in Hofert (2008) in the multivariate one). However, due to upper Fréchet-Hoeffding bound, any diagonal section is necessary below the identity function. This cannot be the case for the functions $\delta_r(x) = \phi(d^r \cdot \phi^{-1}(x))$ when $r < 0$. Self-nested diagonals $\delta_r$ thus cannot be seen as diagonal sections of any copula when $r < 0$.

**Remark 4** (Some expressions of self-nested diagonals). We give here some expressions of self-nested diagonals for some classical copulas that will be considered in numerical illustrations (Section 4.3).

- If $C$ is the independence copula of generator $\phi(t) = \exp(-t)$, then $\delta_r(u) = u^{(d^r)}$.
- If $C$ is a Gumbel copula of generator $\phi(t) = \exp(-t^{1/\theta})$, then $\delta_r(u) = u^{(d^r/\theta)}$, $\theta \geq 1$.
- If $C$ is a Clayton copula of generator $\phi(t) = (1 + \theta t)^{-1/\theta}$, $\delta_r(u) = (1 + d^r(t^{1-\theta} - 1))^{-1/\theta}$, $\theta \in \mathbb{R}^+ \setminus \{0\}$.

From Lemma 3.1 one can obtain the following expression for the self-nested diagonals $\delta_r$ using an interpolation procedure of the discrete self-nested diagonals $\delta_k$.

**Lemma 3.2** (Interpolation of self-nested diagonals). Let $C$ be an Archimedean copula with generator $\phi$. For any real $r \in [k, k + 1)$, $k \in \mathbb{Z}$, any family of self-nested diagonals of $C$ as in Lemma 3.1 satisfies:

$$\delta_r(x) = \phi \left( (\phi^{-1} \circ \delta_k(x))^{1-\alpha} (\phi^{-1} \circ \delta_{k+1}(x))^\alpha \right), \quad , x \in [0, 1],$$

with $\alpha = r - \lfloor r \rfloor$ and $k = \lfloor r \rfloor$, where $\lfloor r \rfloor$ denotes the integer part of $r$.

**Proof:** Consider an Archimedean copula $C$ and an associated family of self-nested diagonals $\delta_r$, for $r \in \mathbb{R}$. By Lemma 3.1, $\delta_r(x) = \phi(d^r \cdot \phi^{-1}(x))$. Define $g_r(x) = r \log d - \log \phi^{-1} \circ \delta_r(x)$. One can easily check that for all $r \in \mathbb{R}$, $g_r(x) = -\log \phi^{-1}(x)$ does not depend on $r$, so that in particular for any $k_1, k_2 \in \mathbb{Z}$ and $\alpha \in [0, 1]$,

$$g_r(x) = (1-\alpha)g_{k_1}(x) + \alpha g_{k_2}(x).$$

When $(1-\alpha)k_1 + \alpha k_2 = r$, this is equivalent to

$$\log \phi^{-1} \circ \delta_r(x) = (1-\alpha) \log \phi^{-1} \circ \delta_{k_1}(x) + \alpha \log \phi^{-1} \circ \delta_{k_2}(x),$$

and the result holds for any $k_1, k_2 \in \mathbb{Z}$ and $\alpha \in [0, 1]$ such that $(1-\alpha)k_1 + \alpha k_2 = r$.

In practice, the interpolation in Lemma 3.2 aims at being used even when $g_k(x)$ is not a constant function of $k$ (e.g. if $g_k$ is estimated, or if the copula is not Archimedean) or when $\phi$ is approximated. For this reason we present it in the particular case where $k_1 = \lfloor r \rfloor$ and $k_2 = \lfloor r \rfloor + 1$. The choice of $\alpha = r - \lfloor r \rfloor$ follows from the condition $(1-\alpha)k_1 + \alpha k_2 = r$, and also ensures that interpolations (9) and (10) are correct for any $r \in \mathbb{R}$, even if $g_r(x)$ is not a constant function of $r$. □

We present in the following a corollary result of Lemma 3.2 in the family of Gumbel-Hougaard copulas.

**Corollary 3.1** (Interpolation in the Gumbel or Independence case). If $C$ is a Gumbel copula with generator $\phi(t) = \exp(-t^{1/\theta})$, for $\theta \geq 1$, then $\delta_r$ can be expressed as a function of $\delta_k$ and $\delta_{k+1}$, and this function does not depend on the parameter $\theta$ of the copula:

$$\delta_r(x) = \exp \left( - (\log \delta_k(x))^{1-\alpha} (\log \delta_{k+1}(x))^\alpha \right), \quad , x \in [0, 1],$$

with $\alpha = r - \lfloor r \rfloor$ and $k = \lfloor r \rfloor$, where $\lfloor r \rfloor$ denotes the integer part of $r$. This result includes also the case of the independent copula, i.e. the Gumbel copula with parameter $\theta = 1$.

In a further estimation section we will use interpolation functions (see Section 4). The interpolation functions satisfying interpolation properties of Lemma 3.2 or Corollary 3.1 will be called perfect interpolation functions, as stated in the following definition.

**Definition 3.3** (Perfect interpolation functions). Let $C$ be an Archimedean copula with generator $\phi$, and $\delta_r$, $r \in \mathbb{R}$ an associated family of self-nested diagonals. A function $z$ is said to be a perfect interpolation function for the copula $C$ if for all $r \in \mathbb{R}$,

$$\delta_r(x) = z \left( (\log \delta_k(x))^{1-\alpha} (\log \delta_{k+1}(x))^\alpha \right), \quad , x \in [0, 1],$$
with \( \alpha = r - \lfloor r \rfloor \) and \( k = \lfloor r \rfloor \), where \( \lfloor r \rfloor \) denotes the integer part of \( r \). As an example, from Lemma 3.2, \( z(x) = \phi(x) \) and \( z(x) = \phi(d^x) \), \( a \in \mathbb{R}^+ \setminus \{0\} \) are perfect interpolation functions. If \( C \) is an Gumbel copula, from Corollary 3.1, \( z(x) = \exp(-x) \) is a perfect interpolation function which does not depend on the parameter of the copula.

**Remark 5** (Identifiability problem). As remarked in Alsina et al. (2006), the diagonal section is not always sufficient to fully determinate an Archimedean copula or its generator, and it may happen that two distinct generators lead to the same diagonal sections. However, one will see that a family of self-nested diagonals is sufficient to fully determinate an Archimedean copula. One may recall here that extended distinct generators lead to the same diagonal sections. However, one will see that a family of self-nested diagonals are not only derived from discrete self-nested diagonal, and thus not only deriving diagonals is sufficient to fully determinate an Archimedean copula. One may recall here that extended self-nested diagonals are not only derived from discrete self-nested diagonal, and thus not only deriving from a diagonal section. One interpolation function is also involved, which is sufficient to ensure the uniqueness of the generator given a whole family of extended self-nested diagonal. As an example, if we select an equivalent generator such that \( \phi(t_0) = \varphi_0 \) for given constants \((t_0, \varphi_0) \in (0, \infty) \times (0, 1)\), then one easily see that \( \delta_r(x) = \phi(d^r \varphi^{-1}(x)) \), so that \( \delta_r(\varphi_0) = \phi(d^r t_0) \), and thus \( \phi(t) = \delta_{\rho(t)}(\varphi_0) \), with \( \rho(t) \) such that \( d^\rho(t_0) = t \).

### 3.2 New expressions of transformations and generators using self-nested diagonals

In this section we present the main result of this paper, i.e. some expressions for the transformations \( T \) (see Proposition 3.1) and for the generators \( \phi \) (see Proposition 3.2 and Corollary 3.2) for Archimedean copulas using the notion of self-nested diagonal previously introduced and discussed in Section 3.1. The expressions introduced below will play a central role in the non-parametric estimation of the associated quantities \((T, \phi)\) (see Section 4).

**Lemma 3.3** (All points of transformation \( T \)). Let \( C_0 \) be an initial Archimedean copula and \( \tilde{C}(u_1, \ldots, u_2) = T \circ C_0(T^{-1}(u_1), \ldots, T^{-1}(u_d)) \) a transformed copula. Let \( \delta_r \) and \( \delta_{\tilde{r}}, r \in \mathbb{R} \), be the two respective self-nested diagonal families of \( C_0 \) and \( \tilde{C} \), as defined in Lemma 3.1. If \( T(x_0) = y_0 \), then \( T(x_r) = y_r \) for all \( r \in \mathbb{R} \), with

\[
\begin{align*}
  x_r &= \delta_r(x_0), \\
  y_r &= \tilde{\delta}_r(y_0).
\end{align*}
\]

**Proof:** Denote by \( \phi \) and \( \tilde{\phi} \) the respective generators of \( C_0 \) and \( \tilde{C} \), where \( \tilde{C}(u, \ldots, u) = T \circ C_0(T^{-1}(u), \ldots, T^{-1}(u)) \). If \( C_0 \) is an Archimedean copula, then \( \delta_r(u) = \phi(d^r \delta^{-1}(u)) \). Since \( \tilde{\phi} = T \circ \phi \), we have \( \tilde{\delta}_r(u) = T \circ \phi(d^r \phi^{-1} \circ T^{-1}(u)) \), so that for all \( u \in [0, 1] \),

\[
T^{-1} \circ \tilde{\delta}_r(u) = \delta_r \circ T^{-1}(u).
\]

From Lemma 2.2, one can choose a transformation within its equivalence class, passing through a point \((x_0, y_0)\). This is equivalent to choose a generator within its equivalence class. Then, setting \( u = y_0 \), we get \( T^{-1} \circ \tilde{\delta}_r(y_0) = \delta_r(x_0) \) since \( T^{-1}(y_0) = x_0 \), and \( T \) is passing through the point \((\delta_r(x_0), \tilde{\delta}_r(y_0))\) for any \( r \in \mathbb{R} \). □

The following result provides an expression for the transformations \( T \) of Archimedean copulas in terms of the self-nested diagonals.

