Beyond univariate Bayes spaces

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Outline

How to decompose multivariate densities?

- Decomposition of multivariate probability density functions (PDFs) in order to reveal dependence structure among random variables belongs to key tasks in probability theory and multivariate statistics
- One well-established approach is represented by copula theory (Sklar, 1959), but other(s) are searched for in context of functional data analysis of PDFs as data objects
- Could Bayes spaces (Egozcue et al., 2006; van den Boogaart, 2014) be of use here?

How to decompose multivariate densities?

Review paper by Petersen, Zhang and Kokoszka (2022):

Looking beyond univariate densities, one often encounters multivariate distributions... Extension of the models and methods discussed in the review to this setting is nontrivial at best... The Bayes space representation (...) provides a sound theoretical base for multivariate densities, although its practical implementation and utility has only been given limited, if any, consideration...

ELSEVIER

Econometrics and Statistics
Volume 21, January 2022, Pages 159-178

Modeling Probability Density Functions as Data Objects

Alexander Petersen [a b], Chao Zhang [b], Piotr Kokoszka [c]

Some inspiration and key ingrediences

- An orthogonal decomposition was constructed for compositional cubes as multi-factorial generalization of compositional data (Fačevicová et al., 2022) – aka *multivariate discrete distributions* – next step is to proceed to the general case and provide a solid theoretical framework

Some inspiration and key ingrediences

- An orthogonal decomposition was constructed for compositional cubes as multi-factorial generalization of compositional data (Fačevicová et al., 2022) – aka *multivariate discrete distributions* – next step is to proceed to the general case and provide a solid theoretical framework
- This is achieved with the help of the Hoeffding-Sobol decomposition formula (Hoeffding, 1948), known from copula theory
- A general framework for orthogonal decomposition of PDFs is developed in Genest et al. (2023) by following previous results in Mercadier et al. (2022)

Bivariate PDFs

- The domain Ω is a Cartesian product of two domains Ω_X and Ω_Y, i.e., $\Omega = \Omega_X \times \Omega_Y$. The reference measure λ can be decomposed as a product measure $\lambda = \lambda_X \times \lambda_Y$ which implies again the *Hilbert space structure* of the Bayes space $\mathcal{B}^2(\lambda)$

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$\Rightarrow$ *Perturbation* and *powering* operations: $f, g \in \mathcal{B}^2(\lambda)$, $\alpha \in \mathbb{R}$

$$(f \oplus g)(x, y) =_{\mathcal{B}^2(\lambda)} f(x, y) \cdot g(x, y), \; (\alpha \odot f)(x, y) =_{\mathcal{B}^2(\lambda)} f(x, y)^{\alpha}$$

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- the *Bayes inner product*:

$$\langle f, g \rangle_{\mathcal{B}^2(\lambda)} = \frac{1}{2\lambda(\Omega)} \iint_\Omega \iint_\Omega \ln \frac{f(x,y)}{f(s,t)} \ln \frac{g(x,y)}{g(s,t)} \, d\lambda(x,y) \, d\lambda(s,t)$$

$\Rightarrow$ $||f||_{\mathcal{B}^2(\lambda)} = \sqrt{\langle f, f \rangle_{\mathcal{B}^2(\lambda)}}, \quad d_{\mathcal{B}^2(\lambda)}(f,g) = ||f \ominus g||_{\mathcal{B}^2(\lambda)}$,
where $f \ominus g = f \oplus [(-1) \odot g]$

Bayes spaces: centred logratio transformation

- Also the *centred logratio (clr) transformation* is easily extendable to the bivariate case

Bayes spaces: centred logratio transformation

- Also the *centred logratio (clr) transformation* is easily extendable to the bivariate case
- The clr transformation of a bivariate density $f(x,y) \in \mathcal{B}^2(\lambda)$ is a real function $f^c : \Omega \to \mathbb{R}$, $f^c \in L_0^2(\lambda)$:

$$\begin{aligned} f^c(x,y) &= \ln f(x,y) - \frac{1}{\lambda(\Omega)} \iint_{\Omega} \ln f(x,y)\, d\lambda = \\ &= \ln f(x,y) - \frac{1}{\lambda(\Omega)} \int_{\Omega_X} \int_{\Omega_Y} \ln f(x,y)\, d\lambda_X d\lambda_Y \end{aligned}$$

