Power-divergence copulas: A new family of Archimedean copulas

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Supplementary Material

This document is supplementary material for the paper named above. In what follows, labels such as Section 1, equation (1), Definition 1, Figure 1, etc., refer to the main text, while Section S1, equation (S1), Definition S1, Figure S1, etc., refer to the contents of this document. In this supplementary material, Section S1 discusses an alternative definition of phi divergences (here labelled 'φ divergences') used by some researchers and its relationship to the one given in Definition 4 ('ϕ divergences'). Section S2 gives an example of a ϕ function that is not continuously differentiable on $(0, \infty)$. Section S3 presents exact formulas for the power-divergence (PD) copulas with $\lambda = -2$, $\lambda = -0.5$ and $\lambda = 1$. In Section S4, we show how to compute and simulate from a bivariate PD copula. Section S5 presents additional results for the analysis of the stock-market indices in the main text, and Section S6 presents an analysis of a Danish fire-insurance dataset. In Section S7, we provide detailed proofs of all results presented in the main text.

S1 Alternative definition of phi divergence

S1.1 A different form of phi (φ) divergence

When defining a phi divergence of one probability distribution from another, alternative definitions have been used other than Definition 4. For clarity, from this point on, we use the symbol ϕ to refer to ϕ divergences and ϕ-divergence generators under Definition 4. We use φ to refer to φ divergences under the alternative definition given below.

The following definition of a φ divergence is sometimes used to define divergences of one probability distribution from another.

Definition S1. Let P and Q be absolutely continuous probability distributions admitting densities p and q with respect to Lebesgue measure. Let $\varphi(x)$ be a convex function for $x > 0$ that satisfies (a) $\varphi(1) = 0$, and (b) $\varphi''(1) > 0$. Then, the φ divergence of P from Q is defined as,

$$D_\varphi(p||q) \equiv \int q(s) \times \varphi\left(\frac{p(s)}{q(s)}\right) \, \mathrm{d}s,$$

where $0 \times \varphi(0/0) = 0$, and $0 \times \varphi(v/0) = v \times \{\lim_{x\to\infty} \varphi(x)/x\}$.

When the probability densities p and q are used as arguments of the ϕ divergence of Definition 4, it is straightforward to show that $D_\phi(p\|q) = \int q(s) \times \phi(p(s)/q(s)) \, \mathrm{d}s$ and $D_\varphi(p\|q) = \int q(s) \times \varphi(p(s)/q(s)) \, \mathrm{d}s$ are exactly equivalent. However, while Definition S1 is only valid when $\int p(s) \, \mathrm{d}s = 1$

and $\int q(s)\,\mathrm{d}s = 1$, Definition 4 is valid for non-negative functions that may not integrate to unity.

S1.2 Relationship to Definition 4

We can recover $\phi(x)$ from $\varphi(x)$ $(x > 0)$ by noting the affine-invariance property of convex functions (e.g., Amari, 2016, p. 56): That is, if $\varphi(x)$ is convex with $\varphi(1) = 0$ and $\varphi''(1) > 0$, the function $\phi^{@}(x) = \varphi(x)+c\times(x-1)$, with real-valued constant c, is also convex with $\phi^{@}(1) = 0$ and $(\phi^{@})''(1) > 0$. Now, following, for example, Cressie and Pardo (2002), take $c = -\varphi'(1)$, and define $\phi(x) \equiv \varphi(x) + \varphi'(1) \times (1 - x)$. Compared to $\varphi(x)$, $\phi(x)$ has the additional property that $\phi'(1) = 0$.

S1.3 Failure of φ to be an Archimedean copula generator

The function $\varphi(x),\ x > 0$, in Definition S1 does not necessarily correspond to an Archimedean-copula generator, though some do. For example, $\varphi(x) = -\log(x)$ satisfies (a) and (b) of Definition S1, and it is a valid Archimedean-copula generator that corresponds to the product copula. However, this does not hold in general. Consider the counterexample below.

Let $\lambda \in (-\infty, \infty)$. Cressie and Read (1984) consider the function,

$$\varphi_\lambda(x) \equiv \frac{x^{\lambda+1} - x}{\lambda(\lambda + 1)},\ \lambda \neq -1, 0,$$

where $x > 0$, and $\varphi_0(x) \equiv \lim_{\lambda\to 0}\phi_\lambda(x)$ and $\varphi_{-1}(x) \equiv \lim_{\lambda\to -1}\varphi_\lambda(x)$. It is straightforward to verify that $\phi_\lambda(x)$ in (3.1) is $\phi_\lambda(x) \equiv \varphi_\lambda(x) + \varphi'_\lambda(1)(1-x)$ for $x > 0$.

Now take $\lambda = 1$, which yields $\varphi_1(x) = 0.5(x^2 - x)$ for $x > 0$, and define $\varphi_1(0) = \lim_{s\downarrow 0}\varphi_1(s)$. The function $\varphi_1(x)$ is not even non-negative for $x \in (0, 1)$, and $\varphi_1(x)$ is not strictly decreasing on $x \in [0, 1]$ since its first derivative, $\varphi'_1(x) = x - 0.5$, is negative for $x \in [0, 0.5)$, zero at $x = 0.5$, and positive for $x \in (0.5, 1]$. This is one example of a φ function that does not satisfy the requirements of an Archimedean-copula generator given in Definition 1.

S2 ϕ function that is not continuously differentiable

Define the piecewise function,

$$\phi_{\text{pw}}(x) = \begin{cases} 0.25 - \exp\{2\} + \exp\{1/x\} & 0 < x < 0.5, \\ (1-x)^2 & 0.5 \le x < \infty. \end{cases}$$

The function $\phi_{\text{pw}} : (0, \infty) \to [0, \infty)$ satisfies (a)-(c) of Definition 4. It is strictly convex for all $x \in (0, \infty)$; it is equal to zero at $x = 1$; it has two derivatives at $x = 1$, with $\phi'_{\text{pw}}(1) = 0$ and $\phi''_{\text{pw}}(1) > 0$; but it lacks a derivative at $x = 0.5$. On defining $\phi_{\text{pw}}(0) = \infty$ since $\lim_{s\downarrow 0}\phi_{\text{pw}}(s) = \infty$, Proposition 1 implies $\phi_{\text{pw}} : [0, 1] \to [0, \infty]$ is a valid Archimedean-copula

generator. The pseudoinverse of $\phi_{\text{pw}}(x)$ is given by,

$$\phi_{\text{pw}}^{[-1]}(t) = \begin{cases} 1 - \sqrt{t} & 0 \leq t < 0.25, \\ [\log(t - 0.25 + \exp\{2\})]^{-1} & 0.25 \leq t \leq \infty. \end{cases}$$

This is a strict inverse, so $\phi_{\text{pw}}^{[-1]}(t) = \phi_{\text{pw}}^{-1}(t)$ for all $t \in [0, \infty]$, but it lacks a derivative at $t = 0.25$, where the two cases meet. Fig. S1 clearly illustrates this point. Since ϕ_{pw}^{-1} is not differentiable for all $t \in (0, \infty)$, ϕ_{pw}^{-1} cannot be d-monotone on $[0, \infty)$ for any $d \geq 3$ (McNeil and Nešlehová, 2009). Therefore, ϕ_{pw} does not generate a valid Archimedean copula in any dimensions $d \geq 3$.

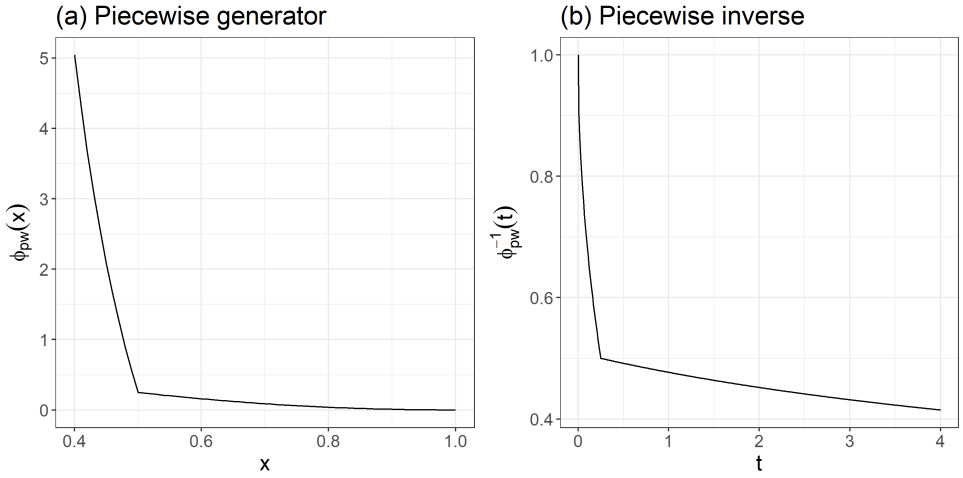

Figure S1: The left panel (a) shows the piecewise ϕ function, $\phi_{\text{pw}}(x)$, $x \in [0, 1]$. Note that $\phi_{\text{pw}}(x)$ has only been plotted for $x \in [0.4, 1]$ to 'zoom in' on the point $x = 0.5$, where the function is continuous but lacks a derivative. The right panel (b) shows the (strict) inverse $\phi_{\text{pw}}^{-1}(t)$ over $t \in [0, 4]$.

