Regularized Multivariate Functional Principal Component Analysis

Mehdi Maadooliat (Joint work with Yue Zhao and Dr. Hossein Haghbin)

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Background: From FPCA to Regularized FPCA

• Performance of FPCA is often enhanced by regularization techniques.



Figure: Estimated first four principal components for the pinch force data. Left: non-smoothed FPCs. Right: smoothed FPCs

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ReMFPCA

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Motivating Example: Cursive Handwriting

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non-noisy handwritings Y coordinate X coordinate

fda - Cursive handwriting samples

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Motivating Example: Cursive Handwriting

Cursive handwriting coordinates vs. time



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- Rice and Silverman (1991) and Silverman (1996) are pioneer works in regularized FPCA (ReFPCA).
 - Studied functions in Hilbert space and developed roughness penalty based on derivative operators.
 - Mathematical foundation of the ReFPCA is developed in Sobolev spaces.
- Huang et al. (2008) proposed an alternative approach from the penalized SVD point of view.
 - Some nice computational properties.
 - A closed form of CV (GCV) criteria can be derived.
- Chiou et al. (2014) and Happ and Greven (2018) extend FPCA methods to multivariate version: Multivariate FPCA (MFPCA).
 - Enables exploring the relationships between multivariate functions.

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As fd object:

@grid:	vector	(x_1, x_2, \ldots, x_m)
@B:	matrix	$\begin{pmatrix} b_{11} & \dots & b_{d1} \\ \vdots & \dots & \vdots \\ b_{1m} & \dots & b_{dm} \end{pmatrix}$
@C:	matrix	

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@C:	matrix	$\begin{pmatrix} c_{11} & c_{21} & c_{31} & \dots \\ \vdots & \vdots & \vdots & \vdots \\ c_{1d} & c_{2d} & c_{3d} & \dots \end{pmatrix}$

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As fd object:

@grid:	matrix	$\begin{pmatrix} x_1, x_2, \dots, x_{m_x}, x_1, x_2, \dots, x_{m_x}, x_1, x_2, \dots, x_{m_x} \\ y_1, y_1, \dots, y_1, y_2, y_2, \dots, y_2, & \dots, y_{m_y} \end{pmatrix}$
@B:	matrix	$\begin{pmatrix} b_{11} & \dots & b_{dx,1} & \dots & b_{d1} \\ \vdots & \cdots & \vdots & \dots & \vdots \\ b_{1\tilde{m}} & \dots & b_{dx,\tilde{m}} & \dots & b_{d\tilde{m}} \end{pmatrix}$
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• How about Multivariate Functional Data (MFD) observed over different dimensional domains?



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• How about Multivariate Functional Data (MFD) observed over different dimensional domains?





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• How about Multivariate Functional Data (MFD) observed over different dimensional domains?









- Regularized MFPCA (ReMFPCA) seems an intuitive next step to enhance the performance of MFPCA.
- Two ReMFPCA approaches are proposed by our research group.
 - Regularized Eigen Decomposition of the Covariance Operator: By extending Silverman (1996) approach into a multivariate framework. (Submitted: https://doi.org/10.48550/arXiv.2306.13980)
 - **Penalized Functional SVD (fSVD) of the Data Operator**: We study theoretical foundations and implementation of fSVD for MFPCA. Specifically we extend Huang et al. (2008) approach to the multivariate setup in Sobolev space with
 - Flexibility in tuning parameters selection, and
 - Computation efficiency.
 - (Ongoing Project: focus of today's talk)

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Preliminary Notations

• Let H_j to be a Hilbert space equipped with the inner product

 $\langle x, y \rangle_{H_j} = \int_{\mathcal{T}_j} x(t)y(t)dt$, where $x, y \in H_j$ and $j = 1, \cdots, p$.

• The Sobolev space W_i^2 is defined as

 $W_j^2 := \{x(\cdot) : x \text{ and } x' \text{ are absolutely continuous on } \mathcal{T}_j \text{ and } x'' \in H_j\}.$

• Given a smoothing parameter $\alpha_j > 0$, we can define the inner product

$$\langle x, y \rangle_{\alpha_j} := \langle x, y \rangle_{H_j} + \alpha_j \langle x'', y'' \rangle_{H_j}.$$

The $lpha_j$ -orthogonality in Sobolev space W_j^2 is

$$\langle x_j, y_j \rangle_{\alpha_j} = 0.$$

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Preliminary Notations cont.

