Dependencies in higher dimensions and in complex data structures

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introduction

example: data on Environmental Quality Index

- available at website of United States Environmental Protection Agency `https://edg.epa.gov/data/Public/ORD/NHEERL/EQI`
- Lobdell *et al.* (2011)
- EQI: variables from five domains – air, water, land, built and sociodemographic
- 3141 observations (representing different locations across the US)

219 variables

consider here variables with more than 90% of unique values

restricting to 3 domains (air, land and water) ...

Table: List of selected variables. Units do not affect analysis and are thus omitted.

Domain	Dimension	Variables
Air	9	Acrolein, Acrylonitrile, Carbon disulfide, Chlorobenzene, Glycol ethers, Methanol, Methyl isobutyl ketone, Polycyclic organic matter/polycyclic aromatic hydrocarbons, Selenium compounds
Water	9	Ammonium, Calcium, Chloride, Magnesium, Nitrate, Potassium, Sodium, Sulfate (all in precipitation), Mercury (deposited)
Land	4	Lead, Zinc, Copper, Herbicides
Combined	22	All the above variables

bivariate association measures and copulas

standard measure of strength of pairwise dependence:

Pearson's correlation coefficient

$$\rho^{(\mathsf{P})}(X_1, X_2) = \frac{\mathsf{Cov}(X_1, X_2)}{\sqrt{\mathsf{Var}(X_1)\mathsf{Var}(X_2)}} = \frac{\mathsf{E}(X_1X_2) - \mathsf{E}(X_1)\,\mathsf{E}(X_2)}{\sqrt{\mathsf{Var}(X_1)\mathsf{Var}(X_2)}}$$

if (X_1, X_2) has a bivariate normal distribution function, then $\rho^{(\mathsf{P})}(X_1, X_2)$ completely characterizes the dependence structure

needs assumption of finite variances

$\Longrightarrow$ need for other association measures

Spearman's rho

Kendall's tau

...

many association measures for measuring **strength of dependency** between X_1 and X_2:

- **Kendall's tau**

with (Y_1, Y_2) an independent copy of (X_1, X_2)

$$\tau(X_1, X_2) = \Pr\left[(X_1 - Y_1)(X_2 - Y_2) > 0\right] - \Pr\left[(X_1 - Y_1)(X_2 - Y_2) < 0\right]$$

- **Spearman's rho**

with (Y_1, Y_2) and (Z_1, Z_2) two independent copies of (X_1, X_2)

$$\begin{aligned}\rho^{(\mathsf{S})}(X_1, X_2) &= 3\left\{\Pr\left[(X_1 - Y_1)(X_2 - Z_2) > 0\right] - \Pr\left[(X_1 - Y_1)(X_2 - Z_2) < 0\right]\right\} \\ &= \frac{\mathsf{Cov}\big(F_1(X_1), F_2(X_2)\big)}{\sqrt{\mathsf{Var}(F_1(X_1))\mathsf{Var}(F_2(X_2))}} = \rho^{(\mathsf{P})}\big(\underbrace{F_1(X_1)}_{=U_1}, \underbrace{F_2(X_2)}_{=U_2}\big)\end{aligned}$$

- **Gini's gamma**
- **Blomqvist beta**

.....

what about the dependence structure?

copula function

joint cumulative distribution function of (X_1, X_2) :

$$F(x_1, x_2) = \Pr(X_1 \leq x_1, X_2 \leq x_2) \qquad (x_1, x_2) \in \mathbb{R}^2$$

marginal cumulative distribution functions :
$F_1(x_1) = P(X_1 \leq x_1) \qquad F_2(x_2) = P(X_2 \leq X_2)$

Sklar's theorem (Sklar (1959)); $\exists$ function $C : [0,1]^2 \to [0,1]$ such that