S3 Exact formulas for $\lambda = -2$, $\lambda = -0.5$ and $\lambda = 1$

For $u_1, u_2 \in [0,1]$, the PD copula with $\lambda = -2$ is,

$$C_{-2}(u_1,u_2) = 1 + 0.5(u_1^{-1} + u_1 + u_2^{-1} + u_2 - 4) - \sqrt{0.25(u_1^{-1} + u_1 + u_2^{-1} + u_2 - 4)^2 + u_1^{-1} + u_1 + u_2^{-1} + u_2 - 4}. \tag{S3.1}$$

The associated copula density, which exists for all $u_1, u_2 \in [0,1]$ due to Theorem 1, is denoted by $c_{-2}(u_1,u_2)$. The expression is not easy to simplify, but it can be obtained in closed form by substituting (S3.1) into (3.11).

The PD copula with $\lambda = -0.5$ is given as follows. For $\{(u_1,u_2) \in [0,1]^2 : 0 \leq (\sqrt{u_1}-1)^2 + (\sqrt{u_1}-1)^2 < 1\}$,

$$C_{-0.5}(u_1,u_2) = 1 + (\sqrt{u_1}-1)^2 + (\sqrt{u_2}-1)^2 - 2\sqrt{(\sqrt{u_1}-1)^2 + (\sqrt{u_1}-1)^2}. \tag{S3.2}$$

Otherwise, $C_{-0.5}(u_1,u_2) = 0$. The copula $C_{-0.5}$ is absolutely continuous by Theorem 1. For $(u_1,u_2) \in [0,1]^2$ such that $0 \leq 2-2(\sqrt{u_1}+\sqrt{u_2})+(u_1+u_2) < 1$, the associated copula density is given by,

$$c_{-0.5}(u_1,u_2) = \frac{(1-(\sqrt{u_1})^{-1})(1-(\sqrt{u_2})^{-1})}{(2-2(\sqrt{u_1}+\sqrt{u_2})+u_1+u_2)^{3/2}}. \tag{S3.3}$$

On the other hand, with $\lambda = 1$, the PD copula is,

$$C_1(u_1,u_2) = \max\left\{1 - \sqrt{u_1^2 - 2u_1 + u_2^2 - 2u_2 + 2}, 0\right\}, \ u_1, u_2 \in [0,1]. \tag{S3.4}$$

The copula $C_1(u_1, u_2)$ has a singular part and an absolutely continuous part. The singular part is supported on the zero curve (the curve in $[0,1]^2$ traced by $u_1^2 - 2u_1 + u_2^2 - 2u_2 + 2 = 1$), and it contains 50% of the probability mass of the bivariate distribution by Theorem 1. On the absolutely continuous part of the copula, over the part of the unit square where $u_1^2 - 2u_1 + u_2^2 - 2u_2 + 2 < 1$, the derivative $\partial^2 C_1(u_1, u_2)/\partial u_1 \partial u_2$ exists and is given by,

$$\frac{\partial^2 C_1}{\partial u_1 \partial u_2} = \frac{(u_1 - 1)(u_2 - 1)}{(u_1^2 - 2u_1 + u_2^2 - 2u_2 + 2)^{3/2}}. \tag{S3.5}$$

Fig. S2 displays the copulas and derivatives for $\lambda = -0.5$ and $\lambda = 1$. Recall that the PD copulas with $\lambda = -2$ and $\lambda = -0.5$ are absolutely continuous, but the PD copula with $\lambda = 1$ is not. Therefore, Fig. S2(b) and S2(d) show copula densities whereas, strictly speaking, Fig. S2(f) is not a density.

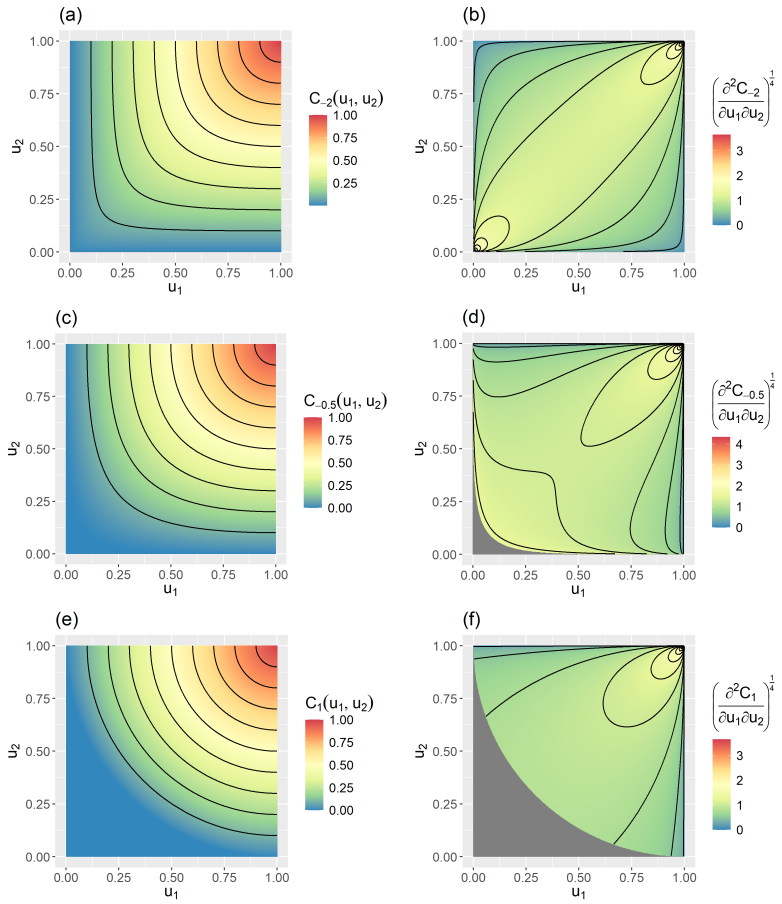

Figure S2: Left column: (a) Power-divergence (PD) copula with $\lambda = -2$; see (S3.1). (c) PD copula with $\lambda = -0.5$; see (S3.2). (e) PD copula with $\lambda = 1$; see (S3.4). Right column: (b) The fourth root of the PD copula density with $\lambda = -2$. (d) The fourth root of the PD copula density with $\lambda = -0.5$; see (S3.3). (f) The fourth root of the derivative $\partial C_1(u_1, u_2)/\partial u_1 \partial u_2$ for $u_1, u_2 \in [0, 1]$; see (S3.5). The fourth-root transformations in (b), (d), and (f) are used for visualisation purposes only.

S4 Computational aspects

S4.1 Computing the PD copula

Algorithm S1 presents a method for computing the PD copula for arbitrary $\lambda \in (-\infty, \infty)$.

Algorithm S1 Computing the power-divergence copula for general $\lambda \in (-\infty, \infty)$.

Let $\lambda \in (-\infty, \infty)$.

Let $u_1, u_2 \in [0, 1]$.

Compute $t = \phi_\lambda(u_1) + \phi_\lambda(u_2)$ using (3.1).

if $t < \phi_\lambda(0)$, **then**

  if $\lambda \neq 0, -1$, **then**

    Compute x^*, the sole solution of (3.9) in $[0, 1]$ by a root-finding algorithm.

    $C_\lambda(u_1, u_2) = x^*$.

  else

    Compute $C_{-1}(u_1, u_2)$ with (3.6) or $C_0(u_1, u_2)$ with (3.8) as appropriate.

  end if

else

  $C_\lambda(u_1, u_2) = 0$.

end if

S4.2 Bivariate simulation

Algorithm S2 below provides details of the conditional distribution method (e.g., Nelsen, 2006, Sec 2.9) for simulating from bivariate PD copulas.

Algorithm S2 The conditional distribution method for simulating from the bivariate power-divergence copula with $\lambda \in (-\infty, \infty)$.

Let $\lambda \in (-\infty, \infty)$.

Simulate u_1 and t independently from the uniform distribution on $[0, 1]$.

if $\lambda = 0$ **then**

    Compute $u_2 = \phi_0^{[-1]}\Big(\phi_0\Big(u_1^{1/t}\Big) - \phi_0(u_1)\Big)$ using (3.1) and (3.7).

else

    if $1 + t^{-1}(u_1^\lambda - 1) < 0$ **then**

        Compute $u_2 = \phi_\lambda^{[-1]}(\phi_\lambda(0) - \phi_\lambda(u_1))$ using (3.1), (3.5), and (3.9).

    else

        Compute $u_2 = \phi_\lambda^{[-1]}\big(\phi_\lambda\big((1 + t^{-1}(u_1^\lambda - 1))^{1/\lambda}\big) - \phi_\lambda(u_1)\big)$; see (3.1), (3.5), and (3.9).

    end if

end if

Return the pair (u_1, u_2). Discard t.

S5 Additional figures for the analysis in Section 5

Figure S3 shows the autocorrelation function (ACF) and partial autocorrelation function (PACF) plots for the residuals of the ARIMA(4, 1, 0)

models fitted to the DJIA and S&P500 time series. The plots show there is effectively no temporal autocorrelation left in the residuals.