**Proposition 3.1** (Transformation \( T \) using self-nested diagonals). Consider an Archimedean copula \( C_0 \) and a transformed copula \( \tilde{C} \), such that \( \tilde{C}(u_1, \ldots, u_d) = T \circ C_0(T^{-1}(u_1), \ldots, T^{-1}(u_d)) \). Consider the two associated families of self-nested diagonals \( \delta_r \) and \( \delta_{\tilde{r}}, r \in \mathbb{R} \) as defined in Lemma 3.1. If \( T(x_0) = y_0 \), then \( T \) is such that \( T(0) = 0, T(1) = 1 \) and for all \( x \in (0, 1) \),

\[
T(x) = \tilde{\delta}_r(x_0)(y_0),
\]

with \( r(x) \) such that \( \delta_r(x_0) = x \),

where \((x_0, y_0) \in (0, 1)^2 \) can be arbitrarily chosen. In the case where \( C_0 \) is the independence copula,

\[
r(x) = \frac{1}{\ln d} \ln \left( -\frac{\ln x}{\ln x_0} \right).
\]
that the copula of \( \widetilde{\phi} \) associated family of self-nested diagonals \( \tilde{\delta}_r \), for \( r \in \mathbb{R} \), as defined in Lemma 3.1. Assume that the copula \( \widetilde{C} \) is reachable by transforming an initial Archimedean copula \( C_0 \) with a strict generator \( \phi \). Then the generator \( \tilde{\phi} \) of \( \widetilde{C} \) is such that, for all \( t \in \mathbb{R}^+ \setminus \{0\} \),

\[
\tilde{\phi}(t) = \frac{1}{\ln - \frac{t}{\ln \phi(x_0)}}.
\]

where \( (x_0, y_0) \in (0,1)^2 \) can be arbitrarily chosen. This expression does only depend on \( \phi \) via the constant \( t_0 = \phi^{-1}(x_0) \). In particular, choosing an initial copula \( C_0 \) and constants \( (x_0, y_0) \) in \( (0,1)^2 \) can be simply reduced to the choice of \( (t_0, \varphi_0) \in \mathbb{R}^+ \setminus \{0\} \times (0,1) \) such that \( \phi(t_0) = \varphi_0 \), with \( t_0 = \phi^{-1}(x_0) \) and \( \varphi_0 = y_0 \).

\textbf{Proof:} Denote by \( \delta_r \), \( r \in \mathbb{R} \), the family of self-nested diagonals of \( C_0 \). By Proposition 3.1 and from \( \tilde{\phi} = T \circ \phi \) (see Remark 1), we can show that \( \tilde{\phi}(t) = \tilde{\delta}_{\rho(t)}(y_0) \), with \( \rho(t) \) such that \( \tilde{\delta}_{\rho(t)}(x_0) = \phi(t) \). Since \( \delta_r(t) = \phi(d\phi^{-1}(t)) \) (see Lemma 3.1), the result holds. \( \square \)

In particular, a suitable generator \( \tilde{\phi} \) is passing through the points

\[
\{(t_r, \varphi_r)\}_{r \in \mathbb{R}} = \left\{ (\phi^{-1} \circ \delta_r(x_0), \tilde{\delta}_r(y_0)) \right\}_{r \in \mathbb{R}}.
\]

If \( \tilde{C} \) is transformed from an independent copula, the suitable generator \( \tilde{\phi} \) is passing through the points

\[
\{(t_r, \varphi_r)\}_{r \in \mathbb{R}} = \left\{ (-d\ln x_0, \tilde{\delta}_r(y_0)) \right\}_{r \in \mathbb{R}}.
\]

Furthermore, if \( \tilde{C} \) is an independent copula, \( \tilde{\delta}_1(u) = u^d \) and \( \tilde{\delta}_r(u) = u^{(d')} \), so that we can easily retrieve

\[
\tilde{\phi}(t) = \exp \left( -\frac{\ln y_0}{\ln x_0} t \right),
\]

which is an equivalent generator of the independence generator \( \phi(t) = \exp(-t) \). From Proposition 3.2 one can easily obtain the following result.

\textbf{Corollary 3.2} (Generator \( \tilde{\phi} \) using self-nested diagonals). Consider an Archimedean copula \( \tilde{C} \) and the associated family of self-nested diagonals \( \tilde{\delta}_r \), for \( r \in \mathbb{R} \), as defined in Lemma 3.1. Denote by \( \tilde{\phi} \) a generator of \( \tilde{C} \). If one assumes furthermore that \( \tilde{\phi}(t_0) = \varphi_0 \), for a given couple of values \( (t_0, \varphi_0) \in \mathbb{R}^+ \setminus \{0\} \times (0,1) \), then the generator \( \tilde{\phi} \) of \( \tilde{C} \) can be written, for all \( t \in \mathbb{R}^+ \setminus \{0\} \),

\[
\tilde{\phi}(t) = \frac{1}{\ln - \frac{t}{\ln \tilde{\phi}(x_0)}}.
\]

\textbf{Proof:} By Lemma 2.1, one can choose one unique equivalent generator such that \( \tilde{\phi}(t_0) = \varphi_0 \). From Proposition 3.2, the result holds directly for a transformed Archimedean copula, since the choice of an initial copula is equivalent to the choice of the constant \( t_0 \). One can also easily check that the result obviously holds for any Archimedean copula since \( \tilde{\phi}(\varphi_0) = \phi(d\phi^{-1}(\varphi_0)) \), for any \( r \in \mathbb{R} \). \( \square \)
4 Non-parametric estimation

4.1 Estimators of transformations and generators

We aim here at finding non-parametric estimators of the generator of a transformed Archimedean copula, when non-parametric shape for the associated generator is assumed, and of the associated transformation $T$. Starting from results of Section 3 for Archimedean families of copulas, we provide some straightforward estimators and some convergence properties of these estimators.

We assume that an estimator of the diagonal of the copula $\delta_1(u) := C(u, \ldots, u)$ and an estimator of the inverse function $\delta_{-1}$ of $\delta_1$ are available. We denote respectively $\hat{\delta}_1$ and $\hat{\delta}_{-1}$ these estimators.

Remark that some consistent estimators for $\delta_1$ and $\delta_{-1}$ are provided in the literature. Deheuvels (1979) investigated the consistency of the empirical copula $\hat{C}$ and Deheuvels (1980) obtained the exact law and the limiting process of $\sqrt{n}(\hat{C} - C)$ when the two margins are independent. Fermanian et al. (2004) extended these results by proving the weak convergence of the process in a more general case. Relevant papers related to the convergence of empirical copula process are also Rüschendorf (1976) and Segers (2012).

Remark 6 (Deheuvels empirical copula estimator). In the literature one can find some different estimators for $\delta_1(u)$. One possible choice is represented by the rank-based estimate proposed of instance by Deheuvels (1979) or by Fermanian et al. (2004). Let $X_j = (X_{j,1}, \ldots, X_{j,d})$, for $1 \leq j \leq n$ be $d$-dimensional sample. Since we work under unknown margins $F_i$, we consider the pseudo-observation based on the ranks of $X_{j,i}$

$$R^n_{j,i} = n \hat{F}_i(X_{j,i}),$$

where $\hat{F}_i$ is the empirical marginal distribution, i.e., $\hat{F}_i(x_i) = \frac{1}{n} \sum^n_{j=1} 1_{[\infty, x_i]}(X_{j,i})$ (see, for instance, Section 3 in Hofert et al. (2011)). Then, in this setting, we get for instance, for $u \in (0,1)$,

$$\hat{\delta}_1(u) = \frac{1}{n} \sum^n_{j=1} 1_{\left(R^n_{j,1} \leq n u, \ldots, R^n_{j,d} \leq n u\right)}.$$ 

However many other possible estimators, including smooth estimators, are available in the literature, see for example Omelka et al. (2009).

In the following, we detail how to build non-parametric estimators of some transformations and of the generator of an Archimedean copula. The methodology is the following one: we start from an empirical copula, which is based only on the data, as seen in the previous Remark 6. This empirical copula does not use any knowledge on the parametric form of the copula or on the underlying margins. Indeed the margins are non-parametrically estimated and thus replaced by pseudo-observations. All following estimations of transformations of non-parametric Archimedean copula rely only on this empirical copula, and thus do not use the underlying parametric structure of margins or joint distribution; they only rely on the data.

We first show how to build estimators of a whole family of self-nested diagonals $\{\delta_r\}_{r \in \mathbb{R}}$ using these two estimators $\hat{\delta}_1$ and $\hat{\delta}_{-1}$.

Definition 4.1 (Estimation of self-nested diagonals). Consider a copula $C$ as in Definition 3.1. Let $\hat{\delta}_1$ be an estimator of $\delta_1$, and $\hat{\delta}_{-1}$ be an estimator of the inverse function $\delta_{-1}$. Estimators of $\delta_k$ and $\delta_{-k}$ can be obtained for any $k \in \mathbb{N} \setminus \{0\}$ by setting

$$\begin{align*}
\hat{\delta}_k(u) &= \hat{\delta}_1 \circ \ldots \circ \hat{\delta}_1(u), \quad (k \text{ times}) \\
\hat{\delta}_{-k}(u) &= \hat{\delta}_{-1} \circ \ldots \circ \hat{\delta}_{-1}(u), \quad (k \text{ times}) \\
\hat{\delta}_0(u) &= u.
\end{align*}$$

(11)

At any order $r \in \mathbb{R}$, an estimator $\hat{\delta}_r$ of $\delta_r$ is

$$\hat{\delta}_r(x) = z \left( z^{-1} \circ \hat{\delta}_k(x) \right)^{1-\alpha} \left( z^{-1} \circ \hat{\delta}_{k+1}(x) \right)^{\alpha}, \quad x \in [0,1],$$

(12)
with $\alpha = r - |r|$ and $k = |r|$, where $|r|$ denotes the integer part of $r$, and where $z$ is a strictly monotone function driving the interpolation, ideally the generator of the considered copula $C$ or any other perfect interpolation function (see Definition 3.3). In particular, $z$ is such that for any $x \in [0,1]$, $z(x) \geq 0$. Note that several interpolation functions may lead to the same interpolation, e.g. $z_1(x)$ and $z_2(x) = z_1(x^n)$, $\alpha \in \mathbb{R}^+ \setminus \{0\}$ are both involving the same interpolation. Such interpolators will be called equivalent interpolators.

This estimation is a plug-in estimation relying on Definition 3.1 and Lemma 3.2. The function $z$ drives the interpolation of $\delta_r$, for $r \in \mathbb{R}$, knowing values of $\delta_k$, for $k \in \mathbb{Z}$. If known, the best choice is the generator $\phi$ of the copula $C$, i.e. $z(x) = \phi(x)$. Otherwise, the identity function $z(x) = x$ (linear interpolation) could be possible, for $x \in [0,1]$. However we recommend, in case of positive dependence, the interpolator $z(x) = \exp(-x)$, $x \in (0,1]$, since it is the best choice for any independence or Gumbel copula, whatever the parameter of the copula, as a consequence of Corollary 3.1.

Using Definition 4.1 we now present two results to easily estimate non-parametrically the transformation $T$ (Definition 4.2) and the generator of an Archimedean copula (Definition 4.3). These two results come down directly from the expressions for the transformations (see Proposition 3.1) and for the generators (see Corollary 3.2) of Archimedean copulas using the notion of self-nested diagonals.