$$F(x_1, x_2) = C(F_1(x_1), F_2(x_2)) \qquad (x_1, x_2) \in \mathbb{R}^2$$

if $F_1(x)$ and $F_2(x)$ are continuous in x, then C is **unique**

C fully describes the dependence structure between X_1 and X_2

C is joint distribution function of $U_1 = F_1(X_1)$ and $U_2 = F_2(X_2)$

copula and association measures

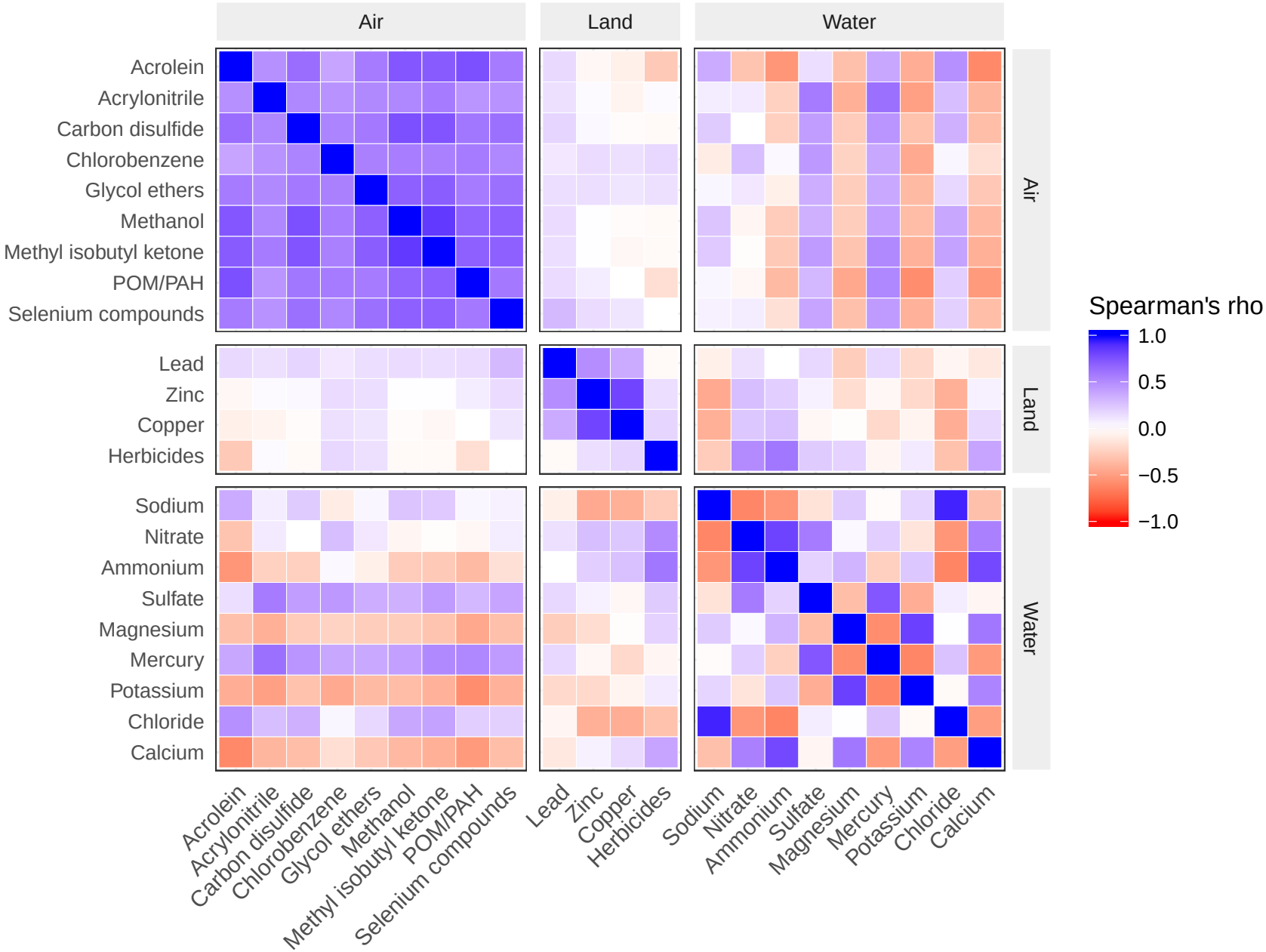
copula	association measure	
C	Kendall's tau	$\tau = 4 \iint C(u_1, u_2)\, dC(u_1, u_2) - 1$
	Spearman's rho	$\rho = 12 \iint C(u_1, u_2)\, du_1\, du_2 - 3$
	Blomqvist's beta	$\beta = 4\, C(0.5, 0.5) - 1$
	Gini's index	$\gamma = 4 \left[\int_0^1 C(u, 1-u) du - \int_0^1 [u - C(u, u)] du \right]$
	...	...

any of these association measures:

functional of the bivariate copula C $(= C_2)$

$\kappa_2(C_2)$

example: heatmap of the empirical pairwise Spearman's rho values



multivariate association measures

d-variate random vector $\mathbf{X} = (X_1, \ldots, X_d)^\top$

aim: how to measure association between the d components ?
which properties ?

what happens if d increases, and eventually tends to infinity ?

F: joint cumulative distribution function of $\mathbf{X}$

$F_1, \ldots, F_d$: continuous marginal distribution functions of $X_1, \ldots, X_d$

applying Sklar's theorem: $\exists$ function $C_d : [0,1]^d \to [0,1]$ such that

$$F(x_1, \ldots, x_d) = C_d(F_1(x_1), \ldots, F_d(x_d)), \quad (x_1, \ldots, x_d)^\top \in \mathbb{R}^d$$

C_d joint cumul. distrib. funct. of $\boldsymbol{U} = (U_1, \ldots U_d)^\top = (F_1(X_1), \ldots, F_d(X_d))^\top$:

$$C_d(\boldsymbol{u}) = \Pr(\boldsymbol{U} \leq \boldsymbol{u}) \qquad \boldsymbol{u} = (u_1, \ldots, u_d)^\top \in [0,1]^d$$

multivariate association measure:

$$\begin{array}{rccl} \kappa_d: & \mathsf{Cop}(d) & \longrightarrow & \mathbb{R} \\ & C_d & \longrightarrow & \kappa_d(C_d) \end{array} \qquad \mathsf{Cop}(d) = \text{set of all } d\text{-variate copulas}$$

what do we expect as properties of such a function ?

some concepts and notations: for a copula C_d of $\boldsymbol{U}$, define

- **survival function** $\overline{C}_d(\boldsymbol{u}) = \Pr(\boldsymbol{U} > \boldsymbol{u})$
- the **survival copula** C_d^S is defined as the copula of $\mathbf{1} - \boldsymbol{U}$, that is

$$C_d^S(\boldsymbol{u}) = \Pr(\mathbf{1} - \boldsymbol{U} \leq \boldsymbol{u}) = \Pr(\boldsymbol{U} > \mathbf{1} - \boldsymbol{u}) = \overline{C}_d(\mathbf{1} - \boldsymbol{u})$$

- **concordance ordering** for copulas $A_d, B_d \in \mathsf{Cop}(d)$:

$$A_d \preceq_C B_d \iff \forall \boldsymbol{u} \in [0,1]^d : A_d(\boldsymbol{u}) \leq B_d(\boldsymbol{u}) \text{ and } \overline{A}_d(\boldsymbol{u}) \leq \overline{B}_d(\boldsymbol{u})$$

- **reflections** of the d-dimensional unit cube $[0,1]^d$:

  a mapping $\xi : [0,1]^d \to [0,1]^d$ is a reflection if $\xi(\boldsymbol{u}) = \boldsymbol{v}$ where for $i \in \{1, \ldots, d\}$ we have $v_i = u_i$ or $v_i = 1 - u_i$

  set of all reflections: $\mathcal{R}_d$

  for any reflection $\xi \in \mathcal{R}_d$, we can define a new copula C_d^{ξ}

  - reflection with respect to all components:

    will be denoted as σ, that is $\sigma(\boldsymbol{u}) = \mathbf{1} - \boldsymbol{u}$

    if C_d is copula of $(X_1, \ldots, X_d)$, then C_d^{σ} is copula of $(-X_1, \ldots, -X_d)$

axioms for multivariate association measures

Rényi (1952), Scarsini (1984), Taylor (2007), Schmid it et al. (2010), ...

(A_1) (Normalization) $\kappa_d(M_d) = 1, \kappa_d(\Pi_d) = 0$.

(A_2) (Continuity) If $\lim_{m\to\infty} C_{d,m}(\boldsymbol{u}) = C_d(\boldsymbol{u}), \forall \boldsymbol{u} \in [0,1]^d$, then $\lim_{m\to\infty} \kappa_d(C_{d,m}) = \kappa_d(C_d)$.