- The *zero integral constraint* is imposed on $f^c(x,y)$ ... $L_0^2(\lambda)$

Orthogonal decomposition of bivariate PDFs

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- Relying on the Bayes space methodology allows one to provide a similar decomposition which is now, however, *orthogonal*
- This enables for an elegant *geometrical representation of the decomposition*, and for a powerful *probabilistic interpretation* with direct *consequences from the statistical viewpoint*

Orthogonal decomposition of bivariate PDFs

⇒ A novel definition of marginals, named *geometric marginals*, built upon marginalizing the bivariate clr transformation:

$$\begin{aligned} f^c_X(x) &= \frac{1}{\lambda_Y(\Omega_Y)} \int_{\Omega_Y} f^c(x,y)\, d\lambda_Y, \\ f^c_Y(y) &= \frac{1}{\lambda_X(\Omega_X)} \int_{\Omega_X} f^c(x,y)\, d\lambda_X; \end{aligned}$$

$f^c_X \in L^2_0(\lambda_X)$ and $f^c_Y \in L^2_0(\lambda_Y)$ (*clr-marginals*)

Orthogonal decomposition of bivariate PDFs

- *Geometric marginals* $f_X \in \mathcal{B}^2(\lambda_X)$ and $f_Y \in \mathcal{B}^2(\lambda_Y)$ are elements of $\mathcal{B}^2(\lambda_X)$ and $\mathcal{B}^2(\lambda_Y)$ associated with the clr-marginals:

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f_X(x) &=_{\mathcal{B}^2(\lambda_X)} \exp\left\{\frac{1}{\lambda_Y(\Omega_Y)}\int_{\Omega_Y} \ln f(x,y)\, d\lambda_Y\right\},\\
f_Y(y) &=_{\mathcal{B}^2(\lambda_Y)} \exp\left\{\frac{1}{\lambda_X(\Omega_X)}\int_{\Omega_X} \ln f(x,y)\, d\lambda_X\right\}
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- The normalizing terms guarantee that the scale of λ (λ_X, λ_Y) does not matter for the construction of geometric marginals
- Geometric marginals are **orthogonal projections** of the bivariate density $f(x,y)$ (Genest et al., 2023)

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- **Independence PDF**: $f_{\mathrm{ind}}(x,y) = f_X(x)f_Y(y),\ (x,y) \in \Omega$
- **Interaction PDF**: $f_{\mathrm{int}}(x,y) = \frac{f(x,y)}{f_X(x)f_Y(y)} = f(x,y) \ominus f_{\mathrm{ind}}(x,y)$,

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$\Rightarrow$ The original bivariate PDF can be decomposed as

$$f(x, y) = f_{\text{ind}}(x, y) \oplus f_{\text{int}}(x, y)$$

Example: a truncated Gaussian density

- We consider a zero-mean bivariate Gaussian density $\mathcal{N}_2(\mu, \Sigma)$ with respect to the (product) Lebesgue measure $\lambda[I] = \lambda[I_1] \times \lambda[I_2]$, truncated on a rectangular domain $I = I_1 \times I_2 \subset \mathbb{R}^2$, with $I_1 = I_2 = [-T, T]$, $T = 5$

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- The PDF is defined, for $\mathbf{x} = (x, y) \in I$, as

$$\begin{aligned} f(x,y) &=_{\mathcal{B}^2(\lambda)} \exp\left\{\mathbf{x}^\top \Sigma^{-1} \mathbf{x}\right\} \\ &= \exp\left\{-\frac{1}{2(1-\rho^2)}\left[\frac{x^2}{\sigma_1^2} - 2\rho\frac{xy}{\sigma_1\sigma_2} + \frac{y^2}{\sigma_2^2}\right]\right\}, \end{aligned}$$

with $\sigma_i^2 = \Sigma_{ii}$ and $\rho \in [0, 1]$ being the correlation coefficient

- Clr transformation of f:

$$f^c(x,y) = -\frac{1}{2(1-\rho^2)}\left[\frac{x^2}{\sigma_1^2} - 2\rho\frac{xy}{\sigma_1\sigma_2} + \frac{y^2}{\sigma_2^2}\right] + \frac{T^2}{6(1-\rho^2)}\left(\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}\right)$$

Example: a truncated Gaussian density

- Independence and interaction (clr-)PDFs in case of Lebesgue reference measure:

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f^c_{\mathrm{ind}}(x,y) &= -\frac{1}{2(1-\rho^2)}\left(\frac{x^2}{\sigma_1^2}+\frac{y^2}{\sigma_2^2}\right)+\frac{T^2}{6(1-\rho^2)}\left(\frac{1}{\sigma_1^2}+\frac{1}{\sigma_2^2}\right);\\
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- In case of independence ($\rho = 0$), f^c_{int} is null, and $f_{\mathrm{int}} = 0_\oplus$.

