Density data analysis: Analyzing samples of probability distributions using Bayes spaces

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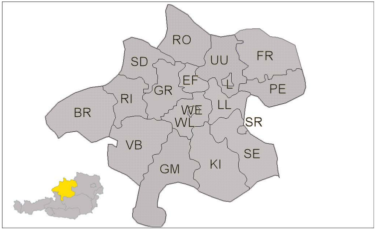
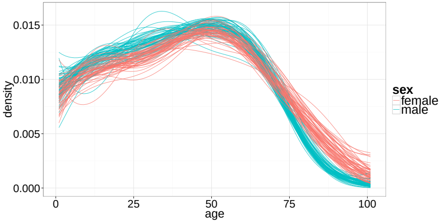
Outline

1. Bayes spaces
2. Exploratory density data analysis
3. SFPCA
4. Applications to simulated and empirical data

Population age distributions in Upper Austria





- 15 political districts, age distributions of men and women living in 114 municipalities of Upper Austria (*population pyramids*)

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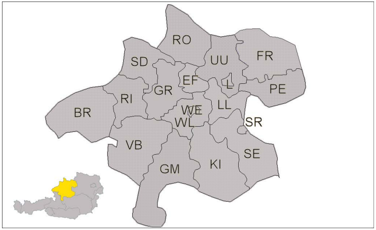
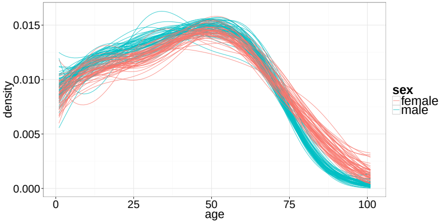
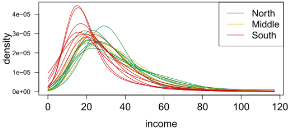
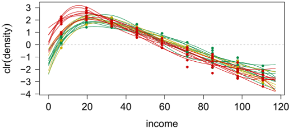




- 15 political districts, age distributions of men and women living in 114 municipalities of Upper Austria (*population pyramids*)
- **Aim**: to describe the available population age densities and perform a dimensionality reduction (PCA)

Income distributions in Italian regions





- Similarly for . . . Italian Survey on Household Income and Wealth (SHIW) income data (income distributions in all 20 Italian regions)

Densities as relative data

- statistical processing of density functions using tools of FDA (Ramsay and Silverman, 2005) is of increasing interest due to the necessity of aggregating massive data while keeping their internal variation and structure
- **examples**: *age distributions*/population pyramids, *income distributions*, *anthropometric distributions (height, weight)*, *particle size distributions*, *concentration distributions*, *metabolite distributions*,...

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- **examples**: *age distributions*/population pyramids, *income distributions*, *anthropometric distributions (height, weight)*, *particle size distributions*, *concentration distributions*, *metabolite distributions*,...
- density functions are inherently characterized by *scale invariance* and *relative scale*
- an infinite-dimensional extension of *compositional data* (Aitchison, 1986), characterized by the Aitchison geometry on the simplex with the Euclidean vector space structure

Densities as relative data

- *scale invariance*: the constant sum constraint $\int_\Omega f(x)\,\mathrm{d}x = 1 = \mathrm{P}(\Omega)$ leads to a representation within a class of functions which provide the same kind of information – namely, the equivalence class of *functions which are proportional to the density function*

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- *relative scale* property: small function values of densities (=relative likelihood) form the main source of variability
- both the scale invariance and the relative scale properties are ignored when probability density functions are considered just like unconstrained functional data

Densities and functional data analysis

- *Functional data analysis* (Ramsay and Silverman, 2005) based on geometry of L^2 Hilbert spaces works well for some well-known examples:

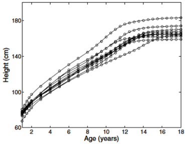
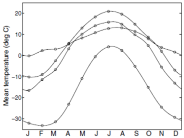


Figure 1.1. The heights of 10 girls measured at 31 ages. The circles indicate the unequally spaced ages of measurement.



