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A trivariate wrapped Cauchy copula

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Abstract

In this paper, we propose a new distribution for data on the three-dimensional torus which we call a trivariate wrapped Cauchy copula. Our trivariate copula has several attractive properties. It has a simple form of density and desirable modality properties. Its parameters allow for an adjustable degree of dependence between every pair of variables and these can be easily estimated. The conditional distributions of the model are well studied bivariate wrapped Cauchy distributions. Furthermore, the distribution can be easily simulated. Parameter estimation via maximum likelihood for the distribution is given and we highlight the simple implementation procedure to obtain these estimates.

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1. Introduction

Angular data occur frequently in domains such as environmental sciences (e.g., wind directions, wave directions), bioinformatics (dihedral angles in protein backbone structures), zoology (animal movement studies), medicine (circadian body clock, secretion times of hormones), or political/social sciences (times of crimes during the day), see for example (1). However, dealing

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with data that are angles requires special care in order to take into account their topology (domain $[0, 2\pi)$ where the end points coincide). Classical statistical concepts from the real line no longer hold for such data (2; 3); in particular, the building blocks of statistical modeling and inference, probability distributions, need to be properly defined. For data involving a single angle, called circular data, a large body of literature proposing circular distributions exists (see for example (4) and (5)), among which are the popular von Mises, wrapped Cauchy and cardioid models. Though less in number, there also exist several interesting distributions for data consisting of two angles, called toroidal data. Popular examples for toroidal distributions are the bivariate von Mises (6), the Sine (7) and Cosine models (8) and the bivariate wrapped Cauchy (9) distributions.

The situation is somewhat different for the case of trivariate distributions. Several models have been introduced in the literature to handle three or more angles, including the multivariate nonnegative trigonometric sums model (10), the copula proposed by (11), the multivariate von Mises distribution (12), the multivariate Generalised von Mises distribution (13), the multivariate wrapped normal distribution (14), the multivariate projected normal distribution (15), and the inverse stereographic normal distribution (16). Such distributions can be used to model datasets, with an important example arising from structural bioinformatics. Predicting the three-dimensional folding structure of a protein from its known one-dimensional amino acid structure is among the most important yet hardest scientific challenges. A cornerstone of this endeavour is the uncertainty quantification of the two dihedral angles ϕ and ψ along with the torsion angle of the side chain ω, meaning that statistical models on the 3-dimensional torus are needed. However, all aforementioned distributions have some limitations that make modelling more challenging, such as intractable normalizing constants, rendering parameter estimation difficult, no clear-cut sampling scheme or unknown/complex marginal distributions.

In order to fill this important gap in the literature, we propose in this paper a trivariate wrapped Cauchy copula. Note that (17) coined the term *circulas* for copulas on the torus. Circulas differ fundamentally from copulas whose domains are rescaled from $[0, 1]^3$ to $[0, 2\pi]^3$ in that they also require the periodicity of the densities, see (17), Section 1. In this paper, we shall consistently use the more classical word copula. Our trivariate wrapped Cauchy copula is given by density (5) and has the following attractive properties: (i) simple form of density, (ii) well-estimable parameters, (iii) adjustable degree of dependence between the variables, enhancing parameter interpretability, (iv) well-known conditional distributions, and (v) a simple data generating mechanism. Thus we are proposing a new model that satisfies the requirements as laid out in (18).

The paper is organized as follows. In Section 2 we review some well-known bivariate distributions which are relevant for our construction before proposing the trivariate wrapped Cauchy copula in Section 3. In Section 4, several properties of the proposed distribution are given, namely conditional distributions, random variate generation, modality and correlation coefficients. Parameter estimation is considered in Section 5. A possible extension to any d-dimensional torus is presented in Section 6, while Section 7 concludes the paper with a discussion. We provide additional information in the Supplementary Material, namely an essential lemma about parameter space, trigonometric moments, further properties, method of moment estimation, Monte Carlo simulation results, and a generalization of our new distribution.

2. Bivariate circular probability distributions and copulas

Before we introduce our trivariate wrapped Cauchy copula, we will first review the most popular bivariate circular distributions.

A popular class of toroidal (circular-circular) distributions that allows specifying the marginal distributions has been put forward by Wehrly and Johnson (19). Their general families have the probability density functions

$$f(\theta_1, \theta_2) = 2\pi g[2\pi\{F_1(\theta_1) - qF_2(\theta_2)\}]f_1(\theta_1)f_2(\theta_2), \tag{1}$$

where q equals 1 or -1 (leading to two distinct families), $0 \leq \theta_1, \theta_2 < 2\pi$, f_1 and f_2 are specified densities on the circle $[0, 2\pi)$, F_1 and F_2 are their distribution functions defined with respect to fixed, arbitrary, origins, and g is also a specified density on the circle. Both families (1) have the nice property that their marginal densities are given by f_1 and f_2.

Let a bivariate circular random vector (Θ_1, Θ_2) have the distribution (1). The families (1) can be readily transformed into copulas for bivariate circular data, assuming $(U_1, U_2)' = (2\pi F_1(\Theta_1), 2\pi F_2(\Theta_2))'$. Throughout this paper, unlike the case of ordinary copulas, we define the domains of the copula variables to be $[0, 2\pi)$ or equivalent domains modulo 2π, rather than $[0, 1]$. Then the density of $(U_1, U_2)'$ is given by

$$c(u_1, u_2) = \frac{1}{2\pi}g(u_1 - qu_2), \quad 0 \leq u_1, u_2 < 2\pi. \tag{2}$$

Simple integration shows that $c(u_1, u_2)$ integrates to 1 and that each marginal is uniform on the circle (see (17) for further properties of the distribution (2)). Therefore the distribution (2) can be viewed as an equivalent of a copula for bivariate circular data. From Sklar's theorem (see page 18 in (20)), the distribution with density (2) can be transformed into a distribution with prespecified marginal distributions, as is the case for the distributions of Wehrly and Johnson (1).

In practice, it is necessary to take specific densities for f_1, f_2 and g in the families (1) of Wehrly and Johnson, or equivalently, the choice of g and marginal distributions is important for the copula-based version (2). Various proposals have been put forward in the literature, many of which are based on the use of the von Mises distribution. We refer the reader to (21), Section 2.4, for a review of these models. Further, (22) and (9) adopted the wrapped Cauchy density, given by

$$f(\theta; \rho, \mu) = \frac{|1-\rho^2|}{1+\rho^2 - 2\rho\cos(\theta-\mu)}, \tag{3}$$

for $\rho \in \mathbb{R} \setminus \{\pm 1\}$, $\mu \in [0, 2\pi)$ as the function g in (2) and fixed $q = 1$. This leads to density (2) being of the form

$$c(u_1, u_2) = \frac{1}{4\pi^2} \frac{|1-\rho^2|}{1+\rho^2 - 2\rho\cos(u_1 - u_2 - \mu)}, \quad 0 \le u_1, u_2 < 2\pi, \tag{4}$$

where $\mu \in [0, 2\pi)$ is the location parameter and $\rho \in \mathbb{R} \setminus \{\pm 1\}$ the dependence parameter between the two variables. The distribution (4) is called a bivariate wrapped Cauchy copula which we label as $\mathrm{BWC}(\mu, \rho)$. In fact, (22) showed that this distribution is derived from a problem in Brownian motion and possesses various tractable properties. Moreover, (9) transformed this model via the Möbius transformation and showed that the transformed distribution (known as Kato–Pewsey model) has the wrapped Cauchy marginal and conditional distributions.

3. Our proposal: the trivariate wrapped Cauchy copula

Having described some of the attractive properties of the bivariate wrapped Cauchy distribution of (9) resulting from the copula (4), we extend (4) to a density on the three-dimensional torus in the following theorem, with anticipation that it will inherit these properties.

