RESEARCH ARTICLE

Cylcop: An R Package for Circular-Linear Copulae with Angular Symmetry

Florian H. Hodel[1] | **John R. Fieberg**[2]

[1]Department of Evolutionary Biology and Environmental Studies, University of Zurich, Zurich, Switzerland

[2]Department of Fisheries, Wildlife, and Conservation Biology, University of Minnesota, St. Paul, MN, USA

Correspondence
Florian H. Hodel, Department of Evolutionary Biology and Environmental Studies, University of Zurich, Zurich, Switzerland
Email: florian.hodel@yahoo.com

Funding information
None

ABSTRACT: The `cylcop` package extends the `copula` package to allow modeling of correlated circular-linear random variables using copulae that are symmetric in the circular dimension. We present and derive several new circular-linear copulae with this property and demonstrate how they can be implemented in the `cylcop` package to model animal movements in discrete time. The package contains methods for estimating copulae parameters, plotting probability density and cumulative distribution functions, and simulating data.

KEYWORDS
copula, circular-linear, R, correlation

1 | INTRODUCTION

Circular-linear data often arise when modeling outcomes with a directional component (e.g., pollutant concentrations with accompanying wind directions; García-Portugués et al., 2013). They are also common in the context of modeling animal movement as a time-series of discrete steps characterized by step lengths (distance between locations) and turn angles (change in direction from the previous step) (Hodel and Fieberg, 2021). Step lengths and turn angles are often correlated, with animals cycling between directed movements with long steps and turn angles near 0 when traveling and short steps with large turn angles when foraging. Movement data are also somewhat unique, in that the circular variable (turn angle) is frequently symmetric, meaning that an animal has no inherent preference to turn left or right. This correlation and symmetry can be captured using a copula, which is a probability distribution with uniform marginals on the interval [0,1]. In this paper, we will only focus on bivariate copulae, but our work can in principle be extended to higher dimensions. We derive several copulae that can be used to model symmetric circular-linear data and and present their implementation in a new `R`-package `cylcop` (R Core Team, 2019),

available on GitHub at `floo66/cylcop`. The `cylcop` package extends the methods available in the `copula`-package (Hofert et al., 2020; Jun Yan, 2007; Ivan Kojadinovic and Jun Yan, 2010; Marius Hofert and Martin Mächler, 2011; Hofert et al., 2018) and also builds on the `circular`-package (Agostinelli and Lund, 2017). We describe the derivation and implementation of new circular-linear copulae here and provide an introduction to circular-linear copulae and their application to movement data elsewhere (Hodel and Fieberg, 2021). Finally, we also provide an app that allows for interactive visualization and exploration of all copulae introduced in this paper which can be accessed at `https://cylcop.shinyapps.io/cylcop-graphs/`.

2 | INTRODUCTION TO COPULAE

A bivariate copula $C(u, v)$ is a cumulative distribution function (CDF) with uniform marginals and its domain restricted to the unit square, $(u, v) \in [0, 1]^2$. Using general properties of CDFs, we can therefore mathematically define a copula to be any function $C(u, v) : [0, 1]^2 \to [0, 1]$ that fulfills

1. $C(u, 0) = C(0, v) = 0, \quad \forall u, v \in [0, 1]$.
2. $C(u, 1) = u$ and $C(1, v) = v, \quad \forall u, v \in [0, 1]$.
3. $C(u, v)$ is 2-increasing.

2-increasing means that for any rectangle $[u, u'] \times [v, v']$ with $u, u', v, v' \in [0, 1]$, $(u \leq u')$ and $(v \leq v')$, the C-volume V_C (i.e. the probability of (U, V) taking a value from the subset of the unit square described by the rectangle) is non-negative

$$V_C([u, u'] \times [v, v']) = C(u', v') - C(u, v') - C(u', v) + C(u, v) \geq 0 . \tag{1}$$

In combination with the first property, i.e. a copula being a grounded function, this means that a copula is non-decreasing in both arguments.

For any two random variables, X and Y, with strictly increasing and continuous CDFs, $F_X(x) = P(X \leq x)$ and $F_Y(y) = P(Y \leq y)$, and their inverses, F_X^{-1} and F_Y^{-1} (defined as $F_X(F_X^{-1}(u)) = u$, and $F_Y(F_Y^{-1}(v)) = v, \quad \forall u, v \in [0, 1]$), we can find a joint CDF where the correlation structure is captured by the chosen copula. Let U and V be uniformly distributed random variables. Then, using the probability integral transform, we have

$$\begin{aligned} C(F_X(x), F_Y(y)) &= \Pr[U \leq F_X(x),\ V \leq F_Y(y)] \\ &= \Pr[F_X^{-1}(U) \leq F_X^{-1}(F_X(x)),\ F_Y^{-1}(V) \leq F_Y^{-1}(F_Y(y))] \\ &= \Pr(X \leq x,\ Y \leq y) \\ &= F_{X,Y}(x, y) . \end{aligned} \tag{2}$$

This is called Sklar's theorem (Sklar, 1959).

The probability density function (PDF), $f_{X,Y}(x, y)$, of that joint distribution is

$$\begin{aligned} f_{X,Y}(x, y) &= \frac{\partial^2}{\partial x \partial y} F_{X,Y}(x, y) \\ &= \frac{\partial^2}{\partial x \partial y} C(F_X(x), F_Y(y)) \\ &= \frac{\partial^2 C(u, v)}{\partial u \partial v} f_X(x) f_Y(y) \\ &= c(u, v) f_X(x) f_Y(y) \\ &= c(F_X(x), F_Y(y)) f_X(x) f_Y(y) \,, \end{aligned} \tag{3}$$

where we made the substitutions $F_X(x) = u$ and $F_Y(y) = v$, and $f_X(x)$ and $f_Y(y)$ denote the marginal PDFs of X and Y, respectively. $c(u, v)$ is the copula density, i.e. a PDF of a distribution with uniform marginals corresponding to the CDF $C(u, v)$. Hereafter, we will use "copula" to refer to $C(u, v)$ and "copula density" to refer to its derivative, $c(u, v) = \frac{\partial^2 C(u,v)}{\partial u \partial v}$.

Besides calculating PDFs and CDFs, we also need to be able to draw samples from joint distributions. This can be done by drawing first a sample from a copula, which can then be transformed via the probability integral transform using the inverses of the marginal CDFs to a sample from the joint distribution. A common approach to sample copulae uses their conditional distributions (Johnson, 2013)

$$\begin{aligned} C_u(v) &= \Pr[V \leq v \mid U = u] \\ &= \frac{\partial}{\partial u} C(u, v) \\ &= \int_0^v c(u, t)\, dt \,. \end{aligned} \tag{4}$$

We can now take 2 independent samples from a uniform distribution, u and z, make the transformation $v = C_u^{-1}(z)$, and thus obtain a sample (u, v) from the copula $C(u, v)$. Finally, we can generate a sample from a joint distribution of a pair of random variables with the correlation structure described by that copula via $(x, y) = (F_X^{-1}(u), F_Y^{-1}(v))$.

Since a copula is a grounded, 2-increasing function, we know that firstly, $C(u, v) \leq C(u, 1) = u$ and $C(u, v) \leq C(1, v) = v$ and secondly, $V_C([u, 1] \times [v, 1]) = 1 - u - v + C(u, v) \geq 0$ and $C(u, v) \geq 0$. From the first statement, we can derive the upper ($M(u, v)$) and from the second the lower ($W(u, v)$) bound of any copula

$$W(u, v) = \max(u + v - 1, 0) \leq C(u, v) \leq \min(u, v) = M(u, v) \,. \tag{5}$$

W and M are called the Fréchet–Hoeffding bounds (Fréchet, 1935; Hoeffding, 1940; Fréchet, 1951) and are themselves copulae (at least in the bivariate case). Not all copulae can describe any degree of correlation and attain both bounds. Finally, the product copula $\Pi(u, v) = uv$, corresponds to independent random variables. For every copula introduced in this paper, we will derive the CDF, PDF, conditional copula and Fréchet–Hoeffding bounds.

2.1 | Empirical Copula

With a sample of n independent and identically distributed (i.i.d.) bivariate observations (x_i, y_i) drawn from a joint distribution, we can calculate the empirical marginal CDFs

$$F_{X,n}(x) = \frac{1}{n+1}\sum_{i=1}^{n} I\left(X_i \leq x\right) \qquad F_{Y,n}(y) = \frac{1}{n+1}\sum_{i=1}^{n} I\left(Y_i \leq y\right) , \tag{6}$$

with I the indicator function. Transforming the observations (x_i, y_i) with the empirical marginal CDFs gives us the so-called pseudo-observations $(F_{X,n}(x_i), F_{Y,n}(y_i))$. Assuming continuous data, and hence a negligible probability for ties, the pseduo-observations are just the ranks (r_i and s_i) of the data divided by a normalization constant, $\left(\frac{r_i}{n+1}, \frac{s_i}{n+1}\right)$. Note that we divide by $n+1$ and not n to have all pseudo-observations inside the open unit square. Doing so helps avoid boundary effects and issues arising when calculating the density. The pseudo-observations can be seen as values drawn from some empirical copula, the CDF of which we can calculate as (Rüschendorf, 1976; Deheuvels, 1979; Genest and Favre, 2007):

$$C_n(u,v) = \frac{1}{n}\sum_{i=1}^{n} I\left(\frac{r_i}{n+1} \leq u,\ \frac{s_i}{n+1} \leq v\right) , \tag{7}$$

The empirical copula density is also easily accessible, but of less importance for the present work. When one of the random variables is circular, we can follow the same procedure, but we will need to define a reference point to determine the ranks of the circular variable. Throughout this paper, we will chose $-\pi$ as our reference.

2.2 | Copula Symmetry and Rotations

The survival function $\bar{F}_X(x)$ of a random variable X is defined as

$$\bar{F}_X(x) = 1 - F_X(x) = \Pr(X > x) , \tag{8}$$

and the joint survival function of two random variables X and Y can be written using de Morgan's laws as

$$\bar{F}_{X,Y}(x,y) = 1 - (F_X(x) + F_Y(y) - F_{X,Y}(x,y)) = \Pr(X > x, Y > y) . \tag{9}$$

Using $C(F_X(x), F_Y(y)) = C(1-\bar{F}_X(x), 1-\bar{F}_Y(y)) = F_{X,Y}(x,y)$, we can rewrite the above equation as

$$\begin{aligned} \bar{F}_{X,Y}(x,y) &= \bar{F}_X(x) + \bar{F}_Y(y) - 1 + C(1-\bar{F}_X(x), 1-\bar{F}_Y(y)) \\ &= \hat{C}(\bar{F}_X(x), \bar{F}_Y(y)) . \end{aligned} \tag{10}$$

$\hat{C}(u,v) = u + v - 1 + C(1-u, 1-v)$ is called the survival copula and is itself a copula Nelsen (2006).