(A_3) (Permutation invariance) $\kappa_d(C_d^\pi) = \kappa_d(C_d)$ for every permutation π.

(A_4) (Ordering) If $C_{d,1} \preceq_C C_{d,2}$, then $\kappa_d(C_{d,1}) \leq \kappa_d(C_{d,2})$.

(A_5) (Duality) $\kappa_d(C_d^\sigma) = \kappa_d(C_d)$.

(A_6) (Reflection principle) $\sum_{\xi\in\mathcal{R}_d} \kappa_d(C_d^\xi) = 0$.

(A_7) (Transition property) There exists a constant r_{d-1} such that

$$\kappa_d(C_d) + \kappa_d(C_d^{\sigma_1}) = r_{d-1}\kappa_{d-1}(C_{d-1}^{(-1)})$$

(A_8) (Independent component addition) For X_{d+1} independent of $(X_1, \ldots, X_d)^\top$

$$\kappa_d(C_d) > \kappa_{d+1}(C_{d+1}) > 0, \quad \text{or} \quad \kappa_d(C_d) < \kappa_{d+1}(C_{d+1}) < 0,$$
$$\text{or} \quad \kappa_d(C_d) = \kappa_{d+1}(C_{d+1}) = 0.$$

how to get to multivariate association meaures ?

does an association measure satisfy these expected, minimal, properties ?

which other properties do they exhibit?

two main approaches towards getting to multivariate association measures:

- pairwise approach: rely on looking at values of bivariate association measures
- copula approach: generalize the bivariate structure to multivariate setting

pairwise approach

- κ_2: bivariate association measure
- create a d-variate association measure as an average of all pairwise measures, i.e.

$$\kappa_d^{\mathsf{PW}}(C_d) = \frac{1}{\binom{d}{2}} \sum_{1 \le i < j \le d} \kappa_2(C_2^{i,j}) \qquad \text{with } C_2^{i,j} \text{ copula of } (X_i, X_j)^\top$$

- does such an approach fullfills the desired properties?

Proposition

Let $\kappa_2 : \mathrm{Cop}(2) \to \mathbb{R}$ be a bivariate measure of association
Define for $d \in \{2, 3, \dots\}$, the measure $\kappa_d^{\mathsf{PW}} : \mathrm{Cop}(d) \to \mathbb{R}$, and set $r_{d-1} = 2(d-2)/d$ in axiom (A_7).
Then $\{(\kappa_d^{\mathsf{PW}}, r_d)\}_{d=3}^{\infty}$ fulfils axioms (A_1) to (A_8).

pairwise approach leads to a 'reasonable' multivariate association measure if the initial bivariate measure is 'reasonable' ...

but : pairwise-constructed measures always assign value 0 to vectors having pairwise independent components no matter if there is an association of higher order ...

copula approach

• multivariate Spearmans's rho

- recall bivariate Spearman's rho:

$$\rho(X_1, X_2) = \frac{\mathsf{cov}(U_1, U_2)}{\sqrt{\mathsf{Var}(U_1)}\sqrt{\mathsf{Var}(U_2)}}$$

- this can be expressed as

$$\begin{aligned}
\rho(C_2) &= \frac{\int_{[0,1]^2} u_1 u_2 \mathrm{d}C_2(u_1, u_2) - (1/2)^2}{\sqrt{(1/12)}\sqrt{(1/12)}} \\
&= \frac{\int_{[0,1]^2} \Pi_2(\boldsymbol{u})\mathrm{d}C_2(\boldsymbol{u}) - \int_{[0,1]^2} \Pi_2(\boldsymbol{u})\mathrm{d}\Pi_2(\boldsymbol{u})}{\underbrace{\int_{[0,1]^2} \Pi_2(\boldsymbol{u})\mathrm{d}M_2(\boldsymbol{u})}_{=1/3} - \underbrace{\int_{[0,1]^2} \Pi_2(\boldsymbol{u})\mathrm{d}\Pi_2(\boldsymbol{u})}_{=1/4}} \qquad \boldsymbol{u} = (u_1, u_2)^\top
\end{aligned}$$

where

$\Pi_2(\boldsymbol{u}) = u_1 u_2$ independence copula

$M_2(\boldsymbol{u}) = \min(u_1, u_2)$ comonotonicity copula, Fréchet upper bound

- a first multivariate generalization (Wolff (1980)) is

$$\begin{aligned}\rho_1(C_d) &= \frac{\int_{[0,1]^d} C_d(\boldsymbol{u})\mathrm{d}\boldsymbol{u} - \int_{[0,1]^d} \Pi_d(\boldsymbol{u})\mathrm{d}\boldsymbol{u}}{\underbrace{\int_{[0,1]^d} M_d(\boldsymbol{u})\mathrm{d}\boldsymbol{u}}_{=1/(d+1)} - \underbrace{\int_{[0,1]^d} \Pi_d(\boldsymbol{u})\mathrm{d}\boldsymbol{u}}_{=1/2^d}} \\ &= h_\rho(d)\left\{2^d \int_{[0,1]^d} C_d(\boldsymbol{u})\mathrm{d}\boldsymbol{u} - 1\right\}\end{aligned}$$

with $h_\rho(d) = (d+1)/\{2^d - (d+1)\}$

- or start from alternative expression in bivariate case, obtained after integration by parts (Schmid *et al.* (2007))

$$\rho(C_2) = \frac{\int_{[0,1]^2} C_2(\boldsymbol{u})\mathrm{d}\Pi_2(\boldsymbol{u}) - \int_{[0,1]^2} \Pi_2(\boldsymbol{u})\mathrm{d}\Pi_2(\boldsymbol{u})}{\int_{[0,1]^2} M_2(\boldsymbol{u})\mathrm{d}\Pi_2(\boldsymbol{u}) - \int_{[0,1]^2} \Pi_2(\boldsymbol{u})\mathrm{d}\Pi_2(\boldsymbol{u})} = \frac{\int [C_2(\boldsymbol{u}) - \Pi_2(\boldsymbol{u})]\,\mathrm{d}\Pi_2(\boldsymbol{u})}{\int [M_2(\boldsymbol{u}) - \Pi_2(\boldsymbol{u})]\,\mathrm{d}\Pi_2(\boldsymbol{u})}$$

standardized average distance between C_2 and Π_2

- leads to an alternative multivariate generalization (Joe (1990), ...)
- two generalizations of bivariate Spearman's rho:

$$\rho_1(C_d) = h_\rho(d)\left\{2^d \int_{[0,1]^d} C_d(\boldsymbol{u})\mathrm{d}\boldsymbol{u} - 1\right\}$$

$$\rho_2(C_d) = h_\rho(d)\left\{2^d \int_{[0,1]^d} \Pi_d(\boldsymbol{u})\mathrm{d}C_d(\boldsymbol{u}) - 1\right\}$$

which of these generalizations is preferable ?