Theorem 1. *For* $\boldsymbol{u} = (u_1, u_2, u_3)'$ *and* $\boldsymbol{\rho} = (\rho_{12}, \rho_{13}, \rho_{23})'$, *let*

$$t(\boldsymbol{u}; \boldsymbol{\rho}) = c_2 \Big[c_1 + 2 \left\{ \rho_{12} \cos(u_1 - u_2) + \rho_{13} \cos(u_1 - u_3) + \rho_{23} \cos(u_2 - u_3) \right\} \Big]^{-1},$$
$$0 \leq u_1, u_2, u_3 < 2\pi, \qquad (5)$$

where $\rho_{12}, \rho_{13}, \rho_{23} \in \mathbb{R} \setminus \{0\}$, $\rho_{12}\rho_{13}\rho_{23} > 0$,

$$c_1 = \frac{\rho_{12}\rho_{13}}{\rho_{23}} + \frac{\rho_{12}\rho_{23}}{\rho_{13}} + \frac{\rho_{13}\rho_{23}}{\rho_{12}}, \qquad (6)$$

and

$$c_2 = \frac{1}{(2\pi)^3} \left\{ \left(\frac{\rho_{12}\rho_{13}}{\rho_{23}} \right)^2 + \left(\frac{\rho_{12}\rho_{23}}{\rho_{13}} \right)^2 + \left(\frac{\rho_{13}\rho_{23}}{\rho_{12}} \right)^2 - 2\rho_{12}^2 - 2\rho_{13}^2 - 2\rho_{23}^2 \right\}^{1/2}. \qquad (7)$$

Suppose that there exists one of the permutations of $(1, 2, 3)$, (i, j, k), *such that*

$$|\rho_{jk}| < |\rho_{ij}\rho_{ik}| / (|\rho_{ij}| + |\rho_{ik}|), \qquad (8)$$

where $\rho_{ji} = \rho_{ij}$ *for* $1 \leq i < j \leq 3$. *Then the following two properties for the function* (5) *hold.*

(i) *The function (5) is a probability density function on the three-dimensional torus* $[0, 2\pi)^3$.

(ii) *A family of distributions with probability density function* (5) *is identifiable under the additional constraint*

$$\rho_{12}\rho_{13}\rho_{23} = 1. \qquad (9)$$

Proof. (i) In order to prove the theorem, it suffices to see that the function (5) satisfies:

(a) $t(\boldsymbol{u}; \boldsymbol{\rho}) \geq 0$ for any $\boldsymbol{u} = (u_1, u_2, u_3)'$;

(b) $\int_{[0,2\pi)^3} t(\boldsymbol{u}; \boldsymbol{\rho}) du_1 du_2 du_3 = 1$.

Proof of (a): Without loss of generality, assume for (8) that $|\rho_{12}| < |\rho_{13}\rho_{23}| / (|\rho_{13}| + |\rho_{23}|)$. We note that

$$\begin{aligned} & c_1 + 2 \left\{ \rho_{12} \cos(u_1 - u_2) + \rho_{13} \cos(u_1 - u_3) + \rho_{23} \cos(u_2 - u_3) \right\} \\ &= \left\| \phi_1 \begin{pmatrix} \cos u_1 \\ \sin u_1 \end{pmatrix} + \phi_2 \begin{pmatrix} \cos u_2 \\ \sin u_2 \end{pmatrix} + \phi_3 \begin{pmatrix} \cos u_3 \\ \sin u_3 \end{pmatrix} \right\|^2, \end{aligned}$$

where

$$\phi_i = \mathrm{sgn}(\rho_{jk}) \left| \frac{\rho_{ij}\rho_{ik}}{\rho_{jk}} \right|^{1/2}, \quad i,j,k = 1,2,3, \quad j,k \neq i, \quad j < k. \tag{10}$$

Then

$$\begin{aligned}
&\left\| \phi_1 \begin{pmatrix} \cos u_1 \\ \sin u_1 \end{pmatrix} + \phi_2 \begin{pmatrix} \cos u_2 \\ \sin u_2 \end{pmatrix} + \phi_3 \begin{pmatrix} \cos u_3 \\ \sin u_3 \end{pmatrix} \right\| \\
&\qquad \geq \left\| \phi_3 \begin{pmatrix} \cos u_3 \\ \sin u_3 \end{pmatrix} \right\| - \left\| \phi_1 \begin{pmatrix} \cos u_1 \\ \sin u_1 \end{pmatrix} + \phi_2 \begin{pmatrix} \cos u_2 \\ \sin u_2 \end{pmatrix} \right\| \\
&\qquad \geq \sqrt{\frac{\rho_{13}\rho_{23}}{\rho_{12}}} - \left(\sqrt{\frac{\rho_{12}\rho_{13}}{\rho_{23}}} + \sqrt{\frac{\rho_{12}\rho_{23}}{\rho_{13}}} \right) > 0.
\end{aligned} \tag{11}$$

Therefore $c_1 + 2\left\{\rho_{12}\cos(u_1 - u_2) + \rho_{13}\cos(u_1 - u_3) + \rho_{23}\cos(u_2 - u_3)\right\} > 0$ for any $(u_1, u_2, u_3)'$.

Next we show that the expression between curly brackets in c_2 given in (7) is positive. It is easy to see that

$$\begin{aligned}
&\rho_{12}^2\rho_{13}^2\rho_{23}^2 \left(\left(\frac{\rho_{12}\rho_{13}}{\rho_{23}} \right)^2 + \left(\frac{\rho_{12}\rho_{23}}{\rho_{13}} \right)^2 + \left(\frac{\rho_{13}\rho_{23}}{\rho_{12}} \right)^2 - 2\rho_{12}^2 - 2\rho_{13}^2 - 2\rho_{23}^2 \right) \\
&\qquad = (\rho_{12}^2 - \rho_{23}^2)^2 \left\{ \rho_{13}^2 - \frac{\rho_{12}^2\rho_{23}^2(\rho_{12}^2 + \rho_{23}^2)}{(\rho_{12}^2 - \rho_{23}^2)^2} \right\}^2 - \frac{4\rho_{12}^6\rho_{23}^6}{(\rho_{12}^2 - \rho_{23}^2)^2}.
\end{aligned} \tag{12}$$

It follows from the assumption $|\rho_{12}| < |\rho_{13}\rho_{23}|/(|\rho_{13}| + |\rho_{23}|)$ that $|\rho_{13}| > |\rho_{12}\rho_{23}|/(|\rho_{23}| - |\rho_{12}|)$. Also, $\rho_{13}^2 > \{|\rho_{12}\rho_{23}|/(|\rho_{23}| - |\rho_{12}|)\}^2$. Then the radicand (12) can be evaluated as

$$\begin{aligned}
&(\rho_{12}^2 - \rho_{23}^2)^2 \left\{ \rho_{13}^2 - \frac{\rho_{12}^2\rho_{23}^2(\rho_{12}^2 + \rho_{23}^2)}{(\rho_{12}^2 - \rho_{23}^2)^2} \right\}^2 - \frac{4\rho_{12}^6\rho_{23}^6}{(\rho_{12}^2 - \rho_{23}^2)^2} \\
&\qquad > (\rho_{12}^2 - \rho_{23}^2)^2 \left\{ \left(\frac{|\rho_{12}\rho_{23}|}{|\rho_{23}| - |\rho_{12}|} \right)^2 - \frac{\rho_{12}^2\rho_{23}^2(\rho_{12}^2 + \rho_{23}^2)}{(\rho_{12}^2 - \rho_{23}^2)^2} \right\}^2 - \frac{4\rho_{12}^6\rho_{23}^6}{(\rho_{12}^2 - \rho_{23}^2)^2} \\
&\qquad = 0.
\end{aligned}$$

Hence $c_2 > 0$. Thus the function (5) satisfies the condition (a) for $|\rho_{12}| < |\rho_{13}\rho_{23}|/(|\rho_{13}| + |\rho_{23}|)$. Due to the symmetry of the function (5), it immediately follows that the condition (a) holds for the other two cases $|\rho_{13}| < |\rho_{12}\rho_{23}|/(|\rho_{12}| + |\rho_{23}|)$ and $|\rho_{23}| < |\rho_{12}\rho_{13}|/(|\rho_{12}| + |\rho_{13}|)$.

Proof of (b): Using the equation (3.613.2.6) of (23), it follows that

$$
\begin{aligned}
&\int_0^{2\pi} t(\boldsymbol{u};\boldsymbol{\rho})du_3 \\
&= \frac{c_2}{c_1+2\rho_{12}\cos(u_1-u_2)}\int_0^{2\pi}\left[1+\frac{2\{\rho_{13}\cos(u_1-u_3)+\rho_{23}\cos(u_2-u_3)\}}{c_1+2\rho_{12}\cos(u_1-u_2)}\right]^{-1}du_3 \\
&= \frac{c_2}{c_1+2\rho_{12}\cos(u_1-u_2)}\int_0^{2\pi}\frac{1}{1+b'\cos(u_3-a')}du_3 \\
&= \frac{c_2}{c_1+2\rho_{12}\cos(u_1-u_2)}\cdot\frac{2\pi}{|1-b'^2|^{1/2}}, \qquad (13)
\end{aligned}
$$

where $b' = 2\{\rho_{13}^2+\rho_{23}^2+2\rho_{13}\rho_{23}\cos(u_1-u_2)\}^{1/2}/\{c_1+2\rho_{12}\cos(u_1-u_2)\}$ and a' satisfies $\tan\alpha' = (\rho_{13}\sin u_1+\rho_{23}\sin u_2)/(\rho_{13}\cos u_1+\rho_{23}\cos u_2)$. The second equality follows from the formula $\alpha\cos u_3+\beta\sin u_3 = \sqrt{\alpha^2+\beta^2}\cos(u_3-\gamma)$, where γ satisfies $\tan\gamma = \beta/\alpha$. In order to see that $|b'|<1$ in the last equality, it suffices to see that