If we reflect a copula density $c(u,v)$ with respect to the lines $u = 0.5$ and $v = 0.5$, we obtain the function $c_\pi = c(1-u, 1-v)$. This is commonly called "rotation" (by 180 degrees) in the copula community, e.g. in Hofert et al.

(2018), (hence the subscript π). The corresponding distribution function can be found by integrating

$$\begin{aligned} C_\pi(u,v) &= \iint c(1-x,1-y)\,dx\,dy \\ &= C(1-u,1-v) + (1-v)K_1 + K_2 \\ &= C(1-u,1-v) - 1 + v + u \end{aligned} \tag{11}$$

where we determined the integration constants $K_1 = -1$ and $K_2 = u$ from the boundary conditions $v = C_\pi(1,v)$ and $u = C_\pi(u,1)$. Note that this is the equation of the survival copula of C and thus, $C_\pi = \hat{C}$. I.e. we have shown that the survival copula can be obtained by rotating the copula density by 180 degrees. "Rotations" by 90 and 270 degrees also lead to valid copulae, which are denoted by $C_{0.5\pi} = v - C(1-u,v)$ and $C_{1.5\pi} = u - C(u,1-v)$. They correspond to orthogonal reflections of the copula density along the line $u = 0.5$ and $v = 0.5$, respectively.

A (continuous) random variable X is symmetric about a if its distribution fulfills

$$F_X(a+x) = P(X \le a+x) = P(X \ge a-x) = 1 - P(X \le a-x) = 1 - F_X(a-x) = \bar{F}_X(a-x) \quad \forall x \in \mathbb{R} \tag{12}$$

which means that $F_X(a+x) + F_X(a-x) = 1$. Hence, it must hold for the density function (if X admits a density) that $f_X(a+x) = f_X(a-x)$. A pair of random variables (X,Y) is marginally symmetric about a point (a,b) if X is symmetric about a and Y is symmetric about b. (X,Y) is furthermore radially symmetric about (a,b) iff

$$F_{X,Y}(a+x,b+y) = \bar{F}_{X,Y}(a-x,b-y) \quad \forall (x,y) \in \mathbb{R}^2 \tag{13}$$

which again means that it must hold for the density function that $f_{X,Y}(a+x,b+y) = f_{X,Y}(a-x,b-y)$. Radial symmetry implies marginal symmetry. From the statements about survival copulae and reflected copula densities made above, we can derive that a pair of random variables that is marginally symmetric is radially symmetric iff its copula density is radially symmetric about $(0.5,0.5)$, i.e.

$$\begin{aligned} C(u,v) &= u + v - 1 + C(1-u,1-v) = \hat{C}(u,v) = C_\pi(u,v) \\ c(u,v) &= c(1-u,1-v), \quad \forall u,v \in [0,1]. \end{aligned} \tag{14}$$

In the following sections, we will often require that pairs of random variables be symmetric in X for any value of Y. With a symmetric marginal distribution of X, this means that the copula must be symmetric in u about $u = 0.5$ and

$$\begin{aligned} C(u,v) &= v - C(1-u,v) = C_{0.5\pi} \\ c(u,v) &= c(1-u,v), \quad \forall u,v \in [0,1]. \end{aligned} \tag{15}$$

3 | CIRCULAR DISTRIBUTIONS AND THEIR IMPLEMENTATION

Let Θ be a continuous circular random variable with support on the unit circle, $\theta \in \mathbb{S}^1$. There are two ways to "unwrap" the density and distribution function. This seems like a minor point, but, in the authors' experience, it can lead to confusion. We will elucidate the issue using the von Mises distribution, one of the most commonly used distributions,

as an example. Functions giving e.g. the von Mises CDF behave differently in different program packages, and since the `cylcop` package makes heavy use of the `circular` package (Agostinelli and Lund, 2017), we will take a closer look at that particular implementation.

The von Mises PDF is usually defined as a function $f : \mathbb{R} \to \mathbb{R}$

$$f_\Theta(\theta \mid \mu, \kappa) = \frac{e^{\kappa \cos(\theta - \mu)}}{2\pi I_0(\kappa)} \tag{16}$$

with $\mu \in \mathbb{R}$, $\kappa \in \mathbb{R}^+$ and support $\text{supp}(f) = [c, 2\pi + c)$, $\forall c \in \mathbb{R}$. This PDF fulfills the boundary condition

$$f_\Theta(\theta = c) = \lim_{t \to 2\pi} f_\Theta(\theta = c + t)\,, \tag{17}$$

and the corresponding CDF is

$$F_\Theta(\theta) = \int_{-\infty}^{\theta} f_\Theta(\omega)\, d\omega. \tag{18}$$

The von Mises PDF and CDF are implemented this way, e.g. in Wolfram Mathematica (Wolfram Research, 2020) (see Figure 1).

Alternatively, we can allow the angle to assume any real value, $\theta \in \mathbb{R}$, and have a PDF with support on the entire real line (which is done e.g. in Mardia and Jupp (2000)). To distinguish it from the "restricted" von Mises density above, we will call it $g_\Theta(\theta \mid \mu, \kappa)$, the only difference to $f_\Theta(\theta \mid \mu, \kappa)$ being that $\text{supp}(g) = \mathbb{R}$, which leads to a periodic PDF with

$$g_\Theta(\theta) = g_\Theta(\theta + 2\pi k) \quad \forall k \in \mathbb{Z} \tag{19}$$

and $g_\Theta(\theta)$ integrating to one over any interval of length 2π. To actually calculate the periodic CDF,

$$G_\Theta(\theta \mid l) = \int_{l}^{\text{mod}(\theta - l, 2\pi) + l} g_\Theta(\omega)\, d\omega \tag{20}$$

we must choose a lower limit of integration l. $g(\theta)$ and $G(\theta \mid l)$ correspond to the functions `pvonmises()` and `dvonmises()`, in the `circular`-package (Agostinelli and Lund, 2017) (see Figure 2).

In summary, we can either allow a circular random variable to have the entire real line as support, which leads to periodic density and distribution functions (which is done e.g. in Mardia and Jupp (2000) and is implemented in the `circular` package), or we restrict the support to an interval of 2π, and have densities that need to fulfill the boundary condition in equation 17. The two approaches of "unwrapping" a circular random variable are of course equivalent. In the context of copulae and turning angles, it is however more natural to think of Θ as being restricted to the interval $[-\pi, \pi)$.

3.1 | Fitting Circular Distributions

We have implemented a function to fit parameters of certain circular distributions to a set of angles in $[-\pi, \pi)$ using a maximum likelihood approach.

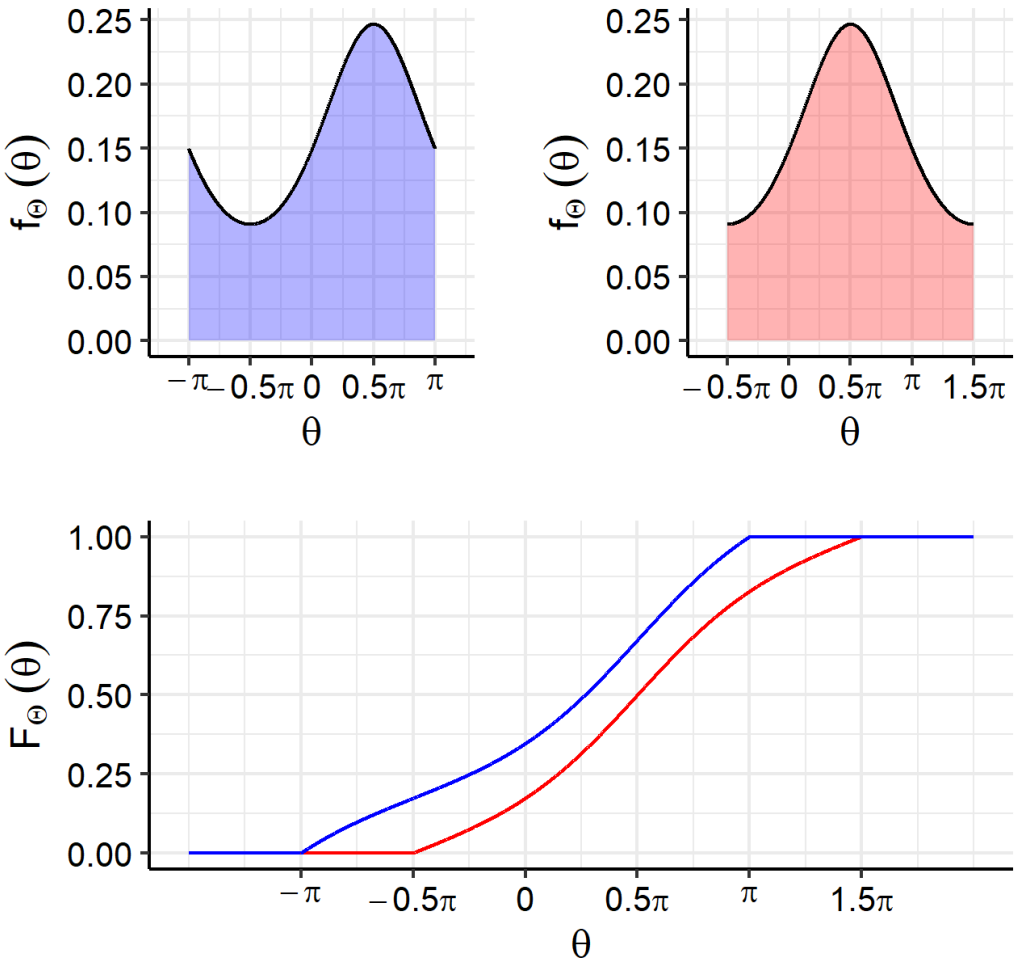

FIGURE 1 Top: PDF of a von Mises distribution with $\mu = 0.5\pi$ and $\kappa = 0.5$. Left: $c = -\pi$, right: $c = -0.5\pi$. Bottom: The corresponding CDFs.

```
fit_angle(theta,
          parametric = c("vonmises", "wrappedcauchy", "mixedvonmises", FALSE),
          bandwidth = NULL,
          mu = NULL)
```