**Definition 4.2 (Non-parametric estimation of a transformation $T$).** Consider two Archimedean copulas $C_0$ and $\tilde{C}$ and their respective self-nested diagonals $\delta_r$ and $\tilde{\delta}_r$, for $r \in \mathbb{R}$. Assume that $\tilde{C}$ is the transformed copula using transformation $T$ and initial copula $C_0$. Denote by $\tilde{\delta}_r$ an estimator of $\delta_r$, for $r \in \mathbb{R}$. A non-parametric estimator of $T$ is defined by $\tilde{T}(0) = 0$, $\tilde{T}(1) = 1$ and for all $x \in (0,1)$ by

$$\tilde{T}(x) = \tilde{\delta}_{r(x)}(y_0),$$

with $r(x)$ such that $\delta_{r(x)}(x_0) = x$,

where $(x_0, y_0) \in (0,1)^2$ can be arbitrarily chosen. In the case where the initial copula $C_0$ is the independence copula, then

$$r(x) = \frac{1}{\ln d} \ln \left( \frac{-\ln x}{-\ln x_0} \right).$$

In particular, the estimator $\tilde{T}$ is passing through the points

$$\{(x_k, y_k)\}_{k \in \mathbb{Z}} = \{ (\delta_k(x_0), \tilde{\delta}_k(y_0)) \}_{k \in \mathbb{Z}}.$$

Remark that no interpolation function $z$ is needed to get $(x_k, y_k)$, for $k \in \mathbb{Z}$.

**Definition 4.3 (Non-parametric estimation of a generator $\tilde{\phi}$).** Consider an Archimedean copula $\tilde{C}$ and associated self-nested diagonals $\tilde{\delta}_r$, for $r \in \mathbb{R}$. Denote by $\tilde{\delta}_r$ the estimator of $\tilde{\delta}_r$, for $r \in \mathbb{R}$. Assume that $\tilde{\phi}(t_0) = \varphi_0$, for a given couple of values $(t_0, \varphi_0) \in \mathbb{R}^+ \setminus \{0\} \times (0,1)$. A non-parametric estimator $\tilde{\phi}$ of $\tilde{\phi}$ is defined by $\tilde{\phi}(0) = 1$ and for all $t \in \mathbb{R}^+ \setminus \{0\}$,

$$\tilde{\phi}(t) = \tilde{\delta}_{\rho(t)}(\varphi_0),$$

with $\rho(t) = \frac{1}{\ln d} \ln \left( \frac{t}{\varphi_0} \right)$,

where $(t_0, \varphi_0) \in \mathbb{R}^+ \setminus \{0\} \times (0,1)$ can be arbitrarily chosen.

In particular, the estimator $\tilde{\phi}$ of $\tilde{\phi}$ is passing through the points

$$\{(t_k, \varphi_k)\}_{k \in \mathbb{Z}} = \{ (d^k t_0, \tilde{\delta}_k(\varphi_0)) \}_{k \in \mathbb{Z}}.$$

Remark that no interpolation function $z$ is needed to get $(t_k, \varphi_k)$, for $k \in \mathbb{Z}$. 

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Assume we have realizations of i.i.d. d-dimensional random vectors. Assume the margins to be continuous and the corresponding copula to be Archimedean. We call Φ the generator associated to \( \hat{C} \). We aim now at providing a non-parametric estimator \( \hat{\phi} \) of \( \Phi \). Using Definitions 4.1-4.3, we directly get an expression for this estimator. Definition 4.2 can also be used to estimate the required transformation \( T \) to transform an initial Archimedean copula \( C_0 \) into \( \hat{C} \).

However, estimating the whole functions \( \Phi \) and \( T \) using some pre-calculations may avoid repeating some steps. Algorithms 1 and 2 show how to store some quantities in order to get readily calculable estimators of \( T \) and \( \Phi \). Some details on the choice of input parameters are summarized in Remark 7 below.

**Remark 7** (On input parameters). We summary here remarks in order to help the choice of initial parameters of the estimation procedure. Unless explicitly mentioned, all proposed default values are those that will be used in our numerical illustrations (see Section 4.3).

- \((x_0, y_0)\) and \((t_0, \varphi_0)\) are arbitrary values respectively in \((0,1)^2\) and \(\mathbb{R}^+ \setminus \{0\} \times (0,1)\), e.g. \(x_0 = y_0 = e^{-1}\) and \(t_0 = 1, \varphi_0 = e^{-1}\). The role of these constants is to select a generator among all equivalent generators. See Remark 8 for more details.

- \(k_{\min}, k_{\max}\) in \(\mathbb{Z}\), indicate a pre-calculation range, e.g. \(k_{\min} = -20, k_{\max} = 20\). As an example, using this small range of 41 values, \(\hat{\phi}(t)\) will rely on pre-calculated values as soon as \(t \in [10^{-6}, 10^6]\) (case \(d = 2\), \(t_0 = 1\)).

- \(C_0\) and \(\Phi\) are the initial Archimedean copula and its associated generator e.g. Independence copula, with \(\hat{\phi}(t) = \exp(-t)\). They are used for the estimation of the transformation \(T\). In the further numerical section, we will see that, on considered data, we get satisfying fits of some multivariate distributions starting from the independence copula. Concerning the impact of the choice of the initial copula \(C_0\) on the transformed copulas, we refer the interested reader to Section 2.3 in Di Bernardino and Rullière (2013). Remark that initial Archimedean copula \(C_0\) is such that the associated \(\delta_\phi\) is known (see Definition 4.2 and Table 2 in Annex).

- \(z(x), x \in \mathbb{R}\), is an interpolation function e.g. \(z(x) = \exp(-x)\). In the further numerical section, we will see that the impact of this choice is quite limited (with maximal relative errors below 1.5% in our applications, see Figure 4). As stated in Corollary 3.1, \(z(x) = \exp(-x)\) is a perfect interpolation function for any Gumbel copula. Another possible choice for \(z\) is an approximation of the generator of the copula, which will lead to a new estimation of this generator at a next step.

- \(\hat{\delta}_1(u)\) and \(\hat{\delta}_{-1}(u)\), for \(u \in [0,1]\), are respective estimators for \(\delta_1(u)\) and its inverse, e.g. the estimator of Deheuvels (1979), or a smooth version, see Remark 6. The problem of estimating the empirical copula (and thus of its diagonal section \(\delta_1\)) has been largely treated in the literature, a comparison of some estimators and some smooth versions are given for example in Omelka et al. (2009).

**Algorithm 1** Detailed procedure for non-parametric estimation of a transformation \(T\)

**Input parameters**

- Choose \(x_0, y_0\), arbitrary values in \((0,1)\), e.g. \(x_0 = y_0 = e^{-1}\)
- Choose \(k_{\min}, k_{\max}\) in \(\mathbb{Z}\), pre-calculation range, e.g. \(k_{\min} = -20, k_{\max} = 20\).
- Choose \(C_0\) and \(\Phi\), initial Archimedean copula and its associated generator, e.g. \(\hat{\phi}(t) = e^{-t}\) (independence).
- Choose \(z\), an interpolation function, e.g. \(z(x) = \exp(-x)\).
- Choose \(\hat{\delta}_1\), an estimator for \(\delta_1\), and its inverse \(\hat{\delta}_{-1}\), e.g. the one of Deheuvels (1979).

**Eventual pre-calculations**

- For \(k \in \{k_{\min}, \ldots, k_{\max}\}\), store \(\hat{\delta}_k(y_0)\) obtained by Equation (11),

**Estimation**

- Define the function \(\hat{\delta}_r(y_0)\) for any \(r \in \mathbb{R}\), using the chosen interpolation function \(z\), by Equation (12), using previous stored values when \(r \in [k_{\min}, k_{\max}]\), or using Equation (11) otherwise.

- Get \(\hat{T}(x)\) for any \(x \in [0,1]\), by Definition 4.2
Let \((\text{Equivalent theoretical generator passing through } (t_0, \varphi_0))\) for any \(r \in \mathbb{R}\), using the chosen interpolation function \(z\), by Equation (12), using previous stored values when \(r \in [k_{\min}, k_{\max}]\), or using Equation (11) otherwise.

Get \(\hat{\Phi}(t)\) for any \(t \in \mathbb{R}^+\), by Definition 4.3.

For a given Archimedean copula, there is a whole family of equivalent generators leading to this copula. As stated in Lemma 2.1, generators \(\phi_1(t)\) and \(\phi_2(t) = \phi_1(at)\) lead to the same copula function, whatever the choice of \(a > 0\). Then two different generators, \(\phi_1\) and \(\phi_2\), which lead to the same copula may have very different graphical shapes, so that a graphical comparison of these generators would have no sense. For these reasons, in Definition 4.3, one can force an estimated generator to pass through an arbitrarily chosen point \((t_0, \varphi_0)\). In the following Remark 8, we also give formulas in order to force a parametric generator to pass through this chosen point \((t_0, \varphi_0)\). This “standardization procedure” will be a first step to compare different generators. However, comparing graphically different generators is a not trivial task. Indeed, as detailed in Section 4.3.1 (“Upper tail dependence”), generators with close appearance but different right derivatives at 0 may lead to different types of asymptotic dependence (see for instance Figures 5-6). Furthermore, for sampling purposes, some algorithms require to invert a Laplace Transform but different right derivatives at 0 may lead to different types of asymptotic dependence (see Remark 8).

\textbf{Remark 8} (Equivalent theoretical generator passing through \((t_0, \varphi_0)\)). Let \((t_0, \varphi_0) \in \mathbb{R}^+ \setminus \{0\} \times (0,1)\).
Let \(\phi\) be a generator of an Archimedean copula. If one set for all \(t \in \mathbb{R}\)
\[
\tilde{\phi}(t) = \phi(at) \quad \text{with} \quad a = \frac{\phi^{-1}(\varphi_0)}{t_0}
\]
then \(\tilde{\phi}\) is an equivalent generator of \(\phi\) such that \(\tilde{\phi}(t_0) = \varphi_0\). This equation is equivalent to \(\tilde{\phi}(t) = \delta_{\phi(t)}(\varphi_0)\), with \(r(t)\) such that \(dr(t) = t/t_0\).

As an example, we give here some standardized generators passing through a given point \((t_0, \varphi_0)\):
- Standardized Gumbel generator: \(\tilde{\phi}(t) = \varphi_0^{(t/t_0)^{1/\theta}}, \theta \geq 1\). If \((t_0, \varphi_0) = (1, e^{-1})\), \(\tilde{\phi}(t) = \exp(-t^{1/\theta})\).
- Standardized independence generator: \(\tilde{\phi}(t) = \varphi_0^{(t/t_0)}\). If \((t_0, \varphi_0) = (1, e^{-1})\), \(\tilde{\phi}(t) = \exp(-t)\).
- Standardized Clayton generator: \(\tilde{\phi}(t) = \left(1 + (\varphi_0^{-\theta} - 1) \frac{t}{t_0}\right)^{-1/\theta}, \theta \in \mathbb{R}^+ \setminus \{0\}\). If \((t_0, \varphi_0) = (1, e^{-1})\), \(\tilde{\phi}(t) = (1 + (e^{\theta} - 1)t)^{-1/\theta}\).