Example: a truncated Gaussian density

- Independence and interaction PDFs in case of Lebesgue reference measure:

$$f_X(x) =_{\mathcal{B}^2(\lambda_X)} \exp\left[-\frac{1}{2(1-\rho^2)}\frac{x^2}{\sigma_1^2}\right], \text{ (likewise } f_Y(y));$$

$$f_{\text{int}}(x,y) =_{\mathcal{B}^2(\lambda)} \exp\left[\frac{1}{(1-\rho^2)}\left(\rho\frac{xy}{\sigma_1\sigma_2}\right)\right].$$

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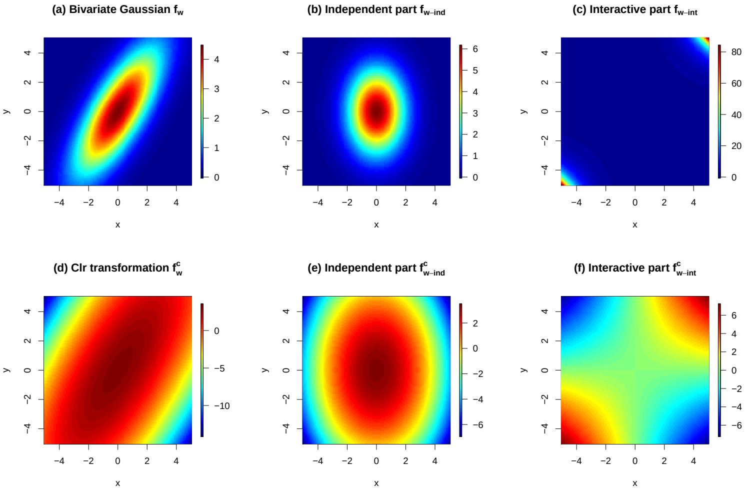
Gaussian example



Conditional probabilities as space quotient (KGvdB)

- Conditional distributions differ by a marginal:

$$f_X(\cdot|y) = g_X(\cdot|y) \Leftrightarrow f(x,y) \ominus g(x,y) \in \mathcal{B}^2(\lambda_Y)$$

which is the definition of equivalence in quotient spaces, i.e.

$$f_X(\cdot|y) \in \frac{\mathcal{B}^2(\lambda_X \times \lambda_Y)}{\mathcal{B}^2(\lambda_Y)}$$

(*spaces of regression models*)

- **Remark**: The difference is the difference of marginal distributions:

$$f(x,y) \ominus g(x,y) =_{\mathcal{B}^2(\lambda_X \times \lambda_Y)} f_Y(y) \ominus g_Y(y)$$

Conditional subspaces (KGvdB)

- The other way around:

$$f_X(\cdot|y) = \frac{f_X(x) \oplus f_Y(y) \oplus f_{\mathrm{int}}(x, y)}{f_Y(y)},$$

i.e., the conditional distribution just misses the marginal part

Conditional subspaces (KGvdB)

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- Conditional distributions are represented by the projection on the orthogonal complement of the conditioning space: $\mathcal{B}^2(\lambda_Y)^{\perp}$

- Any joint structure exists with every combination of marginals

Motivation example: PDFs of chemical elements

- Trivariate densities of (log-transformed) copper (Cu), lead (Pb) and zinc (Zn) soil concentration data in 77 districts of the Czech Republic from the Register of Contaminated Areas (registr kontaminovaných ploch) collected by the Department of Agriculture of the Czech Republic (eAGRI, 2020)
- At least higher hundreds of concentration values available in each district
- Districts are characterized by diverse geological origin and anthropogenic contamination

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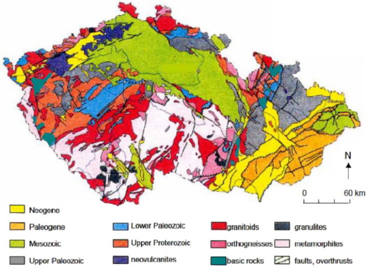