The maximum likelihood estimates with von Mises and wrapped Cauchy distributions or non-parametric kernel density estimates (`parametric=FALSE`) utilize the corresponding functions of the `circular`-package (Agostinelli and Lund, 2017). Our work was motivated by a need to fit circular distributions to animal movement data that exhibited peaks around two different directions (Hodel and Fieberg, 2021). Therefore, we also provide the possibility to perform maximum likelihood estimation for a mixture of two von Mises distributions. The implementation for these mixtures

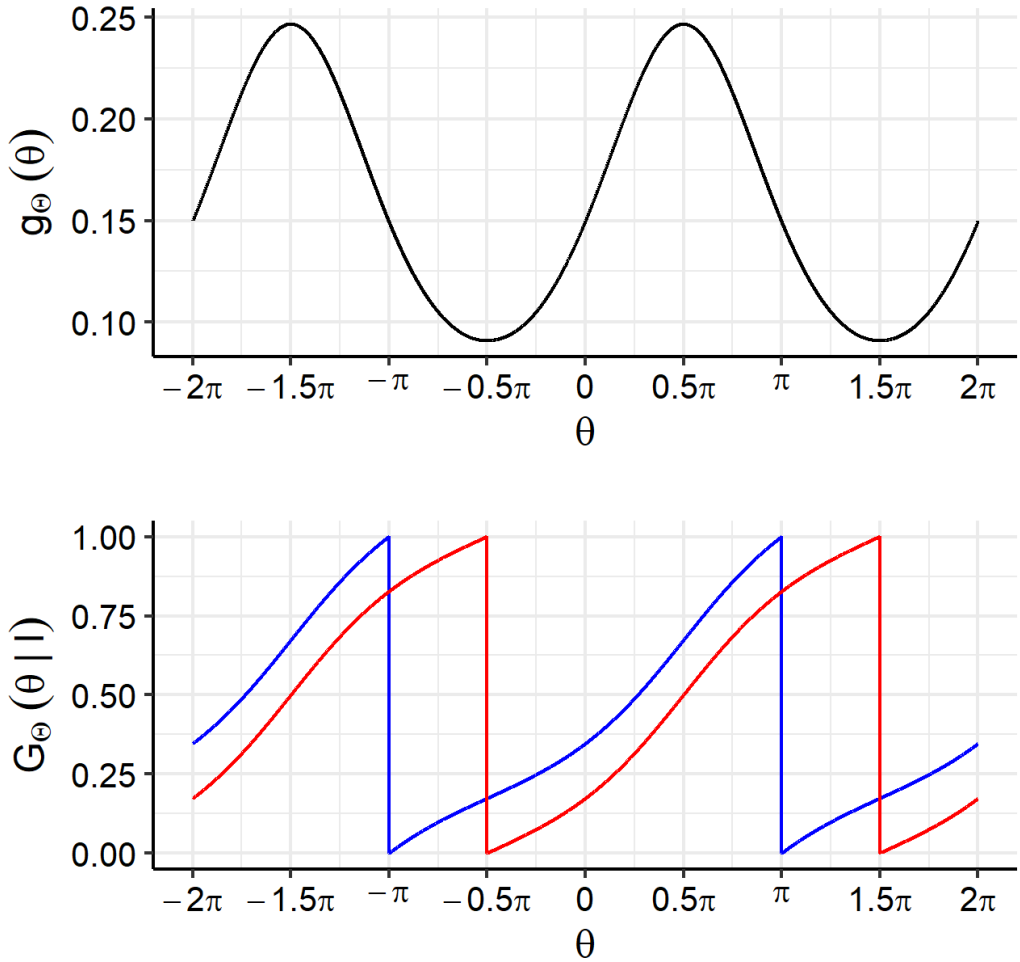

FIGURE 2 Top: PDF of a von Mises distribution with $\mu = 0.5\pi$ and $\kappa = 0.5$. Bottom: The corresponding CDFs. Blue: $l = -\pi$, red: $l = -0.5\pi$.

is derived from the expectation-maximization algorithm of the `movMF`-package (Hornik and Grün, 2014) but with the added ability of fixing and not optimizing the two location parameters (using the `mu` argument to the `fit_angle` function). Fixing the location parameters allows us to accommodate *a priori* assumptions specific to animal movement data (e.g., that there is no inherent bias for an animal to turn left or right). A similar function (`fit_steplength()`) is also available for linear random variables and a variety of common linear distributions.

The quantiles and CDF of the wrapped Cauchy distribution and the quantiles of the mixed von Mises distribution cannot be found analytically, and they are also not part of the `circular`-package (Agostinelli and Lund, 2017). Therefore, we implemented them numerically based on the wrapped G distribution of the `wrapped`-package (Nadarajah and Zhang, 2017) and spline interpolation, respectively (see appendix, section A1). Finally, we also provide PDF, CDF,

random number generation and quantiles for kernel density estimates with the functions

```
rdens(n, density), ddens(x, density), pdens(x, density), qdens(p, density)
```

These functions all take as input a list containing information about the kernel density estimate, i.e. the output of

```
density <- fit_angle(theta, parametric = FALSE)
```

and similar for `fit_steplength()`.

4 | CIRCULAR-LINEAR COPULAE

In the following sections, we will introduce copulae that can be used to model bivariate distributions of circular-linear pairs of random variables, (Θ, X). Such copulae have as their domain not the unit square, but the surface of a cylinder of unit height and unit circumference (hence the name of the package, "cylcop"). This means that they must fulfill a boundary condition analogous to equation 17

$$c(u = 0, v) = c(u = 1, v), \quad \forall v \in [0, 1], \tag{21}$$

where we assumed that u is the dimension of the copula that will be transformed to the circular variable Θ. Since we are concerned with modelling movement data (i.e. joint turn angle and step length distributions), and animals usually do not have an inherent bias to turn left or right, we will focus on turn angle distributions that are symmetric around $\theta = 0$. From section 2.2, we know that this means that the copulae must not only fulfill equation 21, but must also be symmetric in u around $u = 0.5$ (equation 15)

With the `cylcop` package being an extension of the `copula` package (Hofert et al., 2020; Jun Yan, 2007; Ivan Kojadinovic and Jun Yan, 2010; Marius Hofert and Martin Mächler, 2011), we follow their framework and implement the copulae we introduced above as "S4"-classes. For each of them, there are methods to calculate the PDF (`dCopula()`), CDF (`pCopula()`) and (inverse of) the conditional distribution (`cCopula()`), as well as to generate random samples (`rCopula()`).

4.1 | von Mises copula

Johnson and Wehrly (Johnson and Wehrly, 1978) present in section 3 of their paper an approach to obtain a circular-linear PDF with given marginal densities:

$$\begin{aligned} f_{\Theta,X}(\theta, x) &= 2\pi g(2\pi[F_\Theta(\theta) - F_X(x)])f_\Theta(\theta)f_X(x) \\ \theta &\in [-\pi, \pi),\ x \in \mathbb{R}, \end{aligned} \tag{22}$$

where g is some density on the circle. Even though it is not mentioned in that work, a comparison of equations 22 and 3 reveals that $2\pi g(2\pi[u - v]) = c(u, v)$ must be a copula density. This has been recognized by many researchers, see e.g. García-Portugués et al. (2013), who chose as function g the von Mises density and applied this concept to the joint modelling of wind direction and concentration of SO_2. We implement this copula as `cyl_vonmises()` in our `cylcop`-package. In appendix, section A2.1, we demonstrate some properties of the PDF of this circular-linear copula.

Next, we will derive the CDF of the von Mises copula and describe its implementation in the `cylcop` package. We will assume the von Mises density g to have as support the entire real line (see equation 19), a mean μ_0, and a concentration κ_0. Substituting $q = 2\pi t$ and $dt = \frac{dq}{2\pi}$ (in line 4, below), we can integrate the copula density

$$
\begin{aligned}
C(u,v) &= \int_0^u \int_0^v c(s,t)\ dtds \\
&= 2\pi \int_0^u \int_0^v g(2\pi[s-t]\ \mid \mu = \mu_0,\ \kappa = \kappa_0)\ dtds \\
&= 2\pi \int_0^u \int_0^v g(2\pi t\ \mid \mu = 2\pi s - \mu_0,\ \kappa = \kappa_0)\ dtds \\
&= \int_0^u \int_0^{2\pi v} g(q\ \mid \mu = 2\pi s - \mu_0,\ \kappa = \kappa_0)\ dqds \\
&= \int_0^u G(2\pi v\ \mid \mu = 2\pi s - \mu_0,\ \kappa = \kappa_0,\ l = 0)\ ds\,.
\end{aligned}
\tag{23}
$$

Going from the second to the third line, we used the symmetry properties of g, which can be seen in Figure 2. The innermost integral in the fourth line is just the von Mises CDF $G(2\pi v\ \mid\ l = 0)$ with a lower limit of integration $l = 0$ (see equation 20). Since there is no analytic solution, the final integral would have to be solved numerically. As mentioned in section 3, the `cylcop` package implements the von Mises CDF as a periodic function (i.e. following equation 20), and we could implement `pCopula(cyl_vonmises(mu=mu_0, kappa=kappa_0))` by numerically integrating from $u = 0$ to $u = a$ the function

```
circular::pvonmises(q = (2 - .Machine$double.eps) * pi * b,
                    mu = 2 * pi * u - mu_0,
                    kappa = kappa_0,
                    from = 0)
```

Since G is periodic on the half-open interval $[0, 2\pi)$, we multiply not with 2, but a number very close to 2. While this approach is illustrative, it is, however, computationally very slow. Therefore, the actual implementation of the CDF of the von Mises copula in the `cylop` package approximates the double integral in equation 23 with truncated infinite sums of Bessel functions. The function g can be expressed as an infinite series of Bessel functions I_j of increasing order j

$$
g(\omega \mid \mu, \kappa) = \frac{1}{2\pi}\left(1 + \frac{2}{I_0(\kappa)} \sum_{j=1}^{\infty} I_j(\kappa) \cos[j(\omega - \mu)]\right) \tag{24}
$$

From this, we can arrive at the following expression for the bivariate CDF (the derivation can be found in the appendix, section A2.2)

$$
C(u,v) = uv + \frac{1}{2\pi^2 I_0(\kappa)} \sum_{j=1}^{\infty} I_j(\kappa) \left(\frac{\cos[j(2\pi u - 2\pi v - \mu)] - \cos[j(2\pi u - \mu)]}{j^2} + \frac{-\cos[j(-2\pi v - \mu)] + \cos[-j\mu]}{j^2} \right) \tag{25}
$$