- both ρ_1 and ρ_2 satisfy $(A_1) - (A_7)$
  except for the duality axiom (A_5) (see Schmid *et al.* (2010))

  (A_8) is satisfied for ρ_1 and ρ_2 (G. Kika & Omelka (2021))

multivariate Kendall's tau

- bivariate Kendall's tau:

$$\tau(X_1, X_2) = \Pr\{(X_1 - Y_1)(X_2 - Y_2) > 0\} - \Pr\{(X_1 - Y_1)(X_2 - Y_2) < 0\}$$

  where (X_1, X_2) has copula C_2

- can be expressed as

$$\tau(C_2) = 4 \int_{[0,1]^2} C_2(\boldsymbol{u}) \mathrm{d}C_2(\boldsymbol{u}) - 1$$

- can be generalized as (Nelsen (1996), ...)

$$\tau(C_d) = \frac{1}{2^{d-1} - 1} \left\{ 2^d \int_{[0,1]^d} C_d(\boldsymbol{u}) \mathrm{d}C_d(\boldsymbol{u}) - 1 \right\}$$

$\tau(C_d)$ satisfies $(A_1) - (A_8)$

multivariate Gini's gamma

- bivariate Gini's gamma

$$\gamma(C_2) = 2 \int_{[0,1]^2} (M_2(\boldsymbol{u}) + W_2(\boldsymbol{u}) + \overline{M}_2(\boldsymbol{u}) + \overline{W}_2(\boldsymbol{u}))\mathrm{d}C_2(\boldsymbol{u}) - 2$$

$M_2(u_1, u_2) = \min(u_1, u_2)$	comonotonicity copula	Fréchet upper bound
$W_2(u_1, u_2) = \max(u_1 + u_2 - 1, 0)$	countermonotonicity copula	Fréchet lower bound

$$W_2 \leq C \leq M_2$$

- first multivariate generalization (Behboodian *et al.* (2007))

$$\gamma_1(C_d) = \frac{1}{b(d) - a(d)} \left(\int_{[0,1]^d} (M_d(\boldsymbol{u}) + W_d(\boldsymbol{u}) + \overline{M}_d(\boldsymbol{u}) + \overline{W}_d(\boldsymbol{u}))\mathrm{d}C_d(\boldsymbol{u}) - a(d) \right)$$

where

$$a(d) = \frac{2}{d+1} + \frac{1}{(d+1)!} + \sum_{j=0}^{d} (-1)^j \binom{d}{j} \frac{1}{(j+1)!} \qquad b(d) = 2 - \sum_{j=1}^{d-1} \frac{1}{2j}$$

- alternative expression for bivariate Gini's gamma:

$$\gamma(C_2) = 8 \int_{[0,1]^2} C_2(\boldsymbol{u}) \mathrm{d} \left(\frac{M_2(\boldsymbol{u}) + W_2(\boldsymbol{u})}{2} \right) - 2$$

- leads to multivariate generalization (Taylor(2007))

$$\gamma_2(C_d) = \frac{2^d}{2^{d-1}-1} \left(\int_{[0,1]^d} (C_d(\boldsymbol{u}) + C_d^S(\boldsymbol{u})) \mathrm{d} \left(\frac{1}{2^d} \sum_{\xi \in \mathcal{R}_d} M_d^{\xi}(\boldsymbol{u}) \right) - \frac{1}{2^{d-1}} \right)$$

- can conveniently be expressed in terms of reflections

$$\gamma_2(C_d) = \frac{1}{2^{d-1}-1} \left(\sum_{\xi \in \mathcal{R}_d} \int_0^1 (C_d(\xi(u,\ldots,u)) + \overline{C}_d(\xi(u,\ldots,u))) \mathrm{d}u - 2 \right)$$

which involves only calculation of one-dimensional integrals!

which of these two generalizations is preferable ?

- two generalizations of bivariate Gini's gamma:

$$\gamma_1(C_d) = \frac{1}{b(d) - a(d)} \left(\int_{[0,1]^d} (M_d(\boldsymbol{u}) + W_d(\boldsymbol{u}) + \overline{M}_d(\boldsymbol{u}) + \overline{W}_d(\boldsymbol{u})) \mathrm{d}C_d(\boldsymbol{u}) - a(d) \right)$$

$$\gamma_2(C_d) = \frac{1}{2^{d-1} - 1} \left(\sum_{\xi \in \mathcal{R}_d} \int_0^1 (C_d(\xi(u, \ldots, u)) + \overline{C}_d(\xi(u, \ldots, u))) \mathrm{d}u - 2 \right)$$

- has been shown that (G., Kika & Omelka (2021))
  - γ_1: satisfies $(A_1) - (A_3)$

    does NOT satisfy duality axiom (A_5) and (A_8)
  - γ_2: satisfies $(A_1) - (A_8)$

    simpler expression (only one-dimensional integrals)

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bivariate $\Longrightarrow$ multivariate association measures

not so straightforward; which version matters ...

multivariate association measures in increasing dimension

what happens with association measures in case of growing dimension ?