Source: Czech Geological Survey, Prague

Bivariate Cu-Zn densities are depicted:

- the first case corresponds to Nymburk County, where soil contamination is likely low
- the second case corresponds to Louny County, where heavy soil contamination is suspected due to abundant hops culture as well as ore mining and processing

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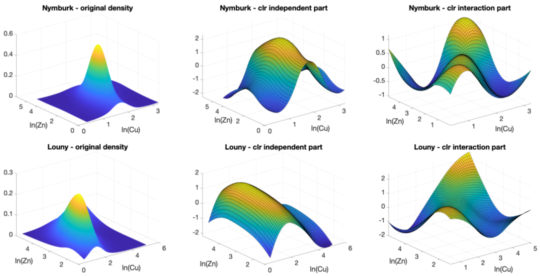

- What information can be obtained from trivariate densities?
- How can we capture interactions between elements?

Notation

- Let $(\Omega, \mathcal{A})$ be now a d-dimensional product space and let λ be a finite product reference measure. Specifically, suppose that for $i \in D$, $(\Omega_i, \mathcal{A}_i)$ is a measurable space and λ_i is a finite, positive, real-valued measure on it. Set

$$\Omega = \Omega_1 \times \cdots \times \Omega_d, \quad \mathcal{A} = \mathcal{A}_1 \otimes \cdots \otimes \mathcal{A}_d, \quad \lambda = \lambda_1 \otimes \cdots \otimes \lambda_d.$$

- For arbitrary non-empty $I \subseteq D$, let

$$\Omega_I = \times_{i \in I} \Omega_i, \quad \mathcal{A}_I = \bigotimes_{i \in I} \mathcal{A}_i, \quad \lambda_I = \bigotimes_{i \in I} \lambda_i.$$

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♡ Necessity of having the product space is the only restriction we need to take into account.

Notation

- For arbitrary $I \subseteq D = \{1, \dots, d\}$, $I \neq \varnothing$, let $\mathcal{B}^2_I(\lambda)$ be the subspace of $\mathcal{B}^2(\lambda)$ given by

$$\mathcal{B}^2_I(\lambda) = \left\{ \mu \in \mathcal{B}^2(\lambda) \,\middle|\, \exists_{\mu_I \in \mathcal{B}^2(\lambda_I)} \forall_{A_i \in \mathcal{A}_i}\ \mu\left(\times_{i \in D} A_i\right) = \prod_{i \notin I} \lambda_i(A_i) \mu_I\left(\times_{i \in I} A_i\right) \right\}$$

$\Rightarrow$ Any λ-density in $\mathcal{B}^2_I(\lambda)$ is a function of arguments with indices in I only

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- Note that when $D = I$, $\mathcal{B}^2_D(\lambda) = \mathcal{B}^2(\lambda)$
- By convention, $\mathcal{B}^2_\emptyset(\lambda)$ is the trivial subspace that contains only the neutral element λ

Geometric marginals

- For $I \subsetneq D$, the *I-th geometric marginal* is

$$f_I = \exp\left\{ \frac{1}{\lambda_{D\setminus I}(\Omega_{D\setminus I})} \int_{\Omega_{D\setminus I}} \ln(f) d\lambda_{D\setminus I} \right\}.$$

and its clr transformation

$$\mathrm{clr}(f_I) = \frac{1}{\lambda_{D\setminus I}(\Omega_{D\setminus I})} \int_{\Omega_{D\setminus I}} \mathrm{clr}(f) d\lambda_{D\setminus I}$$

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♡ It is the unique orthogonal projection of $f (\equiv f_\mu)$ onto $\mathcal{B}_I^2(\lambda)$

- The logarithm of f in f_I can be replaced by its clr transformation due to properties of the exponential (and proportionality of densities in the Bayes space framework)

Decomposition of f

Kuo et al. (2010) reformulated the Hoeffding-Sobol decomposition in terms of projections which was used to derive the following:

Theorem (Decomposition of multivariate densities)

For any $f \in \mathcal{B}^2(\lambda)$,

$$f = f_{\mathrm{ind}} \oplus \bigoplus_{I \subseteq D, |I| \geq 2} f_{I,\mathrm{int}}$$

where the so-called independence and interaction parts are respectively given by

$$f_{\mathrm{ind}} = \bigoplus_{i=1}^{d} f_i, \quad f_{I,\mathrm{int}} = \bigoplus_{J \subseteq I, J \neq \varnothing} \{(-1)^{|I \setminus J|}\} \odot f_J.$$