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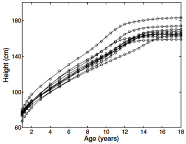

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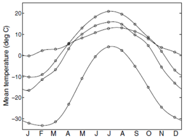


. . . but is not appropriate for density functions

→ **Bayes spaces** ($\mathcal{B}^2$) (Egozcue et al., 2006; van den Boogaart et al., 2014) – Hilbert space structure for densities with square-integrable logarithm

Bayes spaces: geometry

Compact support (interval) $I = [a, b],\ a, b \in R, a < b$ represents the common case in applications, $\eta = b - a$.

- *pertubation* (sum operation)

$$(f \oplus g)(t) =_{\mathcal{B}^2(I)} f(t) \cdot g(t), \quad t \in I,$$

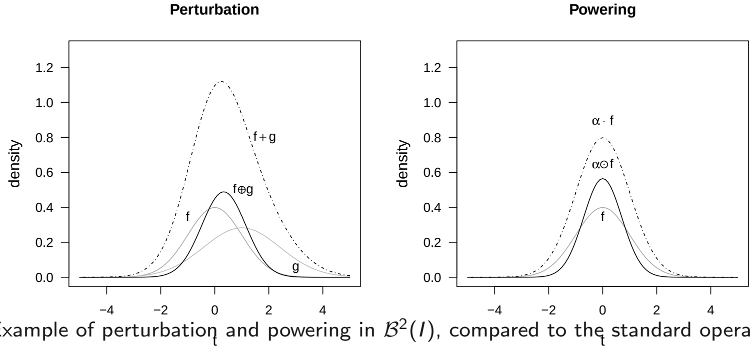
- *powering* (product by a constant)

$$(\alpha \odot f)(t) =_{\mathcal{B}^2(I)} f(t)^{\alpha}, \quad t \in I,$$

- *inner product* between two λ-densities

$$\langle f, g \rangle_{\mathcal{B}^2(I)} = \frac{1}{2\eta} \int_I \int_I \ln \frac{f(t)}{f(u)} \ln \frac{g(t)}{g(u)}\, dt\, du, \quad t, u \in I.$$

Bayes spaces: geometry



Example of perturbation and powering in $\mathcal{B}^2(I)$, compared to the standard operations in $L^2(\lambda)$. Left: Perturbation $f \oplus g$ (solid black line) of two Gaussian densities f, g restricted to $I = [-5, 5]$ (grey lines), and the sum $f + g$ in the space $L^2(\lambda)$ (dot-dashed line). Right: Powering of a Gaussian density f restricted to $I = [-5, 5]$ (grey line) by $\alpha = 2$, $\alpha \odot f$ (solid black line), and the counterpart $\alpha \cdot f$ in L^2 (dot-dashed line).

Representation of PDFs in L^2: clr transformation

- **Goal**: To perform popular FDA methods, developed mostly under the assumption of the L^2 space $\rightarrow$ map PDFs into (a subspace of) the L^2 space . . . the L^2_0 space

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- **Goal**: To perform popular FDA methods, developed mostly under the assumption of the L^2 space $\rightarrow$ map PDFs into (a subspace of) the L^2 space ... the L_0^2 space

$\rightarrow$ centred logratio (clr) transformation:

$$\mathrm{clr}(f)(t) = f^c(t) = \ln f(t) - \frac{1}{\eta}\int_I \ln f(s)\,\mathrm{d}s, \quad \int_I f^c(t)\,\mathrm{d}t = 0;$$

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- the Bayes space geometry transforms accordingly:
  - $clr(f \oplus g)(t) = f^c(t) + g^c(t), \quad clr(\alpha \odot f)(t) = \alpha \cdot f^c(t), \quad t \in I$
  - $\langle f, g\rangle_{\mathcal{B}^2(I)} = \langle clr(f), clr(g)\rangle_{L^2(I)}$

$\Rightarrow$ computations directly in the Bayes space can be avoided

EDDA: sample mean

- . . . any exploratory density data analysis (EDDA) usually starts with . . .
- Given a sample $X_1, ..., X_N$ in $\mathcal{B}^2(I)$, $I = [a, b]$, $a, b \in \mathbb{R}$, $a < b$