With density and distribution functions given above, what remains is the conditional distribution, which can be

derived following equation 23 as

$$
\begin{aligned}
C(v|u) = C_u(v) = \frac{\partial}{\partial u} C(u,v) &= \int_0^v c(u,t)\, dt \\
&= 2\pi \int_0^v g(2\pi(u-t) \mid \mu = \mu_0, \kappa = \kappa_0)\, dt \\
&= G(2\pi v \mid \mu = 2\pi u - \mu_0, \kappa = \kappa_0, l = 0)
\end{aligned}
\tag{26}
$$

Its inverse (which we need for the generation of copula samples) is implemented as

```
1 / (2 * pi) * circular::qvonmises(p = v,
                                   mu = 2 * pi * u - mu_0,
                                   kappa = kappa_0,
                                   from = 0)
```

4.1.1 | Usage and Properties

The von Mises copula (Figure 3) can be instantiated with

```
cylcop::cyl_vonmises(mu = 0, kappa = 1, flip = FALSE)
```

The parameter `mu` shifts the PDF in the v-direction, `kappa` determines the concentration and `flip` indicates whether the copula should represent positive (`flip=FALSE`) or negative (`flip=TRUE`) correlation. With `kappa=0`, we have the independece copula Π. With `kappa=Inf` and `flip=FALSE`, or `flip=TRUE`, we get the upper (M), or lower (W) Fréchet–Hoeffding bound, respectively. While the `cyl_vonmises()` copula is indeed a circular linear copula, and hence periodic, it is not symmetric, which limits its usefulness for the modelling of movement data. The copulae introduced in the following sections, on the other hand, have densities that are both periodic and symmetric in u.

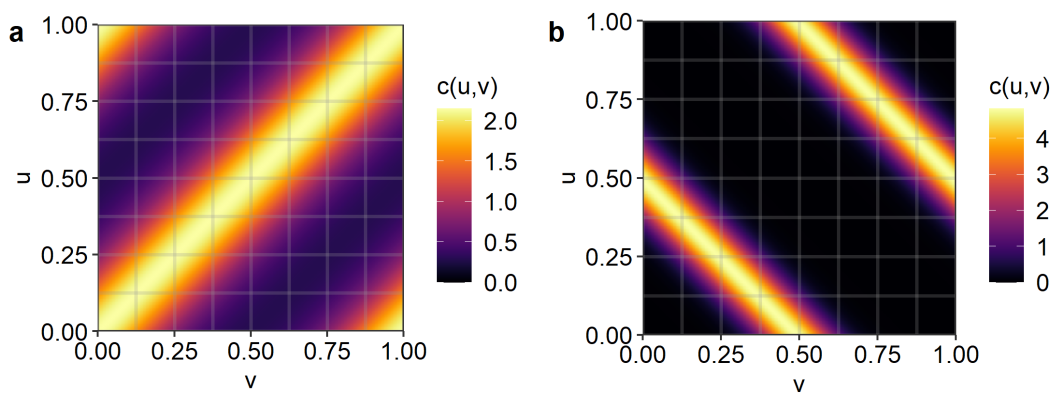

FIGURE 3 PDFs of `cyl_vonmises` copulae. Left: `mu=0,kappa=1`, right: `mu=pi,kappa=4,flip = T`.

4.2 | Copulae with Specific Sections

The sections in v of a copula $C(u,v)$ are defined as a set of functions, $C(u_0,v)$, from $[0,1]$ to $[0,u_0]$: $\{v \mapsto C(u_0,v) \mid u_0 \in [0,1]\}$. Note that the upper bound of the range is u_0 because $C(u_0,1) = u_0$. The section in v at u_0, $C(u_0,v)$, is the curve of intersection of the copula surface with the plane defined by $u = u_0$, which is parallel to the v-axis. Furthermore, it is also proportional to the conditional distribution function $C(u_0,v) = u_0 \Pr[V \leq v \mid U \leq u_0]$ (Nelsen et al., 1997). Below, we show that specific copulae with quadratic or cubic sections in the linear direction v have periodic and symmetric densities in the circular direction u.

4.2.1 | Quadratic Sections

Following section 3.2.5 in Nelsen (2006), we note that copulae with quadratic secitons in v must be of the form

$$C(u,v) = \alpha(u)v^2 + \beta(u)v + \gamma(u)\,. \tag{27}$$

Since $C(u,0) = 0 = \gamma(u)$ and $C(u,1) = u = \alpha(u) + \beta(u)$, we can define $\psi(u) = -\alpha(u) = \beta(u) - u$ to obtain

$$C(u,v) = uv + \psi(u)v(1-v)\,. \tag{28}$$

Due to the constraints that $C(0,v) = 0$ and $C(1,v) = v$, it is necessary that $\psi(0) = \psi(1) = 0$. Additionally, ψ must be chosen so that C is 2-increasing. In Corrolary 3.2.5, Nelsen (2006) states 3 necessary and sufficient conditions for this to be the case. We will now add a fourth one to make $c(u,v)$, the copula density, periodic in u:

1. $\psi(u)$ is absolutely continuous on $[0,1]$.
2. $|\psi'(u)| \leq 1$ almost everywhere on $[0,1]$.
3. $|\psi(u)| \leq \min(u, 1-u) \quad \forall u \in [0,1]$.
4. $\psi'(u)$ must be periodic on $[0,1]$.

The fourth condition is easily derived:

$$\begin{aligned} c(u,v) &= \frac{\partial^2}{\partial u \partial v} C(u,v) \\ &= \frac{\partial^2}{\partial u \partial v}\left[uv + \psi(u)(v - v^2)\right] \\ &= 1 + \psi'(u)(1-2v)\,. \end{aligned} \tag{29}$$

Since $\psi'(u)$ is the only term containing u, requiring $c(u,v)$ to be periodic in u means that $\psi'(u)$ must be also periodic on $[0,1]$. We will therefore choose

$$\begin{aligned} \psi(u) &= a\sin(2\pi u) \\ \psi'(u) &= a\,2\pi\cos(2\pi u)\,. \end{aligned} \tag{30}$$

This function clearly satisfies $\psi(0) = \psi(1) = 0$ and fulfills property 1. It also satisfies properties 2 and 3 but only for certain values of a, $-1/2\pi \leq a \leq 1/2\pi$ (see appendix, section A3). Finally, note that $c(u, v)$ is not only periodic in u on $[0, 1]$, but also symmetric:

$$\begin{aligned} c(u, v) &= 1 + a2\pi \cos(2\pi u)(1 - 2v) \\ &= 1 + a2\pi \cos(2\pi - 2\pi u])(1 - 2v) \\ &= c(1 - u, v) \end{aligned} \tag{31}$$

What remains to derive is the conditional distribution:

$$\begin{aligned} C(v|u) = C_u(v) &= \frac{\partial}{\partial u} C(u, v) = \frac{\partial}{\partial u}[]uv + \psi(u)(v - v^2)] \\ &= v + \psi'(u)(v - v^2) = v + a2\pi \cos(2\pi u)(v - v^2)\,. \end{aligned} \tag{32}$$

The inverse, which we need to generate random samples from the copula, is

$$C_u^{-1}(v) = \frac{\psi'(u) + 1 - \sqrt{(\psi'(u) + 1)^2 - 4\psi'(u)v}}{2\psi'(u)}\,, \tag{33}$$

since

$$\begin{aligned} C_u^{-1}(C_u(v)) &= \frac{\psi'(u) + 1 - \sqrt{\psi'^2(u) + 1 + 2\psi'(u) - 4\psi'(u)v - 4\psi'^2(u)v + 4\psi'^2(u)v^2}}{2\psi'(u)} \\ &= \frac{\psi'(u) + 1 - \sqrt{(\psi'(u) + 1 - 2\psi'(u)v)^2}}{2\psi'(u)} = v\,. \end{aligned} \tag{34}$$

In summary, our circular-linear copulae with quadratic sections have the following properties:

$$C(u, v) = uv + a \sin(2\pi u)v(1 - v) \tag{35}$$

$$c(u, v) = 1 + a2\pi \cos(2\pi u)(1 - 2v) \tag{36}$$

$$C_u(v) = v + a2\pi \cos(2\pi u)(v - v^2) \tag{37}$$

$$a \in [-\frac{1}{2\pi}, \frac{1}{2\pi}] \tag{38}$$

4.2.2 | Cubic Sections

Following an analogous path of reasoning about boundary conditions as in the quadratic case and according to equation 3.2.13 in Nelsen (2006), a copula with cubic sections must be of the form

$$C(u, v) = uv + v(1 - v)[\alpha(u)(1 - v) + \beta(u)v]\,, \tag{39}$$

where $\alpha(0) = \alpha(1) = \beta(0) = \beta(1) = 0$. We will show now that with

$$\alpha(u) = a\sin(2\pi u) \tag{40}$$

$$\beta(u) = -b\sin(2\pi u) \tag{41}$$

and certain values of a and b, C fulfills all requirements of a circular-linear copula with periodic density.

