Journal of Multivariate Analysis 118 (2013) 37–52

Contents lists available at SciVerse ScienceDirect

Journal of Multivariate Analysis

journal homepage: www.elsevier.com/locate/jmva

Densities of nested Archimedean copulas

Marius Hofert[a,*], David Pham[b]

[a] RiskLab, Department of Mathematics, ETH Zurich, 8092 Zurich, Switzerland

[b] Department of Mathematics and Statistics, University of Montreal, H3T 1J4 Montreal, Quebec, Canada

ARTICLE INFO

Article history:
Received 12 April 2012
Available online 26 March 2013

AMS 2010 subject classifications:
62H99
65C60
62H12
62F10

Keywords:
Nested Archimedean copulas
Generator derivatives
Likelihood-based inference

ABSTRACT

Nested Archimedean copulas recently gained interest since they generalize the well-known class of Archimedean copulas to allow for partial asymmetry. Sampling algorithms and strategies have been well investigated for nested Archimedean copulas. However, for likelihood based inference it is important to have the density. The present work fills this gap. A general formula for the derivatives of the nodes and inner generators appearing in nested Archimedean copulas is developed. This leads to a tractable formula for the density of nested Archimedean copulas in arbitrary dimensions if the number of nesting levels is not too large. Various examples including famous Archimedean families and transformations of such are given. Furthermore, a numerically efficient way to evaluate the log-density is presented.

1. Introduction

There has recently been interest in multivariate hierarchical models, that is, models that are able to capture different dependences between and within different groups of random variables. One such class of models is based on nested Archimedean copulas. A *partially nested Archimedean copula* C with two nesting *levels* and d_0 *child copulas* (or *sectors* or *groups*), is given by

$$C(\boldsymbol{u}) = C_0(C_1(\boldsymbol{u}_1), \dots, C_{d_0}(\boldsymbol{u}_{d_0})), \quad \boldsymbol{u} = (\boldsymbol{u}_1, \dots, \boldsymbol{u}_{d_0})^\top, \tag{1}$$

where d_0 denotes the dimension of C_0 and each copula C_s, $s \in \{0, \dots, d_0\}$, is Archimedean with a completely monotone *generator* ψ_s, that is,

$$C_s(\boldsymbol{u}_s) = \psi_s(\psi_s^{-1}(u_{s1}) + \cdots + \psi_s^{-1}(u_{sd_s})) = \psi_s(t_s(\boldsymbol{u}_s)), \tag{2}$$

where

$$t_s(\boldsymbol{u}_s) = \sum_{j=1}^{d_s} \psi_s^{-1}(u_{sj})$$

and $\psi_s : [0, \infty] \to [0, 1]$ is continuous, $\psi_s(0) = 1$, $\psi_s(\infty) = \lim_{t\to\infty} \psi_s(t) = 0$, and $(-1)^k \psi_s^{(k)}(t) \geq 0$ for all $k \in \mathbb{N}_0$, $t \in (0, \infty)$. The set of all completely monotone Archimedean generators is denoted by Ψ_∞ in what follows. The copula C_0 is referred to as the *root copula*. Model (1) provides an intuitive hierarchical structure, since, for example, if $\boldsymbol{U} \sim C$

* Corresponding author.
E-mail addresses: hofertj@math.ethz.ch, marius.hofert@math.ethz.ch (M. Hofert), david-olivier.pham@umontreal.ca (D. Pham).

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http://dx.doi.org/10.1016/j.jmva.2013.03.006

the pair $(U_{sj}, U_{sk})^\top$ $(j \neq k)$ has joint copula C_s whereas the pair $(U_{rj}, U_{sk})^\top$ $(r \neq s)$ follows the root copula C_0. One can therefore directly say what the bivariate margins are and theoretical results about measures of association, for example, directly apply. Furthermore, such a construction provides an explicit form for the copula itself, which is important, for example, in likelihood-based inference for censored data. More complicated nesting structures can be constructed; see Section 6. In general, a *nested Archimedean copula* is an Archimedean copula with arguments possibly replaced by other nested Archimedean copulas.

For statistical applications it is desirable to be able to evaluate the density of a multivariate model, for example, for parameter estimation or when conditional copulas are required (for example, for goodness-of-fit testing via Rosenblatt's transform, see [6]). For Archimedean copulas, the density (if it exists) is theoretically trivial to write down; for (2), one obtains

$$c_s(\boldsymbol{u}_s) = \psi_s^{(d)}(t_s(\boldsymbol{u}_s)) \prod_{j=1}^{d_s} (\psi_s^{-1})'(u_{sj}), \quad \boldsymbol{u}_s \in (0,1)^{d_s}.$$

However, the appearing generator derivatives $\psi_s^{(d)}$ are non-trivial to access theoretically and, even more, computationally. This issue has recently been solved for several well-known Archimedean copulas and transformations of such; see [12,13]. Our goal is to extend these results to the corresponding nested Archimedean copulas. Note that this is more challenging because differentiating (1) is more complicated due to the inner derivatives that appear when applying the Chain Rule; in contrast to Archimedean copulas, these inner derivatives depend on variables with respect to which one has to differentiate again. Already in low dimensions the corresponding formulas for the density c become challenging to write down and, even more, to evaluate in a numerically stable way.

After a brief introduction and overview about nested Archimedean copulas in Section 2, we tackle the problem of computing the density of (1) by first deriving a convenient form for the copula. This will allow us to compute the density; see Section 3. All necessary details for several well-known Archimedean families are provided in Section 4. Section 5 addresses numerical evaluation of the log-density. Section 6 presents the density for three-level nested Archimedean copulas and extensions to higher nesting levels are briefly addressed. For the reader's convenience, proofs are deferred to the Appendix.

2. Nested Archimedean copulas

The class of nested Archimedean copulas was first considered in [14, p. 87] in the three- and four-dimensional cases and later by McNeil [16] in the general d-dimensional case. McNeil [16] and Hofert [9] derive an explicit stochastic representation for nested Archimedean copulas which allows for a fast sampling algorithm of nested Archimedean copulas similar to the Marshall–Olkin algorithm for Archimedean copulas; see [15] for the latter. Hofert [10] provides efficient sampling strategies for the most important ingredients to this algorithm, the random variables responsible for introducing hierarchical dependences. An implementation for several well-known Archimedean families (and transformations of such) is provided by the `R` package `copula`; see [11].

Although nesting is possible in more complicated ways (see Section 6), in the following we focus on nested Archimedean copulas of Type (1) (with some child copulas possibly shrunk to single arguments of C_0). By Bernstein's Theorem, each $\psi \in \Psi_\infty$ is the Laplace–Stieltjes transform of a distribution function F on $[0,\infty)$ with $F(0) = 0$. A sufficient condition under which (1) is indeed a proper copula is then that the *nodes*

$$\mathring{\psi}_{0s} = \psi_0^{-1} \circ \psi_s, \quad s \in \{1, \dots, d_0\},$$

have completely monotone first order derivatives; see [16]. Note that this *sufficient nesting condition* is indeed only sufficient but not necessary. For example, if $\psi_0(t) = -\log(1-(1-e^{-\theta_0})\exp(-t))/\theta_0$ denotes the generator of a Frank copula and $\psi_1(t) = (1+t)^{-1/\theta_1}$ the generator of a Clayton copula, then $C(\boldsymbol{u}) = C_0(u_1, C_1(u_2, u_3))$ is a valid (nested Archimedean) copula for all θ_0, θ_1 such that $\theta_0/(1-e^{-\theta_0}) - 1 \le \theta_1$ although $\mathring{\psi}_{01}$ is not completely monotone for any parameters θ_0, θ_1.

Among the most widely used parametric Archimedean families are those of Ali–Mikhail–Haq, Clayton, Frank, Gumbel, and Joe; see [13] for the corresponding generators, their derivatives, Laplace–Stieltjes inverses, and properties of the copula families. These one-parameter families can easily be extended to allow for more parameters, for example, via outer power transformations. For more details on this and other aspects of nested Archimedean copulas we refer the reader to Hofert [8] and the references therein.

3. Inner generator derivatives and densities for two-level nested Archimedean copulas

3.1. The basic idea

Let C be a d-dimensional nested Archimedean copula of Type (1) (with some child copulas possibly shrunk to single arguments of C_0) and assume the sufficient nesting condition to hold; for the Ali–Mikhail–Haq, Clayton, Frank, Gumbel, and Joe families, this is fulfilled as long as all generators belong to the same family and $\theta_0 \le \theta_s$, $s \in \{1, \dots, d_0\}$. This condition implies that each copula C_s, $s \in \{1, \dots, d_0\}$, is more concordant than C_0.

One of the main ingredients we need in the following is the function

$$\psi_{0s}(t;\,v) = \exp(-v\mathring{\psi}_{0s}(t)) \tag{3}$$

which we refer to as the *inner generator*. It is a proper generator in t for each $v > 0$ as a composition of the completely monotone function $\exp(-v\,\cdot)$ with $\mathring{\psi}_{0s}$ which has a completely monotone derivative. With $F_0 = \mathcal{LS}^{-1}[\psi_0]$, we obtain

$$\begin{aligned} C(\boldsymbol{u}) &= C_0(C_1(\boldsymbol{u}_1), \ldots, C_{d_0}(\boldsymbol{u}_{d_0})) = \int_0^\infty \exp\left(-v_0 \sum_{s=1}^{d_0} \mathring{\psi}_{0s}(t_s(\boldsymbol{u}_s))\right) dF_0(v_0) \\ &= \int_0^\infty \prod_{s=1}^{d_0} \psi_{0s}(t_s(\boldsymbol{u}_s);\, v_0)\, dF_0(v_0). \end{aligned} \tag{4}$$

By our assumption of having completely monotone generators, the density c of C exists and is given by

$$c(\boldsymbol{u}) = \frac{\partial^d}{\partial u_{d_0 d_{d_0}} \cdots \partial u_{11}} C(\boldsymbol{u}).$$

Instead of differentiating (1) directly, the idea is now to use Representation (4). By differentiating under the integral sign, the density c allows for the representation

$$\begin{aligned} c(\boldsymbol{u}) &= \int_0^\infty \prod_{s=1}^{d_0} \psi_{0s}^{(d_s)}(t_s(\boldsymbol{u}_s);\, v_0)\, dF_0(v_0) \cdot \prod_{s=1}^{d_0}\prod_{j=1}^{d_s} (\psi_s^{-1})'(u_{sj}) \\ &= \mathbb{E}\left[\prod_{s=1}^{d_0} \psi_{0s}^{(d_s)}(t_s(\boldsymbol{u}_s);\, V_0)\right] \cdot \prod_{s=1}^{d_0}\prod_{j=1}^{d_s} (\psi_s^{-1})'(u_{sj}). \end{aligned} \tag{5}$$

For the cost of one integral (which will be computed explicitly below!), one can therefore easily compute the density c (theoretically) as a F_0-mixture. This is especially advantageous in large dimensions as the complexity of the problem does not (again, theoretically) depend on the sizes of the child copulas too much, rather on the number of children.