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- Given a sample $X_1, ..., X_N$ in $\mathcal{B}^2(I)$, $I = [a, b]$, $a, b \in \mathbb{R}$, $a < b$
- **Sample mean:** $\overline{X} = \frac{1}{N} \odot \bigoplus_{i=1}^{N} X_i$
- It can be computed through the back-transform of the sample mean in L_0^2 of the clr-transformed data (the latter being defined point-wise)

$$\overline{X} = \mathrm{clr}^{-1}(\overline{X}^c), \quad \overline{X}^c = \frac{1}{N} \sum_{i=1}^{N} X_i^c$$

EDDA: sample covariance function

- Specifies the *covariance* between density values at $t, s \in \Omega$
- Assigned to one FDA object (here PDF, or a *sample* of PDFs)
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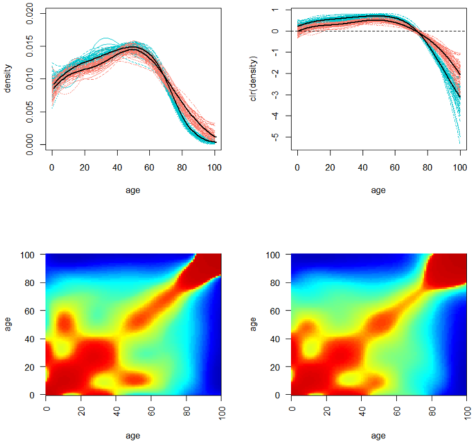
- **Sample covariance function:**

$$v(s,t) = \frac{1}{N}\sum_{i=1}^{N}(X_i^c(s) - \overline{X}^c(s))(X_i^c(t) - \overline{X}^c(t))$$

- Can be visualized as function of two variables (for smoothed clr-transformed densities)

EDDA: Age distributions in Upper Austria



Male and female populations: Sample mean and sample covariance function

Functional principal component analysis (FPCA)

- Consider a *centred* functional random sample $X_1, ..., X_N$ in $L^2(I)$, i.e. from all observations $\overline{X} = \frac{1}{N}\sum_{i=1}^{N} X_i$ is subtracted
- FPCA looks firstly for the main mode of variability, i.e., for the element ξ_1 in $L^2(I)$ – called first functional principal component (FPC)– maximizing over $\xi \in L^2(I)$

$$\frac{1}{N}\sum_{i=1}^{N} \langle X_i, \xi \rangle_2^2 \text{ subject to } \|\xi\|_2 = 1.$$

- **Aim**: to capture the main modes of variability of the data by means of a small number K of linear combinations of the original variables: $X_i \approx \sum_{k=1}^{K} \langle X_i, \xi_k \rangle_2 \xi_k$

Functional principal component analysis (FPCA)

- The remaining FPCs, $\{\xi_j\}_{j\geq 2}$, capture the remaining modes of variability subject to be mutually orthogonal, and are thus obtained by solving problem the previous maximization problem with the additional orthogonality constraint $\langle \xi_k, \xi \rangle_2 = 0, k < j$

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$\rightarrow$ **Outputs**: eigenfunctions of the covariance operator/harmonics ξ_j (interpreted in terms of the original data) and scores (coefficients, representing data structure of the original observations)

FPCA: computational details

- Dealing with FPCA is analogous to the multivariate PCA
- The FPCs $\{\xi_j\}_{j\geq 1}$ coincide with the eigenfunctions of the sample covariance operator $V : L^2(I) \to L^2(I)$, acting on $x \in L^2(I)$ as

$$Vx = \frac{1}{N}\sum_{i=1}^{N}\langle X_i, x\rangle_2 X_i$$

→ The j-th FPC ξ_j and the associated scores $\Psi_{ij} = \langle X_i, \xi_j\rangle_2$, $i = 1, \ldots, N$, are obtained by solving the **eigenvalue equation**

$$V\xi_j = \rho_j \xi_j;$$

ρ_j denotes the j-th eigenvalue, with $\rho_1 \geq \rho_2 \geq \ldots$.

FPCA: computational details

- For each j, the term $\rho_j / \sum_j \rho_j$ is associated with the proportion of total variability explained by the FPC ξ_j.