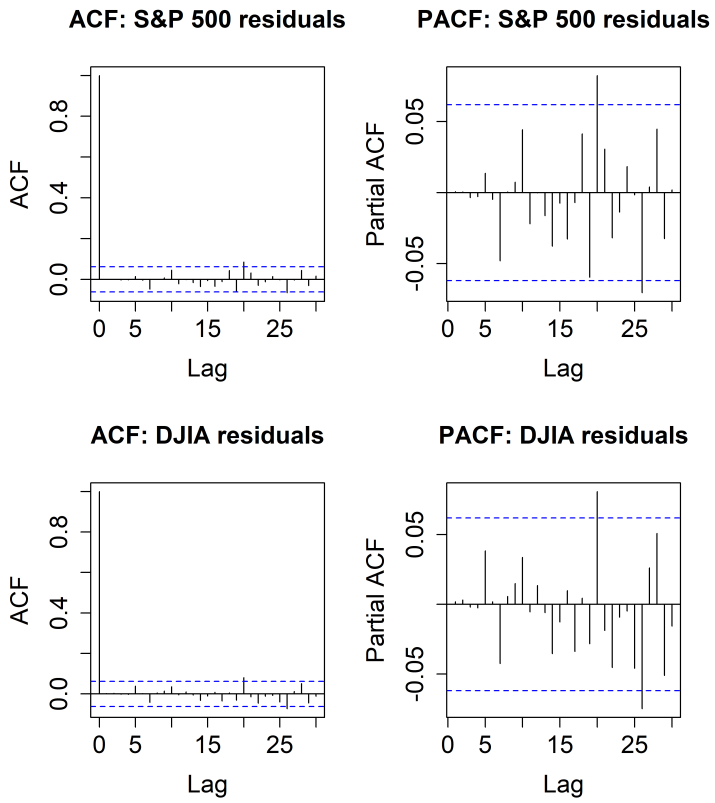

Figure S3: Autocorrelation function (ACF) and partial autocorrelation function (PACF) plots for the residuals of ARIMA(4,1,0) models fitted to time series of the DJIA and S&P500. Left-hand panels: ACF plots. Right-hand panels: PACF plots.

S6 Analysis of the Danish fire insurance data

In this section, we analyse a dataset of Danish insurance claims for businesses experiencing fire-related losses between 1980 and 1990. The dataset comprises 2,167 records of the losses to building, contents, and profits in millions of Danish krone (MDK), adjusted for inflation to the year 1985. The data are available in the R package 'fitdistrplus' (Delignette-Muller and Dutang, 2015). We refer to them as the 'Danish fire insurance data'.

An insurance company or their reinsurers may be interested to know, for example, the joint exceedance probabilities of losses to buildings, contents, and profits to inform pricing of policies, etc. Copulas are uniquely suited to the task of characterising the (potentially complicated) dependence between these variables. In what follows, we evaluate the fit of several copula models, including the PD copulas, to a subset of the Danish fire insurance data and demonstrate the PD copulas are able to achieve the best fit.

Haug et al. (2011) and Kuluratne et al. (2021) also analyse the Danish fire insurance data, focusing on the bivariate relationship between losses to building and losses to contents for small subsets of the data. Here, our analysis instead examines the bivariate relationship between the sum of losses to building and contents, designated as 'material losses', and the loss to profits. Records with no loss to profits are removed, so the following infer-

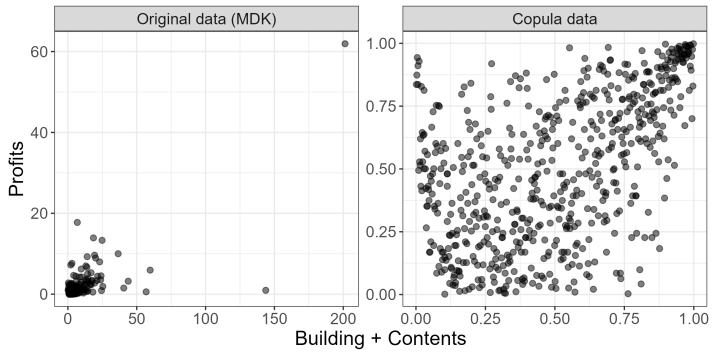

Figure S4: Losses to profits versus total material losses in millions of Danish krone (MDK) (left panel) and as copula data (right panel).

ences are for claims totalling over one MDK in losses with at least some losses to profits. Fig. S4 shows the remaining 616 records, with the losses shown in MDK but also as 'copula data' after a rank-based transformation of the margins. The copula data reveal the dependence structure of the material losses and losses to profits, which appears to have moderate upper tail dependence. The plot also suggests that small losses do not occur together, likely because the dataset only contains records of insurance claims totalling over one MDK in losses and our filtering of records associated with no losses to profits.

For the formal analysis, we fit the PD copula to the Danish fire insurance data, and we compare the fit to those of a suite of Archimedean, extreme-value, and elliptical copulas implemented in the 'copula' R package

(Hofert et al., 2025). The Archimedean copulas used for the comparison are the S-Clayton, Gumbel, Frank, and Joe copulas. The extreme-value copulas are the Galambos, Hüsler-Reiss, and Tawn copulas. A bivariate Gaussian copula is also fitted. Parameters are estimated by maximum likelihood, and Table S1 shows the estimates of the fitted copulas' parameters and the maximised log-likelihood values. The PD copula with $\hat{\lambda} = -0.789$ achieves the highest log-likelihood value among the competing copula models.

Table S1: Copulas fitted to the Danish fire insurance data, their estimated parameters, and maximised log-likelihood values.

Copula	Fitted parameter	Log-likelihood
Power-divergence	**-0.789**	**155.68**
S-Clayton	1.202	145.6
Frank	3.683	94.9
Joe	2.047	147.6
Gumbel	1.603	127.9
Galambos	0.883	125.4
Hüsler-Reiss	1.293	120.8
Tawn	0.897	128.1
Gaussian	0.495	84.2

Downstream analyses using the fitted PD copula may include the calculation of joint exceedance probabilities for extreme material losses and losses

to profits. The PD copula could also be used to simulate future insurance claims, with the fitted model enabling simulation-based decision-making. This is supported by Figure S5, where a synthetic dataset simulated from the fitted PD copula with $\hat{\lambda} = -0.789$ seems to resemble the original data. On the other hand, simulated datasets from the fitted Joe and S-Clayton copulas, which are the next-best competitors of the PD copula in terms of their log-likelihood values, appear to exhibit the correct upper-tail behaviour, but they fail to resemble the real data in the lower tail. In particular, neither the fitted Joe or S-Clayton copulas have a substantial zero set that reflects the fact that very small losses to profits do not occur together with very small material losses (in these fire-related insurance claims over 1 MDK in total losses and non-zero losses to profits).

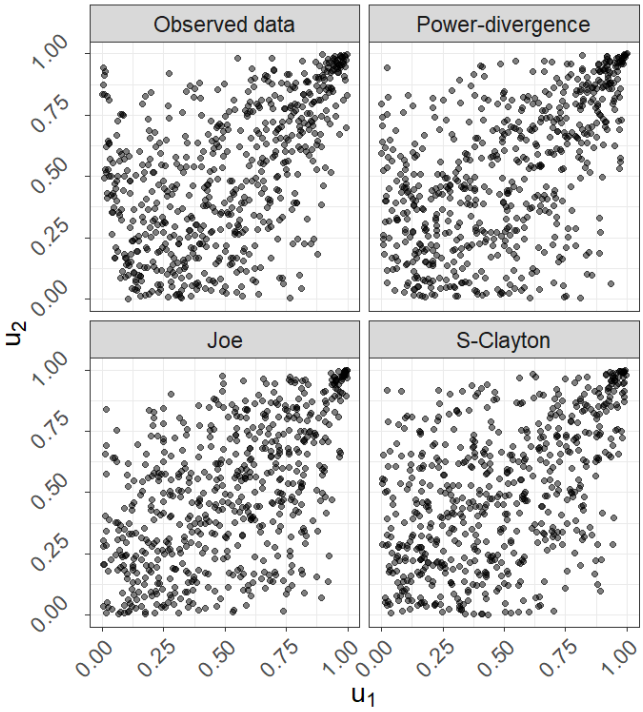

Figure S5: The observed Danish fire insurance data and datasets of the same size ($n = 616$) simulated from the fitted power-divergence, Joe, and S-Clayton copulas.