From Eq. (5), we identify the following key challenges:

Challenge 1 Find the derivatives of the inner generators $\psi_{0s}(t;\, v_0)$;
Challenge 2 Compute their product;
Challenge 3 Integrate it with respect to the mixture distribution function $F_0 = \mathcal{LS}^{-1}[\psi_0]$.

All three challenges will be solved in Section 3.3 with the help of the tools presented in the following section.

3.2. The tools needed: Faà di Bruno's formula and Bell polynomials

One formula which proves to be useful here, is the expression of the nth derivative of a composition of functions; see [5]. Although this formula dates back to the work of Arbogast [1], it is named after the mathematician Faà di Bruno. For suitable functions f and g, Faà di Bruno's formula states that

$$(f \circ g)^{(n)}(x) = \sum_{k=1}^n f^{(k)}(g(x)) \sum_{\boldsymbol{j} \in \mathcal{P}_{n,k}} \binom{n}{j_1, \ldots, j_{n-k+1}} \prod_{l=1}^{n-k+1} \left(\frac{g^{(l)}(x)}{l!}\right)^{j_l}, \tag{6}$$

where $\binom{n}{j_1,\ldots,j_n} = \frac{n!}{j_1!\cdot\cdots\cdot j_n!}$ denotes a multinomial coefficient, $\boldsymbol{j} = (j_1, \ldots, j_n)^\top \in \mathbb{N}_0^n$, and

$$\mathcal{P}_{n,k} = \left\{\boldsymbol{j} \in \mathbb{N}_0^{n-k+1} : \sum_{i=1}^{n-k+1} i j_i = n \text{ and } \sum_{i=1}^{n-k+1} j_i = k\right\}. \tag{7}$$

Alternatively, one can use *Bell polynomials* to reformulate (6). These are defined by

$$B_{n,k}(x_1, \ldots, x_{n-k+1}) = \sum_{\boldsymbol{j} \in \mathcal{P}_{n,k}} \binom{n}{j_1, \ldots, j_{n-k+1}} \prod_{l=1}^{n-k+1} \left(\frac{x_l}{l!}\right)^{j_l}. \tag{8}$$

This implies that (6) can be written as

$$(f \circ g)^{(n)}(x) = \sum_{k=1}^n f^{(k)}(g(x)) B_{n,k}(g'(x), g''(x), \ldots, g^{(n-k+1)}(x)). \tag{9}$$

In the sections to come, we frequently need the following results. Here, $(x)_n = x \cdot (x-1) \cdot \cdots \cdot (x-n+1)$ denotes the *falling factorial*, and $s(n,k)$ and $S(n,k)$ denote the *Stirling numbers of the first* and *the second kind*, respectively, given by the recurrence relations

$$\begin{aligned} s(n+1,k) &= s(n,k-1) - ns(n,k), \\ S(n+1,k) &= S(n,k-1) + kS(n,k), \end{aligned}$$

for all $k \in \mathbb{N}$, $n \in \mathbb{N}_0$, with $s(0,0) = S(0,0) = 1$ and $s(n,0) = s(0,n) = S(n,0) = S(0,n) = 0$ for all $n \in \mathbb{N}$. Note that for $n \in \mathbb{N}$ (in particular $n \neq 0$), the Stirling numbers of the first kind satisfy

$$(x)_n = \sum_{j=1}^{n} s(n,j)x^j. \tag{10}$$

Lemma 3.1. *Let $B_{n,k}$ be the Bell polynomial as in (8) and $n \in \mathbb{N}$. Then*

(1) *for $\boldsymbol{j} \in \mathcal{P}_{n,k}$, $\sum_{l=1}^{n-k+1}(x-l)j_l = xk - n$;*
(2) *$B_{n,k}(x,\ldots,x) = S(n,k)x^k$, $k \in \{0,\ldots,n\}$;*
(3) *$B_{n,k}(-x,\ldots,(-1)^{n-k+1}x) = (-1)^n S(n,k)x^k$, $k \in \{0,\ldots,n\}$;*
(4) *$\operatorname{sign}\big(B_{n,k}(g'(x), g''(x), \ldots, g^{(n-k+1)}(x))\big) = (-1)^{n-k}$ for all x if g' is completely monotone.*

Proposition 3.2. *Let*

$$s_{nk}(x) = \sum_{l=k}^{n} s(n,l)S(l,k)x^l = (-1)^n \sum_{l=k}^{n} |s(n,l)|S(l,k)(-x)^l.$$

Then

(1) *for all $k \in \{0,\ldots,n\}$, $B_{n,k}((x)_1 y^{x-1}, \ldots, (x)_{n-k+1} y^{x-(n-k+1)}) = y^{xk-n} s_{nk}(x)$;*
(2) *$\sum_{k=1}^{n} (-1)_k s_{nk}(x) = (-x)_n$;*
(3) *If $x \in (0,1]$, $\operatorname{sign}(s_{nk}(x)) = (-1)^{n-k}$.*

3.3. The main result

We are now able to derive a general formula for the derivatives of the inner generators and also for the density of nested Archimedean copulas of Type (1). It will follow from Faà di Bruno's formula that the derivatives of the inner generators $\psi_{0s}(t;v_0)$ are the inner generators themselves times a polynomial in $-v_0$. The product of these derivatives can then be computed as a Cauchy product. Interpreting the appearing quantities correctly allows us to compute the expectation with respect to F_0 via the derivatives of ψ_0. This solves all three of the above challenges.

Theorem 3.3. *Let $\psi_s \in \Psi_\infty$, $s \in \{0,\ldots,d_0\}$, such that $\mathring{\psi}_{0s}$ has a completely monotone derivative for all $s \in \{1,\ldots,d_0\}$.*

(1) *For all $n \in \mathbb{N}$,*

$$\psi_{0s}^{(n)}(t;v_0) = \psi_{0s}(t;v_0) \sum_{k=1}^{n} a_{s,nk}(t)(-v_0)^k, \tag{11}$$

where

$$a_{s,nk}(t) = B_{n,k}(\mathring{\psi}_{0s}'(t), \ldots, \mathring{\psi}_{0s}^{(n-k+1)}(t)) \tag{12}$$

with $\operatorname{sign}(a_{s,nk}(t)) = (-1)^{n-k}$ and if $\psi_s = \psi_0$ and $n = k = 1$ then $a_{s,nk}(t) = 1$ for all t.

(2) *The density of (1) is given by*

$$c(\boldsymbol{u}) = \left(\sum_{k=d_0}^{d} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u}))\psi_0^{(k)}(t(\boldsymbol{u})) \right) \cdot \prod_{s=1}^{d_0} \prod_{j=1}^{d_s} (\psi_s^{-1})'(u_{sj}), \tag{13}$$

where

$$\boldsymbol{t}(\boldsymbol{u}) = (t_1(\boldsymbol{u}_1), \ldots, t_{d_0}(\boldsymbol{u}_{d_0}))^\top,$$

$$b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u})) = \sum_{\boldsymbol{j} \in \mathcal{Q}_{\boldsymbol{d},k}^{d_0}} \prod_{s=1}^{d_0} a_{s,d_s j_s}(t_s(\boldsymbol{u}_s)), \tag{14}$$

$$t(\boldsymbol{u}) = \psi_0^{-1}(C(\boldsymbol{u})),$$

with $\boldsymbol{d} = (d_1, \dots, d_{d_0})^\top$ *and*

$$\mathcal{Q}^{d_0}_{\boldsymbol{d},k} = \left\{ \boldsymbol{j} \in \mathbb{N}^{d_0} : \sum_{s=1}^{d_0} j_s = k,\ j_s \le d_s,\ s \in \{1, \dots, d_0\} \right\};$$

that is, $b^{d_0}_{\boldsymbol{d},k}$ *is a coefficient in the Cauchy product of the polynomials* $\sum_{k=1}^{d_s} a_{s,d_s k}(t)(-v_0)^k$.

Remark 3.4. (1) We see from Theorem 3.3 Part (1) that all derivatives of $\psi_{0s}(t; v_0)$ are of similar form in v_0, namely $\psi_{0s}(t; v_0)$ times a polynomial in $-v_0$ where the coefficients $a_{s,d_s k}(t_s(\boldsymbol{u}_s))$ are the Bell polynomials evaluated at the derivatives of the nodes $\mathring{\psi}_{0s}$. This structure is crucial for solving Challenge 3 since it allows one to compute the expectation with respect to F_0 explicitly.

(2) We see from Theorem 3.3 Part (2) how the (log-)density can in general be evaluated. It involves the sign-adjusted derivatives of ψ_0 which are known in many cases; see [13]. Furthermore, the quantities $b^{d_0}_{\boldsymbol{d},k}$, $k \in \{d_0, \dots, d\}$, have to be computed. The remaining parts are comparably trivial to obtain.

(3) If there are *degenerate* child copulas, that is, there exists a subset $\mathcal{S}$ of indices such that $d_s = 1$ for all $s \in \mathcal{S}$, then a straightforward application of Theorem 3.3(1) shows that

$$c(\boldsymbol{u}) = \left(\sum_{k=d'_0}^{d-d_{\mathcal{S}}} b^{d'_0}_{\boldsymbol{d}',k}(\boldsymbol{t}(\boldsymbol{u}))\psi_0^{(k+d_{\mathcal{S}})}(t(\boldsymbol{u})) \right) \cdot \prod_{s=1}^{d_0} \prod_{j=1}^{d_s} (\psi_s^{-1})'(u_{sj}),$$

where $d_{\mathcal{S}} = \sum_{s\in\mathcal{S}} d_s = |\mathcal{S}|$, $d'_0 = d_0 - d_{\mathcal{S}}$ and $\boldsymbol{d}'$ is the vector containing all the dimensions d_s for $s \notin \mathcal{S}$.