• Define the cartesian Hilbert product space $\mathbb{H} := H_1 \times \cdots \times H_p$, where each H_j is a Hilbert space. For $\boldsymbol{x} = (x_1, \cdots, x_p)$ and $\boldsymbol{y} = (y_1, \cdots, y_p) \in \mathbb{H}$,

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\mathbb{H}} = \sum_{j=1}^{p} \langle x_j, y_j \rangle_{H_j}.$$

 Define the cartesian Sobolev product spaces W² := W₁² × ··· × W_p². For *x*, *y* ∈ W² and smoothing parameter *α* = (α₁, α₂, ··· , α_p) ∈ ℝ^p,

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{\alpha}} = \sum_{j=1}^{p} \langle x_j, y_j \rangle_{\alpha_j}.$$

The $oldsymbol{lpha}$ -orthogonality in Sobolev space \mathbb{W}^2 is $\langle oldsymbol{x},oldsymbol{y}
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• Define the cartesian Sobolev product spaces $\mathbb{W}^2 := W_1^2 \times \cdots \times W_p^2$. For $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{W}^2$ and smoothing parameter $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \cdots, \alpha_p) \in \mathbb{R}^p$,

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{lpha}} = \sum_{j=1}^p \langle x_j, y_j \rangle_{\alpha_j}.$$

The $\boldsymbol{\alpha}$ -orthogonality in Sobolev space \mathbb{W}^2 is $\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{\alpha}} = 0$.

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Functional SVD and penalized functional SVD

Theorem

Denote $\boldsymbol{x}_i := [x_{i,j}]_{j=1}^p \in \mathbb{H}$ and the data operator $\boldsymbol{\mathcal{X}} := [\boldsymbol{x}_i]_{i=1}^n \in \mathbb{F}^{p \times n}$ with rank $m \leq n$. There exist linearly independent elements $\boldsymbol{\varphi}_1, \cdots, \boldsymbol{\varphi}_m$ from \mathbb{H} and $\boldsymbol{v}_1, \cdots, \boldsymbol{v}_m$ from \mathbb{R}^n that are orthonormal and

$$oldsymbol{\mathcal{X}} = \sum_{i=1}^m \sqrt{\lambda_i} \; oldsymbol{v}_i \otimes oldsymbol{arphi}_i,$$

where λ_i 's are non-ascending positive scalars.

The goal is to obtain regularized FPCs, which is equivalent to solve the following penalized functional SVD problem:

$$\min_{\boldsymbol{\varphi}:\|\boldsymbol{\varphi}\|_{\boldsymbol{\alpha}}=1, \ \boldsymbol{v}\in\mathbb{R}^n} \|\boldsymbol{\mathcal{X}}-\boldsymbol{v}\otimes\boldsymbol{\varphi}\|_{\mathbb{F}}^2 + \boldsymbol{v}^{\top}\boldsymbol{v}\sum_{j=1}^p \alpha_j \langle \varphi_j'', \varphi_j' \rangle_{H_j}$$
(2)

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Finite dimensional representation of functional data

• In implementation, each functional observations are considered as projection on a finite dimensional subspace $H_j^{d_j} = sp\{v_j^k\}_{k=1}^{d_j} \subseteq H_j$. And we define $\mathbb{H}^d := H_1^{d_1} \times \cdots \times H_p^{d_p}$.