$$
\begin{aligned}
&c_1+2\rho_{12}\cos(u_1-u_2)-2\{\rho_{13}^2+\rho_{23}^2+2\rho_{13}\rho_{23}\cos(u_1-u_2)\}^{1/2} \\
&\qquad = \left|\left\|\phi_1\begin{pmatrix}\cos u_1\\ \sin u_1\end{pmatrix}+\phi_2\begin{pmatrix}\cos u_2\\ \sin u_2\end{pmatrix}\right\|-\left\|\phi_3\begin{pmatrix}\cos u_3\\ \sin u_3\end{pmatrix}\right\|\right|^2>0,
\end{aligned}
$$

holds for any $u_1,u_2,u_3\in[0,2\pi)$. If $|\rho_{12}|<|\rho_{13}\rho_{23}|/(|\rho_{13}|+|\rho_{23}|)$, this inequality is already seen in (11). If $|\rho_{13}|<|\rho_{12}\rho_{23}|/(|\rho_{12}|+|\rho_{23}|)$ or $|\rho_{23}|<|\rho_{12}\rho_{13}|/(|\rho_{12}|+|\rho_{13}|)$, we have

$$
\begin{aligned}
&\left\|\phi_1\begin{pmatrix}\cos u_1\\ \sin u_1\end{pmatrix}+\phi_2\begin{pmatrix}\cos u_2\\ \sin u_2\end{pmatrix}\right\|-\left\|\phi_3\begin{pmatrix}\cos u_3\\ \sin u_3\end{pmatrix}\right\| \\
&\qquad \geq \left|\sqrt{\frac{\rho_{12}\rho_{13}}{\rho_{23}}}-\sqrt{\frac{\rho_{12}\rho_{23}}{\rho_{13}}}\right|-\sqrt{\frac{\rho_{13}\rho_{23}}{\rho_{12}}}>0.
\end{aligned}
$$

The last inequality follows from

$$
\begin{aligned}
&\left|\sqrt{\frac{\rho_{12}\rho_{13}}{\rho_{23}}}-\sqrt{\frac{\rho_{12}\rho_{23}}{\rho_{13}}}\right|^2-\frac{\rho_{13}\rho_{23}}{\rho_{12}} = \frac{1}{\rho_{12}\rho_{13}\rho_{23}}\left[\rho_{12}^2\{\rho_{13}-\rho_{23}\}^2-\rho_{13}^2\rho_{23}^2\right] \\
&\qquad \geq \frac{1}{\rho_{12}\rho_{13}\rho_{23}}\left\{\rho_{12}^2(|\rho_{13}|-|\rho_{23}|)^2-\rho_{13}^2\rho_{23}^2\right\} \\
&\qquad > \frac{1}{\rho_{12}\rho_{13}\rho_{23}}\left\{\left(\frac{\rho_{13}\rho_{23}}{|\rho_{13}|-|\rho_{23}|}\right)^2(|\rho_{13}|-|\rho_{23}|)^2-\rho_{13}^2\rho_{23}^2\right\}=0.
\end{aligned}
$$

Thus we have $c_1+2\rho_{12}\cos(u_1-u_2)-2\{\rho_{13}^2+\rho_{23}^2+2\rho_{13}\rho_{23}\cos(u_1-u_2)\}^{1/2}>0$, which implies $|b'|<1$.

(13) can be simplified as

$$\int_0^{2\pi} t(\boldsymbol{u};\boldsymbol{\rho})du_3 = \frac{2\pi\cdot c_2}{|\rho_{12}\rho_{23}/\rho_{13}+\rho_{12}\rho_{13}/\rho_{23}-\rho_{13}\rho_{23}/\rho_{12}+2\rho_{12}\cos(u_1-u_2)|}$$
$$\equiv t_2(u_1,u_2;\phi_{12}), \tag{14}$$

where ϕ_{12} is defined in (17). Here we show that the denominator of (14) is positive for any $(u_1,u_2)'$. For convenience, write $c_3=\rho_{12}\rho_{23}/\rho_{13}+\rho_{12}\rho_{13}/\rho_{23}-\rho_{13}\rho_{23}/\rho_{12}$. Let $\rho_{12}>0$. For the case $|\rho_{12}|<|\rho_{13}\rho_{23}|/(|\rho_{13}|+|\rho_{23}|)$, it can be seen that

$$\begin{aligned} c_3+2\rho_{12}\cos(u_1-u_2) \le c_3+2\rho_{12} &= \frac{\rho_{12}^2(\rho_{13}+\rho_{23})^2-\rho_{13}^2\rho_{23}^2}{\rho_{12}\rho_{13}\rho_{23}} \\ &< \frac{1}{\rho_{12}\rho_{13}\rho_{23}}\left[\left(\frac{|\rho_{13}||\rho_{23}|}{|\rho_{13}|+|\rho_{23}|}\right)^2(\rho_{13}+\rho_{23})^2-\rho_{13}^2\rho_{23}^2\right]\le 0. \end{aligned}$$

The case $|\rho_{13}|<|\rho_{12}\rho_{23}|/(|\rho_{12}|+|\rho_{23}|)$ or $|\rho_{23}|<|\rho_{12}\rho_{13}|/(|\rho_{12}|+|\rho_{13}|)$ can be proved in a similar manner.

Similarly, when $\rho_{12}<0$, it can be seen that the denominator of (14) remains positive for any $(u_1,u_2)'$.

Note that the discussion above implies $|2\rho_{12}/c_3|<1$. Then it follows from the equation (3.613.2.6) of (23) that, for the parameters satisfying $c_3+2\rho_{12}\cos(u_1-u_2)>0$,

$$\begin{aligned} \int_0^{2\pi} t_2(u_1,u_2;\phi_{12})du_2 &= \int_0^{2\pi}\frac{2\pi c_2}{c_3+2\rho_{12}\cos(u_1-u_2)}du_2 \\ &= \int_0^{2\pi}\frac{2\pi c_2}{c_3\{1+2(\rho_{12}/c_3)\cos(u_1-u_2)\}}du_2 \\ &= \frac{(2\pi)^2c_2}{c_3|1-(2\rho_{12}/c_3)^2|^{1/2}} = \frac{(2\pi)^2c_2}{|c_3^2-4\rho_{12}^2|^{1/2}} = \frac{1}{2\pi}. \end{aligned} \tag{15}$$

Similarly, we can also show $\int_0^{2\pi} t_2(u_1,u_2;\phi_{12})du_2 = 1/(2\pi)$ for the parameters which satisfy $c_3+2\rho_{12}\cos(u_1-u_2)<0$. Finally,

$$\int_{[0,2\pi)^3} t(\boldsymbol{u};\boldsymbol{\rho})du_1du_2du_3 = \int_0^{2\pi}\frac{1}{2\pi}du_1 = 1.$$

Thus the proposed density (5) satisfies the condition (b) as required.

Since the function (5) satisfies both conditions (a) and (b), this function is a probability density function on $[0, 2\pi)^3$. This completes Proof of (i).

(ii) Let $\boldsymbol{\rho} = (\rho_{12}, \rho_{13}, \rho_{23})'$ and $\tilde{\boldsymbol{\rho}} = (\tilde{\rho}_{12}, \tilde{\rho}_{13}, \tilde{\rho}_{23})'$ be two different points in the constrained parameter space of the proposed family (5) with $\rho_{12}\rho_{13}\rho_{23} = \tilde{\rho}_{12}\tilde{\rho}_{13}\tilde{\rho}_{23} = 1$. Assume that $\boldsymbol{\rho}$ and $\tilde{\boldsymbol{\rho}}$ represent the same distribution, namely, $t(\boldsymbol{u}; \boldsymbol{\rho}) = t(\boldsymbol{u}; \tilde{\boldsymbol{\rho}})$ for any $\boldsymbol{u} = (u_1, u_2, u_3)' \in [0, 2\pi)^3$, where t is the density (5). This implies that there exist real-valued constants C and D such that, for any $\boldsymbol{u} \in [0, 2\pi)^3$,

$$\begin{aligned}
&\rho_{12}\cos(u_1 - u_2) + \rho_{13}\cos(u_1 - u_3) + \rho_{23}\cos(u_2 - u_3) \\
&\qquad = D + C\left\{\tilde{\rho}_{12}\cos(u_1 - u_2) + \tilde{\rho}_{13}\cos(u_1 - u_3) + \tilde{\rho}_{23}\cos(u_2 - u_3)\right\}.
\end{aligned}$$