4. Example families and transformations

4.1. Tilted outer power families, Clayton and Gumbel copulas

In order to construct and sample new nested Archimedean copulas it turns out to be useful to consider certain generator transformations; see [8] for more details. One such transformation leads to *tilted outer power generators*

$$\psi_s(t) = \psi((c^{\theta_s} + t)^{1/\theta_s} - c), \tag{15}$$

for a generator $\psi \in \Psi_\infty$, $c \in [0, \infty)$, $\theta_s \in [1, \infty)$, and $s \in \{0, \dots, d_0\}$. Note that generators of this form are elements of Ψ_∞. It follows from Eq. (9) and Proposition 3.2 Part (1) (with $x = 1/\theta_0$ and $y = c^{\theta_0} + t$) that the derivatives of ψ_0 are

$$\psi_0^{(n)}(t) = \sum_{k=1}^{n} \psi^{(k)}((c^{\theta_0} + t)^{1/\theta_0} - c)(c^{\theta_0} + t)^{k/\theta_0 - n} s_{nk}(1/\theta_0). \tag{16}$$

For nesting generators of Type (15), the nodes are given by

$$\mathring{\psi}_{0s}(t) = (c^{\theta_s} + t)^{\alpha_s} - c^{\theta_0}, \quad \alpha_s = \theta_0/\theta_s.$$

This implies that tilted outer power generators of Type (15) fulfill the sufficient nesting condition if $\theta_0 \le \theta_s$. Furthermore,

$$\mathring{\psi}_{0s}^{(k)}(t) = (\alpha_s)_k (c^{\theta_s} + t)^{\alpha_s - k}, \quad k \in \mathbb{N}.$$

By Proposition 3.2 Part (1) (with $x = \alpha_s$ and $y = c^{\theta_s} + t$), this implies that

$$a_{s,nk}(t) = B_{n,k}(\mathring{\psi}'_{0s}(t), \dots, \mathring{\psi}_{0s}^{(n-k+1)}(t)) = (c^{\theta_s} + t)^{\alpha_s k - n} s_{nk}(\alpha_s).$$

By Theorem 3.3 Part (1), this implies that the inner generator

$$\psi_{0s}(t; v_0) = \exp\big(-v_0((c^{\theta_s} + t)^{\alpha_s} - c^{\theta_0})\big),$$

has derivatives

$$\psi_{0s}^{(n)}(t; v_0) = \psi_{0s}(t; v_0) \sum_{k=1}^{n} a_{s,nk}(t)(-v_0)^k = \psi_{0s}(t; v_0) \sum_{k=1}^{n} (c^{\theta_s} + t)^{\alpha_s k - n} s_{nk}(\alpha_s)(-v_0)^k. \tag{17}$$

Note that $(\psi_s^{-1})'(u) = \theta_s(\psi^{-1})'(u)(c + \psi^{-1}(u))^{\theta_s - 1}$. By Eq. (16), Theorem 3.3 Part (2), and slight simplifications, we thus obtain

$$c(\boldsymbol{u}) = \left(\sum_{k=d_0}^{d} b^{d_0}_{\boldsymbol{d},k}(\boldsymbol{t}(\boldsymbol{u})) \left(\sum_{j=1}^{k} \psi^{(j)}\big((c^{\theta_0} + t(\boldsymbol{u}))^{1/\theta_0} - c\big)(c^{\theta_0} + t(\boldsymbol{u}))^{j/\theta_0 - k} s_{kj}(1/\theta_0) \right) \right)$$
$$\cdot \prod_{s=1}^{d_0} \theta_s^{d_s} \prod_{j=1}^{d_s} (\psi^{-1})'(u_{sj})(c + \psi^{-1}(u_{sj}))^{\theta_s - 1}. \tag{18}$$

Remark 4.1 (*Clayton and Gumbel Copulas*).

(1) By taking $\psi(t) = 1/(1+t)$ and $c = 1$ we see that the tilted outer power generator (15) is $\psi_s(t) = (1+t)^{-1/\theta_s}$, that is, a generator of the Clayton family. As a special case of this section, we thus obtain the inner generator derivatives and the densities of nested Clayton copulas. Concerning the former, we obtain from (17) that

$$\psi_{0s}^{(n)}(t; v_0) = \psi_{0s}(t; v_0) \sum_{k=1}^{n} s_{nk}(\alpha_s)(1+t)^{\alpha_s k - n}(-v_0)^k.$$

Concerning the latter, plugging in the corresponding quantities in (18) and simplifying the terms (in particular, the power of $1 + \psi_0^{-1}(C(\boldsymbol{u}))$ can be taken out of the inner sum), we obtain

$$c(\boldsymbol{u}) = \left(\sum_{k=d_0}^{d} (-1)^{d-k} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u}))(1+t(\boldsymbol{u}))^{-(k+1/\theta_0)} \sum_{j=1}^{k} (-1)^{k-j} s_{kj}(1/\theta_0) \right) \cdot \prod_{s=1}^{d_0} \theta_s^{d_s} \left(\prod_{j=1}^{d_s} u_{sj} \right)^{-(1+\theta_s)}.$$

By Proposition 3.2 Part (3), we can further simplify this expression and obtain

$$c(\boldsymbol{u}) = (-1)^d \left(\sum_{k=d_0}^{d} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u}))(-1/\theta_0)_k (1+t(\boldsymbol{u}))^{-(k+1/\theta_0)} \right) \cdot \prod_{s=1}^{d_0} \theta_s^{d_s} \left(\prod_{j=1}^{d_s} u_{sj} \right)^{-(1+\theta_s)}$$

for the density of nested Clayton copulas of Type (1). This formula also follows directly from Theorem 3.3 Part (2) by plugging in the generator derivatives $\psi_0^{(k)}(t) = (-1/\theta_0)_k (1+t)^{-(k+1/\theta_0)}$ and simplifying the expressions.

(2) Interestingly, also the inner generator derivatives and the densities of nested Gumbel copulas of Type (1) follow as a special case of nested tilted outer power families. To see this take $\psi(t) = \exp(-t)$ (the generator of the independence copula) and consider a zero tilt (so $c = 0$). It follows from (17) that

$$\psi_{0s}^{(n)}(t; v_0) = \psi_{0s}(t; v_0) \sum_{k=1}^{n} s_{nk}(\alpha_s) t^{\alpha_s k - n}(-v_0)^k.$$

Concerning the density, a short calculation shows that

$$c(\boldsymbol{u}) = (-1)^d \frac{C(\boldsymbol{u})}{\Pi(\boldsymbol{u})} \left(\sum_{k=d_0}^{d} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u})) \left(\sum_{j=1}^{k} (-t(\boldsymbol{u})^{1/\theta_0})^j s_{kj}(1/\theta_0) \right) \right) \cdot \prod_{s=1}^{d_0} \theta_s^{d_s} \left(\prod_{j=1}^{d_s} -\log u_{sj} \right)^{\theta_s - 1},$$

where C is (1) and Π is the independence copula (hence the product of its arguments). As before, this result can also be directly obtained from 3.3 Part (2) based on Gumbel's generator derivatives $\psi_0^{(k)}(t) = (\psi_0(t)/t^k) \sum_{j=1}^{k} s_{kj}(1/\theta_0)(-1/\theta_0)^j$ as derived in [13].

4.2. Ali–Mikhail–Haq copulas

A nested Archimedean copula of Type (1) with all components $C_s, s \in \{0, \dots, d_0\}$, belonging to the Ali–Mikhail–Haq family is a valid copula according to the sufficient nesting condition if $\theta_0 \le \theta_s$ for all $s \in \{1, \dots, d_0\}$. The generator $\psi_{0s}(t; v_0)$ is given by

$$\psi_{0s}(t; v_0) = \left(\frac{1-\theta_s}{(1-\theta_0)\exp(t) - (\theta_s - \theta_0)} \right)^{v_0} = \left(\frac{1-\theta_{0s}}{\exp(t) - \theta_{0s}} \right)^{v_0},$$

where $\theta_{0s} = (\theta_s - \theta_0)/(1-\theta_0) \in [0, 1)$ and $v_0 \in \mathbb{N}$. It can be shown from (9), Lemma 3.1(2), and (10) that

$$\psi_{0s}^{(n)}(t; v_0) = \psi_{0s}(t; v_0) \sum_{k=1}^{n} s_{nk}\big(1/(1-\theta_{0s}\exp(-t))\big)(-v_0)^k, \tag{19}$$

which reveals that $a_{s,nk}(t) = s_{nk}\big(1/(1-\theta_{0s}\exp(-t))\big)$ in (11).

Hofert et al. [13] showed that

$$\psi_0^{(k)}(t) = (-1)^k \frac{1-\theta_0}{\theta_0} \operatorname{Li}_{-k}(\theta_0 \exp(-t)), \quad t \in (0, \infty),\ k \in \mathbb{N}_0,$$

where $\operatorname{Li}_s(z)$ denotes the *polylogarithm of order s at z*. It follows from Theorem 3.3 Part (2) that

$$c(\boldsymbol{u}) = (-1)^d \frac{1-\theta_0}{\theta_0} \left(\sum_{k=d_0}^{d} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u}))(-1)^k \operatorname{Li}_{-k}\big(\theta_0 \exp(-t(\boldsymbol{u}))\big) \right) \cdot \prod_{s=1}^{d_0} (1-\theta_s)^{d_s} \left(\prod_{j=1}^{d_s} u_{sj}(1-\theta_s(1-u_{sj})) \right)^{-1}.$$

4.3. Joe copulas

The inner generator and its derivatives

Nested Joe copulas of Type (1) are valid copulas if $\theta_0 \le \theta_s$ for all $s \in \{1, \dots, d_0\}$. The generator $\psi_{0s}(t; v_0)$ is given by

$$\psi_{0s}(t; v_0) = (1 - (1 - \exp(-t))^{\alpha_s})^{v_0}, \tag{20}$$

where $\alpha_s = \theta_0/\theta_s$, $s \in \{1, \dots, d_0\}$, and $v_0 \in \mathbb{N}$.

A rather lengthy calculation shows that

$$\begin{aligned}\psi_{0s}^{(n)}(t; v_0) &= \psi_{0s}(t; v_0)(-1)^n \sum_{m=1}^{n} S(n, m)\left(-\frac{e^{-t}}{1 - e^{-t}}\right)^m \sum_{k=1}^{m} v_0^k \sum_{l=k}^{m} s(l, k) s_{ml}(\alpha_s)\left(\frac{x}{1+x}\right)^l \\ &= \psi_{0s}(t; v_0)\sum_{k=1}^{n} a_{s,nk}(t)(-v_0)^k\end{aligned}$$

for

$$a_{s,nk}(t) = \left((-1)^{n-k}\sum_{m=k}^{n} S(n, m)\left(-\frac{\exp(-t)}{1 - \exp(-t)}\right)^m \sum_{l=k}^{m} s(l, k) s_{ml}(\alpha_s)\left(\frac{\psi_{1/\alpha_s}^{\mathrm{J}}(t) - 1}{\psi_{1/\alpha_s}^{\mathrm{J}}(t)}\right)^l\right),$$

where $\psi_{1/\alpha_s}^{\mathrm{J}}(t) = 1 - (1 - \exp(-t))^{\alpha_s}$ denotes Joe's generator with parameter $1/\alpha_s = \theta_s/\theta_0$. This is precisely the form as given in (11).