First, it is immediately clear that $\alpha(0) = \alpha(1) = \beta(0) = \beta(1) = 0$ holds for any values of a and b. Next, we need to show that our choice of α and β leads to a 2-increasing function C. To this end, we use theorem 3.2.8 in Nelsen (2006), which states that $\alpha(u)$ and $\beta(u)$ must both be absolutely continuous, which is clearly satisfied. Furthermore, it is also necessary that the following set be non-empty for almost all $u \in [0,1]$

$$\begin{aligned}&\{(a,b) \in \mathbb{R}\times\mathbb{R} \mid (-1 \le \alpha'(u) \le 2) \wedge (-2 \le \beta'(u) \le 1)\}\\ &\cup \{(a,b) \in \mathbb{R}\times\mathbb{R} \mid [\alpha'(u)]^2 - \alpha'(u)\beta'(u) + [\beta'(u)]^2 - 3\alpha'(u) + 3\beta'(u) \le 0\}\,.\end{aligned} \tag{42}$$

The parameter values in the first set of the union are the ones that fulfill

$$\begin{gathered}\Big(-1 \le a2\pi\cos(2\pi u) \le 2\Big) \wedge \Big(-2 \le b2\pi\cos(2\pi u) \le 1\Big)\\ \Big(-\frac{1}{2\pi} \le a \le \frac{1}{2\pi}\Big) \wedge \Big(-\frac{1}{2\pi} \le b \le \frac{1}{2\pi}\Big)\end{gathered} \tag{43}$$

The second set of the union is somewhat more difficult to derive:

$$\begin{aligned}&[a2\pi\cos(2\pi u)]^2 - [a2\pi\cos(2\pi u)][-b2\pi\cos(2\pi u)] + [-b2\pi\cos(2\pi u)]^2\\ &\quad - 3[a2\pi\cos(2\pi u)] + 3[-b2\pi\cos(2\pi u)]\\ &= (a^2 + ab + b^2)[2\pi\cos(2\pi u)]^2 - 3(a+b)[2\pi\cos(2\pi u)]\\ &\le 0\end{aligned} \tag{44}$$

For given values of a and b, the difference is largest, when $u = 0.5$ and $[2\pi\cos(2\pi 0.5)] = -2\pi$, or when $u = 1$ and $[2\pi\cos(2\pi)] = 2\pi$. Focusing on the first case:

$$\begin{gathered}(a^2 + ab + b^2)4\pi^2 + 3(a+b)2\pi \le 0\\ (a+b) - \frac{ab}{a+b} \le -\frac{3}{2\pi}\,.\end{gathered} \tag{45}$$

The first equation is a quadratic form and describes a closed set bounded by an ellipse. It is easy but tedious to show that its center point is at $(a = -1/(2\pi),\ b = -1/(2\pi))$, the angle between its minor axis and the "a-axis" is 0.25π and the distance between the center and the focal points is $1/\pi$. The length of the semi-minor axis is $\sqrt{0.5}/\pi$. The second case ($u = 1$) leads to

$$(a^2 + ab + b^2)4\pi^2 - 3(a+b)2\pi \le 0\,, \tag{46}$$

an ellipse that has its center point at $(a = 1/(2\pi), b = 1/(2\pi))$. The angle between its minor axis and the "a-axis" is

0.25π, the distance between the center and the focal points is $1/\pi$, and the length of the semi-minor axis is $\sqrt{0.5}/\pi$. From the lengths and directions of their semi-minor axes and their center poisitions, it is clear that the two ellipses only touch at one point $(a = 0, b = 0)$. Finally, the set of admissible parameter values is the union between the closed set bounded by the square described in equation 43 and this set containing only $(a = 0, b = 0)$, which is a subset of the first one (see appendix, figure A1). What remains to show is that $c(u, v)$ is periodic (and symmetric) in u.

$$\begin{aligned} c(u,v) &= \frac{\partial^2}{\partial u \partial v} C(u,v) \\ &= \frac{\partial^2}{\partial u \partial v}\Big((uv + v(1-v)[\alpha(u)(1-v) + \beta(u)v]\Big) \\ &= \frac{\partial}{\partial v}\Big((v + v(1-v)[\alpha'(u)(1-v) + \beta'(u)v]\Big) = \frac{\partial}{\partial v} C_u(v) \\ &= 1 + \alpha'(u)(1 - 4v + 3v^2) + \beta'(u)(2v - 3v^2) \end{aligned} \tag{47}$$

Since for $\alpha'(u) = a2\pi\cos(2\pi u)$ and $\beta'(u) = b2\pi\cos(2\pi u)$ it holds that $\alpha'(u) = \alpha'(1-u)$ and $\beta'(u) = \beta'(1-u)$, the copula density is not only periodic in u, $c(0, v) = c(1, v)$, but also symmetric, $c(u, v) = c(1-u, v)$. The inverse of the conditional distribution (line 3 of the equation above) is implemented analytically in the `cylcop` package. The resulting expression is however very unwieldy and is therefore omitted here.

4.2.3 | Usage and Properties

Quadratic and cubic sections copulae (Figure 4) can be generated using

```
cylcop::cyl_quadsec(a = 1/(2 * pi))
cylcop::cyl_cubsec(a = 1/(2 * pi), b = 1/(2 * pi))
```

The parameters `a` and `b` can take values from $[-1/(2\pi), 1/(2\pi)]$ (see equation 43) and with `a=0` (and `b=0`) we obtain the independece copula Π. The Fréchet–Hoeffding bounds can, however, not be attained. With `a` > 0 (and `b` < 0) the copula captures positive correlation between u and v for $u \in [0, 0.5]$ and negative correlation for $u \in [0.5, 1]$. The opposite is true for `a` < 0 (and `b` > 0).

4.3 | Combinations of Copulae

4.3.1 | Rotated Copulae

We have seen in section 2.2 that orthogonal reflections or "rotations" of copula densities are themselves copula densities. Furthermore, any convex linear combination of copulae is a copula (Nelsen, 2006). We will now show that taking the arithmetic mean between any linear-linear copula $C(u, v)$ and its orthogonal reflection along the line u=0.5, $C_{0.5\pi}$, produces a circular-linear copula

$$\begin{aligned} C_{\text{cyl}}(u,v) &= 0.5[C(u,v) + v - C(1-u,v)]\,, \\ c_{\text{cyl}}(u,v) &= 0.5[c(u,v) + c(1-u,v)]\,. \end{aligned} \tag{48}$$

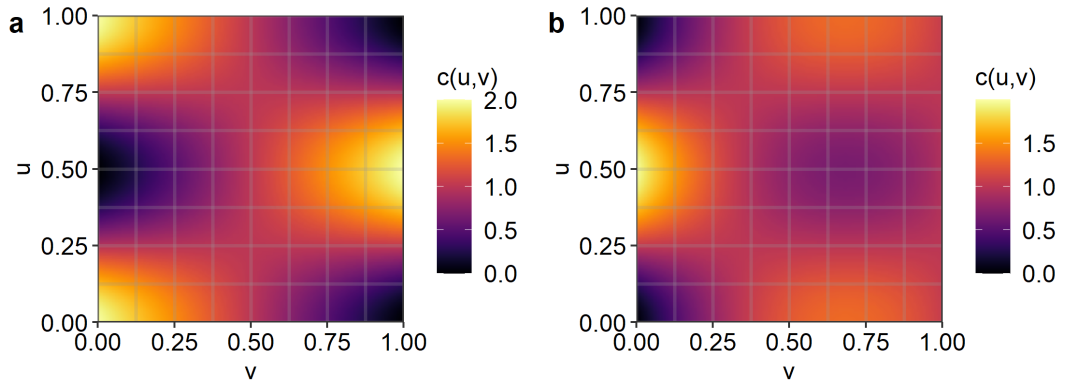

FIGURE 4 PDFs of copulae with specific sections in v. Left: `cyl_quadsec(a=1/(2*pi))`, right: `cyl_cubsec(a=-1/(2*pi),b=0.01)`.

This copula density is not only periodic, but also symmetric in u:

$$\begin{aligned} c_{\text{cyl}}(u,v) &= 0.5[c(u,v) + c(1-u,v)] \\ &= c_{\text{cyl}}(1-u,v)\,. \end{aligned} \tag{49}$$

We can also "periodically shift" the density by 0.5 in u-direction, i.e. $c_{\text{cyl}}((u+0.5) \mod 1, v)$ or

$$c_{\text{cyl,shift}}(u,v) = \begin{cases} c_{\text{cyl}}(u+0.5,v) = 0.5[c(u+0.5,v) + c(0.5-u,v)] & \text{if } u < 0.5 \\ c_{\text{cyl}}(u-0.5,v) = 0.5[c(u-0.5,v) + c(1.5-u,v)] & \text{if } u \geq 0.5 \end{cases} \tag{50}$$

It can be shown with simple geometric arguments that the distribution of such a shifted copula is

$$C_{\text{cyl,shift}}(u,v) = \begin{cases} C_{\text{cyl}}(u+0.5,v) - C_{\text{cyl}}(0.5,v) & \text{if } u < 0.5 \\ C_{\text{cyl}}(u-0.5,v) + v - C_{\text{cyl}}(0.5,v) & \text{if } u \geq 0.5 \end{cases} \tag{51}$$

That this is indeed a copula can be easily proven and $C_{\text{cyl,shift}}$ is in fact a special case of a shuffle of C_{cyl} see, e.g. section 3.2.3 of Nelsen (2006) or section 3.6 of Durante and Sempi (2015).

4.3.2 | Rectangular Patchworks of Copulae

Another method of constructing copulae is from rectangular patchworks (Durante et al., 2009). The unit square, i.e. the domain of the copula, is divided into rectangular regions R_i that can only potentially share points at their boundaries. For points (u,v) outside those rectangles, the copula $C(u,v)$ is equal to some copula $C_{\text{bg}}(u,v)$ ("bg" for background). For points that are an element of rectangle R_i, the copula is equivalent to a 2-increasing function $F_i(u,v) : R_i \to [0,1]$ obtained by some transformation of a copula $C_i(u,v)$ so that $F_i = C_{\text{bg}}$ at the boundaries of R_i. By choosing appropriate rectangles and copulae C_i and C_{bg}, we can construct circular-linear copulae.

Specifically, we define 2 rectangles that are mirror images of each other with respect to the line $u = 0.5$: $R_1 = [u_1, u_2] \times [0, 1]$ and $R_2 = [1 - u_2, 1 - u_1] \times [0, 1]$ with $0 \leq u_1 < u_2 \leq 0.5$. The patchwork-copula is then periodic and symmetric in u if the following two conditions are satisfied

- C_2 is the orthogonal reflection of C_1 with respect to the line $u = 0.5$, i.e. $C_2(u, v) = C_{1,0.5\pi}(u, v) = v - C_1(1-u, v)$.
- C_{bg} is a copula that is periodic and symmetric in u, or $u_1 = 0$ and $u_2 = 0.5$, i.e. the two rectangle cover the entire unit square.

