Exploring wind direction and SO₂ concentration by circular–linear density estimation

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Investigation of the relation between pollutant concentrations from monitoring sites and the emission sources.

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- Investigation of the relation between pollutant concentrations from monitoring sites and the emission sources.
- Circular variables (wind direction) play a relevant role.

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 - Jammalamadaka and Lund (2006), Fernández–Durán (2007): Wind direction and ozone levels.
- ▶ We focus on sulphur dioxide (SO₂) pollutants.

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- Motivation



Figure: Locations of monitoring stations and power plant.

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- Motivation



Distances to power plant

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- ▶ B1: 0.9 km
- ▶ G2: 18.6 km

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Figure: Locations of monitoring stations and power plant.

Distances to power plant

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$\begin{array}{l} \mbox{Goal of the work} \\ \mbox{Study wind direction and SO_2} \\ \mbox{concentration relation}. \end{array}$

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Figure: Rose diagrams for wind direction stations B1 and G2, with average SO_2 concentrations for August 2009.

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Motivation

Circular-linear distributions

Simulation results

Real data application

Some final comments

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Circular distributions

Definition (Mardia and Jupp, 2000)

A circular random variable Θ has its support in \mathbb{S}^1 .

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1.
$$f_{\Theta}(\theta) \ge 0, \forall \theta \in \mathbb{R}.$$

2. $\int_{r}^{2\pi+r} f_{\Theta}(\theta) d\theta = 1, \forall r \in \mathbb{R}.$
3. $f_{\Theta}(\theta) = f_{\Theta}(\theta + 2\pi k), \forall \theta \in \mathbb{R}, \forall k \in \mathbb{Z}.$

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Example (von Mises distribution $vM(\mu,\kappa)$) The von Mises distribution has density

$$\varphi_{vM}(\theta;\mu,\kappa) = (2\pi I_0(\kappa))^{-1} \exp\left[\kappa \cos(\theta-\mu)\right],$$

where $\mu \in [0, 2\pi)$ is the circular mean, $\kappa \ge 0$ is the concentration in μ direction. Its distribution is denoted by Ψ_{vM} .

- Circular-linear distributions

- Circular distributions



Figure: Circular and linear representations of the density and distribution of a von Mises with $\kappa = 0$ (circular uniform distribution).

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- Circular-linear distributions

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Figure: Circular and linear representations of the density and distribution of a von Mises with $\mu = \pi$ and $\kappa = 5$.

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Figure: Circular and linear representations of the density and distribution of a von Mises with $\mu = \pi$ and $\kappa = 10$.

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- $\blacktriangleright~\Theta$ a circular variable with density φ and distribution $\Psi.$
- X a linear variable with density f and distribution F.

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Joint distribution of (Θ,X) ?

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Joint distribution of (Θ,X) ?

Theorem (Johnson and Wehrly, 1978) Let g be a circular density. Then

$$p(\theta, x) = 2\pi g \left[2\pi \left(\Psi(\theta) + F(x) \right) \right] \varphi(\theta) f(x)$$

is a circular-linear density with marginal densities φ and f.

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- \blacktriangleright It is a construction of p from φ and f, not a characterization.
- ▶ Θ and X independent $\Leftrightarrow g(\omega) = (2\pi)^{-1}, \forall \omega \in [0, 2\pi)$

Johnson and Wehrly model

Example (Circular uniform and Normal marginal densities) Densities: $\varphi = (2\pi)^{-1}$, $f = \phi$ and $g = \varphi_{vM}(\mu, \kappa)$.

 $p_1(\theta, x) = (2\pi I_0(\kappa))^{-1} \exp\left[\kappa \cos(\theta - 2\pi \Phi(x) - \mu)\right] \phi(x)$



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Johnson and Wehrly model

Example (von Mises and Normal marginal densities) Densities: $\varphi = \varphi_{vM}(\mu_1, \kappa_1)$, $f = \phi$ and $g = \varphi_{vM}(\mu, \kappa)$.

 $p_2(\theta, x) = I_0(\kappa)^{-1} \exp\left[\kappa \cos\left(2\pi(\Psi_{vM}(\theta) - \Phi(x)) - \mu\right)\right] \varphi_{vM}(\theta)\phi(x)$



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Estimation algorithm

1. Obtain estimators for the marginal densities $\hat{\varphi}$, \hat{f} and the corresponding marginal distributions $\hat{\Psi}$, \hat{F} .