Choosing $(u_1, u_2, u_3)'$ equal to $(\pi/2, \pi/2, 0)'$, $(\pi/2, 0, \pi/2)'$, and $(0, \pi/2, \pi/2)'$, respectively, yields, $\rho_{ij} = D + C\tilde{\rho_{ij}}$ for each couple $(i, j) \in \{(1, 2), (1, 3), (2, 3)\}$. Moreover, $(u_1, u_2, u_3)' = (0, 0, 0)'$ gives $\rho_{12} + \rho_{13} + \rho_{23} = D + C(\tilde{\rho_{12}} + \tilde{\rho_{13}} + \tilde{\rho_{23}})$. Summing the first three equalities and subtracting the last entails $0 = 2D$ and hence $D = 0$, leading to

$$\begin{aligned}
&\rho_{12}\cos(u_1 - u_2) + \rho_{13}\cos(u_1 - u_3) + \rho_{23}\cos(u_2 - u_3) \\
&\qquad = C\left\{\tilde{\rho}_{12}\cos(u_1 - u_2) + \tilde{\rho}_{13}\cos(u_1 - u_3) + \tilde{\rho}_{23}\cos(u_2 - u_3)\right\}.
\end{aligned}$$

Then it follows that, for any (u_1, u_2, u_3),

$$(\rho_{12} - C\tilde{\rho}_{12})\cos(u_1 - u_2) + (\rho_{13} - C\tilde{\rho}_{13})\cos(u_1 - u_3) + (\rho_{23} - C\tilde{\rho}_{23})\cos(u_2 - u_3) = 0.$$

Thus

$$\rho_{12} = C\tilde{\rho}_{12},\ \ \rho_{13} = C\tilde{\rho}_{13},\ \ \rho_{23} = C\tilde{\rho}_{23}.$$

Using this equation and the assumption $\rho_{12}\rho_{13}\rho_{23} = \tilde{\rho}_{12}\tilde{\rho}_{13}\tilde{\rho}_{23} = 1$, we have

$$1 = \rho_{12}\rho_{13}\rho_{23} = C^3\tilde{\rho}_{12}\tilde{\rho}_{13}\tilde{\rho}_{23} = C^3.$$

Thus we have $C = 1$. This implies $\boldsymbol{\rho} = \tilde{\boldsymbol{\rho}}$, which is contradictory to the assumption $\boldsymbol{\rho}$ and $\tilde{\boldsymbol{\rho}}$ are two different points. □

We will refer to this distribution, which has the density of $(U_1, U_2, U_3)'$ given by (5) under condition (8), as the trivariate wrapped Cauchy copula (TWCC or TWC copula). This distribution is also denoted by TWCC($\boldsymbol{\rho}$) in order to specify its parameters.

The proposed family (5) is not identifiable without the constraint (9). This can be seen by noting that $t(\boldsymbol{u};\boldsymbol{\rho}) = t(\boldsymbol{u}; c\boldsymbol{\rho})$ for any constant $c \in \mathbb{R}^+$. However, it is useful to define the TWCC without (9) in order to discuss certain properties, although this constraint needs to be imposed when performing maximum likelihood estimation. Under (9), condition (8) can be re-expressed under simpler form as $\rho_{ij}^2\rho_{ik}^2 > (|\rho_{ij}| + |\rho_{ik}|)$.

In TWCC, different functions of parameters ρ_{12}, ρ_{13} and ρ_{23} control the dependence between the U_i's and the location of the modes, see Theorems 5 and 6 in Section 4. It is also straightforward to incorporate both positive and negative associations by replacing u_i with $q_i u_i$ ($q_i = 1, -1$) and it is possible to extend the distribution to include location parameters by replacing $u_i - u_j$ with $u_i - u_j - \mu_{ij}$ in (5) ($0 \le \mu_{ij} < 2\pi$). Although the parametrization used in the expression (5) for the density is natural in the sense that each parameter ρ_{ij} is multiplied by a function of $u_i - u_j$, this expression does not allow for independence between U_i and U_j. However, an alternative parametrization is available that accommodates independence between the variables; see equation (20) below. A very appealing aspect from both a tractability and computational viewpoint is the closed form of the density which does not include any integrals or infinite sums, unlike most existing distributions on the three-dimensional torus.

The original form of our proposal was derived by modifying the density (4) of the bivariate wrapped Cauchy copula, such that the denominator is replaced by a more general constant term plus a function of the form $\rho_{12}\cos(\theta_1 - \theta_2) + \rho_{13}\cos(\theta_1 - \theta_3) + \rho_{23}\cos(\theta_2 - \theta_3)$; see equation (S.9) of the Supplementary Material. However, the TWCC, which imposes a specific constraint on the constant term, has the appealing property that its bivariate marginals belong to the bivariate wrapped Cauchy copula family. Additionally, it has a simple normalizing constant and a well-known form for the univariate conditional distribution given a single variable. See Theorems 2 and 3 below for further details on the marginals and conditionals.

Next, we show that our model given by TWCC is indeed a copula for trivariate circular data by establishing in Theorem 2 that its univariate marginals are circular uniform distributions. Prior to this, we will show that the bivariate marginals of our new model are bivariate wrapped Cauchy-type copulas as they are of the form (4).

Theorem 2. *Let a trivariate circular random vector* $(U_1, U_2, U_3)'$ *follow the TWCC with density (5) and satisfy the identifiability constraint* (9). *Then* *the following hold for the marginal distributions of* $(U_1, U_2, U_3)'$*:*

(i) The marginal distribution of $(U_i, U_j)'$ *is of the form* (4) *with density*

$$t_2(u_i, u_j; \phi_{ij}) = \frac{1}{4\pi^2} \frac{|1-\phi_{ij}^2|}{1+\phi_{ij}^2 - 2\phi_{ij}\cos(u_i - u_j)}, \quad 0 \le u_i, u_j < 2\pi, \tag{16}$$

where

$$\phi_{ij} = \frac{1}{2\rho_{ij}} \left\{ \frac{\rho_{ik}\rho_{jk}}{\rho_{ij}} - \frac{\rho_{ij}\rho_{ik}}{\rho_{jk}} - \frac{\rho_{ij}\rho_{jk}}{\rho_{ik}} - (2\pi)^3 c_2 \right\}, \tag{17}$$

and c_2 *is as in (7).*

(ii) The marginal distribution of U_i *is the uniform distribution on the circle with density*

$$t_1(u_i) = \frac{1}{2\pi}, \quad 0 \le u_i < 2\pi.$$

Therefore the distribution of $(U_1, U_2, U_3)'$ *is a copula for trivariate circular data.*

Proof. Without loss of generality, we prove the case $(i, j) = (1, 2)$. The other cases can be shown in a similar manner.

(i) It follows from the equation (14) that the marginal density of $(U_1, U_2)'$ can be expressed as

$$\begin{aligned} t_2(u_1, u_2; \phi_{12}) &= \int_0^{2\pi} t(\boldsymbol{u}; \boldsymbol{\rho}) du_3 \\ &= \frac{2\pi \cdot c_2}{|\rho_{12}\rho_{23}/\rho_{13} + \rho_{12}\rho_{13}/\rho_{23} - \rho_{13}\rho_{23}/\rho_{12} + 2\rho_{12}\cos(u_1 - u_2)|}. \end{aligned}$$

This marginal density can be rewritten as

$$t_2(u_1, u_2; \phi_{12}) = \frac{1}{(2\pi)^2} \frac{|1-\phi_{12}^2|}{1+\phi_{12}^2 - 2\phi_{12}\cos(u_1 - u_2)}.$$

The value of ϕ_{12} can be obtained as a solution to the equations $1+\phi_{12}^2 = C \cdot (\rho_{12}\rho_{23}/\rho_{13} + \rho_{12}\rho_{13}/\rho_{23} - \rho_{13}\rho_{23}/\rho_{12})$ and $-2\phi_{12} = 2C\rho_{12}$ for some $C \neq 0$. Specifically, since these equations imply

$$-\frac{1+\phi_{12}^2}{2\phi_{12}} = \frac{c_3}{2\rho_{12}}, \tag{18}$$

where $c_3 = \rho_{12}\rho_{23}/\rho_{13} + \rho_{12}\rho_{13}/\rho_{23} - \rho_{13}\rho_{23}/\rho_{12}$, the solutions of this equation, say $\tilde{\phi}_{12}$, are given by

$$\begin{aligned}\tilde{\phi}_{12} &= \frac{-c_3 \pm \{c_3^2 - 4\rho_{12}^2\}^{1/2}}{2\rho_{12}} \\ &= \frac{\rho_{13}\rho_{23}/\rho_{12} - \rho_{12}\rho_{23}/\rho_{13} - \rho_{12}\rho_{13}/\rho_{23} \pm (2\pi)^3 c_2}{2\rho_{12}}.\end{aligned}$$