S7 Proofs of results

Proof of Proposition 1. We need to show ϕ, with $\phi(0) = \lim_{s\downarrow 0}\phi(s)$ and $\phi(0) = \infty$ when $\lim_{s\downarrow 0}\phi(s) = \infty$, is a convex function with $\phi(1) = 0$, that is strictly decreasing over $[0, 1]$. We immediately have $\phi(1) = 0$ by Definition 4. As for convexity, $\phi(x)$ is a non-negative convex function for all $x > 0$ by Definition 4, and it remains convex for all $x \geq 0$ since $\phi(0) = \lim_{s\downarrow 0}\phi(s)$. As for being strictly decreasing on $[0, 1]$, the fact $\phi'(1) = 0$ and $\phi''(1) > 0$ imply ϕ has a minimum at $x = 1$, where the value of the function is $\phi(1) = 0$. Again using $\phi''(1) > 0$ (by Definition 4), ϕ is strictly convex at $x = 1$, which implies $x = 1$ is the only point in the interval $[0, \infty)$ that satisfies $\phi(x) = 0$. Then convexity of ϕ over $[0, \infty)$ requires ϕ be strictly positive and strictly decreasing for $x \in [0, 1)$, and strictly positive and strictly increasing for $x \in (0, \infty)$. This means ϕ fits the requirements of an Archimedean-copula generator in Definition 1, namely that ϕ (limited to the interval $[0, 1]$) is convex and strictly decreasing, with $\phi(1) = 0$. Therefore, the proposition follows. □

Proof of Proposition 2. First, when $t = 0$, (3.9) becomes $0 = x^{\lambda+1} - (\lambda + 1)x + \lambda$ for $\lambda \neq -1, 0$. Clearly, $x = 1$ is a solution, and the following establishes that it is the only solution. For $\lambda \neq -1, 0$, define $g_\lambda(x) =$

$x^{\lambda+1}-(\lambda+1)x+\lambda$, with first derivative $g'_\lambda(x)=(\lambda+1)(x^\lambda-1)$. For $x=1$, $g_\lambda(1)=0$ and $g'_\lambda(1)=0$. For $x\in[0,1)$, $g'_\lambda(x)<0$ if either $\lambda>0$ or $\lambda<-1$, and $g'_\lambda(x)>0$ if $-1<\lambda<0$. This means $g_\lambda(x)$ is strictly decreasing over $x\in[0,1)$ for $\lambda>0$ and $\lambda<-1$, and it is strictly increasing over $x\in[0,1)$ for $-1<\lambda<0$. Since $x=1$ satisfies $g_\lambda(1)=0$, and since $g_\lambda(x)$ is either strictly decreasing or strictly increasing over $x\in[0,1)$, $x=1$ is the only value of $x\in[0,1]$ that satisfies (3.9) when $t=0$.

Second, let $t\in(0,\phi_\lambda(0))$. Define $h_\lambda(x)=x^{\lambda+1}-(\lambda+1)x+\lambda-\lambda(\lambda+1)t$ for $x\in[0,1]$ and $\lambda\neq-1,0$. The derivative of $h_\lambda(x)$ with respect to x is $h'_\lambda(x)=(\lambda+1)\{x^\lambda-1\}$, and $h'_\lambda(1)=0$ for all $\lambda\neq-1,0$. It is easily verified that $\lim_{x\downarrow0}h_\lambda(x)$ and $\lim_{x\uparrow1}h_\lambda(x)$ are non-zero and have opposite signs for all $\lambda\neq-1,0$ and $t\in(0,\phi_\lambda(0))$. Also, $h'_\lambda(x)<0$ for all $x\in[0,1)$ and $t\in(0,\phi_\lambda(0))$ for $\lambda<-1$ and $\lambda>0$, and $h'_\lambda(x)>0$ for all $x\in[0,1)$ and $t\in(0,\phi_\lambda(0))$ for $-1<\lambda<0$. Since, for all $\lambda\neq-1,0$, $h_\lambda(x)$ is strictly monotone over $x\in[0,1)$ with opposite sign at $x=0$ and $x=1$, the Intermediate Value Theorem implies that $h_\lambda(x_0)=0$ for a unique x_0 in the interval $[0,1)$.

Finally, let $t=\phi_\lambda(0)$ for $\lambda\neq-1,0$. When $\lambda>-1$ and $\lambda\neq0$, we have $\phi_\lambda(0)=1/(\lambda+1)$, and (3.9) becomes $0=x^{\lambda+1}-(\lambda+1)x$. The two solutions are $x=0$ and $x=(1+\lambda)^{1/\lambda}>1$, which means $x=0$ is the unique solution

in $[0, 1]$.

Considering all cases together, the proposition follows. □

Proof of Proposition 3. Recall from (3.3) that $\phi_\lambda(0) = \infty$ for $\lambda \leq -1$ and $\phi_\lambda(0) = 1/(\lambda + 1)$ for $\lambda > -1$. Since the zero curve of the Archimedean copula $C_\lambda(u_1, u_2) \equiv C(u_1, u_2; \phi_\lambda)$ is traced by $(u_1, u_2) \in [0, 1]^2$ that satisfy $\phi_\lambda(u_1) + \phi_\lambda(u_2) = \phi_\lambda(0)$, and since $\phi_\lambda(u) < \infty$ for all $u \in (0, 1]$, it is obvious that only elements of the set $\{(u_1, 0), (0, u_2) : u_1, u_2 \in [0, 1]\}$ satisfy $\phi_\lambda(u_1) + \phi_\lambda(u_2) = \phi_\lambda(0)$ when $\lambda \leq -1$. Thus the zero set of the PD copulas is $\{(u_1, 0), (0, u_2) : u_1, u_2 \in [0, 1]\}$ for $\lambda \leq -1$. When $\lambda > -1$, substitute $\phi_\lambda(x) = (\lambda(\lambda + 1))^{-1}(x^{\lambda+1} - x + \lambda(1 - x))$ into $\phi_\lambda(u_1) + \phi_\lambda(u_2) = \phi_\lambda(0)$ to obtain $(u_1^{\lambda+1} - u_1 + u_2^{\lambda+1} - u_2)/\lambda + 2 - u_1 - u_2 = 1$. The solutions are non-trivial, so the zero set has positive area. Now, the proposition follows. □

Proof of Theorem 1. From Nelsen (2006, Thm 4.3.3), it is sufficient to analyse the limit $-\{\lim_{s\downarrow 0} \phi_\lambda(s)/\phi'_\lambda(s)\}$. If this limit is zero, the copula is absolutely continuous. Otherwise, it has a singular component supported on the zero curve, with probability mass given by the value of the limit. We address this problem in five cases, namely when $\lambda < -1$, $\lambda = -1$, $-1 < \lambda < 0$,

$\lambda = 0$, and $\lambda > 0$. When $\lambda < -1$, we have

$$-\left\{\lim_{s\downarrow 0}\frac{\phi_\lambda(s)}{\phi'_\lambda(s)}\right\} = -\frac{1}{\lambda+1}\left\{\lim_{s\downarrow 0}\frac{s^{\lambda+1}-s+\lambda(1-s)}{s^\lambda-1}\right\} = 0,$$

after two applications of L'Hôpital's rule. When $\lambda = -1$, we have

$$-\left\{\lim_{s\downarrow 0}\frac{\phi_{-1}(s)}{\phi'_{-1}(s)}\right\} = -\left\{\lim_{s\downarrow 0}\frac{s-1-\log(s)}{1-s^{-1}}\right\} = -\left\{\lim_{s\downarrow 0}\frac{s^2-s-s\log(s))}{s-1}\right\} = 0.$$

When $-1 < \lambda < 0$, we have by inspection that

$$-\left\{\lim_{s\downarrow 0}\frac{\phi_\lambda(s)}{\phi'_\lambda(s)}\right\} = -\frac{1}{\lambda+1}\left\{\lim_{s\downarrow 0}\frac{s^{\lambda+1}-s+\lambda(1-s)}{s^\lambda-1}\right\} = 0.$$

When $\lambda = 0$, we have,

$$-\left\{\lim_{s\downarrow 0}\frac{\phi_0(s)}{\phi'_0(s)}\right\} = -\left\{\lim_{s\downarrow 0}\frac{1-s+s\log(s)}{\log(s)}\right\} = -\left\{\lim_{s\downarrow 0}\frac{1-s}{\log(s)}+\lim_{s\downarrow 0}s\right\} = 0.$$

Finally, when $\lambda > 0$, we can evaluate the limit by inspection:

$$-\left\{\lim_{s\downarrow 0}\frac{\phi_\lambda(s)}{\phi'_\lambda(s)}\right\} = -\frac{1}{\lambda+1}\left\{\lim_{s\downarrow 0}\frac{s^{\lambda+1}-s+\lambda(1-s)}{s^\lambda-1}\right\} = \frac{\lambda}{\lambda+1},$$

which is always in the interval $(0,1)$ for finite positive λ. Combining the analysis from all five cases reveals that,

$$-\left\{\lim_{s\downarrow 0}\frac{\phi_\lambda(s)}{\phi'_\lambda(s)}\right\} = \begin{cases} 0 & \lambda \leq 0, \\ \frac{\lambda}{\lambda+1} & \lambda > 0. \end{cases}$$

Theorem 1 of Genest and MacKay (1986) then implies that the power-divergence copulas are absolutely continuous for $\lambda \leq 0$ and have a singular component supported on the zero curve with probability mass $\lambda/(\lambda+1)$ for $\lambda > 0$. Hence the theorem follows. □

Proof of Theorem 2. The PD copula has the generator $\phi_\lambda(x)$ in (3.1) with $\lambda \in (-\infty, \infty)$, which is continuously differentiable over $x \in (0,1)$. Then, per Nelsen (2006, Cor. 4.4.6), it suffices to show that, for $-\infty < \lambda_1 < \lambda_2 < \infty$, $g(x; \lambda_1, \lambda_2) = \phi'_{\lambda_2}(x)/\phi'_{\lambda_1}(x)$ is a non-decreasing function over $x \in (0,1)$. This involves verifying that the derivative of $g(x; \lambda_1, \lambda_2)$ is non-negative in several cases.