Decomposition of f $(d = 3)$

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$\Rightarrow$ Explicit formula for the decomposition using directly marginal densities

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Also recursive formula (cf. Fačevicová et al., 2022) possible:

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$\rightarrow$ Recursive formula:

- $f_{\{1,2\},\text{int}}$, $f_{\{1,3\},\text{int}}$, $f_{\{2,3\},\text{int}}$: no change from before
- $f_{\{1,2,3\},\text{int}} = f \ominus f_1 \ominus f_2 \ominus f_3 \ominus f_{\{1,2\},\text{int}} \ominus f_{\{1,3\},\text{int}} \ominus f_{\{2,3\},\text{int}}$

Decomposition of f $(d = 3)$

- $f_{\mathrm{ind}} = f_1 \oplus f_2 \oplus f_3$

- $f_{\{1,2\},\mathrm{int}} = f_{\{1,2\}} \ominus f_1 \ominus f_2$
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- The recursive formula is important for further derivations

Orthogonality of decomposition

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Orthogonality of decomposition

- Some more notation for $I \subseteq D$ is needed:
- $\mathcal{B}^2_{I,\mathrm{int}}(\lambda)$ is defined as the orthogonal complement of the direct sum $\mathcal{B}^2_{I,\oplus}(\lambda) = \bigoplus_{i\in I} \mathcal{B}^2_{\{i\}}(\lambda) \bigoplus_{J\subsetneq I, |J|\geq 2} \mathcal{B}^2_{J,\mathrm{int}}(\lambda)$ in $\mathcal{B}^2_I(\lambda)$

$\Rightarrow$ $\mathcal{B}^2_{I,\mathrm{int}}(\lambda) = \{f \in \mathcal{B}^2_I(\lambda) \mid \forall_{g\in\mathcal{B}^2_{I,\oplus}(\lambda)} \langle f, g\rangle_{\mathcal{B}^2(\lambda)} = 0\}$

- Independence space:

$$\mathcal{B}^2_{\mathrm{ind}}(\lambda) = \{\mu \in \mathcal{B}^2(\lambda) \mid \exists_{\mu_1\in\mathcal{B}^2(\lambda_1)} \cdots \exists_{\mu_d\in\mathcal{B}^2(\lambda_d)} \mu = \mu_1 \otimes \cdots \otimes \mu_d\}$$

- These subspaces span the corresponding densities from the decomposition of f

Orthogonality of decomposition

Theorem (Orthogonality of decomposition)

For any $f \in \mathcal{B}^2(\lambda)$ and any $I \subseteq D$ with $|I| \geq 2$, $f_{I,\mathrm{int}}$ is the unique orthogonal projection of f on $\mathcal{B}^2_{I,\mathrm{int}}(\lambda)$. Furthermore,

$$\mathcal{B}^2(\lambda) = \bigoplus_{i \in D} \mathcal{B}^2_{\{i\}}(\lambda) \bigoplus_{I \subseteq D, |I| \geq 2} \mathcal{B}^2_{I,\mathrm{int}}(\lambda)$$

and all spaces featuring in the direct sum are mutually orthogonal.

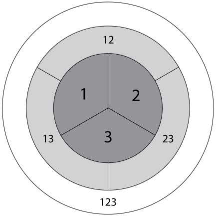
$\Rightarrow$ The independence space can be expressed as

$$\mathcal{B}^2_{\mathrm{ind}}(\lambda) = \mathcal{B}^2_{\{1\}}(\lambda) \oplus \cdots \oplus \mathcal{B}^2_{\{d\}}(\lambda)$$

and for any $f \in \mathcal{B}^2(\lambda)$, the independence part f_{ind} is the unique orthogonal projection of f on $\mathcal{B}^2_{\mathrm{ind}}(\lambda)$.

Orthogonality of decomposition ($d = 3$)

- The situation for $d = 3$ can be depicted as follows:



The sectors marked 1, 2, 3 correspond to the subspaces $\mathcal{B}^2_{\{1\}}(\lambda)$, $\mathcal{B}^2_{\{2\}}(\lambda)$, $\mathcal{B}^2_{\{3\}}(\lambda)$. In light grey the three orthogonal subspaces $\mathcal{B}^2_{I,\mathrm{int}}(\lambda)$ corresponding to the subsets $I = \{1,2\}$, $\{1,3\}$, and $\{2,3\}$ are depicted. The white annulus labeled 123 is $\mathcal{B}^2_{\{1,2,3\},\mathrm{int}}(\lambda)$, i.e., the orthogonal complement of the direct sum $\mathcal{B}^2_{\{1,2,3\},\oplus}(\lambda)$ of the grey zones.