- The eigenvalue equation is solved using basis expansion of each datum X_i, $i = 1, \ldots, N$ using K known basis functions $\phi_1, \ldots, \phi_K$:

$$X_i(\cdot) = \sum_{k=1}^{K} c_{ik} \phi_k(\cdot),$$

where $c_{ik} = \langle X_i, \phi_k \rangle_2$, $k = 1, \ldots, K$

$\rightarrow$ Commonly, smoothing splines are used for this purpose

Simplicial functional principal component analysis

→ **SFPCA**: Reformulate FPCA in terms of Bayes spaces for $X_1, \ldots, X_N$ being a (centred) sample in $\mathcal{B}^2(I)$, i.e., we performed perturbation-subtraction by $\overline{X} = \frac{1}{N} \odot \bigoplus_{i=1}^{N} X_i$

- Maximizing over $\zeta \in \mathcal{B}^2(I)$

$$\frac{1}{N} \sum_{i=1}^{N} \langle X_i, \zeta \rangle_B^2 \text{ subject to } \|\zeta\|_B = 1;\ \langle \zeta_j, \zeta_k \rangle_B = 0,\ k < j$$

→ We can formulate the problem and find the unique solution because $\mathcal{B}^2(I)$ is a separable Hilbert space

→ **Problem**: how to efficiently implement all of this?

Clr transformation and SFPCA

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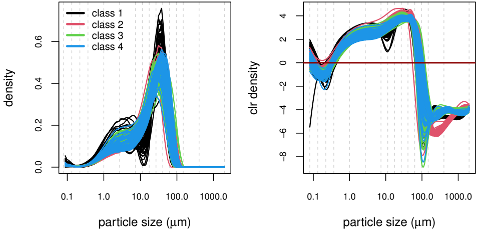
- Consequence for FPCA in clr space: $\xi_0 \equiv 1/\sqrt{b-a}$
- The zero integral constraint needs to be incorporated into the basis expansion → **compositional splines**

Example: Compositional splines

- Unlike the usual case of B-splines, here the basis functions honor the zero intergral constraint
- Example with geological densities (particle size distributions)



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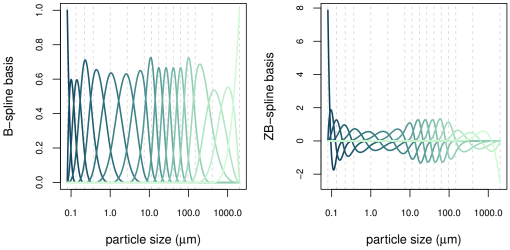


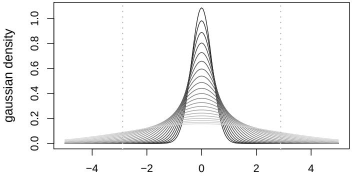
Example: Truncated normal PDFs

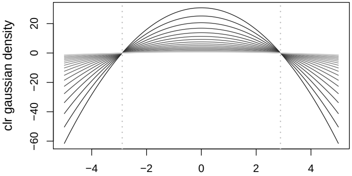
- Normal densities, $\mu = 0, \sigma_i = \exp(-1 + (i-1)/10)$, $i = 1, \ldots, 21$, $I = [-5, 5]$

$$f(t; \sigma_i) =_{\mathcal{B}^2} \exp\left\{-\frac{t^2}{2\sigma_i^2}\right\}, \quad t \in I, \tag{1}$$

$=_{\mathcal{B}^2(I)}$ denotes the equivalence in the space $\mathcal{B}^2(I)$

$$f^c(t; \sigma_i) = -\frac{t^2}{2\sigma_i^2} + \frac{25}{6\sigma_i^2}, \quad t \in I.$$





Dimensionality of PDFs from the exponential family

An important feature of (log-)normal densities in context of Bayes spaces is that they belong to the extended exponential family:

- Recall that a *k-parametric extended exponential family* on Ω, $Exp_{\mathcal{B}^2(I)}(g, \boldsymbol{T}, \vartheta)$ is a collection of densities

$$f(t, \boldsymbol{\alpha}) =_{\mathcal{B}^2(I)} g(t) \cdot \exp\left\{\sum_{j=1}^{k} \vartheta_j(\boldsymbol{\alpha}) T_j(t)\right\}, \quad t \in \Omega,$$

  where $\boldsymbol{\alpha}$ denotes the k-dimensional vector of parameters in a k-dimensional parameter space A, while functions $g : \Omega \to \mathbb{R}$, $\vartheta_j : A \to \mathbb{R}$ and $T_j : \Omega \to \mathbb{R}$, $j = 1, ..., k$, are Borel-measurable