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- 2. Compute an artificial sample $\left\{2\pi \left(\hat{\Psi}(\theta_i) + \hat{F}(x_i)\right)\right\}_{i=1}^n$ and estimate the joining circular density \hat{g} .

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- 2. Compute an artificial sample $\left\{2\pi \left(\hat{\Psi}(\theta_i) + \hat{F}(x_i)\right)\right\}_{i=1}^n$ and estimate the joining circular density \hat{g} .
- 3. Obtain the circular-linear density estimator as

$$\hat{p}(\theta, x) = 2\pi \hat{g} \left[2\pi \left(\hat{\Psi}(\theta) + \hat{F}(x) \right) \right] \hat{\varphi}(\theta) \hat{f}(x).$$

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Estimation approaches

Parametric. Estimate parametrically φ, f and g, for example by ML. Fernández–Durán (2007) estimates the model using ML for the linear density and Nonnegative Trigonometric Sums for the circular densities.

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- Mixed. Estimate φ and f parametrically (some intuition) and g nonparametrically (no intuition) or other possible combinations.

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- Mixed. Estimate φ and f parametrically (some intuition) and g nonparametrically (no intuition) or other possible combinations.
- Nonparametric. Estimate nonparametrically both marginals φ and f and the joining density g by kernel smoothing.

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Kernel estimation

▶ Let f be a linear density and X₁,..., X_n a sample from X ~ f. The kernel estimator of f is

$$\hat{f}_h(x) = \frac{1}{nh} \sum_{i=1}^n K\left(\frac{x - X_i}{h}\right)$$

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For a circular density φ and a sample Θ₁,...,Θ_n, the kernel estimator defined by Hall, Watson and Cabrera (1987) is

$$\hat{\varphi}_{\nu}(\theta) = \frac{c_0(\nu)}{n} \sum_{i=1}^n L\left(\nu \cos(\theta - \Theta_i)\right).$$

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► In the linear case,

$$h_{\mathsf{AMISE}} = \mathcal{O}\left(n^{-rac{1}{5}}
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Circular–linear density estimation Circular–linear distributions Kernel estimation

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- The circular bandwidth parameter ν behaves as $1/h^2$.
- ► Large values of v undersmooth and small ones oversmooth (inverse behaviour of h).
- A possible choice of ν is by LSCV

$$\nu_{\mathsf{LSCV}} = \arg\min_{\kappa \ge 0} \int \hat{f}_{\kappa}(\omega)^2 d\omega - \frac{2}{n} \sum_{i=1}^{n} \hat{f}_{\kappa}^{-i}(\Theta_i).$$

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Figure: Effects of the circular bandwidth in the density estimator. Sample of size n = 100 from an equal mixture of $vM(\frac{\pi}{2}, 2)$ and $vM(\frac{3\pi}{2}, 5)$.

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Figure: LSCV, KL and Taylor bandwidths. Sample of size n = 100 from an equal mixture of $vM(\frac{\pi}{2}, 2)$ and $vM(\frac{3\pi}{2}, 5)$.

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Example 1

- φ a circular uniform.
- $f \sim \mathcal{N}(0, 1)$.
- $g \sim vM(\pi, 2)$.

Example 2

- $\blacktriangleright \varphi \sim vM\left(\frac{\pi}{2},2\right).$
- $f \sim \mathcal{N}(0, 1)$.
- ► $g \sim vM(\pi, 5)$.







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Our model

$$p(\theta, x) = 2\pi g \left[2\pi \left(\Psi(\theta) + F(x) \right) \right] \varphi(\theta) f(x)$$

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Circular-linear density estimation

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$$p(\theta, x) = 2\pi g \left[2\pi \left(\Psi(\theta) + F(x) \right) \right] \varphi(\theta) f(x)$$

In terms of copulas, can be expressed as

$$p(\theta, x) = c(\Psi(\theta), F(x))\varphi(\theta)f(x)$$

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▶ Copula formulation helps for random simulation from p₁ and p₂ (our examples).

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A copula C is a bivariate distribution function with uniform marginals. It allows to express joint distributions in terms of marginal distributions.

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Sklar's Theorem

Let X, Y two random variables with joint distribution F and marginals F_1 and F_2 . There exists a copula C such that

$$F(x,y) = C(F_1(x), F_2(y)), \quad \forall x, y \in \mathbb{R}.$$

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Consider a circular–linear variable (Θ, X) with joint distribution $P = C_{\Theta, X} (\Psi, F)$.