Orthogonality of decomposition ($d = 3$)

- Summing up, one has

$$\mathcal{B}^2(\lambda) = \mathcal{B}^2_{\{1\}}(\lambda) \oplus \mathcal{B}^2_{\{2\}}(\lambda) \oplus \mathcal{B}^2_{\{3\}}(\lambda)$$
$$\oplus \mathcal{B}^2_{\{1,2\},\mathrm{int}}(\lambda) \oplus \mathcal{B}^2_{\{1,3\},\mathrm{int}}(\lambda) \oplus \mathcal{B}^2_{\{2,3\},\mathrm{int}}(\lambda) \oplus \mathcal{B}^2_{\{1,2,3\},\mathrm{int}}(\lambda),$$

$\Rightarrow$ The orthogonal decomposition of any $f \in \mathcal{B}^2(\lambda)$ takes the form

$$f = f_1 \oplus f_2 \oplus f_3 \oplus f_{\{1,2\},\mathrm{int}} \oplus f_{\{1,3\},\mathrm{int}} \oplus f_{\{2,3\},\mathrm{int}} \oplus f_{\{1,2,3\},\mathrm{int}}$$

Consequences of the decomposition (1)

(i) *Pythagoras' Theorem:* One always has

$$\|f_\mu\|^2_{\mathcal{B}^2(\lambda)} = \|f_{\mu,\mathrm{ind}}\|^2_{\mathcal{B}^2(\lambda)} + \sum_{I \subseteq D, |I| \geq 2} \|f_{\mu,I,\mathrm{int}}\|^2_{\mathcal{B}^2(\lambda)},$$

where $\|f_{\mu,\mathrm{ind}}\|^2_{\mathcal{B}^2(\lambda)} = \|f_{\mu,1}\|^2_{\mathcal{B}^2(\lambda)} + \cdots + \|f_{\mu,d}\|^2_{\mathcal{B}^2(\lambda)}$.
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(ii) *Margin-free property:* For any given set $I \subseteq D$ with $|I| \geq 2$, let $f_\nu = f_{\mu,I,\mathrm{int}}$. Then for each $i \in D$, the i-th univariate geometric margin $f_{\nu,i}$ of f_ν satisfies $f_{\nu,i} \propto 1$. Moreover, for any set $J \subsetneq I$ with $|J| \geq 2$, the J-th geometric margin of f_ν satisfies $f_{\nu,J} \propto 1$.

Consequences of the decomposition (2)

(iii) *Independence:* If $f_\mu = f_{\mu_1} \cdots f_{\mu_d} \in \mathcal{B}^2_{\text{ind}}(\lambda)$, then for each $i \in D$, $f_{\mu,i} \propto f_{\mu_i}$ (arith. and geom. margins coincide) and

$$f_\mu \in \mathcal{B}^2_{\text{ind}}(\lambda) \Leftrightarrow f_\mu \propto f_{\mu,1} \oplus \cdots \oplus f_{\mu,d} \Leftrightarrow \forall_{I \subseteq D, |I| \geq 2}\, f_{\mu,I,\text{int}} \propto 1.$$

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(iv) *Yule perturbation:* For $g \propto g_1 \cdots g_d \in \mathcal{B}^2_{\text{ind}}(\lambda)$, set $h = f_\mu \oplus g$. Then the independence and interaction parts of h satisfy

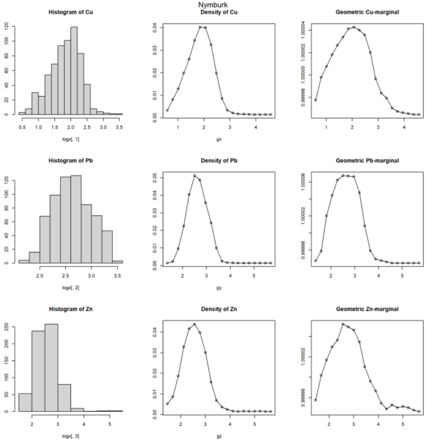
$$h_{\text{ind}} = f_{\mu,\text{ind}} \oplus g, \quad h_{\text{int}} = f_{\mu,\text{int}},$$

where

$$f_{\mu,\text{int}} = \bigoplus_{I \subseteq D, |I| \geq 2} f_{\mu,I,\text{int}}.$$