Begin by noting that, for all $\lambda_1 < \lambda_2$ and $x \in (0,1)$,

$$g'(x; \lambda_1, \lambda_2) = \frac{\phi''_{\lambda_2}(x)\phi'_{\lambda_1}(x) - \phi''_{\lambda_1}(x)\phi'_{\lambda_2}(x)}{[\phi'_{\lambda_1}(x)]^2},$$

by the quotient rule. Then also note that, for given $\lambda \in (-\infty, \infty)$ and $x > 0$, the function $\phi_\lambda(x)$ is non-negative. For $x \in (0,1)$ and $x \in (1, \infty)$, $\phi_\lambda(x)$ is in fact strictly positive since $\phi_\lambda(1) = 0$ represents the unique minimum of the function, and its first two derivatives with respect to x are given by,

$$\phi'_\lambda(x) = \begin{cases} (x^\lambda - 1)/\lambda & \lambda \neq -1, 0, \\ \log(x) & \lambda = 0, \\ 1 - x^{-1} & \lambda = -1, \end{cases} \quad \text{and} \quad \phi''_\lambda(x) = \begin{cases} x^{\lambda-1} & \lambda \neq -1, 0, \\ x^{-1} & \lambda = 0, \\ x^{-2} & \lambda = -1. \end{cases}$$

These facts are needed in the sequel, where we examine the derivative of $g(x; \lambda_1, \lambda_2) = \phi'_{\lambda_2}(x)/\phi'_{\lambda_1}(x)$ for various combinations of λ_1 and λ_2.

If $\lambda_1 = -1$ and $\lambda_2 = 0$, we have,

$$g'(x; -1, 0) = \frac{x - 1 - \log(x)}{(x-1)^2} = \frac{\phi_{-1}(x)}{(x-1)^2}.$$

The derivative is always positive for $x \in (0,1)$ because the numerator is strictly positive for $x \in (0,1)$ by definition, and the denominator is positive for $x \in (0,1)$. Hence, $g(x;-1,0)$ is non-decreasing over $x \in (0,1)$.

If $\lambda_1 = -1$ and $\lambda_2 > -1$, we have to deal with two cases, namely $\lambda_2 = 0$ and $\lambda_2 \neq 0$. We have already dealt with the case where $\lambda_2 = 0$ above. Then, when $\lambda_2 \neq 0$,

$$g'(x;-1,\lambda_2) = \frac{x^{\lambda_2+1} - (\lambda_2^{-1}+1)x^{\lambda_2} + \lambda_2^{-1}}{(x-1)^2} = \frac{\lambda_2^{-1}(\lambda_2^{-1}+1)\phi_{\lambda_2^{-1}}(x^{\lambda_2})}{(x-1)^2}.$$

The denominator is obviously positive for $x \in (0,1)$. The numerator is positive. This follows because, as noted above, $\phi_\lambda(x)$ is strictly positive for all $\lambda \in (-\infty,\infty)$ and $x \in (0,1)$ or $x \in (1,\infty)$. Here, the parameter $\lambda_2 > -1$, and $x^{\lambda_2} \in (1,\infty)$ when $\lambda_2 \in (-1,0)$ and $x^{\lambda_2} \in (0,1)$ when $\lambda_2 > 0$. Similar reasoning applies to all remaining cases. Further, $\lambda_2^{-1}(1+\lambda_2^{-1}) = \lambda_2^{-2}(\lambda_2+1) > 0$ since $\lambda_2 > -1$. Hence, the derivative $g'(x;-1,\lambda_2)$ is positive, and $g(x;-1,\lambda_2)$ is non-decreasing over $x \in (0,1)$.

If $\lambda_1 = 0$ and $\lambda_2 > 0$, we have,

$$g'(x;0,\lambda_2) = \frac{(\lambda_2 x)^{-1}(x^{\lambda_2}\log(x^{\lambda_2}) - x^{\lambda_2} + 1)}{\log(x)^2} = \frac{(\lambda_2 x)^{-1}\phi_0(x^{\lambda_2})}{\log(x)^2}.$$

The numerator is non-negative since $\lambda_2 x > 0$ and $\phi_0(x^{\lambda_2}) > 0$ for $x \in (0,1)$ and $\lambda_2 > 0$. The denominator is positive since $\log(x)^2 > 0$ for $x \in (0,1)$. Therefore, $g'(x;0,\lambda_2) > 0$ for $x \in (0,1)$, which implies that $g(x;0,\lambda_2)$ is

non-decreasing over $x \in (0,1)$.

If $\lambda_1 < -1$ and $\lambda_2 = -1$, we have,

$$g'(x;\lambda_1,-1) = -\frac{\lambda_1^2 x^{-2}(x^{\lambda_1+1} - (\lambda_1^{-1}+1)x^{\lambda_1} + \lambda_1^{-1})}{(x^{\lambda_1}-1)^2} = -\frac{(1+\lambda_1)\phi_{\lambda_1^{-1}}(x^{\lambda_1})}{x^2(x^{\lambda_1}-1)^2}.$$

The denominator is obviously positive for $x \in (0,1)$. The term $\phi_{\lambda_1^{-1}}(x^{\lambda_1})$ in the numerator is positive for all $\lambda_1 < -1$ and $x \in (0,1)$, and $-(1+\lambda_1) > 0$ for $\lambda_1 < -1$. It then follows that $g'(x;\lambda_1,-1) > 0$ for $x \in (0,1)$, which implies $g(x;\lambda_1,-1)$ is non-decreasing over $x \in (0,1)$.

If $\lambda_1 < 0$ and $\lambda_2 = 0$, there are two cases. We have already dealt with the case where $\lambda_1 = -1$ above. Otherwise, for $\lambda_1 \neq -1$, we have,

$$g'(x;\lambda_1;0) = -\frac{\lambda_1 x^{-1}(1 - x^{\lambda_1} + x^{\lambda_1}\log(x^{\lambda_1}))}{(x^{\lambda_1}-1)^2} = -\frac{\lambda_1\phi_0(x^{\lambda_1})}{x(x^{\lambda_1}-1)^2}.$$

The denominator is obviously positive for $x \in (0,1)$. The numerator is positive since $\phi_0(x^{\lambda_1}) > 0$ and $-\lambda_1 x^{-1} > 0$ for $x \in (0,1)$ and $\lambda_1 < 0$. Hence $g'(x;\lambda_1,0)$ is positive, and $g(x;\lambda_1,0)$ is non-decreasing over $x \in (0,1)$.

If $-\infty < \lambda_1 < \lambda_2 < \infty$ and $\lambda_1, \lambda_2 \neq -1, 0$, write $\lambda_2 = \lambda_1 + \kappa$ for some positive constant $\kappa > 0$. Then, we have,

$$\begin{aligned} g'(x;\lambda_1,\lambda_1+\kappa) &= -\frac{\lambda_1 x^{\lambda_1-1}(x^{\kappa} - (1-(\lambda_1+\kappa)^{-1}\lambda_1)x^{\lambda_1+\kappa} - (\lambda_1+\kappa)^{-1}\lambda_1)}{(x^{\lambda_1}-1)^2} \\ &= \frac{\lambda_1 x^{\lambda_1-1}(1-(\lambda_1+\kappa)^{-1}\lambda_1)(\lambda_1+\kappa)^{-1}\lambda_1\phi_{-(\lambda_1+\kappa)^{-1}\lambda_1}(x^{\lambda_1+\kappa})}{(x^{\lambda_1}-1)^2} \end{aligned}$$

In terms of λ_1 and λ_2, this can be written as,

$$g'(x;\lambda_1,\lambda_2) = \frac{\lambda_1 x^{\lambda_1-1}[(1-\lambda_2^{-1}\lambda_1)\lambda_2^{-1}\lambda_1]\phi_{-\lambda_2^{-1}\lambda_1}(x^{\lambda_2})}{(x^{\lambda_1}-1)^2}.$$

It is obvious that the denominator is positive for $x \in (0,1)$. As for the numerator, x^{λ_1-1} is always positive for $x \in (0,1)$ and $\lambda_1 \neq -1, 0$. The term $\phi_{-\lambda_2^{-1}\lambda_1}(x^{\lambda_2}) > 0$ for $x > 0$ for all $\lambda_1, \lambda_2 \neq -1, 0$ by definition. The remaining terms in the numerator can be expressed as,

$$\lambda_1\left(1-\frac{\lambda_1}{\lambda_2}\right)\left(\frac{\lambda_1}{\lambda_2}\right) = (\lambda_2-\lambda_1)\left(\frac{\lambda_1}{\lambda_2}\right)^2.$$

Since $\lambda_2 > \lambda_1$ by definition, this term is always positive for all $\lambda_1, \lambda_2 \neq -1, 0$. Hence, we have shown that all terms in the numerator and denominator are positive, so it follows that $g'(x;\lambda_1,\lambda_2)$ is also positive for all $x \in (0,1)$ and $\lambda_1, \lambda_2 \neq -1, 0$.