- difficult to study in full generality
- study in 2 settings: Archimedean copulas
  meta-elliptical copulas

Archimedian copulas:

* C_d is a d-dimensional Archimedean copula if for any $\boldsymbol{u} \in [0,1]^d$ it permits the representation

$$C_d(\boldsymbol{u}) = \psi\left[\psi^{-1}(u_1) + \cdots + \psi^{-1}(u_d)\right]$$

for some Archimedean generator ψ

$\psi : [0,\infty) \to [0,1]$ a nonincreasing and continuous function
satisfying $\psi(0) = 1$, $\lim_{x\to\infty} \psi(x) = 0$
is strictly decreasing on $[0, \inf\{x : \psi(x) = 0\})$

• Archimedian copulas and multivariate association measures in increasing dimension

- **Spearman's rho** in increasing dimension Wysocki (2015) showed

$$\lim_{d\to\infty} \rho_1(C_d) = c_1 \in [0,1] \quad \Longleftrightarrow \quad \lim_{d\to\infty} (d+1) \int_{[0,1]^d} C_d(\boldsymbol{u}) \mathrm{d}\boldsymbol{u} = c_1$$

$$\lim_{d\to\infty} \rho_2(C_d) = c_2 \in [0,1] \quad \Longleftrightarrow \quad \lim_{d\to\infty} (d+1) \int_{[0,1]^d} \Pi_d(\boldsymbol{u}) \mathrm{d}C_d(\boldsymbol{u}) = c_2$$

  unknown: whether strict positive c_1 and c_2 are possible (achievable)

- **Kendall's tau** in increasing dimension Wysocki (2015) showed

$$\lim_{d\to\infty} \tau(C_d) = 0$$

  or Archimedean copulas are not able to carry any association (measured with Kendall's tau) in very high dimension

- **Gini's gamma** in increasing dimension
  - ◇ established explicit expression for $\gamma_2(\cdot)$ in terms of generator
  - ◇ shown that (Kika, G. & Omelka (2021))

$$\lim_{d\to\infty} \gamma_2(C_d) = 0$$

• meta-elliptical copulas and multivariate association measures in increasing dimension

meta-elliptical copulas are copulas with elliptical contours

- Genest *et al.* (2011): all meta-elliptical copulas with the same correlation matrix also share the same Kendall's tau value

  Kendall's tau depends only on the correlation matrix

- more precisely: C_d copula of $\boldsymbol{U} = (U_1, \ldots U_d)^\top$

  meta-elliptical copula with correlation matrix $\boldsymbol{R} = (\varrho_{i,j})$, with $\varrho_{i,j} \in [-1, 1]$; then

$$\tau(C_d) = \frac{1}{2^{d-1} - 1}\{-1 + 2^d \Pr(\boldsymbol{Z} \geq \boldsymbol{0})\}$$

  $\boldsymbol{Z}$ is d-variate mean zero normal random vector with correlation matrix $\boldsymbol{R}$

- what happens if d increases ?
- so far: answer is known only for some specific correlation structures

- correlation matrix $\boldsymbol{R}$ of the form

$$\varrho_{i,j} = \lambda_i \lambda_j, \quad i \neq j \qquad \lambda_j \in [-1, 1]$$

covers an equicorrelated correlation matrix

for which $\varrho_{i,j} = \varrho$ for all $i \neq j$, with $\varrho \in (-1/(d-1), 1)$

- correlation matrix $\boldsymbol{R}$ of a banded type and $(m+2)$-diagonal (with $m \in \mathbb{Z}_{>0}$), and takes the form

$$\varrho_{i,j} = \begin{cases} 1, & \text{if } i = j \\ c_{i,j} & \text{if } |i-j| \in \{1, \cdots, m\} \\ 0, & \text{if } |i-j| > m \end{cases}$$

where $c_{i,j} = c_{j,i} \in [-1, 1]$ are constants, not all zero, and such that $\boldsymbol{R}$ is a correlation matrix

$$\begin{pmatrix} 1 & * & 0 & 0 & \dots & 0 \\ * & 1 & * & 0 & \dots & 0 \\ 0 & * & 1 & * & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & * & 1 & * & 0 \\ 0 & \dots & 0 & * & 1 & * \\ 0 & \dots & 0 & 0 & * & 1 \end{pmatrix}$$

case $(m = 1)$: tridiagonal matrix; only non-zero values on main diagonal and 2 adjacent diagonals

for both correlation structures Kendall's tau tends to zero as d tends to infinity

Theorem

Let $\{C_d\}$ be a sequence of d-dimensional meta-elliptical copulas with a correlation matrix $\boldsymbol{R} = (\varrho_{i,j})$

(i) first correlation structure: the λ_j satisfy the assumption that there exists $\lambda_0 < 1$ such that $\lambda_j \leq \lambda_0$ for all $j \in \mathbb{Z}_{>0}$

or

(ii) second correlation structure

in both cases, it holds that $\lim_{d\to\infty} \tau(C_d) = 0$

what can happen in case of other correlation structures?

nonparametric estimation of multivariate association measures

$\boldsymbol{X}$ with copula C_d **unknown** (C_d joint distribution of $(\underbrace{F_1(X_1)}_{=U_1}, \ldots, \underbrace{F_d(X_d)}_{=U_d})$)

marginal distributions $F_1, \cdots, F_d$ **unknown**

$\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n$ random sample from $\boldsymbol{X} = (X_1, \ldots, X_d)^\top$

where $\boldsymbol{X}_i = (X_{1,i}, \ldots X_{d,i})^\top$ for $i \in \{1, \ldots n\}$

nonparametric estimation of multivariate association measures

- empirical marginal distribution function F_j for the j-th component

$$\widehat{F}_{j,n}(x) = \frac{1}{n+1} \sum_{i=1}^{n} \mathbb{1}(X_{j,i} \leq x)$$

  lead to pseudo-observations $\widehat{U}_{j,i} = \widehat{F}_{j,n}(X_{j,i})$ from $U_j = F_j(X_j)$
- empirical copula (recall: $C(\boldsymbol{u}) = \Pr(\boldsymbol{U} \leq \boldsymbol{u})$)

$$\widehat{C}_n(\boldsymbol{u}) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}(\widehat{U}_{1,i} \leq u_1, \ldots, \widehat{U}_{d,i} \leq u_d)$$

- and empirical survival function (recall: $\overline{C}_d(\boldsymbol{u}) = \Pr(\boldsymbol{U} > \boldsymbol{u})$)

$$\widehat{\overline{C}}_n(\boldsymbol{u}) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}(\widehat{U}_{1,i} > u_1, \ldots, \widehat{U}_{d,i} > u_d)$$

- nonparametric estimator of an association measure $\kappa(C)$

$$\widehat{\kappa}_n = \kappa(\widehat{C}_n)$$

quality of estimator $\widehat{\kappa}_n$ depends on that of $\widehat{C}_n$ (for the copula C_d)

uniform convergence of empirical copula process
(Tsukahara (2005), Schmid *et al.* (2007), Segers (2012), ...)