Exact analytical formulas for standardized generators, their inverses and theoretical self-nested diagonals \(\delta_r\), in the case of most popular Archimedean families of copulas, are postponed in the Annex.

Remark that the tractable expression for the generator considered in this paper, based on the self-nested diagonal, allows us to easily force the generator to pass through an arbitrarily chosen point. This identifiability-problem of a generator in its equivalent class, under some multiplicative scaling factor (see Lemma 2.1), is not always an elementary problem. For example, for the non-parametric generator
recently proposed by Genest et al. (2011), forcing the generator to pass through a chosen point could be not trivial. We detail this problem in Section 4.3.

In numerical applications (see Section 4.3) we will consider generators passing through \((t_0, \varphi_0) = (1, e^{-1})\). In this case, applying Remark 8, standardized independence and Gumbel generators correspond to the usual Gumbel-generator (see Nelsen (1999)), and standardized Clayton generator becomes \(\tilde{\phi}(t) = (1 + (e^\theta - 1)t)^{-1/\theta}\) which is an equivalent generator of the usual generator \(\phi(t) = (1 + \theta t)^{-1/\theta}\).

4.2 Confidence bands

In this section our goal is to quantify the estimation error of the estimated generator \(\hat{\phi}\) in terms of the error of the estimation of \(\hat{\delta}_1\). To this aim, we proceed in the following way. Firstly, we assume to be able to quantify the estimation error of \(\hat{\delta}_1\) (see Assumption 4.1). From this assumption we derive the estimation error on any \(\hat{\delta}_r(u)\), for \(r \in \mathbb{R}\) (see Proposition 4.1). Finally, we use this last result to control the estimation error of \(\tilde{\phi}\) (see Proposition 4.1). Illustrations of these results, in the particular case of a Gumbel copula, are postponed in Section 4.3.

So, we consider the following assumption on the estimation error of \(\hat{\delta}_1\).

Let \(I\) be a range of \([0, 1]\). We denote \(I_k = \{u \in [0, 1], \hat{\delta}_k(u) \in I\}\), \(k \in \mathbb{Z}\), and \(I_r = I_k \cap I_{k+1}\) for \(k = \lfloor r \rfloor\), \(r \in \mathbb{R} \setminus \mathbb{Z}\). Since \(\delta_0(u) = u\) for all \(u \in [0, 1]\), \(I_0 = I\). In the following we show that confidence bands on \(\hat{\delta}_1(u)\) for all \(u \in I\) induce confidence bands on \(\hat{\delta}_r\) and on \(\tilde{\phi}(u)\). The stronger version, when \(I = [0, 1]\), induce stronger assumptions on \(\hat{\delta}_1\) and may induce larger confidence bands, so that a weaker version, when \(I \subset [0, 1]\) can be useful to get confidence bands of estimators of \(T\) and \(\phi\) on restricted range of values.

**Assumption 4.1 (Estimation error on \(\hat{\delta}_1\)).** For a copula \(\tilde{C}\) as in Definition 3.1, denote \(\hat{\delta}(u) = \hat{\delta}_1(u) = \tilde{C}(u, \ldots, u)\) and \(\delta(u) = \delta_1(u)\) an estimator of \(\tilde{C}\). There exists two nonnegative reals \(\epsilon^-\) and \(\epsilon^+\) and a continuous and strictly monotone function \(h\), from \([0, 1]\) to \(\mathbb{R}\), such that for any \(u \in I\),

\[
h^{-1} \circ L_{\epsilon^-} \circ h \circ \hat{\delta}(u) \leq \hat{\delta}(u) \leq h^{-1} \circ L_{\epsilon^+} \circ h \circ \hat{\delta}(u),
\]

(13)

where \(L_{\epsilon}(u) = \epsilon u\).

This kind of assumption allows a large variety of bounding of the quantity \(\hat{\delta}(u)\), for example:

- \(h(x) = \ln(x)\) leads to assuming \(\hat{\delta}(u)^{\epsilon^-} \leq \hat{\delta}(u) \leq \hat{\delta}(u)^{\epsilon^+}\), where obviously \(\epsilon^+ \leq 1 \leq \epsilon^-\).

- \(h(x) = x\) leads to assuming \(\hat{\delta}(u)^{\epsilon^-} \leq \hat{\delta}(u) \leq \hat{\delta}(u)^{\epsilon^+}\), where obviously \(\epsilon^- \leq 1 \leq \epsilon^+\).

- \(h(x) = \exp(x)\) leads to assuming \(\hat{\delta}(u) + \ln \epsilon^+ \leq \hat{\delta}(u) \leq \hat{\delta}(u) + \ln \epsilon^-\), where obviously \(\epsilon^- \leq 1 \leq \epsilon^+\).

Since this assumption may not be fulfilled in every possible situation, we consider in the following the probability that this assumption is fulfilled and we study the impact on confidence bands for self-nested diagonals.

**Lemma 4.1 (Estimation error on \(\hat{\delta}_r\), for \(r \in \mathbb{R}^+\)).** Consider an Archimedean copula \(\tilde{C}\) with generator \(\tilde{\phi}\). Denote by \(\hat{\delta}\) an estimator of \(\tilde{\delta}\). Denote by \(\tilde{\delta}_{r}\) (resp. \(\delta_r\)) the self-nested diagonal of \(\tilde{\delta}\) (resp. \(\delta\)). Assume that \(\hat{\delta}_{r}\) is interpolated with a perfect interpolation function in Definition 4.1. If the probability that \(\hat{\delta}\) satisfies Assumption 4.1, for the function \(h = \tilde{\phi}^{-1}\), is greater than a given threshold \(\eta \in [0, 1]\), i.e., if there exists reals \(g^-\) and \(g^+\) such that

\[
P \left[ \hat{\delta}_{g^-} \circ \hat{\delta}(u) \leq \hat{\delta}(u) \leq \hat{\delta}_{g^+} \circ \hat{\delta}(u), \forall u \in I \right] \geq \eta,
\]

(14)

then it holds for any \(r \in \mathbb{R}^+\) that

\[
P \left[ \hat{\delta}_{g^-} \circ \hat{\delta}_r(u) \leq \hat{\delta}_r(u) \leq \hat{\delta}_{g^+} \circ \hat{\delta}_r(u), \forall u \in I_r \right] \geq \eta.
\]

(15)
Proof: Assume that there exists a real $\varepsilon$ and such that for all $u \in I$,
\[
\tilde{\delta}(u) \leq h^{-1} \circ L_{\varepsilon} \circ h \circ \tilde{\delta}(u).
\] (16)

By Lemma 3.1, $\tilde{\delta}(u) = \tilde{\phi} \circ L_d \circ \tilde{\phi}^{-1}(u)$, with $L_d(u) = d \cdot u$. It follows
\[
\tilde{\delta}(u) \leq h^{-1} \circ L_{\varepsilon} \circ h \circ \tilde{\phi} \circ L_d \circ \tilde{\phi}^{-1}(u),
\]
and in the case where $h = \tilde{\phi}^{-1}$,
\[
\tilde{\delta}(u) \leq \tilde{\phi} \circ L_{\varepsilon,d} \circ \tilde{\phi}^{-1}(u).
\]

Since Equation (16) holds for any $u \in I$ then in particular for $u = \tilde{\delta}(u_1)$, $u_1 \in I_1$,
\[
\tilde{\delta} \circ \tilde{\delta}(u_1) \leq \tilde{\phi} \circ L_{\varepsilon,d} \circ \tilde{\phi}^{-1} \circ \tilde{\delta}(u_1) \leq \tilde{\phi} \circ L_{(\varepsilon,d)+} \circ \tilde{\phi}^{-1}(u_1).
\]

And, by induction for any $k \in \mathbb{N}^*$,
\[
\tilde{\delta}_k(uk) \leq \tilde{\phi} \circ L_{(\varepsilon,d)+} \circ \tilde{\phi}^{-1}(uk)
\]

holds for any value $u_k$ such that $\tilde{\delta}_k(u_k) = u$ with $u \in I$, that is for all $u_k \in I_k$.

Then
\[
\left[\tilde{\delta}(u) \leq \tilde{\phi} \circ L_{\varepsilon} \circ \tilde{\phi}^{-1} \circ \tilde{\delta}(u), \forall u \in I\right] \implies \left[\tilde{\delta}_k(u) \leq \tilde{\phi} \circ L_{(\varepsilon,d)+} \circ \tilde{\phi}^{-1}(u), \forall u \in I_k\right].
\] (17)

Setting $g^+ = \varepsilon$, from Lemma 3.1, we obtain $\tilde{\phi} \circ L_{(d,\varepsilon)+} \circ \tilde{\phi}^{-1}(u) = \tilde{\delta}_{kg^++k}$ and
\[
\left[\tilde{\delta}(u) \leq \tilde{\delta}_{g^+} \circ \tilde{\delta}(u), \forall u \in I\right] \implies \left[\tilde{\delta}_k(u) \leq \tilde{\delta}_{kg^+} \circ \tilde{\delta}_k(u), \forall u \in I_k\right].
\] (18)

Proceeding the same way for both inequalities, checking the result is obvious when $k = 0$, result in (18) holds for any $k \in \mathbb{N}$. Now assume that $z(x)$ is a perfect interpolation function (see Definition 3.3), $z(x)$ and $\tilde{\phi}(x)$ are equivalent interpolation functions, and both $\tilde{\delta}_r$ and $\tilde{\phi}_r$ are interpolated with the same interpolation function. Without loss of generality, assume $z(x)$ and $z^{-1}(x)$ are decreasing functions of $x$ (would they be increasing, there exists decreasing equivalent interpolation functions). Assume now that for any $k \in \mathbb{N}$, and for all $u \in I_k$, $\tilde{\delta}_{kg^{-}} \circ \tilde{\delta}_k(u) \leq \tilde{\delta}_k(u) \leq \tilde{\delta}_{kg^+} \circ \tilde{\delta}_k(u)$. Since $\delta_r$ and $\tilde{\delta}_r$ are interpolated by the same perfect interpolation function $z(x)$, then for any $\alpha \in [0,1]$, recalling $z^{-1}(x) \geq 0$ for any $x \in [0,1]$, as in Definition 4.1, for all $u \in I_k \cap I_{k+1}$

\[
\left(z^{-1} \circ \tilde{\delta}_{kg^{-}} \circ \tilde{\delta}_k(u)\right)^{1-\alpha} \geq \left(z^{-1} \circ \tilde{\delta}_k(u)\right)^{1-\alpha} \geq \left(z^{-1} \circ \tilde{\delta}_{kg^+} \circ \tilde{\delta}_k(u)\right)^{1-\alpha}
\]

\[
\left(z^{-1} \circ \tilde{\delta}_{(k+1)g^{-}} \circ \tilde{\delta}_{k+1}(u)\right)^{1-\alpha} \geq \left(z^{-1} \circ \tilde{\delta}_{k+1}(u)\right)^{1-\alpha} \geq \left(z^{-1} \circ \tilde{\delta}_{(k+1)g^+} \circ \tilde{\delta}_{k+1}(u)\right)^{1-\alpha}
\]