All cases together show $g(x;\lambda_1,\lambda_2)$ is a non-decreasing function of $x \in (0,1)$ for all $-\infty < \lambda_1 < \lambda_2 < \infty$, and the theorem follows. □

Proof of Proposition 4. For part (i), from Theorem 4.4.7 in Nelsen (2006), it is sufficient to show that $\lim_{\lambda\to\infty} \phi_\lambda(s)/\phi'_\lambda(t) = s-1,\ s,t \in (0,1)$. An application of L'Hôpital's rule gives

$$\lim_{\lambda\to\infty} \phi_\lambda(s)/\phi'_\lambda(t) = \lim_{\lambda\to\infty} (s^{\lambda+1}\log(s)+1-s)/(t^\lambda-1+(\lambda+1)t^\lambda\log(t)) = s-1,$$

where recall $s,t \in (0,1)$. For part (ii), from Theorem 4.4.8 in Nelsen (2006), it is sufficient to show that $\lim_{\lambda\to-\infty} \phi_\lambda(s)/\phi'_\lambda(s) = 0,\ s \in (0,1)$. An

application of L'Hôpital's rule gives

$$\lim_{\lambda\to-\infty}\frac{\phi_\lambda(s)}{\phi'_\lambda(s)}=\lim_{\lambda\to-\infty}\frac{s^{\lambda+1}\log(s)^2}{(\lambda+1)s^\lambda\log(s)^2+2s^\lambda\log(s)},\ s\in(0,1).$$

The limit on the RHS is 0 as $\lambda\to-\infty$. Hence the proposition follows. □

Proof of Theorem 3. For part (i), it is obvious that the lower-tail dependence coefficient is zero for $\lambda>-1$ because, due to Theorem 3, the copula assigns zero probability to any values of $\mathbf{U}\equiv(U_1,U_2)^\top$ below the zero curve; hence $\lim_{u\downarrow0}\Pr(U_1\le u\mid U_2\le u)=0$. When $\lambda\le-1$, we apply the results of Charpentier and Segers (2009) to calculate the lower tail-dependence coefficient. In what follows, we write $\lambda=-\gamma$, where $\gamma\ge1$, for ease of exposition. Now, we calculate $\nu_0(-\gamma)=-\{\lim_{s\downarrow0}s\phi'_{-\gamma}(s)/\phi_{-\gamma}(s)\},\ \gamma\ge1$. First, consider the case where $\gamma=1$ (i.e., $\lambda=-1$): By inspection,

$$\nu_0(-1)=-\left\{\lim_{s\downarrow0}\frac{s-1}{s-1-\log(s)}\right\}=0.$$

Now for the $\gamma>1$ case (i.e., $\lambda>-1$), define

$$\nu_0(-\gamma)=-(1-\gamma)\left\{\lim_{s\downarrow0}\frac{s^{1-\gamma}-s}{s^{1-\gamma}-s-\gamma(1-s)}\right\},\ \gamma>1.$$

After two applications of L'Hôpital's rule, this can be evaluated as $\nu_0(-\gamma)=-(1-\gamma),\ \gamma>1$. Combining the cases yields, $\nu_0(-\gamma)=-(1-\gamma)$ when $\gamma>1$ and $=0$ otherwise. Then, from Theorem 3.1 of Charpentier and Segers (2009), the lower-tail dependence coefficient is zero if $\nu_0(-\gamma)=0$. If $\nu_0>0$,

the lower-tail dependence coefficient is $T_L(-\gamma) = 2^{-1/\nu_0(-\gamma)} = 2^{1/(1-\gamma)}$. Therefore, in terms of λ, we can express the lower tail-dependence coefficient of the PD copulas as,

$$T_L(\lambda) = \begin{cases} 2^{1/(\lambda+1)} & \lambda < -1, \\ 0 & \lambda \geq -1. \end{cases}$$

For part (ii), from Charpentier and Segers (2009), the upper tail-dependence properties of the PD copula can be discovered by calculating $\nu_1(\lambda) = -\{\lim_{s\downarrow 0} s\phi'_\lambda(1-s)/\phi_\lambda(1-s)\}$. We must consider all $\lambda \in (-\infty, \infty)$, so we calculate this quantity for three cases ($\lambda = -1$, $\lambda = 0$, and $\lambda \neq -1, 0$). First, for $\lambda = -1$,

$$\nu_1(-1) = \lim_{s\downarrow 0} \frac{s[1-(1-s)^{-1}]}{s + \log(1-s)} = 2,$$

after two applications of L'Hôpital's rule. Second, for $\lambda = 0$, using the same strategy gives

$$\nu_1(0) = -\left\{\lim_{s\downarrow 0} \frac{s\log(1-s)}{s + (1-s)\log(1-s)}\right\} = 2.$$

Finally, when $\lambda \neq -1, 0$, we have

$$\nu_1(\lambda) = -(\lambda+1)\left\{\lim_{s\downarrow 0} \frac{s[(1-s)^\lambda - 1]}{(1-s)^{\lambda+1} - (\lambda+1)(1-s) + \lambda}\right\}.$$

Two applications of L'Hôpital's rule gives,

$$\nu_1(\lambda) = -(\lambda+1)\left\{\lim_{s\downarrow 0} \frac{\lambda(\lambda-1)s(1-s)^{\lambda-2} - 2\lambda(1-s)^{\lambda-1}}{\lambda(\lambda+1)(1-s)^{\lambda-1}}\right\} = 2,$$

for $\lambda \neq -1, 0$. Finally, from Theorem 4.1 of Charpentier and Segers (2009), since $\nu_1(\lambda) > 0$, the upper tail-dependence coefficient can be expressed as a function of $\nu_1(\lambda)$, namely $T_U(\lambda) = 2 - 2^{1/\nu_1(\lambda)}$. For all $\lambda \in (-\infty, \infty)$, we have seen that $\nu_1(\lambda) = 2$. Therefore, for $C_\lambda(u_1, u_2)$, $T_U(\lambda) = 2 - \sqrt{2}$ for all $\lambda \in (-\infty, \infty)$, as required. □

Proof of Lemma 1. Let $\lambda > 0$. From Definition 1, we have,

$$\phi_\lambda^{[-1]}(t) = \begin{cases} \phi_\lambda^{-1}(t) & 0 \leq t \leq 1/(\lambda+1), \\ 0 & 1/(\lambda+1) \leq t \leq \infty, \end{cases} \tag{S7.6}$$

where $\phi_\lambda^{-1}(t)$ is given by the appropriate solution of (3.9). The function (S7.6) is continuous over $t \in [0, \infty)$. Recall that $\phi_\lambda(x)$ in (3.1) with $\lambda > 0$ has at least one derivative over $x \in (0, \infty)$, which is given by $\phi'_\lambda(x)$ in (3.2). Therefore, the Inverse Function Theorem (IFT) implies that $(\phi_\lambda^{-1})'(t)$ exists over $t \in (0, 1/(\lambda+1))$ and is equal to $(\phi_\lambda^{-1})'(t) = 1/\phi'_\lambda(\phi_\lambda^{-1}(t)) = \lambda/(\phi_\lambda^{-1}(t)^\lambda - 1)$. Then, over $t \in (0, 1/(\lambda+1))$, we have $(\phi_\lambda^{[-1]})'(t) = (\phi_\lambda^{-1})'(t)$. Similarly, over $t \in (1/(\lambda+1), \infty)$, we have $(\phi_\lambda^{[-1]})'(t) = 0$. Now consider the one-sided limit of $(\phi_\lambda^{[-1]})'(t)$ as $t \uparrow 1/(\lambda+1)$: $\lim_{t \uparrow 1/(\lambda+1)} (\phi_\lambda^{[-1]})'(t) = \lim_{t \uparrow 1/(\lambda+1)} (\phi_\lambda^{-1})'(t) = -\lambda$. Also take the other one-sided limit as t approaches $1/(\lambda+1)$ from above (i.e., $t \downarrow 1/(\lambda+1)$): $\lim_{t \downarrow 1/(\lambda+1)} (\phi_\lambda^{[-1]})'(t) = 0$. The limit of the left-derivative and right-derivative do not agree at $t = 1/(\lambda+1)$, so the derivative of (S7.6) does not exist there. □

Proof of Theorem 4. The existence of the derivative of $\phi_\lambda^{[-1]}(t)$ at all $t \in (0,\infty)$ is a necessary condition for $\phi_\lambda^{[-1]}$ to be d-monotone for any $d \geq 3$, which is in turn sufficient and necessary for $\phi_\lambda^{[-1]}(\phi_\lambda(u_1) + \cdots + \phi_\lambda(u_d))$ to be a valid copula (McNeil and Nešlehová, 2009). Lemma 1 establishes that $\phi_\lambda^{[-1]}(t)$ lacks a derivative at $t = 1/(\lambda+1)$ when $\lambda > 0$, so it cannot even be 3-monotone. Hence the theorem follows. □

Proof of Lemma 2. Let $\lambda = 0$. The pseudoinverse $\phi_0^{[-1]}(t)$ is given by (3.7). Then, when $t \in (0,1)$, $(\phi_0^{[-1]})'(t) = (\phi_0^{-1})'(t)$; otherwise, when $t \in (1,\infty)$, $(\phi_0^{[-1]})'(t) = 0$. The derivative $(\phi_0^{-1})'(t)$ exists and, from (3.7), Mathematica (Wolfram Research, Inc., 2024) gives the following result: For $t \in (0,1)$,

$$(\phi_0^{-1})'(t) = \frac{1}{1 + \mathfrak{W}_{-1}((t-1)/\exp\{1\})}, \tag{S7.7}$$

where recall that $\mathfrak{W}_{-1}$ is the lower branch of the Lambert W function. The limit of $(\phi_0^{[-1]})'(t)$ in (S7.7) as $t \uparrow 1$ is 0. Since $\lim_{t\downarrow 1}(\phi_0^{[-1]})'(t) = 0$, $(\phi_0^{[-1]})'(t)$ exists at $t = \phi_0(0) = 1$.