joint weak convergence of empirical copula process and empirical survival copula process

- nonparametric estimators for Spearman's rho (Schmid *et al.* (2007))
- nonparametric estimator for Kendall's tau (Genest *et al.* (2011)):

$$\widehat{\tau}_n = \frac{1}{2^{d-1}-1}\left\{\frac{2^d}{n(n-1)}\left[\sum_{i\neq j}\mathbb{1}\left(\boldsymbol{X}_i \leq \boldsymbol{X}_j\right)\right]-1\right\}$$

asymptotic normality result: as $n \to \infty$

$$\sqrt{n}(\widehat{\tau}_n - \tau(C)) \xrightarrow{D} \mathcal{N}(0, \sigma_\tau^2)$$

where $$\sigma_\tau^2 = \left(\frac{2^d}{2^{d-1}-1}\right)^2 \mathrm{Var}(C(\boldsymbol{U}) + \overline{C}(\boldsymbol{U}))$$

- nonparametric estimator for Gini's gamma (Kika, G. & Omelka (2021)):

$$\sqrt{n}\left(\widehat{\gamma}_{2n} - \gamma_2(C)\right) \xrightarrow{D} \mathcal{N}\left(0, \sigma_{\gamma_2}^2\right) \qquad \text{with } \sigma_{\gamma_2}^2 = ...$$

standard errors of the estimators

- get approximate standard errors by bootstrap procedures
- rely on asymptotic normality results, but focus on the main terms in the i.i.d. representations ...
- for example for CI for the multivariate Kendall's tau:
  - variance $\mathrm{Var}(C(\boldsymbol{U}) + \overline{C}(\boldsymbol{U}))$ can be estimated, using ideas from U-statistics, by the sample variance of $W_1, \ldots, W_n$, i.e.

$$\widehat{\sigma}_n^2 = \frac{1}{n-1} \sum_{i=1}^{n} (W_i - \overline{W}_n)^2, \quad \text{where} \quad \overline{W}_n = \frac{1}{n} \sum_{i=1}^{n} W_i$$

with

$$W_i = \frac{1}{n-1} \sum_{j=1, j \neq i}^{n} \mathbb{1}(\boldsymbol{X}_j \leq \boldsymbol{X}_i) + \frac{1}{n-1} \sum_{j=1, j \neq i}^{n} \mathbb{1}(\boldsymbol{X}_j \geq \boldsymbol{X}_i)$$

  - the standard error of $\widehat{\tau}_n$ is estimated by $\frac{2^d}{2^{d-1}-1} \frac{\widehat{\sigma}_n}{\sqrt{n}}$

real data application: data on Environmental Quality Index (EQI)

Table: Estimated multivariate association measures for EQI dataset (bootstrap SE).

Domain	d	$\widehat{\rho}_{3n}$	$\widehat{\tau}_n$	$\widehat{\gamma}_{2n}$
Air	9	0.44 (0.008)	0.29 (0.007)	0.29 (0.006)
Water	9	0.04 (0.004)	0.03 (0.002)	0.02 (0.002)
Land	4	0.30 (0.011)	0.21 (0.008)	0.23 (0.009)
Combined	22	0.00 (0.000)	0.00 (0.000)	0.00 (0.000)
AirPlus	12	**0.23** (0.008)	**0.15** (0.005)	**0.14** (0.006)

Domain	d	$\widehat{\rho}_n^{\mathrm{PW}}$	$\widehat{\tau}_n^{\mathrm{PW}}$	$\widehat{\gamma}_n^{\mathrm{PW}}$
Air	9	0.60 (0.007)	0.44 (0.006)	0.49 (0.006)
Water	9	0.05 (0.005)	0.04 (0.004)	0.03 (0.004)
Land	4	0.33 (0.011)	0.24 (0.008)	0.27 (0.009)
Combined	22	0.11 (0.003)	0.09 (0.002)	0.09 (0.002)
AirPlus	12	**0.50** (0.007)	**0.36** (0.005)	**0.40** (0.006)

AirPlus: all 9 variables from the air domain, extended with 3 variables from the water domain (Sulfate, Mercury and Chloride)

multivariate tail coefficients

- bivariate lower and upper tail coefficients:

$$\lambda_L(C_2) = \lim_{u \searrow 0} \mathsf{P}(U_2 \leq u | U_1 \leq u) = \lim_{u \searrow 0} \mathsf{P}(U_1 \leq u | U_2 \leq u) = \lim_{u \searrow 0} \frac{C_2(u,u)}{u}$$

$$\lambda_U(C_2) = \lim_{u \nearrow 1} \mathsf{P}(U_2 > u | U_1 > u) = \lim_{u \nearrow 1} \mathsf{P}(U_1 > u | U_2 > u) = \lim_{u \nearrow 1} \frac{1 - 2u + C_2(u,u)}{1-u}$$

- multivariate tail coefficients in the literature ?
  - Frahm's extremal dependence coefficient (Frahm (2006)):
    with $U_{\max} = \max(U_1, \ldots, U_d)$ and $U_{\min} = \min(U_1, \ldots, U_d)$

$$\epsilon_L(C_d) = \lim_{u \searrow 0} \mathsf{P}(U_{\max} \leq u | U_{\min} \leq u) = \lim_{u \searrow 0} \frac{C_d(u, \ldots, u)}{1 - \overline{C}_d(u, \ldots, u)}$$

$$\epsilon_U(C_d) = \lim_{u \nearrow 1} \mathsf{P}(U_{\min} > u | U_{\max} > u) = \lim_{u \nearrow 1} \frac{\overline{C}_d(u, \ldots, u)}{1 - C_d(u, \ldots, u)}$$

    coefficients are not equal to λ_L, λ_U respectively in the bivariate case:

$$\epsilon_L(C_2) = \frac{\lambda_L(C_2)}{2 - \lambda_L(C_2)} \qquad \epsilon_U(C_2) = \frac{\lambda_U(C_2)}{2 - \lambda_U(C_2)}$$

different type of tail dependence coefficient ...