By Lemma 3.2, we get for any $g \in \mathbb{R}$, as in the proof of Lemma 3.2, if $(1-\alpha)(k+\alpha(k+1)) = r$, for all $u \in I_r$.

\[
z \left(\left(z^{-1} \circ \tilde{\delta}_{kg+k}(u)\right)^{1-\alpha} \left(z^{-1} \circ \tilde{\delta}_{(k+1)g+k+1}(u)\right)^{\alpha}\right) = \tilde{\delta}_{(1-\alpha)(kg+k)+\alpha((k+1)g+k+1)}(u) = \tilde{\delta}_{rg}(u)
\] (19)

Finally, setting $k = \lfloor r \rfloor$, and since $z$ is assumed to be decreasing, we get for all $u \in I_r$

\[
\tilde{\delta}_{rg^{-}} \circ \tilde{\delta}_r(u) \leq \tilde{\delta}_r(u) \leq \tilde{\delta}_{rg^+} \circ \tilde{\delta}_r(u)
\]

and the result holds. If $z(x)$ is not an equivalent interpolator as $\tilde{\phi}$, one easily check that the result still holds for integer values $r \in \mathbb{N}$. □

From Proposition 4.1, if all values of $\tilde{\delta}(u), u \in I$ are in a confidence band with a given confidence level $\eta$ (see (17)), then all values of $\tilde{\delta}_r(u), u \in I_r$ will be in a (larger) confidence band (see (18)), for $r \in \mathbb{R}^+$. These last results may be extended to the case where $r \in \mathbb{Z}^-$ or $r \in \mathbb{R}^-$ starting from a bounding assumption for $\tilde{\delta}_{-1}$. For the sake of simplicity, these extensions are omitted here. Using Proposition 4.1, we quantify in the following result the error for the estimated generator $\tilde{\phi}$.
Corollary 4.1. In the following, we apply Proposition 4.1 in the case of a Gumbel copula. then this implies the following bounding for \( \hat{\phi} \)

\[ \begin{align*}
\mathbb{P} \left[ \tilde{\delta}_{g} \circ \tilde{\delta}(u) \leq \tilde{\delta}(u) \leq \tilde{\delta}_{y} \circ \tilde{\delta}(u), \forall u \in I \right] & \geq \eta, \\
\mathbb{P} \left[ \tilde{\delta}_{y} \circ \tilde{\delta}_{-1}(u) \leq \tilde{\delta}_{-1}(u) \leq \tilde{\delta}_{y} \circ \tilde{\delta}_{-1}(u), \forall u \in I \right] & \geq \eta,
\end{align*} \]

(20)

then for all \( t \in \zeta(I) \), with \( \zeta(I) = \{ t \in \mathbb{R}, I_{p(t)(y_{0})} \in I \} \),

\[ \begin{align*}
\mathbb{P} \left[ \tilde{\delta}_{p(t)\gamma} \circ \tilde{\phi}(t) \leq \tilde{\phi}(t) \leq \tilde{\delta}_{p(t)\gamma} \circ \tilde{\phi}(t) \right] & \geq \eta, \quad \text{if } p(t) \geq 0, \\
\mathbb{P} \left[ \tilde{\delta}_{p(t)\gamma} \circ \tilde{\phi}(t) \leq \tilde{\phi}(t) \leq \tilde{\delta}_{p(t)\gamma} \circ \tilde{\phi}(t) \right] & \geq \eta, \quad \text{if } p(t) < 0,
\end{align*} \]

(21)

with \( \tilde{\phi}(t) = \tilde{\delta}_{p(t)}(\varphi_{0}) \) and \( p(t) = \frac{1}{\ln d} \ln \left( \frac{1}{\eta_{0}} \right) \), as in Definition 4.3, and \( (t_{0}, \varphi_{0}) \in \mathbb{R}^{+} \setminus \{ 0 \} \times (0, 1) \).

Proof: As a direct consequence of the Equation (18) in the proof of Proposition 4.1, in all cases where \( \delta_{g} \circ \delta(u) \leq \delta(u) \leq \delta_{y} \circ \delta(u), \forall u \in I \), we get \( \delta_{k_{g}} \circ \delta_{0}(u) \leq \delta_{k}(u) \leq \delta_{k_{y}} \circ \delta_{0}(u), \forall u \in I_{k} \). We can show that the same property holds for \( k \in \mathbb{R}^{+} \). If \( p(t) > 0 \), then in particular for \( k = \rho(t) \) and \( u = y_{0} \), we show that \( \tilde{\delta}_{g} \circ \delta(u) \leq \delta(u) \leq \delta_{y} \circ \delta(u), \forall u \in I \) implies \( \tilde{\delta}_{\rho(t)\gamma} \circ \phi(t) \leq \phi(t) \leq \tilde{\delta}_{\rho(t)\gamma} \circ \phi(t) \), for all \( t \) such that \( y_{0} \in I_{p(t)} \). Proceeding the same way when \( p(t) < 0 \), we get the final result. \( \square \)

Remark 9 (Integer values of \( p(t) \)). Remark that if in Proposition 4.1, the condition on the interpolation function \( z \) does not hold, the result is still available for any \( t \in \zeta(I) \) such that \( p(t) \in \mathbb{Z} \).

Since \( y_{0} \in I_{p(t)} \) is equivalent to \( \tilde{\delta}_{p(t)}(y_{0}) \in I \), then in this case where \( p(t) \in \mathbb{Z} \),

\[ t \in \zeta(I) \iff \tilde{\phi}(t) \in I \]

This last property gives direct confidence bounds for \( \tilde{\phi} \), depending on some constants \( g^{-}, g^{+}, \gamma^{-}, \gamma^{+} \).

One should notice that if the distribution of the process \( \{ \tilde{\delta}(u) \}_{0 \leq u \leq 1} \) is known, and if the family of targeted copula is known, then \( g^{-} \) and \( g^{+} \) can be computed at least numerically, e.g. by simulating paths of the process \( \{ \tilde{\delta}(u) \}_{0 \leq u \leq 1} \). If the family of targeted copulas is unknown, constants \( g^{-} \) and \( g^{+} \) and final confidence bounds can be estimated by replacing \( \tilde{\delta}_{\gamma}, r \in \mathbb{R} \), by their estimators. For example using results of Deheuvels (1980) and Fermanian et al. (2004), i.e. using the law and the limiting process of \( \sqrt{n}(\hat{C} - C) \), one can get suitable constants \( g^{-}, g^{+} \) and \( \gamma^{-}, \gamma^{+} \) for a given confidence level \( \eta \), and thus confidence bounds for \( \hat{\phi} \).

In the following, we apply Proposition 4.1 in the case of a Gumbel copula.

Corollary 4.1 (Estimation errors in the Gumbel case). Consider a Gumbel copula \( \hat{C} \) with generator \( \hat{\phi}(t) = \exp(-t^{1/\beta}) \), and set \( z(x) = \exp(-x) \) as interpolation function. We take as initial non-transformed copula the independent copula, and \( x_{0} = y_{0} = \exp(-1) \), (or equivalently \( t_{0} = 1, \varphi_{0} = \exp(-1) \), see Proposition 3.2). If there exist some reals \( \alpha^{-}, \alpha^{+}, \beta^{-}, \beta^{+} \) such that \( \tilde{\delta}_{\beta} \) and \( \tilde{\delta}_{-1} \) satisfies

\[ \begin{align*}
\mathbb{P} \left[ \tilde{\delta}(u)_{\alpha^{-}} \leq \tilde{\delta}(u) \leq \tilde{\delta}(u)_{\alpha^{+}}, \forall u \in I \right] & \geq \eta, \\
\mathbb{P} \left[ \tilde{\delta}_{-1}(u)_{\beta^{-}} \leq \tilde{\delta}_{-1}(u) \leq \tilde{\delta}_{-1}(u)_{\beta^{+}}, \forall u \in I \right] & \geq \eta,
\end{align*} \]

then this implies the following bounding for \( \tilde{\phi} \), for all \( t \in \zeta(I) \),

\[ \begin{align*}
\mathbb{P} \left[ \tilde{\phi}(t)(\lambda^{-}) \leq \tilde{\phi}(t) \leq \tilde{\phi}(t)(\lambda^{+}) \right] & \geq \eta, \quad \text{if } t \geq 1, \\
\mathbb{P} \left[ \tilde{\phi}(t)(\mu^{-}) \leq \tilde{\phi}(t) \leq \tilde{\phi}(t)(\mu^{+}) \right] & \geq \eta, \quad \text{if } t < 1,
\end{align*} \]

(22)

with \( \lambda^{-} = \frac{\ln \alpha^{-}}{\ln d}, \lambda^{+} = \frac{\ln \alpha^{+}}{\ln d} \) and with \( \mu^{-} = \frac{\ln \beta^{-}}{\ln d}, \mu^{+} = \frac{\ln \beta^{+}}{\ln d} \).
Proof: By direct application of Proposition 4.1, setting \( \alpha^- = d(\theta^- / \theta) \) and \( \alpha^+ = d(\theta^+ / \theta) \), and using Remark 4, that gives in the Gumbel case \( \delta_\kappa(u) = u^{(\theta^- / \theta)} \), we obtain (e.g. when \( k > 0 \))

\[
\mathbb{P}\left[ \hat{\delta}_k(u)^{\alpha^-} \leq \hat{\delta}_k(u) \leq \tilde{\delta}_k(u)^{\alpha^+}, \forall u \in I_k \right] \geq \eta, \quad k \in \mathbb{N}. \tag{23}
\]

The bounding on \( \hat{\phi} \) holds by application of Proposition 4.1. In the case where \( C \) is an independent copula and \( x_0 = y_0 = e^{-1} \), \( \rho(t) = \ln t / \ln d \), so that \( \hat{\delta}(t) = u^{(\theta^- / \theta)} \), and \( \theta^+ = \ln \alpha^+ / \ln d \). Hence the result. \( \square \)

As expected, there is no uncertainty when \( t \) is in a neighbourhood of \( t_0 = 1 \), since transformations are here chosen such that \( (x_0, y_0) = e^{-1} \), implying that \( \phi(t_0) = \varphi_0 \) with \( (t_0, \varphi_0) = (1, e^{-1}) \).