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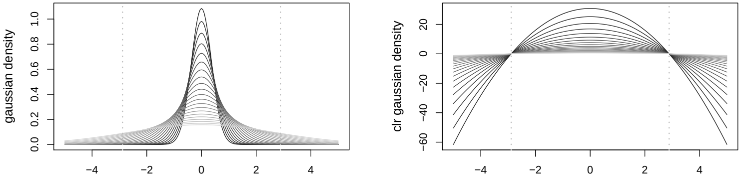
- An extended exponential family on Ω is a **finite dimensional affine subspace** of the Bayes space $\mathcal{B}^2(I)$

Dimensionality of PDFs from the exponential family

- Most routinely used distributions belong to the exponential family
- **Example**: a Gaussian density $N(0, \sigma^2)$ *restricted on* Ω belongs to a 1-parametric extended exponential family, with $\alpha = \sigma$, $\vartheta_1(\alpha) = 1/\sigma^2$, and $T_1(t) = -t^2$



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- A PDF in $Exp_{\mathcal{B}(I)}(g, \boldsymbol{T}, \vartheta)$ can be expressed as a linear combination in $\mathcal{B}^2(I)$:

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- Clr-transformed:

$$f^c(t, \boldsymbol{\alpha}) = \mathrm{clr}(g(t)) + \sum_{j=1}^{k} \left[\vartheta_j(\boldsymbol{\alpha}) \cdot \mathrm{clr}(\exp\{T_j(t)\})\right], \quad t \in \Omega.$$

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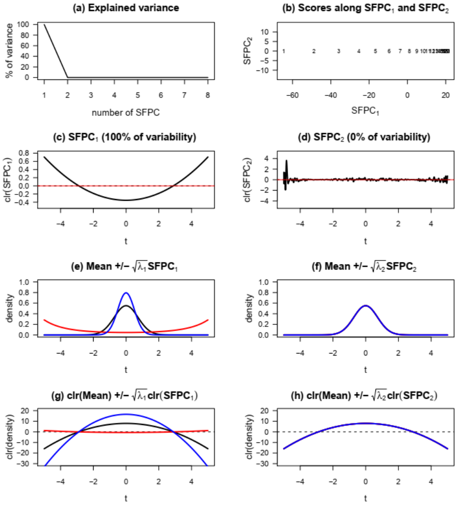
$\Rightarrow$ For $k_0 \leq k$ uncertain parameters, the SFPCA estimates an orthonormal basis of the corresponding k-dimensional affine space in $\mathcal{B}^2(I)$, which is associated to $k_0 \leq k$ non-zero eigenvalues

Dimensionality of PDFs: normal distribution



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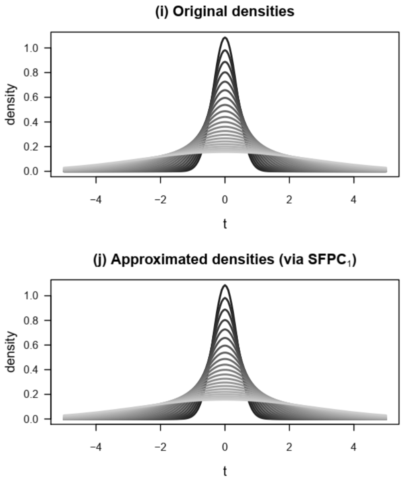
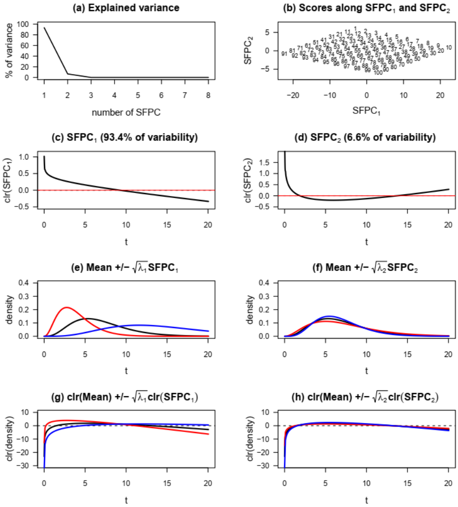