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Consider a circular–linear variable (Θ, X) with joint distribution $P = C_{\Theta, X} (\Psi, F)$.

Simulation from (Θ, X)

- 1. Simulate $(U, V) \sim C_{\Theta, X}$ (U and V are uniforms).
- 2. Compute $\Theta = \Psi^{-1}(U)$ and $X = F^{-1}(V)$.
- **3**. $(\Theta, X) \sim P$.

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- 2. Compute $\Theta = \Psi^{-1}(U)$ and $X = F^{-1}(V)$.
- **3**. $(\Theta, X) \sim P$.
- Simulation by copulas is easier due to the structure of p.
- The copula density is $c(u, v) = 2\pi g(2\pi(u+v))$.

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Circular-linear density estimation

- Parametric: Maximum Likelihood.
- Mixed: φ and f by ML and g by kernel estimation with LSCV bandwidth.
- ► **Nonparametric**: Linear and circular kernel estimation with linear BCV bandwidth and circular LSCV bandwidths.

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- Other bandwidth selectors: Seather & Jones (linear); Kullblack–Leibler and Taylor (circular). Similar results.

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- ► **Nonparametric**: Linear and circular kernel estimation with linear BCV bandwidth and circular LSCV bandwidths.
- Other bandwidth selectors: Seather & Jones (linear); Kullblack–Leibler and Taylor (circular). Similar results.
- ► Sample sizes: n = 50, 200, 500, 1000. Samples generated using copula simulation.

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Simulation setting

Error criterion

$$\mathsf{MISE} = \iint \mathbb{E} \left[\hat{p}(\theta, x) - p(\theta, x) \right]^2 d\theta dx.$$

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Circular-linear density estimation

Error criterion

$$\mathsf{MISE} = \iint \mathbb{E} \left[\hat{p}(\theta, x) - p(\theta, x) \right]^2 d\theta dx.$$

• MISE approximated by Monte Carlo with M = 1000 replicates.

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- Benchmark: Parametric model.
- Relative MISE efficiencies for Mixed and Nonparametric approaches.

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Simulation setting

		Estimation method			Relative efficiency	
	n	Param.	Mixed	Nonpar.	Mixed	Nonpar.
Example 1	50	0.0054	0.0095	0.0168	0.5674	0.3208
	200	0.0013	0.0029	0.0052	0.4802	0.2483
	500	0.0005	0.0012	0.0025	0.4267	0.2078
	1000	0.0003	0.0007	0.0014	0.3897	0.1840
Example 2	50	0.0402	0.0483	0.0977	0.8331	0.4115
	200	0.0104	0.0137	0.0363	0.7595	0.2862
	500	0.0043	0.0060	0.0185	0.7140	0.2296
	1000	0.0021	0.0032	0.0107	0.6783	0.2006

Table: MISE for estimating the circular–linear density in Example 1 and 2.

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-Real data application



Figure: Locations of monitoring stations and power plant.

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Figure: Locations of monitoring stations and power plant.

Raw data

SO₂ measured in µg/m³. Detection limit: > 3µg/m³.

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Wind direction.

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Figure: Locations of monitoring stations and power plant.

Raw data

- ► SO₂ measured in µg/m³. Detection limit: > 3µg/m³.
- Wind direction.

Our data

- Hourly averaged SO₂ and wind direction (circular mean).
- Perturbation to avoid repeated data.

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Box–Cox in SO₂.

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Circular-linear density estimation

Linear case: Azzalini (1981) proposes a perturbation that allows a consistent estimation of the distribution:

$$\widetilde{X}_i = X_i + b\varepsilon_i, \ \varepsilon_i \sim \operatorname{Epanech}\left(-\sqrt{5}, \sqrt{5}\right),$$

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where $b = C^* n^{-\delta}$. Optimum choice of δ is $\frac{1}{3}$, derived from $b_{\text{AMISE}} = \mathcal{O}(n^{-\frac{1}{3}})$. C^* is chosen as $1.3\hat{\sigma}$.