The explicit distribution of a general patchwork-copula (of which the above described copula is a special case) is given in Theorem 2.2 in Durante et al. (2009) and is repeated here for our specific two rectangles:

$$C(u,v) = \begin{cases} \lambda_1 C_1\left(\frac{V_{C_{\text{bg}}}([u_1,u]\times[0,1])}{\lambda_1}, \frac{V_{C_{\text{bg}}}([u_1,u_2]\times[0,v])}{\lambda_1}\right) & \\ +C_{\text{bg}}(u_1, v) & \text{if } (u,v) \in R_1 \\ \lambda_2\Big(\frac{V_{C_{\text{bg}}}([1-u_2,1-u_1]\times[0,v])}{\lambda_2} & \\ -C_1\Big(\frac{V_{C_{\text{bg}}}([1-u_2,u]\times[0,1])}{\lambda_2}, \frac{V_{C_{\text{bg}}}([1-u_2,1-u_1]\times[0,v])}{\lambda_2}\Big)\Big) & \\ +C_{\text{bg}}(1-u_2, v) & \text{if } (u,v) \in R_2 \\ C_{\text{bg}}(u,v)) & \text{if } (u,v) \in [1,0]^2 \setminus (R_1 \cup R_2), \end{cases} \tag{52}$$

with $\lambda_i = V_{C_{\text{bg}}}(R_i)$ (see equation 1 for the definition of the C-volume). In case the two rectangles cover the entire unit square and $C_{\text{bg}}(u, v) = uv$ is the independence copula, this equation drastically simplifies to

$$C(u,v) = \begin{cases} 0.5C_1(2u, v) & \text{if } (u,v) \in R_1 \\ 0.5(v - C_1(2u-1, v)) + 0.5v & \text{if } (u,v) \in R_2 \end{cases} \tag{53}$$

since in this case $\lambda_i = 0.5$, and $V_{C_{\text{indep}}}([0, u] \times [0, v]) = uv$.

The copula PDF is obtained by taking the derivatives of the CDF (see appendix, section A5 for a detailed derivation), which results in

$$c(u,v) = \begin{cases} \frac{1}{\lambda_1}\left(\int_{u_1}^{u_2} c_{\text{bg}}(x,v)\,dx\right) c_1\left(\frac{V_{C_{\text{bg}}}([u_1,u]\times[0,1])}{\lambda_1}, \frac{V_{C_{\text{bg}}}([u_1,u_2]\times[0,v])}{\lambda_1}\right) & \text{if } (u,v) \in R_1 \\ \frac{1}{\lambda_2}\left(\int_{1-u_2}^{1-u_1} c_{\text{bg}}(x,v)\,dx\right) & \\ \times c_1\left(1 - \frac{V_{C_{\text{bg}}}([1-u_2,u]\times[0,1])}{\lambda_2}, \frac{V_{C_{\text{bg}}}([1-u_2,1-u_1]\times[0,v])}{\lambda_2}\right) & \text{if } (u,v) \in R_2 \\ c_{\text{bg}}(u,v)) & \text{if } (u,v) \in [1,0]^2 \setminus (R_1 \cup R_2). \end{cases} \tag{54}$$

As was the case for the distribution, this equation is a lot simpler when the two rectangles cover the entire unit square

and $C_{\text{bg}}(u, v) = uv$:

$$c(u, v) = \begin{cases} 0.5c_1(2u, v) & \text{if } (u, v) \in R_1 \\ 0.5c_1(2 - 2u, v) & \text{if } (u, v) \in R_2 \end{cases} \tag{55}$$

To sample from the patchwork-copula, we follow the algorithm described in section 2 of Durante et al. (2009): Generate a sample (u, v) from $C_{\text{bg}}(u, v)$. If this point does not fall within any rectangle, take it as a sample from C. If it falls within rectangle i, generate a sample (x_i, y_i) from C_i and transform it to $(\psi_u^{-1}(x_i), \psi_v^{-1}(y_i))$, where $\psi_u^{-1}(u) = \frac{V_{C_{\text{bg}}}([u_1,u]\times[0,1])}{V_{C_{\text{bg}}}(R_i)}$ and $\psi_v^{-1}(v) = \frac{V_{C_{\text{bg}}}([u_1,u_2]\times[0,v])}{V_{C_{\text{bg}}}(R_i)}$. In the special case where the two rectangles cover the entire unit square and $C_{\text{bg}}(u, v) = uv$, the transformation simplifies to $(x_1/2, y_1)$ for R_1 and $((x_2 + 1)/2, y_2)$ for R_2.

With the algorithm described above, it is not necessary to find the inverse of the conditional distribution of the patchwork-copula to generate samples from it. Nevertheless, we implemented the conditional distribution and its inverse using numeric integration of the copula density and numeric inversion.

4.3.3 | Usage and Properties

A copula-object consisting of a linear combination of a linear-linear copula and its "90 degrees rotation" can be obtained as

```
cyl_rot_combine(copula, shift = FALSE)
```

where `copula` must be a copula-object from the `copula` package (Hofert et al., 2020; Jun Yan, 2007; Ivan Kojadinovic and Jun Yan, 2010; Marius Hofert and Martin Mächler, 2011). This gives a copula with a correlation structure that leads to an X-shaped PDF. With `shift = TRUE`, the same copula, but with its PDF "periodically shifted" by 0.5 in u-direction is obtained. It has a diamond-shaped density (see Figure 5 a and b).

A copula-object generated from a patchwork of copulae can be obtained as

```
cyl_rect_combine(copula,
  background = indepCopula(),
  low_rect = c(0, 0.5),
  up_rect = "symmetric",
  flip_up = TRUE
)
```

`copula` is the copula on which the functions in the two rectangles are based and must be a copula-object from the `copula`-package (Hofert et al., 2020; Jun Yan, 2007; Ivan Kojadinovic and Jun Yan, 2010; Marius Hofert and Martin Mächler, 2011), or a `cylvon_mises`-object, whereas the copula outside the two rectangle (`background`) can be any circular-linear or linear-linear copula. The direction of correlation can be tuned by "rotating" the copulae on which the functions in the rectangles are based using `flip_up` and by changing the corrleation structure of the background-copula (see Figure 5 c and d).

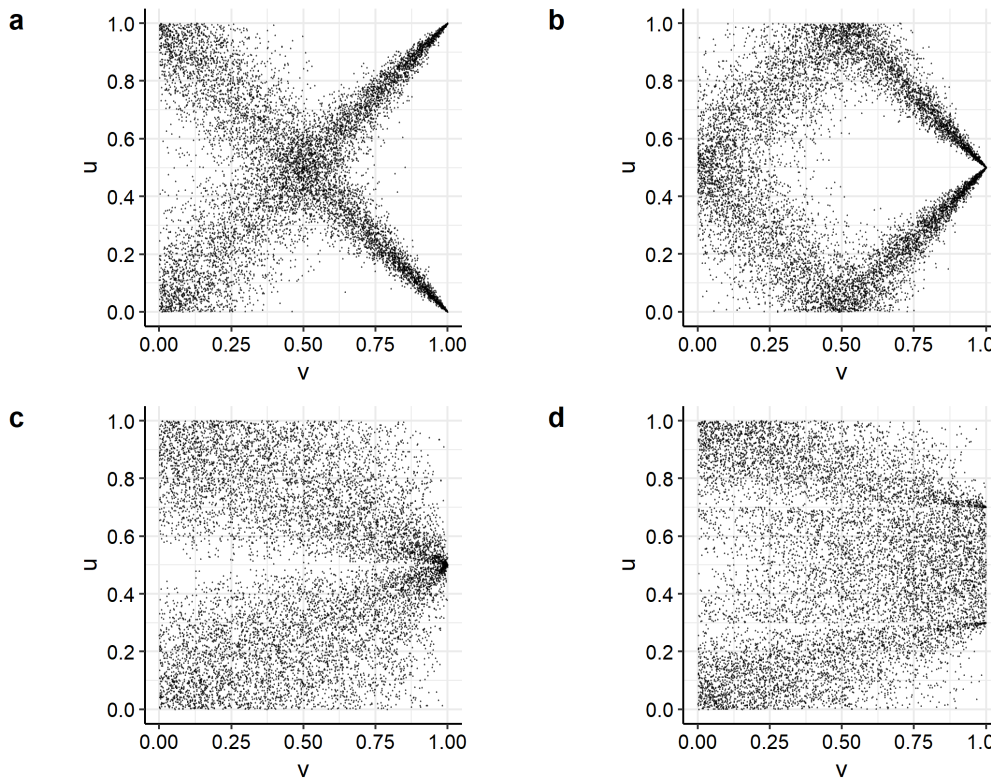

FIGURE 5 Scatterplots of 10,000 samples drawn from the following copulae.
a: `cyl_rot_combine(copula::rotCopula(claytonCopula(8),flip=T))`,
b: `cyl_rot_combine(copula::rotCopula(claytonCopula(8),flip=T),shift = T)`,
c: `cyl_rect_combine(copula::rotCopula(claytonCopula(1.1),flip=T))`,
d: `cyl_rect_combine(copula::rotCopula(claytonCopula(1.1),flip=T),background = cyl_quadsec(), low_rect = c(0,0.3))`.

5 | DEPENDENCE AND PARAMETER ESTIMATES

5.1 | Parameter Estimation

Given a set of n i.i.d. observations of a pair of circular and linear variables (θ_i, x_i), an assumed copula family, $C(u, v; \boldsymbol{\alpha})$, and assumed marginal distributions, $F_\Theta(\theta; \boldsymbol{\beta})$ and $F_X(x; \boldsymbol{\gamma})$, we could, in principle, estimate the parameter vector $(\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma})$ by maximizing the log-likelihood based on the joint PDF of equation 3. However, this approach would require optimizing a large number of parameters simultaneously, and mis-specification of the marginal distributions would lead to biased estimators of the copula parameters and vice versa.

If we knew the true marginal distributions, we could transform our data to observations from the copula and

maximize the log-likelihood

$$\ell(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \log[c(F_\Theta(\theta_i),\, F_X(x_i);\, \boldsymbol{\alpha})]\,. \tag{56}$$

This leads to two alternative approaches for estimating copulae parameters, in which estimates of F_Θ and F_X are plugged into equation 56. These estimates, $\hat{F}_\Theta(\theta)$ and $\hat{F}_X(x)$, can either be obtained parametrically via maximum likelihood (Joe and Xu, 1996; Joe, 1997, 2005), or non-parametrically as pseudo-observations, i.e. draws from the empirical copula (section 2.1).

Note that in the parametric case, misspecified marginal distributions still lead to biased estimators of copula parameters (Fermanian and Scaillet, 2005). The number of parameters that have to be simultaneously optimized is, however, reduced in both cases. When using estimates, $(\hat{F}_\Theta(\theta_i), \hat{F}_X(x_i))$, instead of the true marginal distributions in equation 56, $\ell(\boldsymbol{\alpha})$ is no longer a true log-likelihood. Further, when using the empirical copula (eq. 7), observations are also no longer i.i.d. since the non-parametric estimates of the marginal distributions clearly depend on the entire data set (Hofert et al., 2018). The estimation of copula parameters using non-parametrically estimated marginals is referred to as maximum pseudo likelihood estimation (MPLE, see Oakes, 1994; Genest et al., 1995; Shih and Louis, 1995; Tsukahara, 2005) and is implemented in the `cylcop`-package as

```
optML(copula, theta, x, parameters, start)
```

The arguments of this function, which are based on `copula::fit_copula()` from the `copula`-package, are a circular linear copula object (`copula`), the circular (`theta`) and linear (`x`) components of the measurements, the parameters of the copula that are to be optimized (`parameters`), and their initial values for that optimization (`start`).