Now let $-1 < \lambda < 0$, and write $\lambda = -\gamma$ with $0 < \gamma < 1$. The pseudoinverse $\phi_{-\gamma}^{[-1]}(t)$ is given by (S7.6) for $-1 < \lambda < 0$ (i.e., $0 < \gamma < 1$). For $t \in (1/(1-\gamma),\infty)$, $(\phi_{-\gamma}^{[-1]})'(t) = 0$. For $t \in (0, 1/(1-\gamma))$, $(\phi_{-\gamma}^{[-1]})'(t) = (\phi_{-\gamma}^{-1})'(t)$. Since $\phi_{-\gamma}(x)$ has infinitely many derivatives on $x \in (0,\infty)$, the

IFT implies that $(\phi_{-\gamma}^{-1})'(t)$ exists for $t \in (0, 1/(1-\gamma))$ and is given by,

$$(\phi_{-\gamma}^{-1})'(t) = \frac{1}{\phi'_{-\gamma}(\phi_{-\gamma}^{-1}(t))} = -\frac{\gamma}{\phi_{-\gamma}^{-1}(t)^{-\gamma} - 1} = -\frac{\gamma \phi_{-\gamma}^{-1}(t)^{\gamma}}{1 - \phi_{-\gamma}^{-1}(t)^{\gamma}}. \tag{S7.8}$$

Note that $\lim_{t \uparrow 1/(1-\gamma)} (\phi_{-\gamma}^{-1})'(t) = 0$. For the other one-sided limit, we have $\lim_{t \downarrow 1/(1-\gamma)} (\phi_{-\gamma}^{[-1]})'(t) = 0$. These two limits agree, so $(\phi_{-\gamma}^{[-1]})'(t)$ exists at $t = 1/(1-\gamma)$.

Combining the cases for $\lambda = 0$ and $-1 < \lambda < 0$ gives the result. □

Proof of Lemma 3. Let $\lambda = 0$. Recall that $(\phi_0^{-1})'(t)$ for $t \in (0, 1)$ is given by (S7.7). Now, for the second derivative, Mathematica gives,

$$(\phi_0^{-1})''(t) = \frac{\mathfrak{W}_{-1}((t-1)/\exp\{1\})}{(1-t)(1+\mathfrak{W}_{-1}((t-1)/\exp\{1\}))^3}, \tag{S7.9}$$

where recall $t \in (0, 1)$. We see that (S7.9) is positive over all $t \in (0, 1)$ since $(1-t) > 0$ and $-\infty < \mathfrak{W}_{-1}(s) < -1$ for all $s \in (-\exp\{-1\}, 0)$. Since (S7.9) is positive over its domain, the first derivative of $-(\phi_0^{-1})'(t)$, which is simply -1 times (S7.9), is negative over its domain, demonstrating that $-(\phi_0^{-1})'(t)$ is non-increasing, as required. As for convexity over $t \in (0, 1)$, Mathematica gives,

$$(\phi_0^{-1})^{(3)}(t) = \frac{\mathfrak{W}_{-1}((t-1)/\exp\{1\})^2(4+\mathfrak{W}_{-1}((t-1)/\exp\{1\}))}{(t-1)^2(1+\mathfrak{W}_{-1}((t-1)/\exp\{1\}))^5}, \tag{S7.10}$$

This is the second derivative of (S7.7), so $-(\phi_0^{-1})^{(3)}(t)$ is the second derivative of $-(\phi_0^{-1})'(t)$. To refute that $-(\phi_0^{-1})'(t)$ is convex for all $t \in (0, 1)$,

it suffices to find a value of $t \in (0,1)$ where $-(\phi_0^{-1})^{(3)}(t)$ is negative and hence where $-(\phi_0^{-1})'(t)$ is concave. To give one example, at $t = 0.9$, we have $-1(\phi_0^{-1})^{(3)}(0.9) = -2.389074$, so $-(\phi_0^{-1})'(t)$ is concave there.

Now let $-1 < \lambda < 0$, and write $\lambda = -\gamma$ for $0 < \gamma < 1$. Then recall that $(\phi_{-\gamma}^{-1})'(t)$ is given by (S7.8). On $t \in (0, 1/(1-\gamma))$, the second and third derivatives exist and are,

$$(\phi_{-\gamma}^{-1})''(t) = \frac{\gamma^3 \phi_{-\gamma}^{-1}(t)^{2\gamma-1}}{(1-\phi_{-\gamma}^{-1}(t)^{\gamma})^3}. \tag{S7.11}$$

$$(\phi_{-\gamma}^{-1})^{(3)}(t) = -\left\{ \frac{\gamma^4 \phi_{-\gamma}^{-1}(t)^{3\gamma-2}((1+\gamma)\phi_{-\gamma}^{-1}(t)^{\gamma} + 2\gamma - 1)}{(1-\phi_{-\gamma}^{-1}(t)^{\gamma})^5} \right\} \tag{S7.12}$$

Observe that (S7.11) is non-negative for all $t \in (0, \infty)$ since $0 \leq \phi_{-\gamma}^{-1}(t) \leq 1$. Then, $-(\phi_{-\gamma}^{-1})'(t)$ must have non-positive first derivative given by -1 times (S7.11), so $-(\phi_{-\gamma}^{-1})'(t)$ is non-increasing, as required, for $0 < \gamma < 1$ (equivalently, $-1 < \lambda < 0$). As for convexity, consider the second derivative of $-(\phi_{-\gamma}^{-1})'(t)$, which is simply -1 times (S7.12). Therefore, the function $-(\phi_{-\gamma}^{-1})'(t)$ is convex on $t \in (0, 1/(1-\gamma))$ if and only if $(\gamma^4 \phi_{-\gamma}^{-1}(t)^{3\gamma-2}((1+\gamma)\phi_{-\gamma}^{-1}(t)^{\gamma} + 2\gamma - 1))/((1-\phi_{-\gamma}^{-1}(t)^{\gamma})^5) \geq 0$, for all $t \in (0, 1/(1-\gamma))$. Note that the denominator on the left-hand side (LHS) of the inequality is always non-negative since $0 \leq \phi_{-\gamma}^{-1}(t) \leq 1$. But, in the numerator, the term $((1+\gamma)\phi_{-\gamma}^{-1}(t)^{\gamma} + 2\gamma - 1)$ will be negative for some $t \in (0, 1/(1-\gamma))$ if $\gamma < 0.5$ (i.e., $\lambda > -0.5$). If $\gamma \geq 0.5$ (i.e., $\lambda \leq -0.5$), then non-negativity is guaranteed.

Therefore, $-(\phi_{-\gamma}^{-1})'(t)$ is convex when $0.5 \leq \gamma < 1$ (equivalently, $-1 < \lambda \leq -0.5$), but not when $0 < \gamma < 0.5$ (equivalently, $-0.5 < \lambda < 0$). It then follows that $-(\phi_{\lambda}^{[-1]})'(t)$ is convex when $-1 < \lambda \leq -0.5$ but not when $-0.5 < \lambda < 0$.

Combining the two cases gives the result. □

Proof of Theorem 5. This follows from Lemmas 2 and 3 and Proposition 2.3 of McNeil and Nešlehová (2009). □

Proof of Lemma 4. Recall $\lambda < -1$, and write $\lambda = -\gamma$ for $\gamma > 1$. By the IFT, the first, second, and third derivatives of $\phi_{-\gamma}^{-1}(t)$ exist for all $t \in (0, \infty)$ since $\phi'_{-\gamma}(x)$, $\phi''_{-\gamma}(x)$, and $\phi^{(3)}_{-\gamma}(x)$ exist for all $x \in (0, \infty)$. The derivatives of $\phi_{-\gamma}^{-1}(t)$ are respectively given by (S7.8), (S7.11), and (S7.12) for $t \in (0, \infty)$ and $\gamma > 1$. Now we need to show $-(\phi_{-\gamma}^{-1})'(t)$ is positive and convex for all $t \in (0, \infty)$. For positivity, simply inspect -1 times (S7.8) with the knowledge that $0 < \phi_{-\gamma}^{-1}(t) < \infty$ for $t \in (0, \infty)$ and $\gamma > 1$. For convexity, note that $(\phi_{-\gamma}^{-1})^{(3)}(t)$ in (S7.12) is strictly negative for $t \in (0, \infty)$ and $\gamma > 1$, so $-(\phi_{-\gamma}^{-1})^{(3)}(t)$ is strictly positive for $t \in (0, \infty)$ and $\gamma > 1$, which shows $-(\phi_{-\gamma}^{-1})'(t)$ is convex over $(0, \infty)$ for $\gamma > 1$. This gives the result. □

Proof of Theorem 6. This follows from Lemma 4 and Proposition 2.3 of McNeil and Nešlehová (2009). □