These results (Proposition 4.1 and Corollary 4.1) are theoretical results. In practice, it is not trivial to choose constants such as \( \alpha^- \), \( \alpha^+ \), \( \beta^- \), \( \beta^+ \). One can propose two ways for trying to determine such constants:

- The theoretical way: for given values \( \alpha^- \), \( \alpha^+ \), \( \beta^- \), \( \beta^+ \), when the joint law of the whole empirical process \( \{\hat{\delta}(u), u \in [0, 1]\} \) is given, probabilities in Equation (22) can be calculated explicitly, so that sets of constants such that this assumption is fulfilled can be determined precisely. However, even when results on this process \( \{\hat{\delta}(u), u \in [0, 1]\} \) are available (see Rüschendorf (1976), Feramzian et al. (2004), Segers (2012)), it is not easy to calculate these probabilities, and would require more theoretical analysis.

- The numerical way: it is possible to randomly draw some paths of an empirical copula (e.g. when the copula is given). For given coefficients \( \alpha^- \), \( \alpha^+ \), \( \beta^- \), \( \beta^+ \), it is possible to estimate the probability in Equation (22), and to select coefficients leading to a target probability level. This can be time consuming, since we both have to simulate paths and to find coefficients leading to a target probability level. For some usual Archimedean copulas like the Gumbel copula, requiring that \( \hat{\delta}(u)^{\alpha^-} \leq \hat{\delta}(u) \leq \hat{\delta}(u)^{\alpha^+} \) for all \( u \in I \) is requiring that \( a(u) = \ln \hat{\delta}(u) / \ln \delta(u) \) is belonging to the interval \([\alpha^-, \alpha^+]\) for all \( u \) in the given subinterval \( I \) of \([0, 1]\). By drawing one or several trajectories of \( a(u) \), we can interpret more clearly the meaning of these coefficients (see Figure 1).

A precise estimation of coefficients \( \alpha^- \), \( \alpha^+ \), \( \beta^- \), \( \beta^+ \) is still to be investigated, and illustrations such as further Figures 7-8 mainly aim at showing the theoretical link between estimation errors of \( \hat{\delta}(u) \) and estimation errors of \( \hat{\phi}(u) \), not at providing the best confidence bands for \( \hat{\phi}(u) \).

### 4.3 Numerical illustrations

In this section we provide some numerical illustrations of the proposed non-parametric estimation procedure for the transformation \( T \) (Definition 4.2) and the generator \( \phi \) (Definition 4.3). The impact of the choice of the function \( z \) driving the interpolation is also analyzed (see Definition 4.1). Furthermore, we estimate the diagonal of the copula \( \delta_i(u) \) := \( C(u, \ldots, u) \) and its inverse function \( \delta_{-1} \) using the consistent empirical copula \( \hat{C} \) in Deheuvels (1979).

#### 4.3.1 Simulated data illustration

**Estimation of a self-nested diagonal**

In Figure 2 we provide an illustration of the estimation of self-nested diagonals (see Definition 4.1): we generate a sample of size \( n = 1500 \) from a Clayton copula with parameter \( \theta = 6 \) (left) or a Gumbel copula with parameter \( \theta = 3 \) (right). We consider \( k = -3, -2, -1, 0, 1, 2, 3 \) and we estimate the self-nested diagonal \( \delta_k(u) \), for \( u \in [0, 1] \).

**Estimation of the transformation \( T \)**

Following Definition 4.2, in Figure 3 we have drawn the non-parametric estimation for the transformation \( T \) starting from the independence initial copula \( C_0 \), i.e. \( \hat{T}(x) = \hat{\delta}_{r(x)}(y_0) \), with \( r(x) = \frac{1}{\ln} \left( \frac{\ln x}{\ln y_0} \right) \). We have chosen here \( x_0 = y_0 = 0.5 \). We generate two samples of size \( n = 1500 \) from a Clayton (Figure 3, left)
Figure 1: 100 paths of ratios \( a(u) = \ln \delta(u) / \ln \tilde{\delta}(u) \), for simulated bivariate data with Gumbel copula of parameter \( \theta = 2 \) (Kendall’s \( \tau = 0.5 \)) in the case where the data size is \( n = 3500 \) (left) or \( n = 2000 \) (right). Here we choose bounds \( \alpha^+ = 0.9 \) and \( \alpha^- = 1.1 \) (dashed horizontal lines) and \( \alpha^+ = 0.95 \) and \( \alpha^- = 1.05 \) (full horizontal lines). The blue vertical lines represents the considered interval \( I = [0.05, 0.95] \subset [0, 1] \).

Figure 2: Estimation of self-nested diagonal \( \hat{\delta}_k(u) \) as in Definition 4.1 in the Clayton-case with parameter \( \theta = 6 \) (left), or in the Gumbel-case with parameter \( \theta = 3 \) (right) for \( k = -3, -2, -1, 0, 1, 2, 3 \). The estimated \( \hat{\delta}_k(u) \) are represented using full lines, the theoretical one’s using dotted lines. The black upper curve corresponds to \( k = -3 \), the yellow lower curve to \( k = 3 \).

and a Gumbel (Figure 3, right) copulas for different Kendall’s \( \tau \). In both cases we take as interpolation function \( z(x) = \exp(-x) \), \( x \in (0, 1] \).

Evaluation of the interpolation function impact

In order to evaluate the impact of the interpolation function \( z(x) \) in the evaluation of \( \hat{\delta}_r \), \( r \in \mathbb{R} \), we define the theoretical self-nested diagonal using a (possibly wrong) interpolator \( z \) as

\[
\delta^*_r(x) = z \left( (z^{-1} \circ \delta_k(x))^{1-\alpha} \left( z^{-1} \circ \delta_{k+1}(x) \right)^\alpha \right), \quad x \in [0, 1]
\]

where \( k = \lfloor r \rfloor \) and \( \alpha = r - \lfloor r \rfloor \).
In Figure 4 we analyse the impact of the choice of the function $z$. Indeed this function drives the interpolation of $\delta_k$, for $r \in \mathbb{R}$, knowing values of $\delta_k$, for $k \in \mathbb{Z}$ (see Definition 4.1). By Lemma 3.2, if known, the best choice for $z$ is the generator $\phi$ of the copula $C$.

However we illustrate the error obtained by using another interpolation function. In particular, we denote

- $\delta^{3d}$ theoretical self-nested diagonal in (24) where $z$ is the identity function $z(x) = x$ (linear interpolator),
- $\delta^{Ga}$ theoretical self-nested diagonal in (24) where $z(x) = \exp(-x)$ (Gumbel interpolator),
- $\delta^{Cl}$ theoretical self-nested diagonal in (24) where $z(x) = (1 + (e^\theta - 1)x)^{-1/\theta}$ (Clayton interpolator).

In Figure 4 we consider a Clayton copula with parameter $\theta = 1$. In this case, by Lemma 3.2, the true theoretical self-nested diagonals in (24) are $\delta^z = \delta^{Cl}$, for $r \in \mathbb{R}$. We have drawn the theoretical errors $| \delta^{Cl}(u) - \delta^{Cl}(u)|$ (Figure 4, left) and $| \delta^{Cl}(u) - \delta^{Ga}(u)|$ (Figure 4, right), for $u = 0.5$, as a function of $r \in [-15, 15]$. Trivially for $r = k \in \mathbb{N}$ the error is null since there is no interpolation procedure. For $r \in \mathbb{R} \setminus \mathbb{N}$ this error is not zero but however it is really small ($< 0.01$). In all cases, the induced relative error is less than 1.5%.

As a consequence, there are no visual differences in graphical representations of $\hat{\phi}$ if using an interpolator or another (and such figures are omitted here). It should be noticed that, even if interpolation error is small, it can be easily reduced, if necessary, by replacing $z$ by a previous estimation of $\hat{\phi}$ at a step $\nu$, then giving an estimation of $\hat{\phi}$ at a step $\nu + 1$, $\nu \in \mathbb{N}$.

**Estimation of the generator**

Using Definition 4.3, we illustrate the finite sample properties of the non-parametric estimation of the generator for an Archimedean copula. We take the independence initial copula $C_0$. Then $\hat{\phi}(t) = \hat{\rho}_t(y_0)$ where $\rho(t) = \frac{1}{\ln m} \ln \left( \frac{1}{\ln x } \right)$ and $d$ is the dimension of the problem. We have chosen here $x_0 = y_0 = e^{-1}$ (or equivalently $t_0 = 1$, $\varphi_0 = \exp(-1)$, see Proposition 3.2), and in this case

$$\hat{\phi}(t) = \hat{\delta}_{(\ln t / \ln d)}(e^{-1}).$$

The values of $\hat{\delta}_r$, $r \in \mathbb{R}$ are interpolated from values of $\hat{\delta}_k$, $k \in \mathbb{Z}$. As a consequence, in the dimension $d = 2$, for $t \in [1000^{-1}, 1000]$, $\hat{\phi}(t)$ does only depend on $\hat{\delta}_k$, with $k \in \{-10, \ldots, 10\}$. For $t \in [30^{-1}, 30]$,
Figure 4: Theoretical errors $| \delta^{G}_{r}(u) - \delta^{D}_{r}(u) |$ (left) and $| \delta^{C}_{r}(u) - \delta^{Gu}_{r}(u) |$ (right), for $u = 0.5$, as a function of $r \in [-15, 15]$. For $r = k \in \mathbb{N}$ the error is null (red points) since there is no interpolation procedure.

\(\hat{\phi}(t)\) does only depend on \(\hat{\delta}_k\), with $k \in \{-5, \ldots, 5\}$. In practice, we thus only need to compute values of \(\hat{\delta}_k\) for a small range of values of $k$.

In Figures 5, we generate two bivariate samples of size $n = 150$ and $n = 1500$ from a Gumbel copula. Three different levels of (bivariate) dependence are considered, i.e., Kendall’s $\tau = 0.25$, 0.5 and 0.75. We have drawn the estimated generators on these two different samples for each level of dependence. We compare the obtained \(\hat{\phi}(t)\) with the theoretical standardized Gumbel-generator, i.e., \(\bar{\phi}(t) = \exp(-t^{1/\theta})\), since \((t_0, \varphi_0) = (1, e^{-1})\). In this case, we take as function $z$ driving the interpolation, $z(x) = \exp(-x)$, $x \in (0, 1]$, since it is the best choice for any independence or Gumbel copula, whatever the parameter of the copula, as a consequence of Corollary 3.1.

Analogously, in Figure 6, we generate two sample of size $n = 150$ and $n = 1500$ from a Clayton copula with Kendall’s $\tau = 0.25$, 0.5 and 0.75. We compare the obtained $\hat{\phi}(t)$ with the theoretical standardized Clayton-generator, i.e., \(\bar{\phi}(t) = (1 + (e^\theta - 1)t)^{-1/\theta}\), since \((t_0, \varphi_0) = (1, e^{-1})\). Also in this case we take as interpolation function $z(x) = \exp(-x)$, $x \in (0, 1]$.