For many linear-linear copulae, parameter estimates can be derived analytically from estimates of a correlation measure, such as Spearman's rho or Kendall's tau (Oakes, 1982; Genest, 1987; Genest and Rivest, 1993); analytical solutions are not possible, however, for most of the copulae introduced in this paper, and we therefore had to resort to using numerical optimization methods. The exception are patchwork copulae, where the rectangles span the entire unit square. Their parameters can be estimated using Kendall's tau implemented with the function

```
optTau(copula, theta, x)
```

For all other circular-linear copulae, we carried out a grid-search to determine the copula parameters that minimize the difference in a correlation measure (section 5.2) between the empirical and parametric copula. This approach assumes the absolute values of copula parameters increase monotonously with increasing circular-linear correlation and is implemented as

```
optCor(copula, theta, x, method = c("cor_cyl", "mi_cyl"))
```

The two methods `"cor_cyl"` and `"mi_cyl"` refer to a non-parametric estimate of a circular-linear correlation coefficient and mutual information, respectively (see section 5.2). The parameter values obtained in this way serve as reasonable starting values for MPLE, the choice of which is especially important when the parameter-hypersurface is rugged and high-dimensional.

Finally, model selection can be performed according to Akaike's information criterion, which is a common (e.g. Chen and Fan, 2005; McNeil et al., 2015; Joe, 2014), but for MPLE not uncontroversial approach (see Grønneberg and Hjort 2014, but also Jordanger and Tjøstheim 2014).

5.2 | Measures of Correlation

Parametric measures of circular-linear correlation require normally distributed linear random variables (Johnson and Wehrly, 1977; Mardia, 1976) and are therefore not generally applicable to all circular-linear data. Instead, we used a non-parametric estimate of a circular-linear correlation coefficient, D, that was introduced by Mardia (1976) and applied by Solow et al. (1988) or, more recently, Tu (2015). It is estimated by ranking the data, i.e. from the pseudo-observations

$$D = k\left(\left(\sum_i s_i \cos\frac{2\pi r_i}{n}\right)^2 + \left(\sum_i s_i \sin\frac{2\pi r_i}{n}\right)^2\right), \tag{57}$$

where k is a normalization constant, r_i is the circular (with $-\pi$ as reference) and s_i the linear rank of observation i. However, this coefficient can only take values between 0 and 1 and thus cannot distinguish between positive and negative correlation.

We also implemented a correlation measure based on mutual information, i.e. the Kullback-Leibler divergence of the product of the marginal distributions from the joint distribution (see e.g. Leguey et al., 2019).

$$\begin{aligned} I(\Theta, X) &= \int_{-\pi}^{\pi}\int_0^{\infty} f_{\Theta,X}(\theta, x)\log\left(\frac{f_{\Theta,X}(\theta,x)}{f_\Theta(\theta)f_X(x)}\right)\,d\theta\,dx \\ &= \int_{-\pi}^{\pi}\int_0^{\infty} c(F_\Theta(\theta), F_X(x))\,f_\Theta(\theta)f_X(x)\,\log\left(c(F_\Theta(\theta), F_X(x))\right)\,d\theta\,dx \\ &= \int_0^1\int_0^1 c(u,v)\log\left(c(u,v)\right)\,du\,dv. \end{aligned} \tag{58}$$

The last equality was obtained by setting $u = F_\Theta(\theta)$ and $v = F_X(x)$. From this expression, it is immediately clear that the mutual information is the negative of the differential entropy associated with $c(u, v)$ (Jian and Zengqi, 2011; Calsaverini et al., 2009). If we could easily carry out the integration in the last line of equation 58, we could directly determine the parameter values of the chosen copula family that give the correct mutual information. Unfortunately, the integral is computationally difficult to calculate in most cases. However, Tenzer and Elidan (2016) have demonstrated that the mutual information is monotonous in the dependence parameter for a wide range of bivariate copulae. The rough optimization framework described above can therefore be expected to work well with mutual information as a criterion for dependence. We can obtain an estimate of the mutual information by binning the data (measurements of the circular and the linear random variable) and taking the average of the point-wise mutual information (based on the frequency of data points in the bins) over all bin combinations. Note also that the mutual information of the data is equal to the mutual information of the empirical copula. If required, the mutual information can be normalized to an interval $[0, 1]$ (zero meaning independence copula and 1 meaning upper Fréchet-Hoeffding copula) with the entropy H:

$$I_{\text{norm}}(u, v) = \frac{I(u, v)}{\sqrt{H(u)H(v)}} \tag{59}$$

Finally, if we take it as fact that the true copula is symmetric in u, we can symmetrize the empirical copula (set the values of u that are larger than 0.5 to $1 - u$). The two correlation measures are implemented as

```
cor_cyl(theta, x)
mi_binned(theta, x, normalize = T, symmetrize = F)
```

6 | CODED EXAMPLES

To begin with, we will load the necessary packages and generate two `cylcop` objects with which we will demonstrate the functionality of the `cylcop` package. First, we generate a copula with cubic sections

```
library(copula)
library(cylcop)
copula_1 <- cyl_cubsec(a = 0.05, b = -1 / (2 * pi))
```

Secondly, to demonstrate the level of complexity in the correlation structure that can be captured, we generate a copula consisting of a rectangular patchwork with rectangles $[0.1, 0] \times [0.4, 1]$ and $[0.6, 0] \times [0.9, 1]$. Inside of the rectangles, the copula is derived from a Gumbel copula rotated by 180 degrees (first rectangle) and a Gumbel copula rotated by 180 and 90, i.e. 270, degrees. Outside the rectangles, the copula consists of the linear combination of a Frank copula and its 90 degree rotation.

```
copula_2 <- cyl_rect_combine(
    copula = copula::rotCopula(gumbelCopula(1.2), flip = T),
    background = cyl_rot_combine(frankCopula(10), shift = F),
    low_rect = c(0.1, 0.4),
    up_rect = c(0.6, 0.9),
    flip_up = T)
```

The densities of these two copulae are shown in Figure 6 and were produced using the `cop_plot` function in our package

```
cop_plot(copula_1, type = "pdf", plot_type = "ggplot", resolution = 200)
```

Similarly, we could plot the CDF by setting `type="cdf"`, and we can also plot 3-dimensional surfaces using the `rgl` package (Murdoch and Adler (2021); `plot_type="rgl"`) or the `plotly` package (Sievert (2020); `plot_type="plotly"`).

As we mentioned in the introduction, our motivation for deriving new copulae for correlated circular-linear data and for developing software for their implementation stems from a desire to model animal movement in discrete time (Hodel and Fieberg, 2021). Thus, we also provide functions for simulating movement trajectories using copulae in the package. Selecting the first copula (`copula_1`), we can now generate a trajectory from 10,000 step lengths (distances between consecutive locations) and turn angles (changes in direction between successive locations) drawn from a joint distribution with a correlation structure described by that copula. As marginal distributions, we chose a gamma distribution for the step lengths and a mixed von Mises distribution for the turn angles.

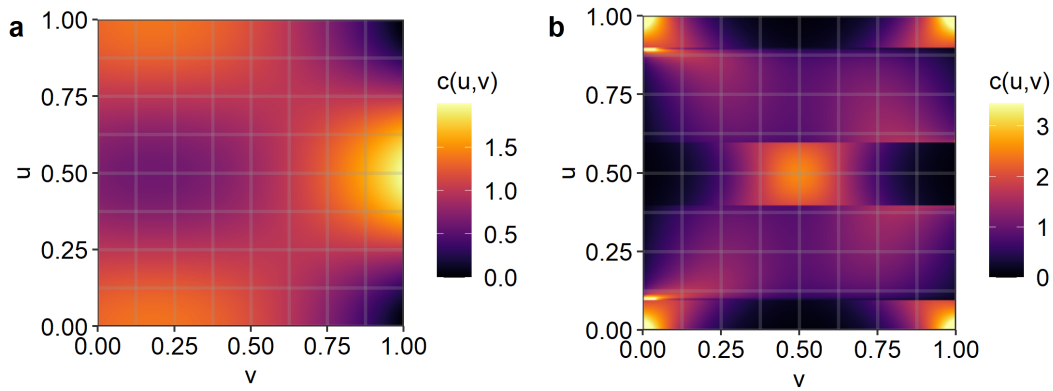

FIGURE 6 PDFs of a: cubic sections copula `copula_1` and b: rectangular patchwork copula `copula_2`.

```
traj <- make_traj(
  n = 10000,
  copula = copula_1,
  marginal_circ = "mixedvonmises",
  parameter_circ = list(mu1 = 0, mu2 = pi, kappa1 = 2, kappa2 = 1, prop = 0.7),
  marginal_lin = "gamma",
  parameter_lin = list(shape = 3)
)
```

Any distribution for which a quantile function is available can be used when specifying the linear marginal distribution (using argument `marginal_lin`). For the circular marginal distribution, the von Mises, the wrapped Cauchy, and a mixture of 2 von Mises distributions are available.

The ouput of `make_traj()` is a `data.frame` that contains the draws from the copula, the step lengths and turn angles, i.e. the draws from the copula transformed by the inverse CDFs of the marginal distributions, and the positions in space the animal would visit by moving according to those step lengths and turn angles. We have implemented several functions, below, to visualize simulated trajectories (e.g. Fig. 7).

```
scat_plot(traj, periodic = TRUE)
traj_plot(traj)
cop_scat_plot(traj)
circ_plot(traj)
```

The argument `periodic` determines whether the plot is periodically extended past the angles $-\pi$ and π.

We provide several options for quantifying the correlation between circular and linear variables, which we demonstrate with our simulated data. The first available option is the circular-linear correlation coefficient described in section 5.2.