Application

• The minimization problem given in (2) becomes

$$\min_{\substack{\boldsymbol{b},\boldsymbol{v}}\\\boldsymbol{\omega}} \| \boldsymbol{B} - \boldsymbol{v} \boldsymbol{b}^{\top} \|_{F}^{2} + \boldsymbol{v}^{\top} \boldsymbol{v} \boldsymbol{b}^{\top} \boldsymbol{\Omega}_{\boldsymbol{\alpha}} \boldsymbol{b},$$
(3)
where $\underset{\sim}{B} = BG^{\frac{1}{2}}$, $\underset{\sim}{b} = G^{\frac{1}{2}}b$, $\boldsymbol{\Omega}_{\boldsymbol{\alpha}} = G^{-\frac{1}{2}}D_{\boldsymbol{\alpha}}G^{-\frac{1}{2}}$, and

 B is the matrix associated to the projection coefficients of X on ℍ^d,

Methodology

• $\boldsymbol{G} := \operatorname{diag} \{ \boldsymbol{G}_1, \cdots, \boldsymbol{G}_p \},$ where $\boldsymbol{G}_j = \left[\langle v_j^l, v_j^k \rangle_{H_j} \right]_{l,k=1}^{d_j}$, b is the vector corresponding to the projection coefficients of φ on H^d,

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•
$$D_{\alpha} := \text{diag}\{\alpha_1 D_1, \cdots, \alpha_p D_p\},\$$

where $D_j = \left[\langle v_j^{l}{}'', v_j^{k}{}'' \rangle_{H_j}\right]_{l,k=1}^{d_j}.$

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where $\boldsymbol{B} = \boldsymbol{B} \boldsymbol{G}^{\frac{1}{2}}$, $\boldsymbol{b} = \boldsymbol{G}^{\frac{1}{2}} \boldsymbol{b}$, $\boldsymbol{\Omega}_{\boldsymbol{\alpha}} = \boldsymbol{G}^{-\frac{1}{2}} \boldsymbol{D}_{\boldsymbol{\alpha}} \boldsymbol{G}^{-\frac{1}{2}}$, and

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Methodology

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Conclusion and Future work

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References



Implementation Strategy: Power algorithm

- To optimize (3), one may use the following iterative power algorithm:
 Initialize b.
 - Initialize **o**.
 - 2 Repeat until convergence:
 - (a) $v \leftarrow BGb$,

$$b \leftarrow \mathrm{S}^2_{\alpha} GB^{\dagger} v$$

Inormalize b.

Here $\mathbf{S}_{oldsymbol{lpha}} = (oldsymbol{G} + oldsymbol{D}_{oldsymbol{lpha}})^{-rac{1}{2}}$ is referred to a half-smoothing matrix.

• For a fixed *v*, the penalized SVD in (3) becomes a penalized regression problem:

$$\|\bar{\boldsymbol{y}} - \bar{\boldsymbol{X}} \underline{\boldsymbol{b}}\|^2 + \underline{\boldsymbol{b}}^\top (\boldsymbol{v}^\top \boldsymbol{v} \boldsymbol{\Omega}_{\boldsymbol{\alpha}}) \underline{\boldsymbol{b}}, \qquad (4)$$

where

$$ar{m{y}} := egin{bmatrix} m{B}^{ op}_{-1}, m{B}^{ op}_{-2}, \dots, m{B}^{ op}_{N-d} \end{bmatrix}^{ op} \in \mathbb{R}^{nd}, \ ar{m{X}} := egin{bmatrix} m{v} & m$$

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Implementation Strategy: Power algorithm

- To optimize (3), one may use the following iterative power algorithm:
 - 1 Initialize **b**.
 - 2 Repeat until convergence:

$$v \leftarrow BGb, \\ S^2 GB^2$$

$$b \leftarrow \mathbf{S}^2_{\boldsymbol{\alpha}} GB'v$$

) normalize **b**.

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$$b \leftarrow \mathbf{S}^{\mathbf{z}}_{\boldsymbol{\alpha}} GB'v$$

normalize **b**

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Tuning parameters selection based on GCV