Proof of Lemma 5. Let $\lambda = -1$. To show that ϕ_{-1}^{-1} in (3.5) is completely monotone on $[0, \infty)$, rewrite (3.5) as $\phi_{-1}^{-1}(t) = \mathfrak{V}(\exp\{-(t+1)\})$, where $\mathfrak{V}(r) \equiv -\mathfrak{W}_0(-r)$ for $r \in (0, \exp\{-1\})$. It is obvious that $\exp\{-(t+1)\}$ is completely monotone on $[0, \infty)$ since the function is positive, and the chain rule shows its k-th derivative is $(-1)^k \exp\{-(t+1)\}$ for $t \in (0, \infty)$ and $k = 1, 2, \ldots$. As for $\mathfrak{V}(r)$, this function is absolutely monotone on $r \in (0, \exp\{-1\})$, as shown below. The function itself is non-negative, from the properties of the principal branch of the Lambert W function. The first derivative is $\mathfrak{V}'(r) = \mathfrak{W}_0'(-r)$. It has previously been shown (Kalugin et al., 2012) that $\mathfrak{W}_0'(r)$ is completely monotone on $r \in (-\exp\{-1\}, \infty)$, so it is also completely monotone on the subinterval $r \in (0, \exp\{-1\})$. Therefore, $\mathfrak{W}_0'(-r)$ is absolutely monotone on $r \in (0, \exp\{-1\})$ (Widder, 1946, p. 145). Therefore, being non-negative and having absolutely monotone first derivative, it follows that $\mathfrak{V}(r)$ is absolutely monotone on $r \in (0, \exp\{-1\})$. Now Theorem 2b of Widder (1946, p. 145) implies $\phi_{-1}^{-1}(t) = -\mathfrak{W}_0(-\exp\{-(t+1)\})$ is completely monotone on $[0, \infty)$ since this is the composition of an absolutely monotone function and a completely monotone function. □

Proof of Lemma 6. From Definition 6, each summand in $\mathfrak{B}_{k,j}$ is,

$$\frac{k!}{c_1!c_2!\cdots c_{k-j+1}!}\prod_{l=1}^{k-j+1}\left(\frac{x_l}{l!}\right)^{c_l}. \tag{S7.13}$$

The term (S7.13) is non-negative if k is even and non-positive if k is odd. To see this, observe that the number $l \times c_l$ is even if and only if c_l is even or l is even (hence $x_l \geq 0$). It follows that, if $l \times c_l$ is even, then $(x_l/l!)^{c_l} \geq 0$ since either $x_l \geq 0$ or its exponent is even. As for the only remaining case, observe that the number $l \times c_l$ is odd if and only if c_l is odd and l is odd (hence $x_l \leq 0$). Hence, if $l \times c_l$ is odd, then $(x_l/l!)^{c_l} \leq 0$ since odd powers of a non-positive value are also non-positive. From (3.15), we see that $\sum_{l=1}^{k-j+1}(l \times c_l) = k$. If the integer k is even, then the sum in (3.15) must consist of any number of terms where $l \times c_l$ is even, and an even number of terms where $l \times c_l$ is odd. Therefore, the product (S7.13) must be non-negative if k is even because it will be a product of non-negative terms (since $(x_l/l!)^{c_l} \geq 0$ when $l \times c_l$ is even) and an even number of non-positive terms (since $(x_l/l!)^{c_l} \leq 0$ when $l \times c_l$ is odd). On the other hand, if k is odd, then the sum in (3.15) consists of any number of terms where $l \times c_l$ is even, and an odd number of non-positive terms where $l \times c_l$ is odd. This implies the product (S7.13) is a product of some non-negative terms as well as, crucially, an odd number of non-positive terms (since $(x_l/l!)^{c_l} \leq 0$ if $l \times c_l$ is odd). Thus, if k is odd, (S7.13) is non-positive.

Finally, returning to the definition of $\mathfrak{B}_{k,j}$ in (3.13), we see that (3.13) is a sum of (S7.13). Since only the value of k, not j, determines whether (S7.13) is non-negative or non-positive, it follows that, for any given k, (3.13) is a sum of only non-negative terms if k is even and a sum of only non-positive terms if k is odd. Therefore, if $(-1)^l x_l \geq 0$ for all $l = 1, ..., k-j+1$, then, for all $j = 1, ..., k$, $\mathfrak{B}_{k,j} \geq 0$ if k is even and $\mathfrak{B}_{k,j} \leq 0$ if k is odd, as required. □

Proof of Lemma 7. Let $z = 1$, and set $\lambda = -(z+1) = -2$. For $\lambda = -2$, (3.1) has the form, $\phi_{-2}(x) = 0.5(x^{-1} + x - 2)$. The derivatives are $\phi_{-2}^{(1)}(x) = -0.5(x^{-2} - 1)$, $\phi_{-2}^{(2)}(x) = x^{-3}$, and $\phi_{-2}^{(k)}(x) = (-1)^k \times \left(\prod_{j=3}^{k} j\right) \times x^{-(k+1)}$ for $k = 3, 4, ...$ Then, the IFT implies $\phi_{-2}^{-1}(t)$ has derivatives of all orders over $t \in (0, \infty)$ since $\phi_{-2}(x)$ is continuous and has derivatives of all orders for all $x \in (0, \infty)$. For the signs of these derivatives, rearrange (3.9) into the form,

$$0 = x(t)^2 - 2[t+1]x(t) + 1, \tag{S7.14}$$

where $x(t) \in [0, 1]$ is the function of $t \in [0, \infty)$ that solves this equation. Hence, $x(t)$ is precisely $\phi_{-2}^{-1}(t)$. Letting $k \geq 1$ be a positive integer, differentiate both sides of (S7.14) $(k+1)$ times with respect to t. On the RHS of (S7.14), the $(k+1)$-th derivative of $x(t)^2$ is given by Faà di Bruno's formula,

and the $(k+1)$-th derivative of $2[t+1]x(t)$ can be obtained by applying the general Leibniz rule. This yields,

$$0 = 2x(t)\mathfrak{B}_{k+1,1}(t) + 2\mathfrak{B}_{k+1,2}(t) - 2(k+1)x^{(k)}(t) - 2[t+1]x^{(k+1)}(t),$$

where the two terms $\mathfrak{B}_{k+1,1}(t) \equiv B_{k+1,1}(x^{(1)}(t), ..., x^{(k+1)}(t))$ and $\mathfrak{B}_{k+1,2}(t) \equiv B_{k+1,2}(x^{(1)}(t), ..., x^{(k)}(t))$ are incomplete exponential Bell polynomials per Definition 6 (e.g., Comtet, 1974, pp. 133-137). Importantly, the definition in (3.13) and conditions in (3.14) and (3.15) imply that $\mathfrak{B}_{k+1,1}(t) = x^{(k+1)}(t)$. Hence, after some algebra, we obtain, $0 = (x(t) - [t+1])\, x^{(k+1)}(t) + \mathfrak{B}_{k+1,2}(t) - (k+1)x^{(k)}(t)$. By rearranging to isolate $x^{(k+1)}(t)$ on the LHS, we obtain,

$$x^{(k+1)}(t) = -\left(\frac{(k+1)x^{(k)}(t) - \mathfrak{B}_{k+1,2}(t)}{t+1-x(t)}\right). \tag{S7.15}$$

From this point, the proof is completed by induction on k. The inductive hypothesis is that, for given positive integer k, the derivatives $x^{(j)}(t)$ all satisfy $(-1)^j x^{(j)}(t) \geq 0$ for $j = 1, ..., k$. Now examine the terms on the RHS of (S7.15). There is a prefactor of -1; the denominator is $t+1-x(t) \geq 0$, since $t \in (0, \infty)$ and $x(t) \in [0, 1]$; in the numerator, we have $(k+1)x^{(k)}(t) - \mathfrak{B}_{k+1,2}(t)$. By the inductive hypothesis, $x^{(k)}(t)$ has sign $(-1)^k$ (i.e., positive if k is even and negative if k is odd) and, also by Lemma 6, we have $\mathfrak{B}_{k+1,2}(t) \geq 0$ if $k+1$ is even (k is odd) and $\mathfrak{B}_{k+1,2}(t) \leq 0$ if

$k+1$ is odd (k is even). Therefore, $(k+1)x^{(k)}(t)$ and $\mathfrak{B}_{k+1,2}(t)$ have opposite signs, and $(k+1)x^{(k)}(t) - \mathfrak{B}_{k+1,2}(t)$ has the same sign as $x^{(k)}(t)$, namely $(-1)^k$. Hence $x^{(k+1)}(t)$ has the opposite sign to $x^{(k)}(t)$ for any given $k = 1, 2, \ldots$. In other words, if $(-1)^k x^{(k)}(t) \geq 0$, then $(-1)^{k+1} x^{(k+1)}(t) \geq 0$.

The base case for the induction is provided by explicitly calculating $x^{(1)}(t)$ and verifying that $(-1)x^{(1)}(t) \geq 0$. By the IFT, $x(t) \equiv \phi_{-2}^{-1}(t)$ has first derivative, $x^{(1)}(t) = -2\{x(t)^2/(1-x(t)^2)\}$, which is negative since $0 \leq x(t)^2 \leq 1$, which in turn indicates that $(-1)x^{(1)}(t) \geq 0$. This provides the base case. Therefore, by induction, it follows that $(-1)^k x^{(k)}(t) \geq 0$ for all $t \in (0, \infty)$ and $k = 1, 2, \ldots$. Hence $x(t) \equiv \phi_{-2}^{-1}(t)$ is completely monotone on $[0, \infty)$. □

Proof of Theorem 7. This follows immediately from Lemmas 5 and 7 in combination with the result of Kimberling (1974); see also Theorem 4.6.2 in Nelsen (2006). □

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