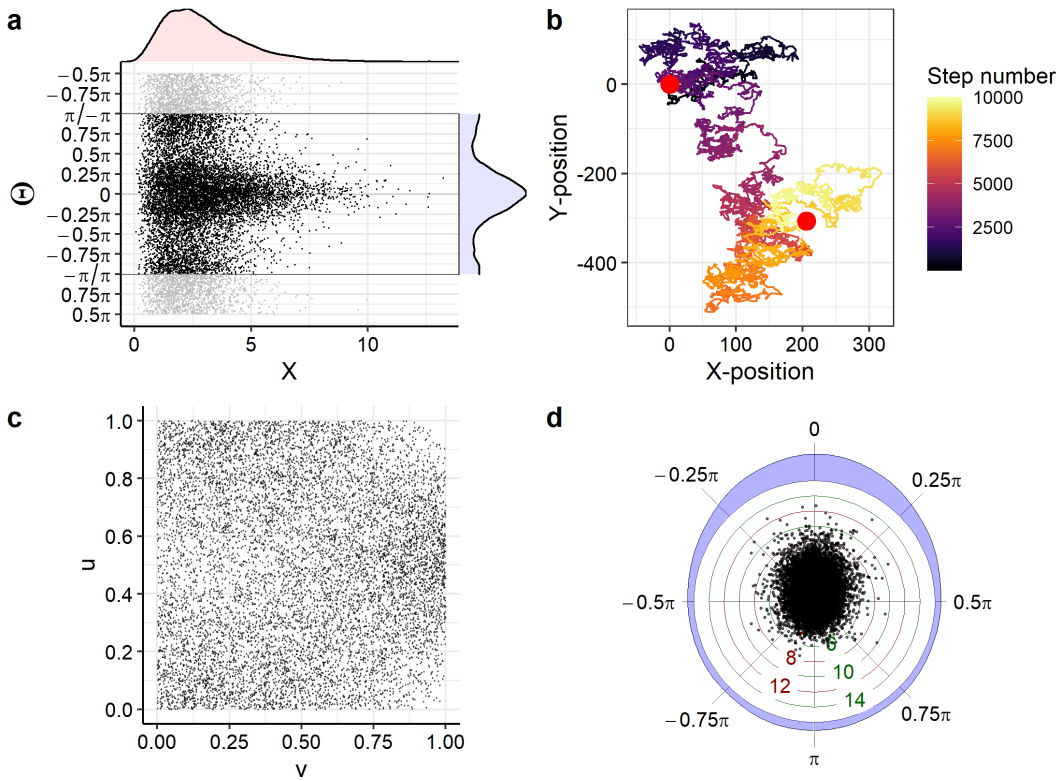

FIGURE 7 Circular-linear data representing turn angles and step lengths were simulated using `copula_1`, a copula with cubic sections, and marginal distributions given by gamma and mixed von Mises distributions. a: scatterplot of turn angles (Θ) and step lengths (X) with non-parametric density estimates in blue and red, respectively, obtained with `scat_plot()`. b: Plot of the trajectory derived from the sequence of turn angles and step lengths obtained with `traj_plot()`. c: scatterplot of the draws from `copula_1` obtained with `cop_scat_plot()`. d: circular scatterplot of turn angles and step lengths obtained with `circ_plot()`.

```
cor_cyl(theta = traj$angle, x = traj$steplength)
[1] 0.07428712
```

The second option is to calculate the mutual information between the step lengths and turn angles. The mutual information can be normalized to lie in $[0, 1]$ by dividing by the square root of the product of the entropies of the two random variables (see equation 59). By specifying `symmetrize = T`, we set the values of u of the empirical copula that are larger than 0.5 to $1 - u$, ensuring that a symmetric circular-linear copula with perfect correlation has a normalized mutual informaiton of 1 (see appendix A6)

```
mi_cyl(theta = traj$angle, x = traj$steplength, normalize = T, symmetrize = T)
[1] 0.0223797
```

As described in section 5.2, neither correlation measure depends on the marginal distributions, which means that

we obtain the same output, whether we take step lengths and turn angles as input, or the corresponding untransformed draws from the copula.

To facilitate model selection, we have written a function, `opt_auto`, to autonomously fit 15 different circular-linear copulae (see appendix A7) to the data. The function returns a list containing descriptions of the copulae, `cylcop`-objects, and AIC values associated with the fitted copulae.

```
guess_fit <- opt_auto(theta = traj$angle, x = traj$steplength)
```

The copula with the lowest AIC (-932.50) is a cubic sections copula with parameters $a = 0.048$ and $b = -0.15$, i.e. the copula with which we have generated the data (`copula_1`). The copulae with the second and third lowest AIC are a quadratic sections copula ($a = 0.11$, AIC $= -754.10$, see Figure 8 a) and a rectangular patchwork copula with symmetric rectangles spanning the entire unit square and the copula inside the rectangles based on a Frank copula with parameter $\alpha = 1.65$ (AIC $= -732.19$, see Figure 8 b).

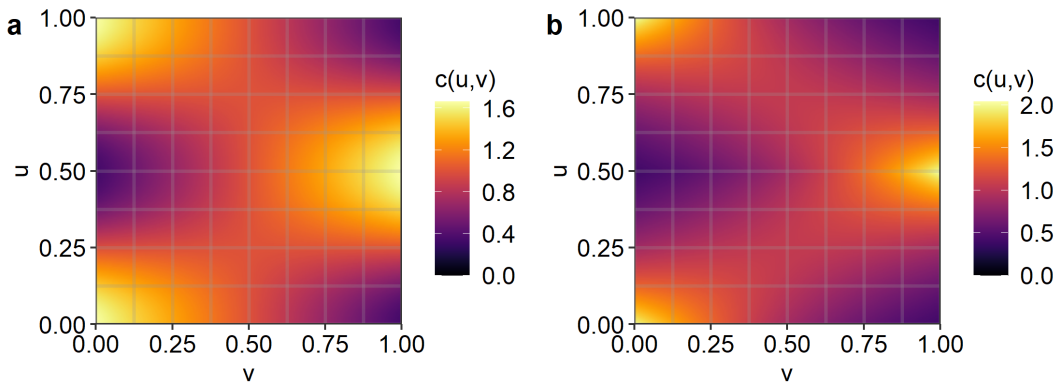

FIGURE 8 a: PDF of a quadratic sections copula with $a = 0.11$. b: PDF of a rectangular patchwork copula with symmetric rectangles spanning the entire unit square and the copula inside the rectangles based on a Frank copula with parameter $\alpha = 1.65$.

To fit a chosen copula to the data "by hand" we can first calculate starting values for MPLE using a correlation measure. `optCor` first calculates the circular linear correlation coefficient or the mutual information (specified by the argument `method`). Next, `n` samples are drawn from `copula` and the corresponding correlation measure is calculated. The parameters of the copula are changed and the process repeated until the copula parameters giving the lowest difference between the correlation of the data and the correlation of the sample drawn from that copula are found with an accuracy specified by the argument `acc`. The parameter search is implemented as an exponential followed by a binary search.

```
start_val <- optCor(
  copula = cyl_cubsec(0,0),
  theta = traj$angle,
  x = traj$steplength,
  acc = 0.01,
  n = 10000,
```

```
  method = "cor_cyl",
  parameter = "both"
)
```

Finally, copula parameters can be fit to the data via MPLE with the output of `optCor` as starting value. The function `optML()` is based on `copula::fitCopula()` and returns a list containing the `cylcop` object with the optimized parameters, the maximum likelihood value and the corresponding AIC.

```
optimized <- optML(
 copula = cyl_cubsec(),
 theta = traj$angle,
 x=traj$steplength,
 parameters = c("a","b"),
 start = start_val,
 lower = c(-0.1, -1 / (2 * pi)),
 traceOpt = T,
 optim.method = "L-BFGS-B",
 optim.control = list(maxit = 100)
)
```

We also provide functions to fit the parameters of linear (`fit_steplength()`) and circular (`fit_angle()`) marginal distributions to the data using maximum likelihood. The `circular` (Agostinelli and Lund, 2017) and `MASS` packages (Venables and Ripley, 2002) provide excellent methods and functions for fitting almost any circular or linear distribution; our functions are basically just wrappers to these functions with some simplifications for easier usage. One exception is the mixed von Mises distribution, for which there was no method available to obtain maximum likelihood estimates in the `circular` package. We based our implementation on code from the `movMF` package (Hornik and Grün, 2014) with the added feature of optionally fixing the mean directions.

```
angle_distr <- fit_angle(theta = traj$angle, parametric = "mixedvonmises", mu = c(0, pi))
```

For both linear and circular marginal distributions, we can also obtain non-parameteric density estimates by setting `parametric = FALSE`, and passing a bandwidth (in this case, obtained using the `opt_circ_bw` function)

```
bw <- cylcop::opt_circ_bw(theta = traj$angle, loss = "adhoc", kappa.est = "trigmoments")
angle_non_param <- fit_angle(theta = traj$angle, parametric = FALSE, bandwidth = bw)
```

Further details can be found in Agostinelli and Lund (2017). As is also described there, an adhoc estimation of the bandwidth used for the non-parameteric density estimate can give wrong results, especially with multimodal distributions, and we compare density estimates obtained with different bandwidths in section A8 in the appendix). Finally, the non-parametric density estimates can be used to simulate trajectories

```
steplength_distr <- fit_steplength(x = traj$steplength, parametric = "gamma")
traj_fit <- make_traj(
  n = 10000,
```

```
  copula = optimized$copula,
  marginal_circ = "dens",
  parameter_circ = angle_non_param,
  marginal_lin = "gamma",
  parameter_lin = steplength_distr$coef
)
```

7 | CONCLUSIONS

We derived new copulae and implemented them in our `cylcop` package to facilitate modeling correlated circular-linear data where the circular variable is expected to be symmetric. We aimed to provide a thorough derivation of our circular-linear copulae together with a package that is easy to use, even as a black-box. This should, on the one hand, allow application-oriented researchers to easily and quickly use these copulae to visualize and model their data and, on the other hand, provide statisticians and modellers with a starting point to further develop new methods.

In the future, we hope to integrate non-parametric copulae obtained from smoothing the empirical copula using e.g. Bernstein polynomials (Sancetta and Satchell (2004); Janssen et al. (2012); Carnicero et al. (2013); García-Portugués et al. (2013, 2014)) into our package. The addition of conditional copulae (Patton, 2006; Fermanian and Wegkamp, 2012) would also allow tackling issues, such as temporal autocorrelation, or performing time series analysis and regression.

Acknowledgements

JF received partial salary support from the Minnesota Agricultural Experimental Station.

Conflict of Interest

None

references

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