It follows from Hofert et al. [13] that

$$\psi_0^{(k)}(t) = (-1)^k \frac{(1 - \exp(-t))^{1/\theta_0}}{\theta_0} P_{k,\theta_0}^{\mathrm{J}}\left(\frac{\exp(-t)}{1 - \exp(-t)}\right), \quad t \in (0, \infty),\ n \in \mathbb{N},$$

where $P_{k,\theta_0}^{\mathrm{J}}(x) = \sum_{l=1}^{k} S(k, l)(l - 1 - 1/\theta_0)_{l-1} x^l$. We obtain from Theorem 3.3 Part (2) that

$$c(\boldsymbol{u}) = \frac{(-1)^d}{\theta_0}\big(1 - \exp(-t(\boldsymbol{u}))\big)^{1/\theta_0}\left(\sum_{k=d_0}^{d}(-1)^k b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u})) P_{k,\theta_0}^{\mathrm{J}}\left(\frac{\exp(t(\boldsymbol{u}))}{1 - \exp(-t(\boldsymbol{u}))}\right)\right)\cdot \prod_{s=1}^{d_0}\theta_s^{d_s}\prod_{j=1}^{d_s}\frac{(1 - u_{sj})^{\theta_s - 1}}{1 - (1 - u_{sj})^{\theta_s}}.$$

Note that $\exp(-t(\boldsymbol{u})) = \prod_{s=1}^{d_0}\big(1 - (1 - C_s(\boldsymbol{u}_s))^{\theta_0}\big)$.

4.4. Frank copulas

Nested Frank copulas of Type (1) are valid copulas according to the sufficient nesting condition if $\theta_0 \le \theta_s$ for all $s \in \{1, \dots, d_0\}$. The generator $\psi_{0s}(t; v_0)$ is given by

$$\psi_{0s}(t; v_0) = \left(\frac{1 - (1 - p_s\exp(-t))^{\alpha_s}}{p_0}\right)^{v_0},$$

where $\alpha_s = \theta_0/\theta_s$, $p_j = 1 - e^{-\theta_j}$, $j \in \{0, s\}$, and $v_0 \in \mathbb{N}$. Note that this inner generator is a shifted (and appropriately scaled) inner Joe generator, that is,

$$\psi_{0s}(t; v_0) = \frac{\psi_{0s}^{\mathrm{J}}(h + t; v_0)}{\psi_{0s}^{\mathrm{J}}(h; v_0)},$$

where $h = -\log p_s$; see [8, p. 104] for more details about such generators. In particular, with the representation for the generator derivatives for the inner Joe generator, this implies that

$$\begin{aligned}\psi_{0s}^{(n)}(t; v_0) &= \frac{\psi_{0s}^{\mathrm{J}\,(n)}(h + t; v_0)}{\psi_{0s}^{\mathrm{J}}(h; v_0)} = \frac{\psi_{0s}^{\mathrm{J}}(h + t; v_0)}{\psi_{0s}^{\mathrm{J}}(h; v_0)}\sum_{k=1}^{n} a_{s,nk}^{\mathrm{J}}(t + h)(-v_0)^k \\ &= \psi_{0s}(t; v_0)\sum_{k=1}^{n} a_{s,nk}^{\mathrm{J}}(t + h)(-v_0)^k\end{aligned}$$

and thus that $a_{s,nk}(t) = a_{s,nk}^{\mathrm{J}}(t + h)$, that is, the coefficients of the polynomial in $-v_0$ for the derivatives of the inner Frank generator are the ones of the inner Joe generator, appropriately shifted.

It follows from Hofert et al. [13] that

$$\psi_0^{(k)}(t) = (-1)^k \frac{1}{\theta_0} \operatorname{Li}_{-(k-1)}(p_0 \exp(-t)), \quad t \in (0, \infty),\ k \in \mathbb{N}_0.$$

Theorem 3.3 Part (2) then implies that

$$c(\boldsymbol{u}) = (-1)^d \left(\sum_{k=d_0}^{d} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u}))(-1)^k \operatorname{Li}_{-(k-1)}\big(p_0 \exp(-t(\boldsymbol{u}))\big) \right) \cdot \prod_{s=1}^{d_0} \theta_s^{d_s} \prod_{j=1}^{d_s} \frac{\exp(-\theta_s u_{sj})}{1-\exp(-\theta_s u_{sj})}.$$

4.5. A nested Ali–Mikhail–Haq ∘ Clayton copula

If ψ_0 is the generator of an Ali–Mikhail–Haq copula and $\psi_s, s \in \{1, \dots, d_0\}$, generate Clayton copulas, then Hofert [8, p. 115] showed that the sufficient nesting condition holds if $\theta_s \in [1, \infty), s \in \{1, \dots, d_0\}$, so one can build nested Archimedean copulas of Type (1) with the root copula C_0 being of Ali–Mikhail–Haq and the child copulas C_s being of Clayton type under this condition (referred to as Ali–Mikhail–Haq ∘ Clayton copulas). In this case, a short calculation shows that

$$\psi_{0s}(t; v_0) = \psi((1+t)^{1/\theta_s} - 1)$$

for $\psi(t) = (1 + (1-\theta_0)t)^{-v_0}$. We can thus apply (16) with $c = 1$ to see that

$$\psi_{0s}^{(n)}(t; v_0) = \sum_{j=1}^{n} \psi^{(j)}((1+t)^{1/\theta_s} - 1)(1+t)^{j/\theta_s - n} s_{nj}(1/\theta_s), \tag{21}$$

where

$$\psi^{(j)}((1+t)^{1/\theta_s} - 1) = (1-\theta_0)^j \psi_{0s}(t; v_0)\psi_{0s}(t; j) \sum_{k=1}^{j} s(j,k)(-v_0)^k.$$

Plugging this result into (21) and interchanging the order of the two summations, we obtain

$$\psi_{0s}^{(n)}(t; v_0) = \psi_{0s}(t; v_0) \sum_{k=1}^{n} \left(\sum_{j=k}^{n} s(j,k) s_{nj}(1/\theta_s) \psi_{0s}(t; j)(1-\theta_0)^j (1+t)^{j/\theta_s - n} \right) (-v_0)^k,$$

which provides the structure of the coefficients $a_{s,nk}$ in (11), namely,

$$a_{s,nk}(t) = \sum_{j=k}^{n} s(j,k) s_{nj}(1/\theta_s) \left(\frac{1-\theta_0}{\theta_0 + (1-\theta_0)(1+t)^{1/\theta_s}} \right)^j (1+t)^{j/\theta_s - n}.$$

It is clear from Theorem 3.3 Part (2) that the density for the nested Ali–Mikhail–Haq ∘ Clayton copula basically consists of the corresponding pieces of the Ali–Mikhail–Haq and the Clayton density we have already seen earlier. It is given by

$$c(\boldsymbol{u}) = (-1)^d \frac{1-\theta_0}{\theta_0} \left(\sum_{k=d_0}^{d} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u}))(-1)^k \operatorname{Li}_{-k}\big(\theta_0 \exp(-t(\boldsymbol{u}))\big) \right) \prod_{s=1}^{d_0} \theta_s^{d_s} \left(\prod_{j=1}^{d_s} u_{sj} \right)^{-(1+\theta_s)}.$$

Note that $\exp(t(\boldsymbol{u})) = \prod_{s=1}^{d_0} \frac{C_s(\boldsymbol{u}_s)}{1-\theta_0(1-C_s(\boldsymbol{u}_s))}$.

5. Numerical evaluation

5.1. The log-density

In statistical applications one typically aims at computing the log-density. From a numerical point of view, this is typically not as trivial as computing the density and taking the logarithm afterwards. Often, the density cannot be computed without running into numerical problems; hence taking the logarithm of the density faces the same problem. However, an intelligent implementation of the log-density is possible (and often even required); see the implementation in the `R` package `copula`.

We now briefly explain how one can efficiently compute the log-density of a nested Archimedean copula of Type (1). Recall from (13) that

$$c(\boldsymbol{u}) = \left(\sum_{k=d_0}^{d} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u}))\psi_0^{(k)}(t(\boldsymbol{u})) \right) \cdot \prod_{s=1}^{d_0} \prod_{j=1}^{d_s} (\psi_s^{-1})'(u_{sj}).$$

Let us first think about the signs of the terms $b^{d_0}_{\boldsymbol{d},k}(\boldsymbol{t}(\boldsymbol{u}))$, $k \in \{d_0, \dots, d\}$. By Theorem 3.3(1) we know that sign $\big(a_{s,d_sj_s}(t_s(\boldsymbol{u}_s))\big) = (-1)^{d_s-j_s}$, thus

$$\operatorname{sign}\prod_{s=1}^{d_0} a_{s,d_sj_s}(t_s(\boldsymbol{u}_s)) = (-1)^{\sum_{s=1}^{d_0} d_s - \sum_{s=1}^{d_0} j_s}.$$

Recall from (14) the structure of $b^{d_0}_{\boldsymbol{d},k}(\boldsymbol{t}(\boldsymbol{u}))$, which is the sum in $\boldsymbol{j} \in \mathcal{Q}^{d_0}_{\boldsymbol{d},k}$ over $\prod_{s=1}^{d_0} a_{s,d_sj_s}(t_s(\boldsymbol{u}_s))$. For such $\boldsymbol{j}$, it follows from the definition of $\mathcal{Q}^{d_0}_{\boldsymbol{d},k}$ that $\sum_{s=1}^{d_0} j_s = k$. Furthermore, note that $\sum_{s=1}^{d_0} d_s = d$; hence

$$\operatorname{sign} b^{d_0}_{\boldsymbol{d},k}(\boldsymbol{t}(\boldsymbol{u})) = (-1)^{d-k}.$$

This implies that

$$c(\boldsymbol{u}) = \left(\sum_{k=d_0}^{d} (-1)^{d-k} b^{d_0}_{\boldsymbol{d},k}(\boldsymbol{t}(\boldsymbol{u}))(-1)^k \psi_0^{(k)}(t(\boldsymbol{u}))\right) \cdot \prod_{s=1}^{d_0}\prod_{j=1}^{d_s} (-\psi_s^{-1})'(u_{sj}) \tag{22}$$

where we note that $\prod_{s=1}^{d_0}\prod_{k=1}^{d_s}(-1) = (-1)^d$.

We see from (22) that all appearing quantities are positive which is quite convenient for computing the log-density

$$\log c(\boldsymbol{u}) = \log\left(\sum_{k=d_0}^{d} (-1)^{d-k} b^{d_0}_{\boldsymbol{d},k}(\boldsymbol{t}(\boldsymbol{u}))(-1)^k \psi_0^{(k)}(t(\boldsymbol{u}))\right) + \sum_{s=1}^{d_0}\sum_{j=1}^{d_s} \log(-\psi_s^{-1})'(u_{sj}).$$

Since the latter double sum is typically trivial to compute, let us focus on the first sum. To compute the (intelligent) logarithm of this sum, let

$$x_k = \log\big((-1)^{d-k} b^{d_0}_{\boldsymbol{d},k}(\boldsymbol{t}(\boldsymbol{u}))\big) + \log\big((-1)^k \psi_0^{(k)}(t(\boldsymbol{u}))\big), \quad k \in \{d_0, \dots, d\},$$

and note that

$$\begin{aligned}\log \sum_{k=d_0}^{d} (-1)^{d-k} b^{d_0}_{\boldsymbol{d},k}(\boldsymbol{t}(\boldsymbol{u}))(-1)^k \psi_0^{(k)}(t(\boldsymbol{u})) &= \log \sum_{k=d_0}^{d} \exp(x_k)\\ &= x_{\max} + \log \sum_{k=d_0}^{d} \exp(x_k - x_{\max}),\end{aligned}$$

where $x_{\max} = \max_{d_0 \le k \le d} x_k$. Since all summands in the latter sum are in $(0, 1]$, the corresponding logarithm can easily be computed. It remains to discuss how the x_k, $k \in \{d_0, \dots, d\}$, can be computed.