- Li's tail dependence parameter (Li (2009), De Luca & Rivieccio (2012),...)

  consider a subset of indices: $\emptyset \neq I_h \subset \{1, \ldots, d\}$ such that $|I_h| = h$ and $J_{d-h} = \{1, \ldots, d\} \backslash I_h$

  lower and upper tail dependence parameters:

$$\lambda_L^{I_h|J_{d-h}}(C_d) = \lim_{u \searrow 0} \mathrm{P}(U_i \leq u, \forall i \in I_h | U_j \leq u, \forall j \in J_{d-h})$$

$$\lambda_U^{I_h|J_{d-h}}(C_d) = \lim_{u \nearrow 1} \mathrm{P}(U_i > u, \forall i \in I_h | U_j > u, \forall j \in J_{d-h})$$

  heavily depends on the choice of the set I_h

  includes the bivariate tail coefficients as special cases

  ($h = 1$, $I_1 = \{1\}$ and $J_1 = \{2\}$)

- Schmid's and Schmidt's tail dependence measure (Schmid & Schmidt (2007))

- ....

additional study:

- in case of extreme value copulas: tail dependence measures in terms of Pickands dependence function
- tail dependence using subvectors (compare with pairwise approach)
- set of desirable for multivariate tail coefficients
- investigate the properties of the tail coefficients, starting from these
- how do they behave when d increases ?

..., Kika, G. & Omelka (2020), ...

- how to estimate them nonparametrically ?

let's have a look at one multivariate tail coefficient ....

- problem when estimating tail coefficients: need to deal with the limits
- Frahm's lower tail and upper tail dependence

$$\epsilon_L(C) = \lim_{u \searrow 0} \frac{C_d(u, \ldots, u)}{1 - \overline{C}_d(u, \ldots, u)}$$

- consider $u_n > 0$
  nonparametric estimator of ϵ_L is

$$\widehat{\epsilon}_L(u_n) = \frac{\widehat{C}_n(u_n, \ldots, u_n)}{1 - \widehat{\overline{C}}_n(u_n, \ldots, u_n)}$$

  assumptions on sequence: such that $u_n \to 0$ and $nu_n \to \infty$, as $n \to \infty$
- in univariate setting: nu_n can be interpreted as number of extreme observations
- **how to choose u_n ?** (G. Kika & Omelka (2022))

application in variable clustering

suppose d objects, denoted $X_1, \ldots, X_d$

n observations on these objects

aim: find clusters in the d objects

- using agglomerative clustering methods
- see e.g. Di Lascio, Durante & Pappadà (2017), ...
  - start: each variable is one cluster (of size 1)
  - in each step: two clusters are merged together
  - example of approach: using linkage method
    - for each pair (X_j, X_k) calculate a bivariate similarity measure s_{jk}
    - translate this into dissimilarity measures: $g : [-1.1] \to [0, +\infty)$ decreasing function with $g(1) = 0$

$$\text{diss}_{j,k} = g(s_{j,k})$$

examples: $g(x) = \sqrt{1-x}$, or $g(x) = \sqrt{1-x^2}$

    - linkage method: describes how dissimilarity between 2 clusters can be based on dissimilarities among elements of the cluster

approach using multivariate dissimilarities: see Fuchs, Lascio & Durante (2021) ....

using multivariate dissimilarities ....

- two vectors $\boldsymbol{Y}$ and $\underline{Z}$, of dimensions d_1 and d_2
  consider $(\boldsymbol{Y}^\top, \boldsymbol{Z}^\top)^\top$, of dimension say d, with copula C_d
- example of dissimilarity function

$$\text{diss}_\tau(C_d) = \left(\frac{2^{d-1}-1}{2^d}\right)(1-\tau(C_d))$$

- (iterative) clustering procedure
  - ⋆ suppose r clusters in the current iteration
  - ⋆ for each pair of clusters $\boldsymbol{M}_k$ and $\boldsymbol{M}_\ell$, $k, \ell = 1, \ldots, r$, $k \neq \ell$, calculate dissimilarity
  - ⋆ merge 2 clusters with smallest dissimilarity measure
  - ⋆ continue to do this until all variables are in one cluster
- stopping rules can be considered, e.g. impose an upper bound for dissimilarity (no longer merge when this is exceeded)