Denote these solutions by $\tilde{\phi}_{12}^+ = \{-c_3 + \{c_3^2 - 4\rho_{12}^2\}^{1/2}\}/(2\rho_{12})$ and $\tilde{\phi}_{12}^- = \{-c_3 - \{c_3^2 - 4\rho_{12}^2\}^{1/2}\}/(2\rho_{12})$. Then by definition of ϕ_{12} it is straightforward to see $\tilde{\phi}_{12}^- = \phi_{12}$, $\tilde{\phi}_{12}^+\tilde{\phi}_{12}^- = 1$ and $\tilde{\phi}_{12}^+ = 1/\phi_{12}$. Note that $t_2(u_1, u_2; \phi_{12})$ in equation (16) with the parameter $\phi_{12} (\neq 0)$ satisfies

$$t_2(u_1, u_2; \phi_{12}) = t_2(u_1, u_2; 1/\phi_{12}), \quad 0 \leq u_1, u_2 < 2\pi. \tag{19}$$

This expression implies that the two solutions of (18), i.e., $\tilde{\phi}_{12}^+$ and $\tilde{\phi}_{12}^-$, correspond to the parameters of the same distribution. Using the parameters derived from the solution $\tilde{\phi}_{12}^-$, we have

$$t_2(u_1, u_2; \phi_{12}) \propto \left\{1 + \phi_{12}^2 - 2\phi_{12}\cos(u_1 - u_2)\right\}^{-1}.$$

Since the functional form of this marginal density is essentially the same as that of (4), it follows that the marginal density is given by (16) with $(i, j) = (1, 2)$.

(ii) It immediately follows from equation (15) that the marginal distribution of U_1 is the uniform distribution on the circle.

□

Note that the ϕ_{ij} are invariant under ρ_{ij} replaced by $c\rho_{ij}$ for some constant $c \in \mathbb{R}^+$, implying that they do not depend on any identifiability condition on ρ_{ij}. We draw the reader's attention to the fact that the constant c_1 has to be of the form (6), which guarantees that the bivariate marginal distribution belongs to the bivariate wrapped Cauchy-type family. See equality (14).

In order to investigate the properties of the TWCC, it is often convenient to express its density using complex variables. Let $(U_1, U_2, U_3)'$ have the TWCC density (5), and assume that $(Z_1, Z_2, Z_3)' = (e^{\mathrm{i}U_1}, e^{\mathrm{i}U_2}, e^{\mathrm{i}U_3})'$. Then some simple algebra yields that the TWCC density can be expressed as

$$tc(\boldsymbol{z}; \boldsymbol{\phi}) = \frac{1}{(2\pi)^3} \frac{\{\phi_1^4 + \phi_2^4 + \phi_3^4 - 2\phi_1^2\phi_2^2 - 2\phi_1^2\phi_3^2 - 2\phi_2^2\phi_3^2\}^{1/2}}{|\phi_1 z_1 + \phi_2 z_2 + \phi_3 z_3|^2}, \tag{20}$$

where $\boldsymbol{z} = (z_1, z_2, z_3)' \in \Omega = \{z \in \mathbb{C}\,;\, |z| = 1\}$ is the unit circle in the complex plane and $\boldsymbol{\phi} = (\phi_1, \phi_2, \phi_3)'$ and ϕ_i is defined as in (10). We call this the complex TWCC. Note that, in terms of the original parameters, we have $\rho_{12} = \phi_1\phi_2$, $\rho_{13} = \phi_1\phi_3$ and $\rho_{23} = \phi_2\phi_3$. The inequality (8) on the parameters in Theorem 1 then simplifies to $|\phi_i| > |\phi_j| + |\phi_k|$ for (i, j, k) a certain permutation of $(1, 2, 3)$. In fact, this is equivalent to the condition that the denominator of (20) satisfies $\phi_1 z_1 + \phi_2 z_2 + \phi_3 z_3 \neq 0$ for all $(z_1, z_2, z_3)'$, see Lemma 1 in Section S.1 of the Supplementary Material for a statement and proof. Equivalently, the condition on the parameter $|\rho_{jk}| < |\rho_{ij}\rho_{ik}|/(|\rho_{ij}| + |\rho_{ik}|)$ for some (i, j, k) is necessary to guarantee the boundedness of the TWCC($\boldsymbol{\rho}$) for all $(u_1, u_2, u_3)'$. The identifiability constraint (9) turns into $(\phi_1\phi_2\phi_3)^2 = 1$.

If the parameter space is extended to include $(\phi_i\phi_j)^2 = 1$ and $\phi_k = 0$, the complex TWCC includes the case where Z_k is independent of both Z_i and Z_j. The additional assumptions $\phi_i = 1 + \varepsilon$ and $\phi_j = -(1 + \varepsilon)^{-1}$ for small $\varepsilon > 0$ imply strong positive dependence between Z_i and Z_j. As $\varepsilon \to \infty$, the complex TWCC converges to the circular equivalent of the comonotonic copula of (Z_i, Z_j), that is, $P(Z_i = Z_j) = 1$.

The parameter space can also be extended to include $\phi_i = 1$ and $\phi_j = \phi_k = 0$, which corresponds to the independence copula. In this case, the random variables Z_1, Z_2, Z_3 are exchangeable in the sense that (Z_1, Z_2, Z_3) has the same distribution as (Z_i, Z_j, Z_k) for any permutation (i, j, k) of $(1, 2, 3)$.

4. Properties of the TWC copula

We will investigate distinct properties of our new copula distribution TWCC($\boldsymbol{\rho}$). In the next sections, we will study and discuss conditional distributions, random variate generation, modality, and correlation coefficients; in Sections S.2 and S.3 of the Supplementary Material we further investigate trigonometric moments, the shapes of our distribution, and limiting cases.

4.1. Conditional distributions and regression

In this subsection we consider the conditional distributions of the model TWCC($\boldsymbol{\rho}$). As we will show, just like the bivariate and univariate marginal distributions, all conditional distributions belong to well-known families, namely to wrapped Cauchy distributions on the circle and to the Kato–Pewsey distribution on the torus. This property also highlights the versatility of the TWCC.

Theorem 3. *Let $(U_1, U_2, U_3)'$ be a trivariate random vector having the distribution TWCC($\boldsymbol{\rho}$). Then the conditional distributions of $(U_1, U_2, U_3)'$ are given below.*

(i) The conditional distribution of $(U_i, U_j)'$ given $U_k = u_k$ is a reparametrized version of the Kato-Pewsey distribution of (9) with density

$$\begin{aligned} & t_{2|1}(u_i, u_j | u_k; \boldsymbol{\rho}) \\ &= 2\pi c_2 \Big[c_1 + 2 \left\{ \rho_{ij} \cos(u_i - u_j) + \rho_{ik} \cos(u_i - u_k) + \rho_{jk} \cos(u_j - u_k) \right\} \Big]^{-1} \qquad (21) \\ &= 2\pi c_2 \Big[c_1 + 2 \{ \rho_{ik} \cos(u_i - u_k) + \rho_{jk} \cos(u_j - u_k) \\ &\qquad + \rho_{ij} \cos(u_i - u_k) \cos(u_j - u_k) + \rho_{ij} \sin(u_i - u_k) \sin(u_j - u_k) \} \Big]^{-1}, \qquad (22) \\ &\qquad 0 \le u_i, u_j < 2\pi. \end{aligned}$$

(ii) The conditional distribution of U_i given $U_j = u_j$ is the wrapped Cauchy distribution (3) *with density*

$$t_{1|1}(u_i | u_j; \phi_{ij}) = \frac{1}{2\pi} \frac{|1 - \phi_{ij}^2|}{1 + \phi_{ij}^2 - 2\phi_{ij} \cos(u_i - u_j)}, \quad 0 \le u_i < 2\pi, \quad (23)$$

where ϕ_{ij} is as in (17)*.*

(iii) The conditional distribution of U_i given $(U_j, U_k)' = (u_j, u_k)'$ is the wrapped Cauchy distribution (3) *with density*

$$t_{1|2}(u_i | u_j, u_k; \eta_{i|jk}, \delta_{i|jk}) = \frac{1}{2\pi} \frac{|1 - \delta_{i|jk}^2|}{1 + \delta_{i|jk}^2 - 2\delta_{i|jk} \cos(u_i - \eta_{i|jk})}, \quad (24)$$

where $0 \le u_i < 2\pi$, and, for $\phi_{i|jk} = -\rho_{jk}(\rho_{ik}^{-1} e^{\mathrm{i}u_j} + \rho_{ij}^{-1} e^{\mathrm{i}u_k})$,

$$\eta_{i|jk} = \arg(\phi_{i|jk}) \quad \textit{and} \quad \delta_{i|jk} = |\phi_{i|jk}|. \quad (25)$$

Proof. Without loss of generality, we consider the case $(i, j, k) = (1, 2, 3)$.