For computing the x_k, $k \in \{d_0, \dots, d\}$, efficient implementations for the functions $\log((-1)^k \psi_0^{(k)}(t))$ in the R package `copula` can be used. Computing the quantities $\log\big((-1)^{d-k} b^{d_0}_{\boldsymbol{d},k}(\boldsymbol{t}(\boldsymbol{u}))\big)$ is more challenging. Recall from (14) that

$$b^{d_0}_{\boldsymbol{d},k}(\boldsymbol{t}(\boldsymbol{u})) = \sum_{\boldsymbol{j} \in \mathcal{Q}^{d_0}_{\boldsymbol{d},k}} \prod_{s=1}^{d_0} a_{s,d_sj_s}(t_s(\boldsymbol{u}_s)),$$

where $a_{s,d_sj_s}(t_s(\boldsymbol{u}_s))$ is given in (12). For computing the function $s_{d_sj_s}$ that often appears in $a_{s,d_sj_s}(t_s(\boldsymbol{u}_s))$, the function `coeffG` in `copula` can be used; to be more precise, `(-1)^(`d_s `-` j_s `) * copula:::coeffG(`d_s `,x)` computes $s_{d_sj_s}$`(x)`. For the summation over the set $\mathcal{Q}^{d_0}_{\boldsymbol{d},k}$, the R package `partitions` provides the function `blockparts`. With `blockparts` `(`$\boldsymbol{d}$ `-rep(1L,` d_0 `),` k `-` d_0 `)+1L` one can then obtain a matrix with d_0 rows where each column gives one $\boldsymbol{j} \in \mathcal{Q}^{d_0}_{\boldsymbol{d},k}$.

5.2. The −log-likelihood of two-parameter nested Gumbel copulas

In this section, we compute the −log-likelihood (based on a sample of size $n = 100$) of two nested Gumbel copulas with parameters θ_0 and θ_1 such that Kendall's tau equals 0.25 and 0.5, respectively. In order to be able to provide graphical insights, we focus on two-parameter nested copulas of the form

$$C(\boldsymbol{u}) = C_0(u_1, C_1(u_2, \dots, u_d)) \tag{23}$$

where $d \in \{3, 10\}$.

Note that we obtain nested Archimedean copulas of Type (23) from (1) by artificially thinking of u_1 as a child copula $\psi_0(\psi_0^{-1}(u_1))$ of dimension 1, that is, as a degenerate child copula. For such s, note that $a_{s,d_sj_s}(t_s(\boldsymbol{u}_s)) = a_{s,11}(t_s(\boldsymbol{u}_s))$ and $t_s(\boldsymbol{u}_s)$ equals ψ_0^{-1} at the corresponding (one-dimensional) argument, which is u_1 in (23). It follows from the last statement in Theorem 3.3(1) that $a_{s,d_sj_s}(t_s(\boldsymbol{u}_s)) = 1$ for degenerate children. This implies that these terms drop out of the product in (14). The set $\mathcal{Q}^{d_0}_{\boldsymbol{d},k}$ shrinks accordingly since $1 \le j_s \le d_s = 1$ for degenerate children s.

Fig. 1 displays the −log-likelihoods as level plots for the nested Gumbel copulas as described above based on a sample of size $n = 100$ (note the restriction $\theta_0 \le \theta_1$). The parameters from which the samples were drawn and the minima based on the grid points as displayed in the wireframe plots are included. It is interesting to see the behavior of the −log-likelihood in the child parameter θ_1 when the dimension of the child copula C_1 is increased (with C_0 and its dimension fixed). As can be seen from the plots, the −log-likelihood is easier to minimize in θ_1-direction. This behavior was already observed by Hofert et al. [13] for Archimedean copulas and can be expressed by the empirical observation that the mean squared error behaves like $1/(nd)$ which is decreasing in d for fixed n. To see a similar behavior here for the −log-likelihoods of the nested Gumbel copulas is not surprising since the marginal copula for $u_1 = 1$ is the Archimedean copula C_1. Finally, let us remark that the optimization procedure used to generate Fig. 1 can also be found in the R package `copula` as a demo. This can directly be used for fitting a two-level nested Archimedean copula to a real life data set. Furthermore, similar figures as Fig. 1 are provided in the demo for a nested Clayton copula.

6. Densities for three- (and higher-) level nested Archimedean copulas

In this section, a density formula analogous to (13) is derived for three-level nested Archimedean copulas and extensions to higher nesting levels are briefly addressed.

When working with three or more nesting levels, it turns out to be convenient to (slightly) change the notation used in the previous sections. Consider a three-level nested Archimedean copula of the form

$$C(\boldsymbol{u}) = C_1\big(C_{11}(C_{111}(\boldsymbol{u}_{111}), \ldots, C_{11d_{11}}(\boldsymbol{u}_{11d_{11}})), \ldots, C_{1d_1}(C_{1d_11}(\boldsymbol{u}_{1d_11}), \ldots, C_{1d_1d_{1d_1}}(\boldsymbol{u}_{1d_1d_{1d_1}}))\big), \tag{24}$$

where $\boldsymbol{u}_{s_1s_2s_3} = (u_{s_1s_2s_31}, \ldots, u_{s_1s_2s_3d_{s_1s_2s_3}})^\top$ denotes the argument of $C_{s_1s_2s_3}$ (the copula generated by $\psi_{s_1s_2s_3}$), $d_{s_1s_2s_3}$ denotes the dimension of $C_{s_1s_2s_3}$, and $d_{s_1s_2}$ denotes the dimension of $C_{s_1s_2}$ (the copula generated by $\psi_{s_1s_2}$). Here and in the following, s_1 always equals 1, $s_2 \in \{1, \ldots, d_{s_1}\}$, and $s_3 \in \{1, \ldots, d_{s_1s_2}\}$. Note that it is convenient to think of (24) as a tree; see Fig. 2. Furthermore, let

$$\begin{aligned}
t_{s_1s_2s_3}(\boldsymbol{u}_{s_1s_2s_3}) &= \sum_{s_4=1}^{d_{s_1s_2s_3}} \psi^{-1}_{s_1s_2s_3}(u_{s_1s_2s_3s_4}) = \psi^{-1}_{s_1s_2s_3}(C_{s_1s_2s_3}(\boldsymbol{u}_{s_1s_2s_3})),\\
\boldsymbol{u}_{s_1s_2} &= (\boldsymbol{u}^\top_{s_1s_21}, \ldots, \boldsymbol{u}^\top_{s_1s_2d_{s_1s_2}})^\top,\\
\boldsymbol{t}_{s_1s_2}(\boldsymbol{u}_{s_1s_2}) &= (t_{s_1s_21}(\boldsymbol{u}_{s_1s_21}), \ldots, t_{s_1s_2d_{s_1s_2}}(\boldsymbol{u}_{s_1s_2d_{s_1s_2}}))^\top,\\
C^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2}) &= C_{s_1s_2}(C_{s_1s_21}(\boldsymbol{u}_{s_1s_21}), \ldots, C_{s_1s_2d_{s_1s_2}}(\boldsymbol{u}_{s_1s_2d_{s_1s_2}}))\\
&= \psi_{s_1s_2}\left(\sum_{s_3=1}^{d_{s_1s_2}} \mathring{\psi}_{s_1s_2,s_1s_2s_3}\big(t_{s_1s_2s_3}(\boldsymbol{u}_{s_1s_2s_3})\big)\right),\\
t^{*s_1s_2}(\boldsymbol{u}_{s_1s_2}) &= \psi^{-1}_{s_1s_2}(C^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2})) = \sum_{s_3=1}^{d_{s_1s_2}} \mathring{\psi}_{s_1s_2,s_1s_2s_3}\big(t_{s_1s_2s_3}(\boldsymbol{u}_{s_1s_2s_3})\big),
\end{aligned}$$

where

$$\mathring{\psi}_{s_1s_2,s_1s_2s_3} = \psi^{-1}_{s_1s_2} \circ \psi_{s_1s_2s_3}$$

and $C^*_{s_1s_2}$ denotes the (marginal) nested Archimedean copula with root $C_{s_1s_2}$. Note that the dimension of the root copula $C_{s_1s_2}$ of the nested Archimedean copula $C^*_{s_1s_2}$ is $d_{s_1s_2}$ which is in general not equal to the dimension $d_{s_1s_2\cdot} = \sum_{s_3=1}^{d_{s_1s_2}} d_{s_1s_2s_3}$ of $C^*_{s_1s_2}$. Furthermore, the root copula C_1 ($=C_{s_1}$) of the nested Archimedean copula C has d_1 ($=d_{s_1}$) arguments, the s_2th of which has $d_{s_1s_2}$-many arguments. Overall, $d_{s_1\cdot\cdot} = \sum_{s_2=1}^{d_{s_1}} \sum_{s_3=1}^{d_{s_1s_2}} d_{s_1s_2s_3}$ equals d, the dimension of C.

In order to compute the density c of C, we use a similar idea as in Section 3.1.