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• Circular case: **open problem**. Our perturbation:

$$\widetilde{\theta}_i = \theta_i + d\varepsilon_i, \, \varepsilon_i \sim v M(0, 1),$$

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• Circular case: **open problem**. Our perturbation:

$$\widetilde{\theta}_i = \theta_i + d\varepsilon_i, \, \varepsilon_i \sim v M(0,1),$$

with $d = n^{-\frac{1}{5}}$. Analogy with the bidimensional (S¹) linear $b_{\text{AMISE}} = \mathcal{O}(n^{-\frac{1}{5}})$ (Liu and Yang, 2008).

-Real data application

L Testing independence

Are wind direction and SO₂ independent?

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Circular-linear density estimation

Are wind direction and SO₂ independent?

Circular-linear correlation coefficients (Mardia, 1976):

- ρ_{CL} : R^2 for $X \sim \cos(\Theta) + \sin(\Theta)$.
- D_n : ranks correlation. Test for $H_0: D_n = 0$.

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Uniformity tests (Mardia and Jupp, 2000):

- Kuiper: Kolmogorov-type test.
- Watson: Cramer-von Mises test.
- Rayleigh: Alternative hypothesis is a unimodal distribution.
- Rao's Spacing test.

Circular-linear density estimation

Station B1



Figure: SO_2 concentration (Box–Cox) in B1.



Figure: Wind direction in B1.

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Circular-linear density estimation

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Circular-linear density estimation

Station B1



Figure: Estimation of g in B1.

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Circular-linear density estimation Real data application

Station B1



Test	Statistic	p–value
Kuiper	2.8196	< 0.01
Watson	0.6425	< 0.01
Rayleigh	0.1552	< 0.01
Rao	140.8554	< 0.05

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Table: Uniformity tests for g.

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Circular-linear density estimation

Station B1



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Circular-linear correlation

- $\rho_{CL} = 0.1515.$
- ▶ D_n = 0.1422 with p-value=0.

Circular-linear density estimation

Station B1



Figure: Surface and contourplot of the estimated circular-linear density in B1.

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Another exploratory tool: circular regression.

• Consider a circular regression model:

$$Y = m(\Theta) + \varepsilon, \quad m(\theta) = \mathbb{E}\left(Y|\Theta = \theta\right)$$

with ε a zero-mean variable independent from Θ .

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Circular-linear density estimation

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The circular Nadaraya–Watson, with von Mises kernel, is

$$\hat{m}(\theta;\nu) = \frac{\sum_{i=1}^{n} y_i \cdot \varphi_{vM}(\theta - \theta_i; 0, \nu)}{\sum_{i=1}^{n} \varphi_{vM}(\theta - \theta_i; 0, \nu)}$$

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Possible selection of ν:

$$\nu_{\mathsf{LSCV}} = \arg\min_{\kappa \ge 0} \sum_{i=1}^{n} \left(y_i - \hat{m}^{-i}(\theta_i; \kappa) \right)^2$$

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Circular-linear density estimation

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Circular-linear density estimation

Station B1



Figure: Circular regression of SO₂ (Box–Cox) in wind direction for B1.

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Circular-linear density estimation

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Circular-linear density estimation

Station G2



Figure: Circular regression of SO₂ (Box–Cox) in wind direction for G2.

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Circular-linear density estimation

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Circular	-linea	nr density	estimation
Real	data	applicatio	on

Station G2



Figure: Estimation of g in G2.

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Figure: Estimation of g in G2.

Test	Statistic	p–value
Kuiper	1.2042	> 0.15
Watson	0.0748	> 0.10
Rayleigh	0.0259	0.737
Rao	130.7370	> 0.10

Table: Uniformity tests for g.

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Circular-linear density estimation

Station G2



Figure: Estimation of g in G2.

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Kuiper	1.2042	> 0.15
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Table: Uniformity tests for g.

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Circular-linear correlation

- $\rho_{CL} = 0.0103.$
- ▶ D_n = 0.0124 with p-value=0.0622.

Station G2



Figure: Right: contourplot of the estimated density in G2. Left: contourplot under independence.

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Circular-linear density estimation

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Conclusions

- ► B1:
 - Moderate dependence between wind direction and SO_2 .
 - ► Higher SO₂ concentrations linked to the NE and N wind, opposite direction to the power plant.
- ► G2: independence between wind direction and SO₂.

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Open problems

- 1. Circular data perturbation.
- 2. Goodness-of-fit test for the Johnson and Wehrly family of circular-linear distributions.

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Exploring wind direction and SO₂ concentration by circular–linear density estimation

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