(i) It is straightforward to derive the first expression of the conditional density (21) from the equation $t_{2|1}(u_1, u_2 | u_3; \boldsymbol{\rho}) = t(\boldsymbol{u}; \boldsymbol{\rho})/t_1(u_3)$, where $t(\boldsymbol{u}; \boldsymbol{\rho})$ is the trivariate density (5) and $t_1(u_3)$ is the density of U_3, namely, the circular uniform density (see Theorem 2(ii)). It follows from equation (2) of (9) that the second expression of the conditional density (22) has the same functional form apart from parametrization.

(ii) Theorem 2 implies that the density of $(U_1, U_2)'$ is given by (16) and the density of U_2 is the circular uniform density. Then it follows from the expression $t_{1|1}(u_1|u_2; \phi_{12}) = t_2(u_1, u_2; \phi_{12})/t_1(u_2)$ that the conditional density of U_1 given $U_2 = u_2$ is the wrapped Cauchy density (23).

(iii) Using the complex expression of the density (20), the conditional density of Z_1 given $(Z_2, Z_3)' = (z_2, z_3)'$ is of the form

$$tc_{1|2}(z_1|z_2, z_3) \propto \left| z_1 + \frac{\phi_2 z_2 + \phi_3 z_3}{\phi_1} \right|^{-2}, \quad z_1 \in \Omega.$$

Note that the density of the wrapped Cauchy distribution can be expressed as

$$f(z) = \frac{1}{2\pi} \frac{|1 - \delta^2|}{|z - \delta e^{\mathrm{i}\eta}|^2}, \quad z \in \Omega,$$

where $\eta \in [0, 2\pi)$ is the location parameter and $\delta \geq 0$ is the concentration parameter (see (24)). It follows that the conditional of Z_1 given $(Z_2, Z_3)' = (z_2, z_3)'$ is the wrapped Cauchy distribution with the location parameter $\arg(\phi_{1|23})$ and concentration parameter $|\phi_{1|23}|$, where $\phi_{1|23} = -\phi_1^{-1}(\phi_2 z_2 + \phi_3 z_3) = -\rho_{23}(\rho_{13}^{-1} e^{\mathrm{i}u_2} + \rho_{12}^{-1} e^{\mathrm{i}u_3})$.

$\square$

As this theorem shows, the univariate conditionals in Theorem 3(ii) and (iii) have the wrapped Cauchy distributions. Note that the univariate conditional given in Theorem 3(ii) does not follow the wrapped Cauchy in general if c_1 is not defined as in (6). The bivariate conditional in Theorem 3(i) has various tractable properties as discussed in (9).

The well-known form of the conditional distributions paves the way for regression purposes with one angular dependent variable and one or two angular regressors as well as two angular dependent variables and one angular regressor. Indeed, if we wish to predict one angular component based on two angular components, then from Theorem 3(iii) we find that the mean direction and circular variance of U_i given $(U_j, U_k)'$ are simply $\eta_{i|jk}$ and $1 - \delta_{i|jk}$, respectively. Similarly, if we wish to predict two angular components based on a third angular component, then from Theorem 3(i) we see that the toroidal mean and variance of $(U_i, U_j)'$ given U_k can be calculated in the same way as in Section 2.5 of (9). Note that circular-circular regression of, for example, U_i given U_j can also be obtained in a straightforward way from Theorem 3(ii). These properties are not explored here but we emphasize that they can be used in practice easily.

4.2. Random variate generation

The fact that all the marginal and conditional distributions belong to existing tractable families lays the foundations for random variate generation. Indeed, random variates from the proposed trivariate model TWCC($\boldsymbol{\rho}$) can be efficiently generated from uniform random variates on $(0,1)$.

Theorem 4. *The following algorithm generates random variates from the distribution TWCC($\boldsymbol{\rho}$).*

Step 1. Generate uniform $(0,1)$ *random variates* ω_1, ω_2 *and* ω_3*.*

Step 2. Compute

$$\begin{aligned} u_1 &= 2\pi\omega_1, \\ u_2 &= u_1 + \arg(\phi_{12}) + 2\arctan\left[\left(\frac{1-|\phi_{12}|}{1+|\phi_{12}|}\right)\tan\left\{\pi(\omega_2 - 0.5)\right\}\right], \\ u_3 &= \eta_{3|12} + 2\arctan\left[\left(\frac{1-\delta_{3|12}}{1+\delta_{3|12}}\right)\tan\left\{\pi(\omega_3 - 0.5)\right\}\right], \end{aligned}$$

where ϕ_{12} *is as in* (17) *and* $(\eta_{3|12}, \delta_{3|12})$ *are as in* (25)*.*

Step 3. Output $(u_1, u_2, u_3)'$ *as the random variate from the distribution TWCC($\boldsymbol{\rho}$).*

Proof. The trivariate density (5) can be decomposed as

$$t(\boldsymbol{u}; \boldsymbol{\rho}) = t_{1|2}(u_3|u_1, u_2; \eta_{3|12}, \delta_{3|12}) t_{1|1}(u_2|u_1; \phi_{12}) t_1(u_1).$$

Theorems 2 and 3 imply that $t_{1|2}(u_3|u_1, u_2; \eta_{3|12}, \delta_{3|12})$ is the wrapped Cauchy density (24), $t_{1|1}(u_2|u_1; \phi_{12})$ is also the wrapped Cauchy density (23), and $t_1(u_1)$ is the circular uniform density. This expression implies that the random variate generation from the proposed trivariate distribution (5) is equivalent to that from the circular uniform and wrapped Cauchy distributions.

It is straightforward to see that u_1 computed in Step 2 is a random variate from the circular uniform distribution. In order to generate random variates u_2 and u_3 from the conditional wrapped Cauchy distributions, we apply the following result: if a random variable U follows the circular uniform distribution on $(-\pi, \pi)$, then the random variable defined by

$$\Theta = \eta + 2\arctan\left\{\left(\frac{1-\delta}{1+\delta}\right)\tan\left(\frac{U}{2}\right)\right\}$$

has the wrapped Cauchy distribution (3) with location parameter $\eta \in [0, 2\pi)$ and concentration parameter $\delta \in \mathbb{R}^+ \backslash \{1\}$. See (24) and (9) for details. Using this result, it is straightforward to see that u_2 and u_3 computed in Step 2 are variates from the conditional wrapped Cauchy distributions with location parameters $u_1 + \arg(\phi_{12})$ and $\eta_{3|12}$ and concentration parameters $|\phi_{12}|$ and $\delta_{3|12}$, respectively. $\square$

We note the simplicity and efficiency of the algorithm in which a variate from the proposed distribution can be generated through a transformation of three uniform random variates without rejection.

4.3. Modality

In this section we investigate the modes of TWCC($\boldsymbol{\rho}$).

Theorem 5. *For $\rho_{ij} > 0$ and $\rho_{ik}, \rho_{jk} < 0$, the modes of the density TWCC($\boldsymbol{\rho}$) are given by*

$$\begin{array}{lll} (i) & u_i = u_j = u_k & \text{if } |\rho_{ij}| < |\rho_{ik}\rho_{jk}|/(|\rho_{ik}| + |\rho_{jk}|), \\ (ii) & u_i = u_j + \pi = u_k + \pi & \text{if } |\rho_{ik}| < |\rho_{ij}\rho_{jk}|/(|\rho_{ij}| + |\rho_{jk}|), \end{array} \tag{26}$$

and the antimodes of the density TWCC($\boldsymbol{\rho}$) are given by

$$u_i = u_j = u_k + \pi. \tag{27}$$

If $\rho_{ij}, \rho_{ik}, \rho_{jk} > 0$, then u_k in the modes (26) and antimodes (27) is replaced by $u_k + \pi$.