By replacing $\psi_1(=\psi_{s_1}) = \mathcal{LS}[F_1]$ with the corresponding integral, we obtain

$$\begin{aligned}
C(\boldsymbol{u}) &= \int_0^\infty \prod_{s_2=1}^{d_1} \exp\big(-v_1\psi^{-1}_{s_1}(C^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2}))\big)\, dF_1(v_1)\\
&= \int_0^\infty \prod_{s_2=1}^{d_1} \psi_{s_1,s_1s_2}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2});\, v_1)\, dF_1(v_1)
\end{aligned}$$

where

$$\psi_{s_1,s_1s_2}(t;\, v_1) = \exp\big(-v_1\mathring{\psi}_{s_1,s_1s_2}(t)\big)$$

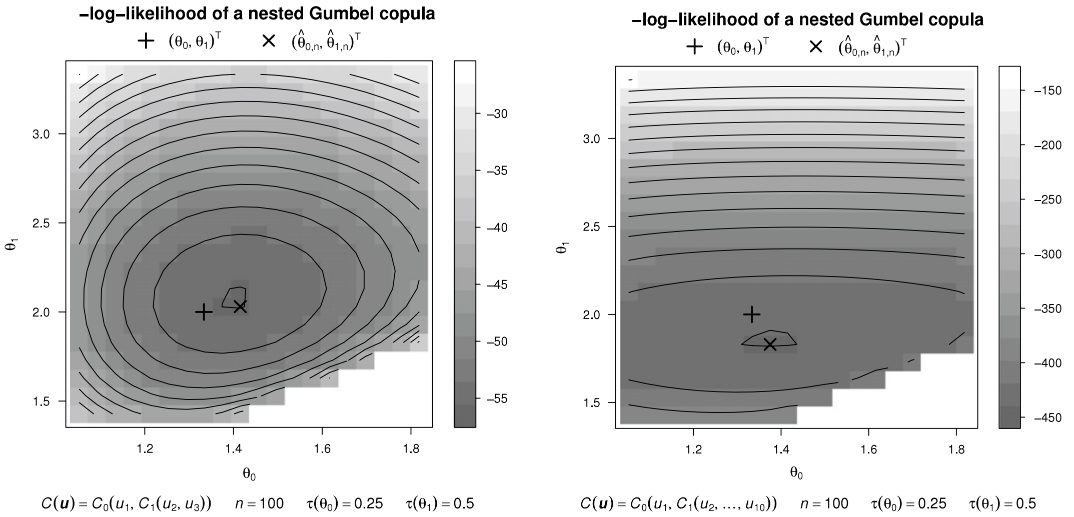

Fig. 1. Wireframe plots of the −log-likelihood of a three-dimensional (left) and a ten-dimensional (right) nested Gumbel copula $C(\boldsymbol{u}) = C_0(u_1, C_1(u_2, u_3))$ with parameters $\theta_0 = 4/3$ (Kendall's tau equals 0.25) and $\theta_1 = 2$ (Kendall's tau equals 0.5) based on a sample of size $n = 100$.

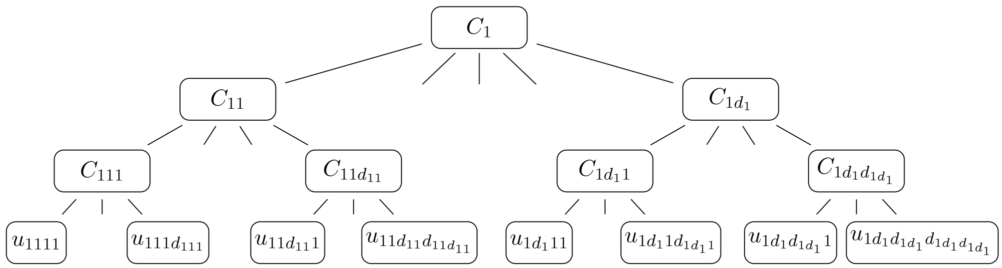

Fig. 2. Tree structure (some arguments are omitted) for a three-level nested Archimedean copula of Type (24).

and thus

$$c(\boldsymbol{u}) = \int_0^\infty \prod_{s_2=1}^{d_1} \frac{\partial}{\partial \boldsymbol{u}_{s_1 s_2}} \psi_{s_1, s_1 s_2}(t^*_{s_1 s_2}(\boldsymbol{u}_{s_1 s_2}); v_1)\, dF_1(v_1), \tag{25}$$

where $\frac{\partial}{\partial \boldsymbol{u}_{s_1 s_2}}$ denotes the derivative with respect to all components of $\boldsymbol{u}_{s_1 s_2}$ (which is a vector of length $d_{s_1 s_2 \cdot}$).

Similar as in Section 3.1, we observe the following key challenges:

Challenge 1 Find the derivatives in the integrand;
Challenge 2 Compute their product;
Challenge 3 Integrate it with respect to the mixture distribution function $F_1 = \mathcal{LS}^{-1}[\psi_1]$.

We will first solve Challenge 1 by considering a multivariate version of Faà di Bruno's formula. For suitable functions $f : \mathbb{R} \to \mathbb{R}$ and $g : \mathbb{R}^n \to \mathbb{R}$, it follows from Hardy [7] that

$$\frac{\partial}{\partial \boldsymbol{x}} f(g(\boldsymbol{x})) = \sum_{k=1}^{n} f^{(k)}(g(\boldsymbol{x})) \sum_{\pi : |\pi| = k} \prod_{B \in \pi} \frac{\partial^{|B|}}{\prod_{i \in B} \partial x_i} g(\boldsymbol{x}), \quad \boldsymbol{x} = (x_1, \ldots, x_n)^\top, \tag{26}$$

where the last sum extends over all partitions π of $\{1, \ldots, n\}$ with k elements and the last product over all blocks B of π. Observe that, if $x_1 = \cdots = x_n = x$, then the univariate Faà di Bruno's formula (9) can be restated as

$$(f \circ g)^{(n)}(x) = \sum_{k=1}^{n} f^{(k)}(g(x)) \sum_{\pi : |\pi| = k} \prod_{B \in \pi} g^{(|B|)}(x),$$

where π is a partition of $\{1, \ldots, n\}$. Comparing this identity with (9) yields

$$B_{n,k}(g'(x), \ldots, g^{(n-k+1)}(x)) = \sum_{\pi : |\pi| = k} \prod_{B \in \pi} g^{(|B|)}(x). \tag{27}$$

This will be used in the following lemma, which is a special case of (26) with stronger assumptions on the function g. It will then lead us to a solution for Challenge 1 by choosing suitable functions f and g.

Lemma 6.1. *Suppose there exists a partition $\{B_1,\dots,B_m\}$ of $\{1,\dots,n\}$ with $|B_l|=d_l$ for $l\in\{1,\dots,m\}$ (with $\sum_{l=1}^m d_l=n$), such that for any indices $k_1\in B_i$ and $k_2\in B_j$, for $i,j\in\{1,\dots,m\}$ with $i\neq j$, the partial derivative of $g(x_1,\dots,x_n)$ with respect to x_{k_1} and x_{k_2} equals zero, that is*

$$\frac{\partial^2}{\partial x_{k_1}\partial x_{k_2}}g(\boldsymbol{x})=0,\quad \text{for all } k_1\in B_i,\ k_2\in B_j,\ i,j\in\{1,\dots,m\},\ i\neq j. \tag{28}$$

Moreover, suppose that for any $l\in\{1,\dots,m\}$ and any subset B of B_l, there exist functions h_{l1} and h_{l2} such that

$$\frac{\partial^{|B|}}{\prod_{i\in B}\partial x_i}g(\boldsymbol{x})=h_{l1}^{(|B|)}(h_{l2}(\boldsymbol{x}))\prod_{i\in B}\frac{\partial}{\partial x_i}h_{l2}(\boldsymbol{x}). \tag{29}$$

Then one has, for any suitable function f,

$$\frac{\partial}{\partial\boldsymbol{x}}f(g(\boldsymbol{x}))=\left(\prod_{l=1}^m\prod_{i\in B_l}\frac{\partial}{\partial x_i}h_{l2}(\boldsymbol{x})\right)\cdot\sum_{k=1}^n f^{(k)}(g(\boldsymbol{x}))\sum_{\boldsymbol{j}\in\mathcal{Q}_{\boldsymbol{d},k}^m}\prod_{l=1}^m B_{d_l,j_l}\big(h_{l1}'(h_{l2}(\boldsymbol{x})),\dots,h_{l1}^{(d_l-j_l+1)}(h_{l2}(\boldsymbol{x}))\big),$$

where $\mathcal{Q}_{\boldsymbol{d},k}^m$ is defined as in Theorem 3.3(2) and $\boldsymbol{d}=(d_1,\dots,d_m)^\top$.

We are now in the position to solve Challenge 1. By applying Lemma 6.1 with $\boldsymbol{x}=\boldsymbol{u}_{s_1s_2}$, $n=d_{s_1s_2\cdot}$, $m=d_{s_1s_2}$, $B_l=\{s_1s_2l1,\dots,s_1s_2ld_{s_1s_2l}\}$ (slightly abusing the notation), $\boldsymbol{d}_{s_1s_2}=(d_{s_1s_21},\dots,d_{s_1s_2d_{s_1s_2}})^\top$, $f(t)=\psi_{s_1,s_1s_2}(t;v_1)$, $g(\boldsymbol{x})=t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2})$, $h_{l1}(t)=\mathring{\psi}_{s_1s_2,s_1s_2l}(t)$, and $h_{l2}(\boldsymbol{u})=t_{s_1s_2l}(\boldsymbol{u}_{s_1s_2l})=\sum_{s_4=1}^{d_{s_1s_2l}}\psi^{-1}_{s_1s_2l}(u_{s_1s_2ls_4})$, the derivative in the integrand in (25) is given by

$$\frac{\partial}{\partial\boldsymbol{u}_{s_1s_2}}\psi_{s_1,s_1s_2}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2});v_1)=\left(\prod_{s_3=1}^{d_{s_1s_2}}\prod_{s_4=1}^{d_{s_1s_2s_3}}(\psi^{-1}_{s_1s_2s_3})'(u_{s_1s_2s_3s_4})\right)\sum_{l=1}^{d_{s_1s_2\cdot}}\psi^{(l)}_{s_1,s_1s_2}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2});v_1)$$
$$\cdot\left(\sum_{\boldsymbol{j}\in\mathcal{Q}^{d_{s_1s_2}}_{\boldsymbol{d}_{s_1s_2},l}}\prod_{s_3=1}^{d_{s_1s_2}}B_{d_{s_1s_2s_3},j_{s_3}}\big((\mathring{\psi}^{(k)}_{s_1s_2,s_1s_2s_3}(t_{s_1s_2s_3}(\boldsymbol{u}_{s_1s_2s_3})))_{k\in\{1,\dots,d_{s_1s_2s_3}-j_{s_3}+1\}}\big)\right).$$

By applying Theorem 3.3(1), this derivative can be written as

$$\begin{aligned}\frac{\partial}{\partial\boldsymbol{u}_{s_1s_2}}\psi_{s_1,s_1s_2}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2});v_1)&=\left(\prod_{s_3=1}^{d_{s_1s_2}}\prod_{s_4=1}^{d_{s_1s_2s_3}}(\psi^{-1}_{s_1s_2s_3})'(u_{s_1s_2s_3s_4})\right)\psi_{s_1,s_2s_2}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2});v_1)\\&\quad\cdot\sum_{l=1}^{d_{s_1s_2\cdot}}\sum_{k=1}^{l}a_{s_1s_2,lk}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2}))(-v_1)^k\\&\quad\cdot\left(\sum_{\boldsymbol{j}\in\mathcal{Q}^{d_{s_1s_2}}_{\boldsymbol{d}_{s_1s_2},l}}\prod_{s_3=1}^{d_{s_1s_2}}B_{d_{s_1s_2s_3},j_{s_3}}\big((\mathring{\psi}^{(k)}_{s_1s_2,s_1s_2s_3}(t_{s_1s_2s_3}(\boldsymbol{u}_{s_1s_2s_3})))_{k\in\{1,\dots,d_{s_1s_2s_3}-j_{s_3}+1\}}\big)\right).\end{aligned}$$