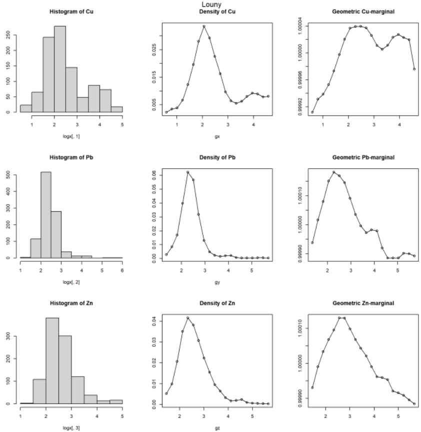
In particular, the geometric margins of h satisfy $h_i \propto f_{\mu,i} g_i$ for all $i \in D$.

PDFs of chemical elements: univariate analysis



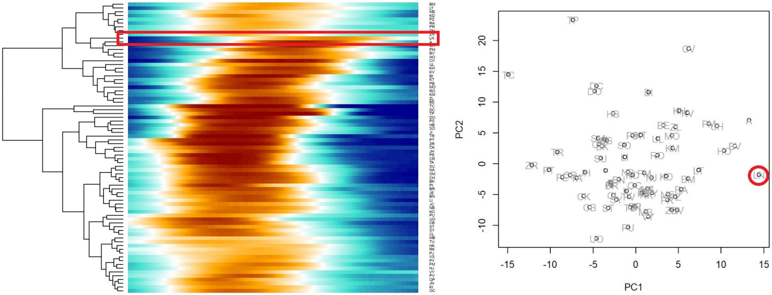
Geometric marginals capture also interelemental relationships!

PDFs of chemical elements: univariate analysis



Geometric marginals capture also interelemental relationships!

PDFs of chemical elements: “univariate” analysis

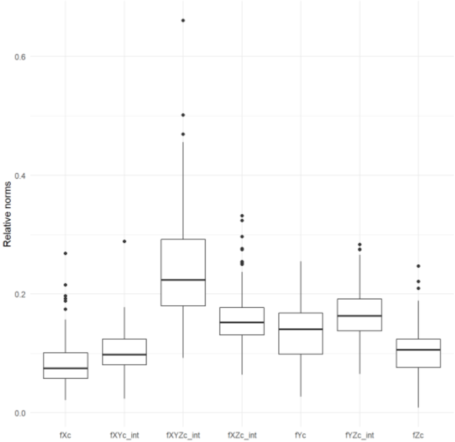


Cu geometric marginals, clr space

left: clustering, right: scores of functional principal component analysis

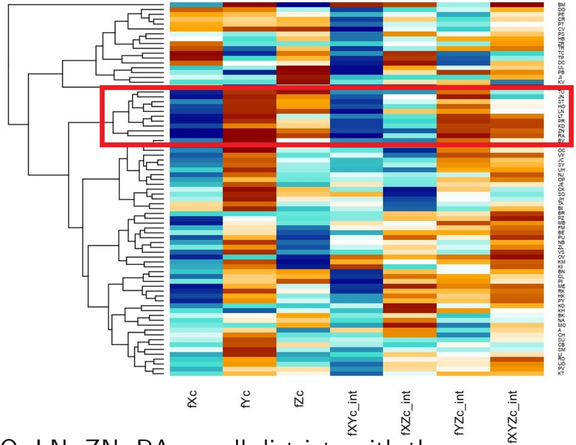
Louny . . . LN, Nymburk . . . NB

PDFs of chemical elements: decomposition



X . . . Cu, Y . . . Pb, Z . . . Zn

PDFs of chemical elements: decomposition (clr)



LN, LT, HO, LN, ZN, RA are all districts with the same source of contamination (agricultural spraying due to intensive land use)

Exploratory FDA of multivariate PDFs: R code

https://github.com/uradojic/EFDA-of-multivariate-densities.git

(with special thanks to Una Radojičić and Ivana Pavlů)

Outlook

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- A great potential of multivariate Bayes spaces further in Bayesian inference (Barfoot and D'Eleuterio, 2023; Wynne, 2023), graphical models, conditional distributions, generalized regression. . .

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