Proof. First we consider the case $\rho_{ij}, \rho_{ik}, \rho_{jk} > 0$. Without loss of generality, assume $(i, j, k) = (1, 2, 3)$. It is clear that the antimodes of the density (5) are $u_1 = u_2 = u_3$ because $\cos(u_i - u_j)$ $(1 \leq i < j \leq 3)$ is maximized at $u_i = u_j$. In order to derive the modes of the density (5), we first note that the density (5) can be expressed as

$$t(\boldsymbol{u}; \boldsymbol{\rho}) \propto \Big[c_1 + 2\rho_{12} \cos(u_1 - u_2) \\ + 2\{\rho_{13}^2 + \rho_{23}^2 + 2\rho_{13}\rho_{23} \cos(u_1 - u_2)\}^{1/2} \cos(u_3 - \tilde{\eta}_{3|12}) \Big]^{-1},$$

where $\tilde{\eta}_{3|12} = \arg\{\rho_{13} \cos u_1 + \rho_{23} \cos u_2 + \mathrm{i}(\rho_{13} \sin u_1 + \rho_{23} \sin u_2)\}$. It immediately follows from this expression that the density (5) is maximized at $u_3 = \tilde{\eta}_{3|12} + \pi$. Then the maximization of the density (5) reduces to the minimization of its functional part

$$B(x) = \rho_{12} x - \{\rho_{13}^2 + \rho_{23}^2 + 2\rho_{13}\rho_{23} x\}^{1/2},$$

where $x = \cos(u_1 - u_2) \in [-1, 1]$. The first derivative of this function is

$$\frac{d}{dx}B(x) = \rho_{12} - \rho_{13}\rho_{23}(\rho_{13}^2 + \rho_{23}^2 + 2\rho_{13}\rho_{23}x)^{-1/2}. \tag{28}$$

Now it is straightforward to see that this derivative can be upper bounded by $\rho_{12} - \rho_{13}\rho_{23}/(\rho_{13} + \rho_{23})$ (by replacing x with 1 in (28)), and that the derivative is thus negative if $\rho_{12} < \rho_{13}\rho_{23}/(\rho_{13} + \rho_{23})$, leading to a minimization of $B(x)$ at $x = 1$ if $\rho_{12} < \rho_{13}\rho_{23}/(\rho_{13} + \rho_{23})$. By using similar arguments, one can show that $B(x)$ is minimized at $x = -1$ if $\rho_{12} > \rho_{13}\rho_{23}/|\rho_{13} - \rho_{23}|$. It then follows that the modes of the density (5) are given at $u_1 = u_2$ for $\rho_{12} < \rho_{13}\rho_{23}/(\rho_{13} + \rho_{23})$ and at $u_1 = u_2 + \pi$ for $\rho_{12} > \rho_{13}\rho_{23}/|\rho_{13} - \rho_{23}|$. Finally, $u_3 = \tilde{\eta}_{3|12} + \pi$ implies that $u_3 = u_1 + \pi$ if $\rho_{12} < \rho_{13}\rho_{23}/(\rho_{13} + \rho_{23})$. If $\rho_{12} > \rho_{13}\rho_{23}/|\rho_{13} - \rho_{23}|$, then we have $u_3 = u_1$ for $\rho_{13} - \rho_{23} < 0$. Noticing that $\rho_{12} > \rho_{13}\rho_{23}/|\rho_{13} - \rho_{23}|$ and $\rho_{13} - \rho_{23} < 0$ imply $\rho_{13} < \rho_{12}\rho_{23}/(\rho_{12} + \rho_{23})$, we obtain the modes of the density (5) for the case $(i, j, k) = (1, 2, 3)$. If $\rho_{12} > \rho_{13}\rho_{23}/|\rho_{13} - \rho_{23}|$ and $\rho_{13} - \rho_{23} > 0$, the modes of the density (5) can be obtained by setting $(i, j, k) = (2, 1, 3)$ rather than $(i, j, k) = (1, 2, 3)$ due to the symmetry of the density (5) with respect to the permutation of (ρ_{ik}, ρ_{jk}).

The modes and antimodes of the density (5) for the case $\rho_{ij} > 0$ and $\rho_{ik}, \rho_{jk} < 0$ can be obtained in the same manner by noticing the straightforward equality $t(u_i, u_j, u_k; \rho_{ij}, \rho_{ik}, \rho_{jk}) = t(u_i, u_j, u_k + \pi; \rho_{ij}, -\rho_{ik}, -\rho_{jk})$. □

Since the conditions in (26) are the same as (8) in Theorem 1, one of them is always satisfied, which makes the result very strong as it shows that our trivariate copula has modes lying on a single line. Moreover, the modes of TWCC($\boldsymbol{\rho}$) have the most natural form in the case (i) of equation (26), and very simple forms in the other cases. This property simplifies working with mixtures.

4.4. Correlation coefficients

We consider three well-known correlation coefficients for bivariate circular data. Let $(U_i, U_j)'$ be a bivariate circular random vector and $X_k = (\cos U_k, \sin U_k)'$ $(k = i, j)$. Then the correlation coefficients of Johnson and Wehrly (25), Jupp and Mardia (26) and Fisher and Lee (27) are respectively defined by

$$\rho_{\mathrm{JW}} = \lambda^{1/2}, \quad \rho_{\mathrm{JM}} = \mathrm{tr}(\Sigma_{ii}^{-1}\Sigma_{ij}\Sigma_{jj}^{-1}\Sigma_{ij}'),$$

$$\rho_{\mathrm{FL}} = \frac{\det\{E(X_i X_j')\}}{[\det\{E(X_i X_i')\}\det\{E(X_j X_j')\}]^{1/2}},$$

where λ is the largest eigenvalue of $\Sigma_{ii}^{-1}\Sigma_{ij}\Sigma_{jj}^{-1}\Sigma_{ij}'$ and $\Sigma_{k\ell} = E(X_k X_\ell') - E(X_k)E(X_\ell)'$ $(k,\ell = i,j)$. The correlation coefficients of our bivariate marginal distributions are given in the following theorem.

Theorem 6. *Let a trivariate random vector $(U_1, U_2, U_3)'$ follow the model TWCC($\boldsymbol{\rho}$). Then, for any pair of random variables $(U_i, U_j)'$, the correlation coefficients of Johnson and Wehrly (25), Jupp and Mardia (26) and Fisher and Lee (27) are given by*

$$\rho_{\mathrm{JW}} = \gamma_{ij}, \quad \rho_{\mathrm{JM}} = 2\gamma_{ij}^2 \quad \textit{and} \quad \rho_{\mathrm{FL}} = \gamma_{ij}^2,$$

respectively, where $\gamma_{ij} = \min(|\phi_{ij}|, |\phi_{ij}|^{-1})$ and ϕ_{ij} is given in (17).

Proof. If follows from Theorem 2(i) that $(U_i, U_j)'$ has the density (16). This density is equivalent to a special case of the distribution of (9) with circular uniform marginals. Then the three correlation coefficients ρ_{JW}, ρ_{JM} and ρ_{FL} of our model can be immediately calculated from those of the distribution of (9) given in Section 2.6 of their paper. Note that $t_2(u_i; u_j; \phi_{ij}) = t_2(u_i; u_j; \phi_{ij}^{-1})$ in (16), and either form of the parameter, ϕ_{ij} or ϕ_{ij}^{-1}, should be used to obtain the same parameter range as the distribution of (9). $\square$

Note the simplicity of the expressions for all the three correlation coefficients. Further, these all depend on the parameter ϕ_{ij}, implying that it is a good measure of dependence of the model. Recall in this context the agreeable fact that ϕ_{ij} remains invariant under ρ_{ij} being replaced by $c\rho_{ij}$ for some constant c, hence does not depend on the identifiability condition on ρ_{ij}.

5. Parameter Estimation

In this section we consider maximum likelihood estimation, and method of moment estimation is discussed in Section S.4 of the Supplementary Material. Parameter estimation is described for model (5), whose marginal distributions are uniformly distributed. Further developments would be needed for fitting non-uniform marginals, which is a topic we do not deal with in this paper. Throughout this section, let $\{(u_{1m}, u_{2m}, u_{3m})'\}_{m=1}^n$ be a realization of a random sample $\{(U_{1m}, U_{2m}, U_{3m})'\}_{m=1}^n$ from the distribution TWCC($\boldsymbol{\rho}$).