Interchanging the order of summation in the double sum yields

$$\begin{aligned}\frac{\partial}{\partial\boldsymbol{u}_{s_1s_2}}\psi_{s_1,s_1s_2}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2});v_1)&=\left(\prod_{s_3=1}^{d_{s_1s_2}}\prod_{s_4=1}^{d_{s_1s_2s_3}}(\psi^{-1}_{s_1s_2s_3})'(u_{s_1s_2s_3s_4})\right)\psi_{s_1,s_2s_2}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2});v_1)\\&\quad\cdot\sum_{k=1}^{d_{s_1s_2\cdot}}(-v_1)^k\sum_{l=k}^{d_{s_1s_2\cdot}}\Bigg(a_{s_1s_2,lk}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2}))\\&\quad\cdot\left(\sum_{\boldsymbol{j}\in\mathcal{Q}^{d_{s_1s_2}}_{\boldsymbol{d}_{s_1s_2},l}}\prod_{s_3=1}^{d_{s_1s_2}}B_{d_{s_1s_2s_3},j_{s_3}}\big((\mathring{\psi}^{(k)}_{s_1s_2,s_1s_2s_3}(t_{s_1s_2s_3}(\boldsymbol{u}_{s_1s_2s_3})))_{k\in\{1,\dots,d_{s_1s_2s_3}-j_{s_3}+1\}}\big)\right)\Bigg)\end{aligned}$$

which can be written as

$$\frac{\partial}{\partial \boldsymbol{u}_{s_1s_2}}\psi_{s_1,s_1s_2}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2});\,v_1) = \left(\prod_{s_3=1}^{d_{s_1s_2}}\prod_{s_4=1}^{d_{s_1s_2s_3}}(\psi^{-1}_{s_1s_2s_3})'(u_{s_1s_2s_3s_4})\right)\psi_{s_1,s_2s_2}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2});\,v_1) \cdot \sum_{k=1}^{d_{s_1s_2\cdot}} a_{s_1s_2,d_{s_1s_2\cdot}k}(\boldsymbol{t}_{s_1s_2}(\boldsymbol{u}_{s_1s_2}))(-v_1)^k, \tag{30}$$

for

$$a_{s_1s_2,d_{s_1s_2\cdot}k}(\boldsymbol{t}_{s_1s_2}(\boldsymbol{u}_{s_1s_2})) = \sum_{l=k}^{d_{s_1s_2\cdot}}\left(a_{s_1s_2,lk}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2}))\cdot\left(\sum_{\boldsymbol{j}\in\mathcal{Q}^{d_{s_1s_2}}_{\boldsymbol{d}_{s_1s_2},l}}\prod_{s_3=1}^{d_{s_1s_2}}B_{d_{s_1s_2s_3},j_{s_3}} \times\left((\mathring{\psi}^{(k)}_{s_1s_2,s_1s_2s_3}(t_{s_1s_2s_3}(\boldsymbol{u}_{s_1s_2s_3})))_{k\in\{1,\ldots,d_{s_1s_2s_3}-j_{s_3}+1\}}\right)\right)\right). \tag{31}$$

With this notation, the connection with Theorem 3.3(1) is clearly visible.

Finally, in order to solve Challenges 2 and 3, one introduces

$$b^{d_{s_1}}_{\boldsymbol{d}_{s_1},k}(\boldsymbol{t}(\boldsymbol{u})) = \sum_{\boldsymbol{j}\in\mathcal{Q}^{d_1}_{\boldsymbol{d}_{s_1},k}}\prod_{s_2=1}^{d_{s_1}} a_{s_1s_2,d_{s_1s_2\cdot}j_{s_2}}(\boldsymbol{t}_{s_1s_2}(\boldsymbol{u}_{s_1s_2})), \tag{32}$$

with

$$\begin{aligned}
&\boldsymbol{t}(\boldsymbol{u}) = (\boldsymbol{t}_1(\boldsymbol{u}_1)^\top,\ldots,\boldsymbol{t}_{d_1}(\boldsymbol{u}_{d_1})^\top)^\top,\\
&\boldsymbol{t}_{s_1}(\boldsymbol{u}_{s_1}) = (\boldsymbol{t}_{s_11}(\boldsymbol{u}_{s_11})^\top,\ldots,\boldsymbol{t}_{s_1d_{s_1}}(\boldsymbol{u}_{s_1d_{s_1}})^\top)^\top,\\
&\boldsymbol{d}_{s_1} = (\boldsymbol{d}^\top_{s_11},\ldots,\boldsymbol{d}^\top_{s_1d_{s_1}})^\top.
\end{aligned}$$

Similarly to Theorem 3.3(2), one then obtains (with $t(\boldsymbol{u}) = \psi_1^{-1}(C(\boldsymbol{u}))$ as before)

$$\begin{aligned}
c(\boldsymbol{u}) &= \int_0^\infty \prod_{s_2=1}^{d_{s_1}} \frac{\partial}{\partial \boldsymbol{u}_{s_1s_2}}\psi_{s_1,s_1s_2}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2});\,v_1)\,dF_1(v_1)\\
&= \left(\prod_{s_2=1}^{d_{s_1}}\prod_{s_3=1}^{d_{s_1s_2}}\prod_{s_4=1}^{d_{s_1s_2s_3}}(\psi^{-1}_{s_1s_2s_3})'(u_{s_1s_2s_3s_4})\right)\sum_{k=d_{s_1}}^{d} b^{d_{s_1}}_{\boldsymbol{d}_{s_1},k}(\boldsymbol{t}(\boldsymbol{u}))\\
&\quad\cdot\int_0^\infty\left(\prod_{s_2=1}^{d_{s_1}}\psi_{s_1,s_1s_2}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2});\,v_1)\right)(-v_1)^k dF_1(v_1)\\
&= \left(\prod_{s_2=1}^{d_{s_1}}\prod_{s_3=1}^{d_{s_1s_2}}\prod_{s_4=1}^{d_{s_1s_2s_3}}(\psi^{-1}_{s_1s_2s_3})'(u_{s_1s_2s_3s_4})\right)\sum_{k=d_{s_1}}^{d} b^{d_{s_1}}_{\boldsymbol{d}_{s_1},k}(\boldsymbol{t}(\boldsymbol{u}))\,\psi_1^{(k)}(t(\boldsymbol{u})).
\end{aligned} \tag{33}$$

Remark 6.2. The pattern to compute the density of nested Archimedean copulas with more than three levels can be deduced from the previous computations, the following heuristic argument shows how. In order to understand the reasoning, it is useful to remind ourselves that the structure of nested Archimedean copulas can be depicted by trees; see Fig. 2 for a tree representation of (24). Let L denote the number of levels (with (24) having $L = 3$). Thanks to our notation, we can easily identify a certain branch of the tree with the corresponding sequence of indices. Each time a nesting level is added, for each branch $s_1s_2\cdots s_l$, $l\in\{1,\ldots,L\}$, finite sequences of coefficients a's and b's (similar to $a_{s_1s_2,d_{s_1s_2\cdot}k}$ and $b^{d_{s_1}}_{\boldsymbol{d}_{s_1},k}$ above) will appear and their structure can be deduced from Eq. (31). More precisely, as in Eqs. (14) and (32), the sequence of b's can always be interpreted as the coefficients of the Cauchy product of the polynomials with a's as coefficients.

The structure of the a's at each branch $s_1\cdots s_l$ is more complicated. For any branch $s_1\cdots s_L$, that is on the ultimate level of nesting, the a's are simply the Bell polynomials applied to the function $\mathring{\psi}_{s_1\cdots s_{L-1},s_1\cdots s_L}$ and its derivatives. For any other branch $s_1\cdots s_l$, $l\in\{1,\ldots,L-1\}$, the coefficients a's are the (Euclidean) inner product of the vector of all Bell polynomials applied to the function $\mathring{\psi}_{s_1\cdots s_l,s_1\cdots s_{l+1}}$ and its derivatives with the vector of all coefficients b's, the exact structure of Eq. (31). In

Eq. (31), the level l is equal to $1 = L-2$ and the term $a_{s_1s_2,lk}(t^*_{s_1s_2}(\boldsymbol{u}_{s_1s_2}))$ stands for the Bell polynomial applied to $\mathring{\psi}_{s_1\cdots s_l,s_1\cdots s_{l+1}}$ and its derivatives, while the lth member of the sequence of b's is defined by

$$\sum_{\boldsymbol{j}\in\mathcal{Q}^{d_{s_1s_2}}_{\boldsymbol{d}_{s_1s_2},l}} \prod_{s_3=1}^{d_{s_1s_2}} B_{d_{s_1s_2s_3},j_{s_3}}\left(\left(\mathring{\psi}^{(k)}_{s_1s_2,s_1s_2s_3}(t_{s_1s_2s_3}(\boldsymbol{u}_{s_1s_2s_3}))\right)_{k\in\{1,\dots,d_{s_1s_2s_3}-j_{s_3}+1\}}\right),$$

the term appearing in (31).

Acknowledgments

The authors would like to thank Paul Embrechts (ETH Zurich) for giving them feedback and the opportunity to work on this topic. The first author (Willis Research Fellow) thanks Willis Re for financial support while this work was being completed.

Appendix

Proof of Lemma 3.1. (1) $\sum_{l=1}^{n-k+1}(x-l)j_l = x\sum_{l=1}^{n-k+1} j_l - \sum_{l=1}^{n-k+1} lj_l = xk - n$.
(2) The identity $B_{n,k}(1,\dots,1) = S(n,k)$ can be found, for example, in [4, p. 135] or [3, p. 87]. It then follows that

$$\begin{aligned} B_{n,k}(x,\dots,x) &= \sum_{\boldsymbol{j}\in\mathcal{P}_{n,k}} \binom{n}{j_1,\dots,j_{n-k+1}} \prod_{l=1}^{n-k+1}\left(\frac{x}{l!}\right)^{j_l} \\ &= x^k B_{n,k}(1,\dots,1) = S(n,k)x^k, \end{aligned}$$

since $\sum_{l=1}^{n-k+1} j_l = k$ by definition of $\mathcal{P}_{n,k}$.
(3) By definition of $\mathcal{P}_{n,k}$ it follows from $\sum_{l=1}^{n-k+1} lj_l = n$ and (2) that

$$\begin{aligned} B_{n,k}(-x,\dots,(-1)^{n-k+1}x) &= \sum_{\boldsymbol{j}\in\mathcal{P}_{n,k}} \binom{n}{j_1,\dots,j_{n-k+1}} \prod_{l=1}^{n-k+1}\left(\frac{(-1)^l x}{l!}\right)^{j_l} \\ &= (-1)^n B_{n,k}(x,\dots,x) = (-1)^n S(n,k)x^k. \end{aligned}$$