Since in these estimations we use the consistent empirical copula \(\hat{C}\) in Deheuvels (1979), presented in Remark 6, then, as expected, the greater $n$ is, the better the estimations are (see in Figures 5-6 the quality of the estimation in the plots on the left-hand, for $n = 150$, with respect to that on the right-hand, for $n = 1500$).

**Illustration for theoretical confidence bands**

At last, we are looking for theoretical confidence bands for the estimated generator, in the Gumbel case, as detailed in Corollary 4.1. Let \(\hat{C}\) be a Gumbel copula of parameter $\theta = 2$ (i.e., Kendall’s $\tau = 0.5$). Corresponding estimators $\hat{\delta}_1$ and $\hat{\delta}_{-1}$ were build as previously, using a bivariate sample of size $n = 2000$. We just aim here at showing the shape of the confidence bands, so that we did not estimate constants.
\( \alpha^-, \alpha^+, \beta^-, \beta^+ \) such that

\[
\begin{align*}
\mathbb{P} \left[ \hat{\alpha}(u) \leq \hat{\delta}(u) \leq \tilde{\delta}(u), \forall u \in I \right] & \geq \eta, \\
\mathbb{P} \left[ \hat{\beta}_{-1}(u) \leq \hat{\delta}_{-1}(u) \leq \tilde{\delta}_{-1}(u), \forall u \in I \right] & \geq \eta,
\end{align*}
\]

We have chosen for these constants some values \( \alpha^- = \beta^- = 1.05, \alpha^+ = \beta^+ = 0.95, \) (Figure 7) and \( \alpha^- = \beta^- = 1.1, \) (Figure 8). These constants are corresponding to horizontal (full and dashed) lines in Figure 1, which illustrate the behavior of \( a(u) = \ln \hat{\delta}(u) / \ln \tilde{\delta}(u) \) for 100 paths of process, for \( u \in [0, 1] \).

For these chosen constants, the confidence bands for \( \hat{\delta} \) and \( \hat{\delta}_{-1} \) are given in Figures 7-8 (left). These figures give one path of \( \hat{\delta}(u) \) (resp. \( \hat{\delta}_{-1} \)) and band \([\hat{\alpha}(u)^\alpha, \delta(u)^\alpha] \) (resp. \([\hat{\alpha}_{-1}(u)^\alpha, \delta_{-1}(u)^\alpha] \)) for chosen constants \( \alpha^- \) and \( \alpha^+ \) (resp. \( \beta^- \) and \( \beta^+ \)). The resulting theoretical confidence bands for \( \phi \) using Equation (22) are given in Figures 7-8 (right). Obviously, the confidence band around \( \hat{\phi}(t) \) gets narrow when \( t \) is close to \( t_0 = 1 \), since \( \hat{\phi}(t) \) is the chosen equivalent generator passing through \( (t_0, \varphi_0) = (1, e^{-1}) \).
Figure 5: Estimated versus theoretical Gumbel-generator with Kendall’s $\tau = 0.25$, 0.5 and 0.75. Size of simulated samples $n = 150$ (left column) and $n = 1500$ (right column). Estimated $\hat{\varphi}(t) = \hat{\delta}_\rho(t)(y_0)$ as in Definition 4.3 (full line). The theoretical standardized Gumbel-generator, i.e., $\bar{\varphi}(t) = \exp(-t^{1/\theta})$, is drawn using a dashed line. We force the generators to pass through the point $(t_0, \varphi_0) = (1, e^{-1})$ (black point).
Figure 6: Estimated versus theoretical Clayton-generator with Kendall’s $\tau = 0.25$, 0.5 and 0.75. Size of simulated samples $n = 150$ (left column) and $n = 1500$ (right column). Estimated $\hat{\phi}(t) = \hat{\delta}_{\phi(t)}(y_0)$ as in Definition 4.3 (full line). The theoretical standardized Clayton-generator, i.e., $\bar{\phi}(t) = (1 + (e^{\theta} - 1)t)^{-1/\theta}$, is drawn using a dashed line. We force the generators to pass through the point $(t_0, \varphi_0) = (1, e^{-1})$ (black point).
Figure 7: (Left) Confidence bands for $\hat{\delta}$ and $\hat{\delta}_{-1}$ for chosen parameters $\alpha^- = \beta^- = 1.05$, $\alpha^+ = \beta^+ = 0.95$. (Right) Resulting confidence band for $\hat{\phi}$. The considered copula is a Gumbel copula of parameter $\theta = 2$ (i.e., Kendall’s $\tau = 0.5$), the size of generated sample is $n = 2000$. Horizontal blue lines are indicative chosen thresholds $0.05$ and $0.95$ of Figure 1 (see Remark 9).

Figure 8: (Left) Confidence bands for $\hat{\delta}$ and $\hat{\delta}_{-1}$ for chosen parameters $\alpha^- = \beta^- = 1.1$, $\alpha^+ = \beta^+ = 0.9$. (Right) Resulting confidence band for $\hat{\phi}$. The considered copula is a Gumbel copula of parameter $\theta = 2$ (i.e., Kendall’s $\tau = 0.5$), the size of generated sample is $n = 2000$. Horizontal blue lines are indicative chosen thresholds $0.05$ and $0.95$ of Figure 1 (see Remark 9).
Upper tail dependence

As Embrechts and Hofert (2011) explain, a possible limitation of a non-parametric estimation of the generator of an Archimedean copula is the loss of the upper tail dependence. Indeed if $\phi$ has a finite right-hand derivative at zero, the Archimedean copula generated by $\phi$ has upper tail independent bivariate marginal copulas, i.e., $\lambda_U = 0$ (see Section 3 in Embrechts and Hofert (2011)).

For instance Embrechts and Hofert (2011) prove that the estimator $\hat{\phi}_n$ of generator proposed by Genest et al. (2011) is such that $\lim_{t \to 0} -\hat{\phi}'_n(t) < \infty$. This means that the copula generated by $\hat{\phi}_n$ can never have upper tail dependence for $d > 2$. In other word in the context of the estimator presented by Genest et al. (2011) one can obtain a generator function as close as wanted to the underlying, unknown one, but the corresponding Archimedean copula will never have upper tail dependence.

On the other hand, we remark that constructions based on the diagonal section of an Archimedean copula can have some identifiability-problem in the case when $|\hat{\phi}'(0)| = +\infty$ (see Remark 3 based on Theorem 3.5 in Erdely et al. (2013)). Indeed in this case the function $\phi$ can not be reconstructed in a unique way from the only diagonal $\hat{\delta}$ (see also discussion in Segers (2011)). As a consequence, in previous Figures 5 and 6, it is important to remark that the global shape of the generator does not reflect perfectly the asymptotic dependency structure. Generators with close appearance but different right derivatives at 0 may lead to different asymptotic dependency.

In the following we construct an illustration study in order to investigate this interesting and problematic behavior of our estimator as well as well of the estimator by Genest et al. (2011).

Let, for instance, $(x_0, y_0) = (0.5, 0.5)$. From Definition 4.3, if $\tilde{C}$ is transformed from an independent copula (or equivalently if we set $t_0 = -\ln x_0$ and $\varphi_0 = y_0$), our generator $\tilde{\phi}$ is passing through the points

$$\{(t_k, \varphi_k)\}_{k \in \mathbb{N}} = \left\{\left(-d^k \ln(x_0), \hat{\delta}_k(y_0)\right)\right\}_{k \in \mathbb{R}}.$$

We are thus interested to analyse the behaviour of the Newton’s difference quotient for $t_k > 0$:

$$\hat{\phi}'(t_k) := \frac{\hat{\delta}_{k+1}(y_0) - \hat{\delta}_k(y_0)}{t_{k+1} - t_k}. \tag{25}$$

Checking that $t_k$ is an increasing function of $k$, with $\lim_{k \to \infty} t_k = 0$, and recalling that at the limit $\hat{\phi}(0) = 1$, one can also define another difference quotient at the limit:

$$\hat{\phi}'(0) := \lim_{k \to \infty} \frac{1 - \hat{\delta}_k(y_0)}{d^k \ln(x_0)}. \tag{26}$$

Under the assumption of the continuity of derivatives of $\hat{\delta}$, which implies conditions on interpolation function $z$, this coefficient correspond to the right-hand derivative of $\phi$ at $t = 0$, so that one can write $\hat{\phi}'(0) = \lim_{t \to 0^+} \frac{d}{dt} \hat{\phi}(t)$.

Considering the non-parametric estimator of $\phi(t)$ proposed in this paper, it is indeed expressed as a composition of functions, and the number of composition increases infinitely when $t$ gets closer to 0 (but stays inferior to 20 as soon as $t$ is greater to $10^{-6}$ for example, which ensure practical use of this estimator). Our estimator and the Genest et al. (2011)’s one do not appear to be well-adapted to describe the upper tail dependency in the Archimedean multivariate structures (see Remark 3 for our estimator, and Embrechts and Hofert (2011) for the Genest et al. (2011)’s one).

In Figure 9 we propose the ratio of the estimated derivative of $\phi$ divided by the true value of the derivative. To construct these ratios we use our estimator (with derivative as in Equations (25) and (26)) and the estimator by Genest et al. (2011). These ratios seem to tend to 0 for values of $k$ less than 30, which indicates, on this data and for very small values of $t$, around $10^{-13}$, that the estimated derivative using
our estimator as well the estimator by Genest et al. (2011), may become negligible compared to the theoretical one. So the unboundedness of the derivative is not guaranteed with our estimator or with Genest et al. (2011)'s estimator (as established theoretically in Embrechts and Hofert (2011) for this last estimator).

Figure 9: Ratio $\hat{\phi}'(t_k)/\phi'(t_k)$ in terms of $k$, for $k \in [-40, +1]$, i.e. $t_k \in [6.3e-13, 1.39]$. Case of a Gumbel copula with parameter $\theta = 4$ (i.e., Kendall’s $\tau = 0.75$), $n = 2000$, $d = 3$. Black dots: Ratio for our estimator using Equation (25) for $\hat{\phi}'$. Blue crosses: Ratio for our estimator using Equation (26) for $\hat{\phi}'$. Green full dots: Ratio using estimator of $\phi'$ introduced by Genest et al. (2011).

**Lambda function**

We present here the $\lambda$ function, as originally introduced in Genest and Rivest (1993) for inferential purposes,

$$
\lambda(u) = \phi^{-1}(u) \cdot \phi'\left(\phi^{-1}(u)\right),
$$

where $\phi'$ denotes the derivative of the generator $\phi$. One can easily see, after some calculations, that this coefficient is identical for any generator belonging to the same equivalent class (see Lemma 2.1), and on the contrary of the generator itself, does not depend on the choice of some arbitrarily point $(t_0, \varphi_0)$.