For the original model (5), the likelihood function for $\{\boldsymbol{u}_m\}_{m=1}^n = \{(u_{1m}, u_{2m}, u_{3m})'\}_{m=1}^n$ is given by

$$\log L(\boldsymbol{\rho}) = \log \prod_{m=1}^{n} t(\boldsymbol{u}_m) = n \log c_2 - \sum_{m=1}^{n} \log F_m, \tag{29}$$

where $F_m = c_1 + 2\{\rho_{12}\cos(u_{1m}-u_{2m}) + \rho_{13}\cos(u_{1m}-u_{3m}) + \rho_{23}\cos(u_{2m}-u_{3m})\}$. Its score function is

$$\frac{\partial}{\partial \rho_{ij}} \log L(\boldsymbol{\rho}) = n \frac{\frac{\partial c_2}{\partial \rho_{ij}}}{c_2} - \sum_{m=1}^{n} \frac{\frac{\partial c_1}{\partial \rho_{ij}} + 2\cos(u_{im} - u_{jm})}{F_m}$$

where

$$\frac{\partial c_1}{\partial \rho_{ij}} = \frac{\rho_{ik}}{\rho_{jk}} + \frac{\rho_{jk}}{\rho_{ik}} - \frac{\rho_{jk}\rho_{ik}}{\rho_{ij}^2},$$
$$\frac{\partial c_2}{\partial \rho_{ij}} = \frac{1}{(2\pi)^3} \left\{ \rho_{ij} \left(\left(\frac{\rho_{ik}}{\rho_{jk}} \right)^2 + \left(\frac{\rho_{jk}}{\rho_{ik}} \right)^2 \right) - \frac{(\rho_{jk}\rho_{ik})^2}{\rho_{ij}^3} - 2\rho_{ij} \right\} \left((2\pi)^3 c_2\right)^{-1}.$$

The maximum likelihood estimates $\hat{\rho}_{12}, \hat{\rho}_{13}, \hat{\rho}_{23}$ are obtained by equating the score function to zero and numerically solving the system of three equations, see below. For the reader's convenience, we provide in Section S.5 in the Supplementary Material the associated expected Fisher information matrix.

Although the proposed density (5) has a simple and closed form, it is essential to keep the parameter constraints (8) and (9) in mind. The simplified constraint $|\rho_{ij}| + |\rho_{ik}| < |\rho_{ij}|^2|\rho_{ik}|^2$ can further be turned into

$$|\rho_{ij}| > \frac{1 + \{1 + 4|\rho_{ik}|^3\}^{1/2}}{2|\rho_{ik}|^2}$$

by solving an inequality of the second order. Using the expression

$$\zeta_{ij} = \frac{1 + \{1 + 4|\rho_{ik}|^3\}^{1/2}}{2|\rho_{ik}|^2} \frac{1}{\rho_{ij}}, \quad \zeta_{ij} \in (-1, 0) \cup (0, 1),$$

it is straightforward to see that the parameters of the model (5) can be expressed in terms of ρ_{ik} and ζ_{ij} alone (remember that this holds for one choice of i, j, k). The parameter space of this reparametrized model under the constraint $|\rho_{jk}| < |\rho_{ij}\rho_{ik}|/(|\rho_{ij}| + |\rho_{ik}|)$ and $\rho_{12}\rho_{13}\rho_{23} = 1$ is thus

$$\tilde{\Omega} = \{(\zeta_{ij}, \rho_{ik})\,;\, \zeta_{ij} \in (-1, 0) \cup (0, 1)\,, \rho_{ik} \in \mathbb{R} \setminus \{0\}\}.$$

For notational convenience, write $\log L(\rho_{12}, \rho_{13}, \rho_{23}) = \log L(\zeta_{ij}, \rho_{ik})$ if the log-likelihood function (29) is represented in terms of (ζ_{ij}, ρ_{ik}). Then maximum likelihood estimation for the proposed model can be carried out as follows:

Step 1. For (j, k) successively being equal to $(1, 2), (2, 3), (3, 1)$, obtain the following estimates

$$(\tilde{\zeta}_{ij}, \tilde{\rho}_{ik}) = \underset{(\zeta_{ij}, \rho_{ik}) \in \tilde{\Omega}}{\arg\max} \log L(\zeta_{ij}, \rho_{ik}).$$

Step 2. Among the three obtained maximized quantities, calculate

$$(\hat{\zeta}_{i^*j^*}, \hat{\rho}_{i^*k^*}) = \underset{(\tilde{\zeta}_{ij}, \tilde{\rho}_{ik})}{\arg\max} \log L(\tilde{\zeta}_{ij}, \tilde{\rho}_{ik}).$$

Step 3. Record the maximum likelihood estimate $(\hat{\rho}_{12}, \hat{\rho}_{13}, \hat{\rho}_{23})'$ as

$$\hat{\rho}_{i^*k^*} = \hat{\rho}_{i^*k^*}, \quad \hat{\rho}_{i^*j^*} = \frac{1 + \{1 + 4|\hat{\rho}_{i^*k^*}|^3\}^{1/2}}{2|\hat{\rho}_{i^*k^*}|^2} \frac{1}{\hat{\zeta}_{i^*j^*}}, \quad \hat{\rho}_{j^*k^*} = \frac{1}{\hat{\rho}_{i^*j^*} \hat{\rho}_{i^*k^*}},$$

where (i^*, j^*, k^*) is a permutation of $(1, 2, 3)$.

The algorithm is repeated with different initial values, to make sure that the global maximum is achieved. The initial values for the parameters ζ_{ij} and ρ_{ik} are uniformly chosen from the intervals they are allowed to take values in (where of course the infinite intervals for ρ_{ik} are limited to a large maximal value). The function for calculating the ML estimates was written in the programming language R, using the optimizer solnp from the library Rsolnp (28) and is available in the GitHub repository `https://github.com/Sophia-Loizidou/Trivariate-wrapped-Cauchy-copula`. The consistency of this approach is shown and its finite-sample performance is investigated by means of Monte Carlo simulations, which we provide in Section S.6 in the Supplementary Material.

6. An extension to the *d*-dimensional torus

It is natural albeit challenging to extend the model presented here to any d-dimensional torus. An adequate treatment requires the space of an entire paper. A potential model could be of the form

$$t(\boldsymbol{u}; \boldsymbol{\rho}) \propto \left\{ c_4 + 2 \sum_{1 \le i < j \le d} \rho_{ij} \cos(u_i - u_j) \right\}^{-1} \tag{30}$$

where $\boldsymbol{u} = (u_1, \ldots, u_d)'$, $\boldsymbol{\rho} \in \mathbb{R}^{d(d-1)/2}$ contains the parameters $\rho_{ij} \in \mathbb{R}$, which need to satisfy certain conditions and c_4 depends on them. To make this a valid density, it suffices that c_4 is greater than $2\sum_{1 \le i<j \le d} |\rho_{ij}|$, and we need to find the normalizing constant as well as, afterwards, conditions on the parameters in the style of (8). Note that the general form of (30) has been proposed in (29), Equation (106); no properties were investigated. One of the key properties of the model (30) and certain extensions thereof are given in the following theorem.

Theorem 7. *Let a $[0, 2\pi)^d$-valued random vector $(U_1, \ldots, U_d)'$ have the probability density function $t_d(\boldsymbol{u})$ for $\boldsymbol{u} = (u_1, \ldots, u_d)'$. Suppose that t_d is a function of $\{u_i - u_j\,;\, 1 \le i < j \le d\}$, namely,*

$$t_d(\boldsymbol{u}) = h(u_1 - u_2, u_1 - u_3, \ldots, u_{d-1} - u_d), \quad 0 \le u_1, \ldots, u_d < 2\pi.$$

Then the marginal distribution of U_i $(1 \le i \le d)$ has the uniform distribution on the circle.

Proof. Without loss of generality, we calculate the marginal distribution of U_d. The marginal density of U_d can be expressed as

$$f_{u_d}(u_d) = \int_{[0,2\pi)^{d-1}} h(u_1 - u_2, u_1 - u_3, \ldots, u_{d-1} - u_d) du_1 \cdots du_{d-1}. \qquad (31)$$

Putting $v_i = u_i - u_d$ $(i = 1, \ldots, d-1)$, it follows that $u_i - u_j = v_i - v_j$ for $j = 1, \ldots, d-1$ and therefore $\{u_i - u_j\,;\, 1 \le i < j \le d\}$ can be expressed using $d-1$ variables $v_1, \ldots, v_{d-1}$. Thus the marginal density (31) can be expressed as

$$f_{u_d}(u_d) = \int_{[0,2\pi)^{d-1}} h(v_1 - v_2, v_1 - v_3, \ldots, v_{d-1}) dv_1 \cdots dv_{d-1} = C.$$

Since $f_{u_d}(u_d)$ is a constant which does not depend on u_d, it follows that the marginal distribution of U_d is the uniform distribution on the circle. $\square$

This general result makes it appealing to work on the extension of TWCC to (30) in the future.

7. Discussion

In this paper we have proposed a new distribution on the three-dimensional torus, a trivariate wrapped Cauchy copula. The marginal and conditional distributions of the copula are known distributions and random variate generation is simple and efficient through a transformation of uniform random variates without rejection. We have explicit expressions for the locations of the modes of our distribution as well as for correlation coefficients, enhancing parameter interpretability. Parameter estimation can be performed via maximum likelihood estimation. In future work, besides the d-dimensional extension, we intend to explore choices of marginal distributions which will extend the domain of potential applicability of our new copula.

Code availability: The relevant code of the paper is available in `https://doi.org/10.5281/zenodo.15675162` as well as in `https://github.com/Sophia-Loizidou/Trivariate-wrapped-Cauchy-copula`.

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