Dimensionality of PDFs: gamma distribution

Data: $n = 100$ densities with kernel Gamma $\Gamma(\theta_i, \kappa_j)$, with $\theta_i = 1/9 + (i-1)/9$ and $\kappa_j = 2 + (j-1)/4$ for $i, j = 1, \ldots, 10$, and domain $I = [e^{-7}, e^3]$

- A Gamma distribution $\Gamma(\theta, \kappa)$ on I belongs to a 2-parametric extended exponential family with $\boldsymbol{\alpha} = (\theta, \kappa)$, $\vartheta_1(\boldsymbol{\alpha}) = \theta$, $\vartheta_2(\boldsymbol{\alpha}) = \kappa$, $T_1(t) = -t$, and $T_2(t) = \ln(t)$, for $t \in I$
- We expect now that a sensible dimensionality reduction method will single out the dimension $k = 2$ of these densities
- A comparison with FPCA for the original densities is performed as well

Dimensionality of PDFs: gamma distribution



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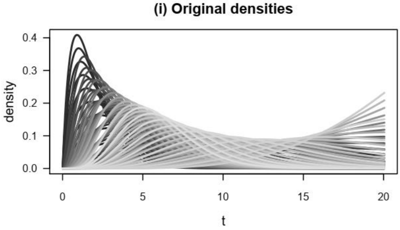
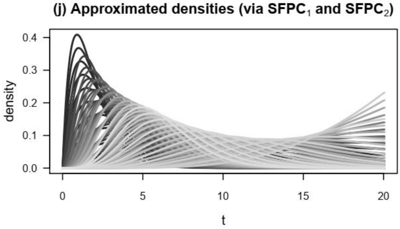
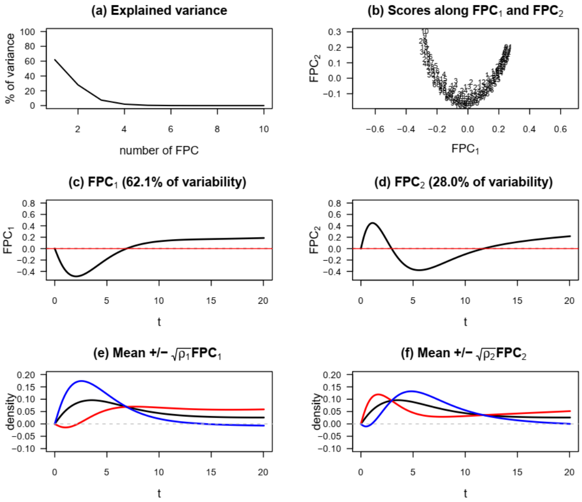
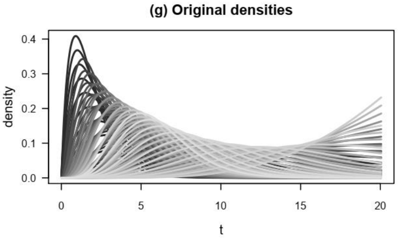


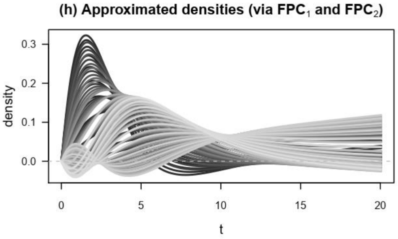


Dimensionality of PDFs: gamma distribution (L^2)

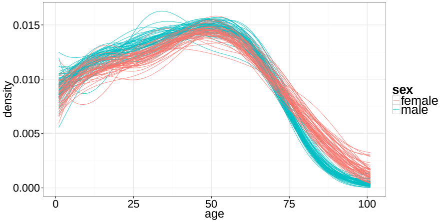


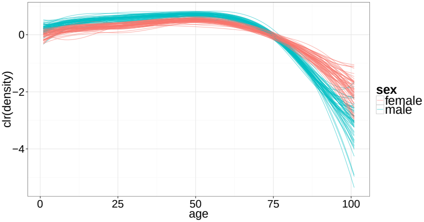
Dimensionality of PDFs: gamma distribution (L^2)