Following the same methodology as Genest et al. (2011), we have estimated the $\lambda$ function, for our estimator and for the estimator of Genest et al. (2011). For our estimator, complicated analytical expressions using derivatives of the function $z$ can be calculated. More simply, an approximation of the derivative by finite differences leads to following estimator of $\lambda$, for a small value of $h$, $u \in (0, 1)$, $h < \phi^{-1}(u)$:

$$
\hat{\lambda}(u) = \phi^{-1}(u) \cdot \frac{\phi(\phi^{-1}(u) + h) - \phi(\phi^{-1}(u) - h)}{2h}.
$$

This estimator however relies on the knowledge of both $\phi$ and $\phi^{-1}$, and thus involve numerical resolutions of root to get the inverse function of $\phi$. A more simple estimator of $\lambda$ permit to avoid function inversions. It is based on the fact that $\lambda(u) = \frac{1}{\ln d} \frac{\partial}{\partial r} \delta_r(u) |_{r=0}$, so that we can simply propose

$$
\hat{\lambda}^*(u) = \frac{1}{\ln d} \frac{\hat{\delta}_h(u) - \hat{\delta}_{-h}(u)}{2h}.
$$

Remark that $\hat{\lambda}^*(u)$ only relies on self-nested diagonals $\hat{\delta}_r$. The estimation of $\lambda$ function is also possible using the Genest et al. (2011)'s estimator of $\phi$ and $\phi'$ as detailed in Section 4.3 in Genest et al. (2011)). In the following, we denote this estimator $\hat{\lambda}_G(u)$.
Figure 10: Estimation of $\lambda$ function. Black: theoretical $\lambda$ function. Dark green dashed line: $\hat{\lambda}_G(u)$ (estimator proposed by Genest et al. (2011)), Black dotted line: $\hat{\lambda}(u)$ (i.e., our estimator using Equation (28)). Violet dotted-dashed line: $\hat{\lambda}^*(u)$ (i.e. our estimator using Equation (29)). Parameters setting : $n = 200$, (right column) and $n = 1000$ (left column), $d = 2$. Kendall’s tau parameter is $\tau = 0.75$ ($\theta = 4$) (upper row) and $\tau = 0.25$ ($\theta = 1.333$) (bottom row).

In Figures 10 and 11, we have estimated the $\lambda$ function, we get $\hat{\lambda}(u)$ and $\hat{\lambda}^*(u)$ for our estimator, and $\hat{\lambda}_G(u)$ for the estimator by Genest et al. (2011). The chosen parameter setting in Figures 10 and 11 is exactly as in Figure 2 in Genest et al. (2011). The results show that, empirically on this data-set, all these estimators are very close. The violet dashed line $\hat{\lambda}^*(u)$ seems performing a little bit better especially in upper illustrations of Figure 10, in the dimension $d = 2$.

On tested data, no estimator seems to perform significantly better. Despite it would require more numerical studies to compare all available estimators. However, in our case, estimators relying on self-nested diagonals have several advantages among which:

- For the generator itself, the facility to get generators passing through a given point (see Definition 4.3 and Remark 8), contrary to the estimator in Genest et al. (2011) which relies on the choice of a radius $r_m$. As remarked by Genest et al. (2011), if we are interested in the estimation of the $\lambda$ function then the choice of $r_m$ in their procedure is completely arbitrary. For instance we can easily set $r_m = 1$. However in order to compare other estimated values (which depend on $r_m$) and theoretical one (which does not), like $\phi$ or $\phi'$, the choice of $r_m$ is not trivial. For instance, in Figure 9 we illustrate the behavior of the ratio $\hat{\phi}'(t)/\phi'(t)$ and we had to find of the Genest et al. (2011)’s estimator the value $r_m = 5500$ to get a correct result.
Both estimators of $T$ or $\phi$ are relying on direct analytical expressions, whereas the estimator in Genest et al. (2011) rely on a large number of root resolution procedures. Indeed in the Genest et al. (2011)’s estimator we have to solve a triangular non-linear system containing $m$ equations. For instance, if the sample size is $n = 2000$ the value $m$ is approximately around 1200 − 1300.

Some first theoretical results on confidence bands. Such results would probably be difficult to get with estimators relying on successive optimization procedures or root resolutions.

4.3.2 Real data illustration

We now propose the non-parametric estimation $\hat{\phi}(t)$ using two real-data set (see Definition 4.3). Firstly, we consider the Loss-ALAE data (for details see Frees and Valdez (1998)). The data size is $n = 1500$. Each claim consists of an indemnity payment (the loss, $X$) and an allocated loss adjustment expense (ALAE, $Y$). Examples of ALAE are the fees paid to outside attorneys, experts, and investigators used to defend claims. As remarked in Kojadinovic and Yan (2010), there is a non-negligible number of ties in this data set. The presence of ties can be attributed to monetary rounding and precision issues, and may require a specific treatment in operational studies.
We take the independence initial copula $C_0, x_0 = y_0 = e^{-1}$ (or equivalently $t_0 = 1, \varphi_0 = \exp(-1)$, see Proposition 3.2), and $z(x) = \exp(-x)$ (Gumbel interpolator). The obtained non-parametric generator $\hat{\phi}(t)$ is represented in Figure 12 (left). Different authors, in the recent literature, agree that a satisfying fit on these data can be represented by the Gumbel-Hougaard copula with parameter $\theta = 1.453$ (see for instance Frees and Valdez (1998) and Genest et al. (2009)). Then the standardized Gumbel generator with parameter $\theta = 1.453$ is also represented in Figure 12 in order to exhibit the quality of our non-parametric estimation.

Secondly, we consider a subset of the Framingham Heart study data (http://www.framingham.com/heart/). We focus on the dependence structure underlying the diastolic (DBP) and the systolic (SBP) blood pressures (in mm Hg) measured on 663 male subjects at their first visit (see Qu and Yin (2012)). Lambert (2007) proposed a ratio approximation of the Archimedean copula generator and he found that the Gumbel copula was appropriate for this data without being fully satisfactory. The estimated parameter of this Gumbel copula, $\theta = 2.11$, is given in Qu and Yin (2012). Then, in Figure 12 (right), we represent our estimation $\hat{\phi}(t)$ and the standardized Gumbel generator with parameter $\theta = 2.11$. As we can see the non-parametric generator has a slightly different form (in particular a different concavity) with respect to the analytical function $\phi(t) = \exp(-t^{1.11})$.

**Conclusions**

We described some properties on transformations of Archimedean copulas, among which the characterization of an equivalence class for both transformations and generators. This characterization was necessary to build transformations and generators as function of what we called self-nested diagonals functions. Using their properties we proposed a non-parametric estimator for the self-nested diagonal functions, as well as for the transformations and the generators. This estimation is straightforward and does not rely on any optimization procedure. Then we can easily get convergence properties of such estimators. Numerical illustrations showed the simplicity of these estimators, the good fit to theoretical values in simulated example, the good fit to literature parametric adjustments in real-data problems.

Some perspectives are the following ones: using results in Di Bernardino and Rullière (2013), we can
get easily a whole parametric copula estimation, with a tunable number of parameters and without optimization procedures.

One limitation of the presented transformations is that they transform Archimedean copulas into other Archimedean copulas. The resulting copula is thus symmetric in the sense that it does not vary if margins are permuted. However, on real data, copulas may not be symmetrical. A way to cope with this problem is to work with nested copulas, as defined in Hofert and Pham (2013), or hierarchical Kendall copulas, as defined in Brechmann (2013). Considering nested Archimedean copulas, non-parametric estimation of child Archimedean copulas can be done using presented transformations, so as the estimation of root Archimedean copulas on resulting pseudo-data. Complex parametric dependence structures with many parameters can be derived from non-parametric estimation, as detailed in Di Bernardino and Rullière (2013). The choice of the right nested structure and the analysis of the resulting dependencies are interesting perspectives.

Such development may also ease the inversion and smoothing of the empirical copula as well as its tail estimation. Furthermore, a whole benchmark study would be required to compare different available estimators of the generator of an Archimedean copula. In this sense a development of \( \lambda \) function study started in Section 4.3.1 could be an important future work. At last, the measure of the goodness of fit and the construction of specific tests, based on the non-parametric estimated generator of a copula, are interesting perspectives.

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Annex

In this Annex we give the analytical formulas for standardized generators \( \tilde{\phi}(t) \), their inverses \( \tilde{\phi}^{-1}(t) \) and theoretical self-nested diagonals \( \delta_r \), in the case of most popular Archimedean families of copulas.

In Table 1 we present some classical generators and their associated inverses (see Equation (1)), well known in the literature (see for instance Nelsen (1999)).

In Table 2 we also provide the expressions for the theoretical self-nested diagonals for all \((\delta_r, \tilde{\phi}, \tilde{\phi}^{-1}(t))\) in the case of most popular Archimedean families of copulas.

### Table 1: Classical generators and their associated inverses in the case of most popular Archimedean families of copulas.

| Copula          | \( \phi(t) \)                                  | \( \phi^{-1}(t) \)                          | parameter \( \theta \)        |
|-----------------|------------------------------------------------|---------------------------------------------|-----------------------------|
| Ali-Mikhail-Haq | \( \frac{1 - e^{-\theta \phi}}{t - \theta} \) | \( \ln \left( \frac{1 - e^{-\theta \phi}}{t - \theta} \right) \) | \( \theta \in (0, 1) \) |
| Clayton         | \( (1 + \theta t)^{-1/\theta} \)              | \( \frac{1}{\theta} (t^{-\theta} - 1) \)   | \( \theta \in (0, \infty) \) |
| Frank           | \( -\frac{1}{\theta} \ln(1 - (1 - \exp(-\theta))e^{-t}) \) | \( -\ln \left( \frac{\exp(-\theta t) - 1}{\exp(-\theta t) - 1} \right) \) | \( \theta \in (0, \infty) \) |
| Gumbel          | \( \exp(-t^{1/\theta}) \)                     | \( (-\ln(t))^{\theta} \)                   | \( \theta \in [1, \infty) \) |
| Independence    | \( \exp(-t) \)                                | \( (-\ln(t))^{\theta} \)                   | none                        |
| Joe             | \( 1 - (1 - \exp(-t))^{1/\theta} \)          | \( -\ln \left( 1 - (1 - t)^{\theta} \right) \) | \( \theta \in [1, \infty) \) |

Table 2: Standardized generators \( \tilde{\phi} \), such that \( \tilde{\phi}(t_0) = \varphi_0 \), their associated inverses and theoretical self-nested diagonals in the case of most popular Archimedean families of copulas.
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