example: data on Environmental Quality Index

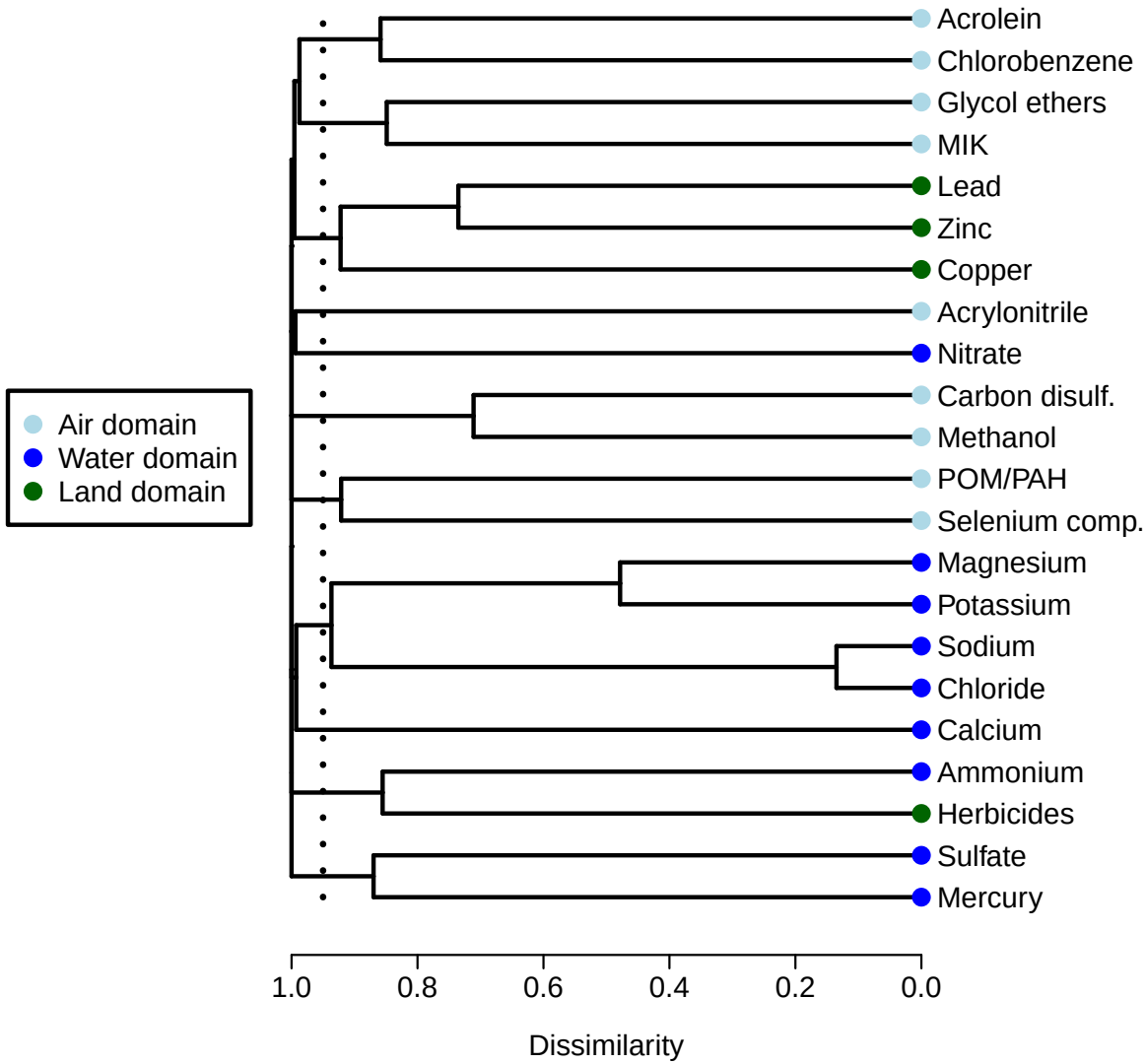

Figure: Clustering of chemical substances in EQI by extreme high concentraties. Vertical dotted line: dissimilarity of 0.95.

11 clusters; mostly of size 2; 1 cluster of size 3; 1 cluster of size 4; ...

measuring associations between random vectors

.... based on comparing clusters pairwise ....

what is we want to look at say k clusters simultaneaously ?

- need association measure between k random vectors, not only 2
- how to measure association between k random vectors ?

some recent approaches:

- ϕ-divergences (cf information theory) (De Keyser & G. (2022), ...)
- based on optimal transport ideas (Mordant & Segers (2022), ...)
- ....

measuring associations in more complex (different) data structures

- what if random variables are not real values, but curves, images, ... ?
- what if data live on a circle, a torus, ...?
- ...

how to measure (strength of) dependence in these cases?

for circular data: bivariate case

- random angles Θ_1, Θ_2, with joint (circular) cum. distr, function F and marginals F_1 and F_2
- a bivariate circula is defined as
  (Kato *et al.* (2022), Ameijeiras-Alonso & G. (2022), ...)

$$F(\theta_1, \theta_2) = C\left(2\pi F_1(\theta_1) - \pi, \ldots, 2\pi F_d(\theta_d) - \pi\right) \quad (\theta_1, \theta_2) \in [-\pi, \pi)^2$$

with $C : [-\pi, \pi)^2 \mapsto [0, 1]$, a bivariate circular distribution whose marginals are circular uniform distributions
(circular periodicity, i.e. $F_j(\theta + 2\pi) - F_j(\theta) = 1$)

- consider

$$\mathbf{X}_1 = (\cos(\Theta_1), \sin(\Theta_1))^\top \qquad \mathbf{X}_2 = (\cos(\Theta_2), \sin(\Theta_2))^\top$$

  $\mathbf{X}_1, \mathbf{X}_2$ values in $[-1,1]^2 \subset \mathbb{R}^2$

- since circular uniform marginals: for $s \in \{1,2\}$

$$E(\mathbf{X}_s) = \mathbf{0}^\top \qquad \text{and} \qquad E\left(\mathbf{X}_s \mathbf{X}_s^\top\right) = \mathbf{I}_2/2$$

  where $\mathbf{I}_2$ is the identity matrix of size 2

- furthermore

$$\begin{aligned}
&\boldsymbol{\Sigma}_{12} \\
&= E\left(\mathbf{X}_1 \mathbf{X}_2^\top\right) - E(\mathbf{X}_1)\, E(\mathbf{X}_2)^\top \\
&= \begin{pmatrix} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \sin\theta_1 \sin\theta_2\, \mathbf{C}(\boldsymbol{\theta_1, \theta_2}) d\theta_1 d\theta_2 - 1 & -\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \cos\theta_1 \sin\theta_2\, \mathbf{C}(\boldsymbol{\theta_1, \theta_2}) d\theta_1 d\theta_2 \\ -\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \cos\theta_1 \sin\theta_2\, \mathbf{C}(\boldsymbol{\theta_1, \theta_2}) d\theta_1 d\theta_2 & \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \cos\theta_1 \cos\theta_2\, \mathbf{C}(\boldsymbol{\theta_1, \theta_2}) d\theta_1 d\theta_2 \end{pmatrix}
\end{aligned}$$

available dependence measures in terms of this matrix ....

notation: $\lambda_1(\boldsymbol{\Sigma})$ and $\lambda_2(\boldsymbol{\Sigma})$: eigenvalues of matrix $\boldsymbol{\Sigma}$

Table: *Dependence measures when applied to circulas.*

Expression	Reference
$\tau_{\mathsf{FL}} = 4\det(\boldsymbol{\Sigma}_{12})$	Lee & Fisher (1983)
$\tau_{\mathsf{JW}} = \sqrt{\max\{\lambda_1(4\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{12}^\top), \lambda_2(4\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{12}^\top)\}}$	Johnson (1977)
$\tau_{\mathsf{JM}} = \mathsf{trace}(4\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{12}^\top)$	Jupp (1980)
$\tau_{\mathsf{R}} = 2\mathsf{sign}(\det(\boldsymbol{\Sigma}_{12}))\min\{\lvert\lambda_1(\boldsymbol{\Sigma}_{12})\rvert, \lvert\lambda_2(\boldsymbol{\Sigma}_{12})\rvert\}$	Rivest (1982)

further issues

- what happens with dependence structures/strengths when variables are added to a vector:
  - an independent vector
  - or a canonical combination of components already included .. ?
  - or a set of arbitrary components ?
  -
- what are reasonable association measures, in particular in high dimensions ?
- how to measure dependence for complex data structures ?
-
-

Thank you