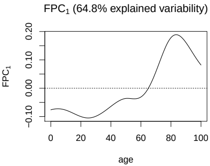


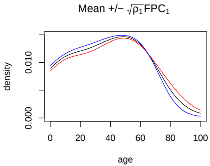


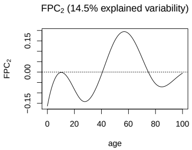
SFPCA: Population age distributions

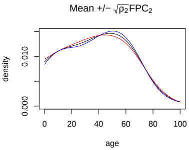




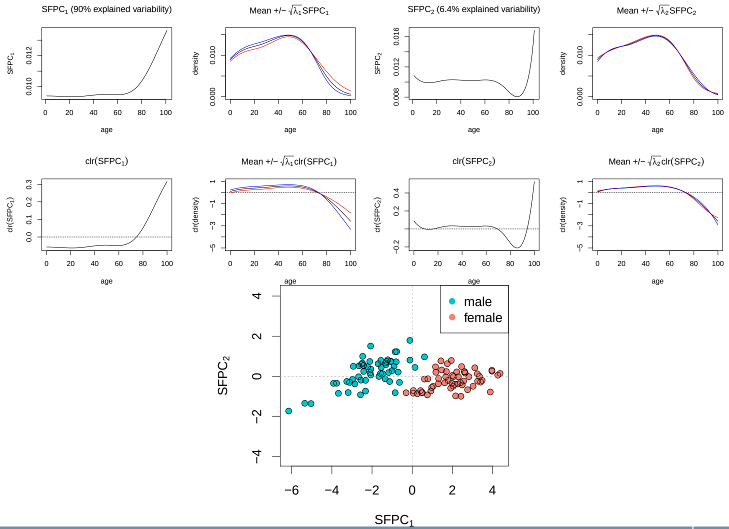




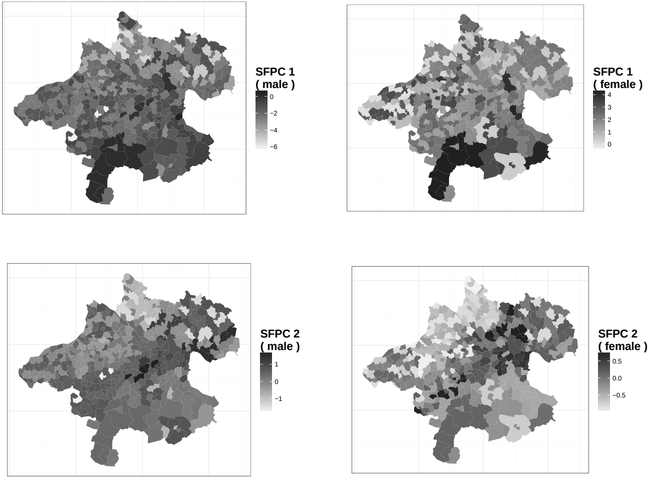




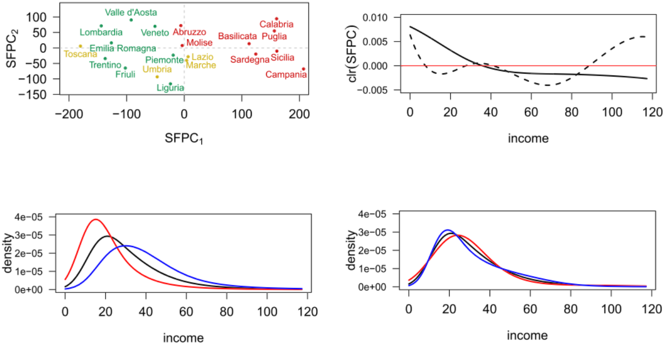
SFPCA: Population age distributions



SFPCA: Population age distributions



SFPCA: Income distributions



SFPC$_1$ . . . 66.08% variability, SFPC$_2$ . . . 18.14% variability

SFPCA: R code

https://github.com/AMenafoglio/BayesSpaces-codes

(with special thanks to Ivana Pavlů, *Palacký University*)

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- Classification (Pavlů et al., 2023), outlier detection (Lei et al., 2023)
- Change point analysis (Kutta et al., 2025)

Extension to the multivariate case

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- Related to this, also the spline representation in Bayes spaces (Machalová et al., 2021; Hron et al., 2022) can be extended to the multivariate case
- A great potential of Bayes spaces further in Bayesian inference (Barfoot and D'Eleuterio, 2023; Wynne, 2023), graphical models, conditional distributions, generalized regression...

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