(4) By (8),

$$B_{n,k}(g'(x), g''(x),\dots,g^{(n-k+1)}(x)) = \sum_{\boldsymbol{j}\in\mathcal{P}_{n,k}} \binom{n}{j_1,\dots,j_{n-k+1}} \prod_{l=1}^{n-k+1}\left(\frac{g^{(l)}(x)}{l!}\right)^{j_l}. \tag{34}$$

Note that $\operatorname{sign}(g^{(l)}(x)) = (-1)^{l-1}$ for all x and $l \in \{1,\dots,n-k+1\}$, so that the sign of the lth factor in the product in (34) is $(-1)^{(l-1)j_l}$. This implies that

$$\operatorname{sign}\prod_{l=1}^{n-k+1}\left(\frac{g^{(l)}(x)}{l!}\right)^{j_l} = (-1)^{\sum_{l=1}^{n-k+1}(l-1)j_l} = (-1)^{\sum_{l=1}^{n-k+1} lj_l - \sum_{l=1}^{n-k+1} j_l}.$$

Now since we sum over $\boldsymbol{j} \in \mathcal{P}_{n,k}$, we see from (7) that

$$\operatorname{sign}\prod_{l=1}^{n-k+1}\left(\frac{g^{(l)}(x)}{l!}\right)^{j_l} = (-1)^{n-k}$$

and thus the whole sum in (34) has this sign. □

Proof of Proposition 3.2. (1) Let $h(t) = \exp((yt)^x)$. It follows from Faà di Bruno's formula ((6) and (9) with $f(x) = \exp(x)$ and $g(t) = (yt)^x$) and Lemma 3.1 Part (1) that

$$\begin{aligned} h^{(n)}(t) &= h(t)\sum_{k=1}^{n}\sum_{\boldsymbol{j}\in\mathcal{P}_{n,k}} \binom{n}{j_1,\dots,j_{n-k+1}} \prod_{l=1}^{n-k+1}\left(\frac{(x)_l y^x t^{x-l}}{l!}\right)^{j_l} \\ &= h(t)\sum_{k=1}^{n}\sum_{\boldsymbol{j}\in\mathcal{P}_{n,k}} \binom{n}{j_1,\dots,j_{n-k+1}} \prod_{l=1}^{n-k+1}\left(\frac{(x)_l y^x}{l!}\right)^{j_l} t^{xk-n} \end{aligned}$$

$$= h(t)\sum_{k=1}^{n} y^n \sum_{\boldsymbol{j}\in\mathcal{P}_{n,k}} \binom{n}{j_1,\ldots,j_{n-k+1}} \prod_{l=1}^{n-k+1}\left(\frac{(x)_l y^{x-l}}{l!}\right)^{j_l} t^{xk-n}$$

$$= \frac{h(t)}{t^n}\sum_{k=1}^{n} y^n B_{n,k}((x)_1 y^{x-1},\ldots,(x)_{n-k+1}y^{x-(n-k+1)})t^{xk}.$$

On the other hand, we may differentiate the series expansion of h and use the identity $e^{-x}\sum_{k=0}^{\infty} k^l x^k/k! = \sum_{k=0}^{l} S(l,k)x^k$, see [2], with x being $(yt)^x$. With (10), it then follows that

$$h^{(n)}(t) = \sum_{k=0}^{\infty}(xk)_n \frac{t^{xk-n}}{k!}y^{xk} = \frac{1}{t^n}\sum_{k=0}^{\infty}\left(\sum_{l=1}^{n} s(n,l)(xk)^l\right)\frac{(yt)^{xk}}{k!}$$

$$= \frac{1}{t^n}\sum_{l=1}^{n} s(n,l)x^l \sum_{k=0}^{\infty} k^l \frac{(yt)^{xk}}{k!} = \frac{\exp((yt)^x)}{t^n}\sum_{l=1}^{n} s(n,l)x^l\sum_{k=0}^{l} S(l,k)(yt)^{xk}$$

$$= \frac{h(t)}{t^n}\sum_{k=0}^{n}\left(y^{xk}\sum_{l=k}^{n} x^l s(n,l)S(l,k)\right)t^{xk} = \frac{h(t)}{t^n}\sum_{k=1}^{n}\left(y^{xk}\sum_{l=k}^{n} x^l s(n,l)S(l,k)\right)t^{xk}.$$

Comparing the two representations for $h^{(n)}$ leads to the result as stated.

(2) Since $\sum_{k=1}^{j}(x)_k S(j,k) = x^j$ and by (10), one obtains that

$$\sum_{k=1}^{n}(-1)_k s_{nk}(x) = \sum_{j=1}^{n} s(n,j)x^j\sum_{k=1}^{j}(-1)_k S(j,k) = \sum_{j=1}^{n} s(n,j)(-x)^j = (-x)_n.$$

(3) For all $x\in(0,1]$, $s_{nk}(x) = (-1)^{n-k}p(n;k)n!/k!$, where the probability mass function $p(n;k) > 0$ (in $n\in\{k,k+1,\ldots\}$) corresponds to the distribution function whose Laplace–Stieltjes transform is the inner generator appearing in a nested Joe copula; consider Hofert [8, p. 99] with $V_0 = k$ and $\theta_0/\theta_1 = x$ to see this. This representation implies that $\operatorname{sign}(s_{nk}(x)) = (-1)^{n-k}$. □

Proof of Theorem 3.3. (1) Apply (9) with $f(x) = \exp(-v_0 x)$ and $g(t) = \mathring{\psi}_{0s}(t)$. For the statement about the signs, apply Lemma 3.1(4). For the last statement, note that by Lemma 3.1(2), $a_{s,11}(t) = B_{1,1}(\mathring{\psi}_{0s}'(t)) = B_{1,1}(1) = S(1,1)\cdot 1^1 = 1$ if $\psi_s = \psi_0$.

(2) Given the form (11) we see that the product appearing as integrand in (5) can be computed via

$$\prod_{s=1}^{d_0}\psi_{0s}^{(d_s)}(t_s(\boldsymbol{u}_s);v_0) = \prod_{s=1}^{d_0}\sum_{k=1}^{d_s} a_{s,d_s k}(t_s(\boldsymbol{u}_s))(-v_0)^k\cdot\prod_{s=1}^{d_0}\psi_{0s}(t_s(\boldsymbol{u}_s);v_0)$$

$$= \sum_{k=d_0}^{d} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u}))(-v_0)^k\cdot\prod_{s=1}^{d_0}\psi_{0s}(t_s(\boldsymbol{u}_s);v_0).$$

Now note that $\prod_{s=1}^{d_0}\psi_{0s}(t_s(\boldsymbol{u}_s);v_0) = \exp(-v_0 t(\boldsymbol{u}))$. Hence, we obtain

$$\prod_{s=1}^{d_0}\psi_{0s}^{(d_s)}(t_s(\boldsymbol{u}_s);v_0) = \sum_{k=d_0}^{d} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u}))(-v_0)^k\exp(-v_0 t(\boldsymbol{u})).$$

By replacing v_0 by V_0 and taking the expectation, one obtains

$$\mathbb{E}\left[\prod_{s=1}^{d_0}\psi_{0s}^{(d_s)}(t_s(\boldsymbol{u}_s);V_0)\right] = \sum_{k=d_0}^{d} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u}))\mathbb{E}\big[(-V_0)^k\exp(-V_0 t(\boldsymbol{u}))\big]$$

$$= \sum_{k=d_0}^{d} b_{\boldsymbol{d},k}^{d_0}(\boldsymbol{t}(\boldsymbol{u}))\psi_0^{(k)}(t(\boldsymbol{u})),$$

so that, by (5), the density is of the form as stated. □

Proof of Lemma 6.1. Due to Eq. (28), observe that the second sum in (26) may be rewritten as

$$\sum_{\pi:|\pi|=k}\prod_{B\in\pi}\frac{\partial^{|B|}}{\prod_{i\in B}\partial x_i}g(\boldsymbol{x}) = \sum_{\boldsymbol{j}\in\mathcal{Q}_{\boldsymbol{d},k}^m}\prod_{l=1}^{m}\left(\sum_{\pi_l:|\pi_l|=j_l}\prod_{B\in\pi_l}\frac{\partial^{|B|}}{\prod_{i\in B}\partial x_i}g(\boldsymbol{x})\right),$$

where π_l is a partition of B_l with j_l elements, $l\in\{1,\ldots,m\}$; note that $j_l\le d_l$, because $|B_l| = d_l$. Both sides are equal because the remaining terms in the sum on the left-hand side are zero as derivatives with respect to two or more variables belonging to different partitions vanish. Combining this result with (29), it follows from (26) that

$$\frac{\partial}{\partial \boldsymbol{x}} f(g(\boldsymbol{x})) = \sum_{k=1}^{n} f^{(k)}(g(\boldsymbol{x})) \sum_{\boldsymbol{j} \in \mathcal{Q}^{m}_{\boldsymbol{d},k}} \prod_{l=1}^{m} \left(\sum_{\pi_l : |\pi_l| = j_l} \left(\prod_{B \in \pi_l} \left(h_{l1}^{(|B|)}(h_{l2}(\boldsymbol{x})) \prod_{i \in B} \frac{\partial}{\partial x_i} h_{2l}(\boldsymbol{x}) \right) \right) \right).$$

Observe that for any partition π_l of B_l, $l \in \{1, \ldots, m\}$, we have that

$$\prod_{B \in \pi_l} \prod_{i \in B} \frac{\partial}{\partial x_i} h_{l2}(\boldsymbol{x}) = \prod_{i \in B_l} \frac{\partial}{\partial x_i} h_{l2}(\boldsymbol{x}),$$

so that

$$\begin{aligned} \frac{\partial}{\partial \boldsymbol{x}} f(g(\boldsymbol{x})) &= \sum_{k=1}^{n} f^{(k)}(g(\boldsymbol{x})) \sum_{\boldsymbol{j} \in \mathcal{Q}^{m}_{\boldsymbol{d},k}} \prod_{l=1}^{m} \left(\left(\prod_{i \in B_l} \frac{\partial}{\partial x_i} h_{l2}(\boldsymbol{x}) \right) \sum_{\pi_l : |\pi_l| = j_l} \prod_{B \in \pi_l} h_{l1}^{(|B|)}(h_{l2}(\boldsymbol{x})) \right) \\ &= \left(\prod_{l=1}^{m} \prod_{i \in B_l} \frac{\partial}{\partial x_i} h_{l2}(\boldsymbol{x}) \right) \sum_{k=1}^{n} f^{(k)}(g(\boldsymbol{x})) \sum_{\boldsymbol{j} \in \mathcal{Q}^{m}_{\boldsymbol{d},k}} \prod_{l=1}^{m} \sum_{\pi_l : |\pi_l| = j_l} \prod_{B \in \pi_l} h_{l1}^{(|B|)}(h_{l2}(\boldsymbol{x})). \end{aligned}$$

Finally, applying identity (27) completes the proof. □

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