The GCV criteria can be simply nested within the power algorithm

$$GCV_{\boldsymbol{\alpha}} = \frac{1}{d} \sum_{k=1}^{p} \frac{\|(\boldsymbol{I}_{k} - \boldsymbol{\tilde{S}}_{\alpha_{k}})(\boldsymbol{\tilde{B}}_{k}^{\top} \boldsymbol{v})\|^{2}}{(1 - \frac{1}{d} tr\{\boldsymbol{\tilde{S}}_{\alpha_{k}}\})^{2}},$$

where $\tilde{S}_{\alpha_{k}}$ is k^{th} diagonal block of $\boldsymbol{\tilde{S}}_{\boldsymbol{\alpha}} \coloneqq \boldsymbol{G}^{\frac{1}{2}} \boldsymbol{S}_{\boldsymbol{\alpha}}^{2} \boldsymbol{G}^{\frac{1}{2}}$

a) v ← BGb

Simply nest GCV selection of α inside step (b)

b) $\boldsymbol{b} \leftarrow \boldsymbol{S}_{\boldsymbol{\alpha}}^2 \boldsymbol{G} \boldsymbol{B}^T \boldsymbol{v}$

c) Normalize b

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Two flexible choices in power algorithm

- Simultaneous power algorithm:
 - Obtaining FPCs jointly where all FPCs share the same tuning parameter.
 - Preserves the α -orthogonality in Sobolev space.
 - Since we compute the (p > 1)-dimensional subspace simultaneously, a QR factorization is needed in step 2(b).
- Sequential power algorithm:
 - Obtaining FPCs sequentially where different tuning parameter is allowed for each FPC.
 - The flexibility of having different level of smoothness for FPCs.
 - Losing the α-orthogonality property in Sobolev space.

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Simulation setup

• Let $\mathbf{X}(t)$ be a bivariate functional observation. We define a bivariate orthonormal basis system $\psi_m(t)$, where

$$\psi_m^{(1)}(t) = \sin\left((2m-1)\pi t\right) \text{ and } \psi_m^{(2)}(t) = \sin\left(\frac{(4m-3)\pi}{2}t\right).$$

We adopt the following functional data generating model:

$$\boldsymbol{X}_{i}(\boldsymbol{t}) = \sum_{m=1}^{M} \rho_{i,m} \boldsymbol{\psi}_{m}(\boldsymbol{t}), \qquad \rho_{i,m} \sim \mathbb{N}(0, \lambda_{m}), \quad i = 1, \dots, n.$$
 (5)

- The goal is to examine scenarios where varying levels of noise are added to each $\psi_m(t)$, where $\tilde{\psi}_m(t) = \psi_m(t) + \epsilon_m(t)$.
- We simulate our observations, using

$$\boldsymbol{Y}_{i}(\boldsymbol{t}) = \sum_{m=1}^{M} \rho_{i,m}(\tilde{\boldsymbol{\psi}}_{m}(\boldsymbol{t})), \qquad (6)$$



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Simulation: Comparison

- To assess the performance of our sequential and joint approach, we compare them with two other methods: non-regularized MFPCA and Happ's approach (Happ and Greven, 2018).
- The accuracy of the estimated eigenvalue and eigenfunction pairs, denoted as $\hat{\lambda}_m$ and $\hat{\psi}_m$ respectively, was evaluated by comparing them to their original counterparts:

$$Err(\hat{\lambda}_m) = |\hat{\lambda}_m - \lambda_m| / |\lambda_m|$$
 and $Err(\hat{\psi}_m) = \|\hat{\psi}_m - \psi\|_{\mathbb{H}}.$

• Furthermore, the accuracy of the estimates for each replication is assessed using the mean relative absolute error (MRAE), defined as

$$\mathsf{MRAE} = \frac{1}{n} \sum_{i=1}^{n} (\|\hat{\boldsymbol{x}}_{i} - \boldsymbol{x}_{i}\|_{\mathbb{H}}) / \|\boldsymbol{x}_{i}\|_{\mathbb{H}},$$

where
$$\hat{\pmb{x}}_i = \sum_{m=1}^J \langle \pmb{y}_i, \hat{\pmb{\psi}}_m
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Household electric power consumption data

• Consider a bivariate functional data that include active power and voltage consumption of one household in Sceaux (7km of Paris, France) between December 2006 and November 2010.



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Interpretation of PC scores: FPC1





Left top: Average temperature heatmap; Left bottom: Clustering based on PC1 scores; Right: Clustering details on original data.

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Interpretation of PC scores: FPC3



Figure: Boxplot of PC3 scores

Figure: Clustering details on original data.

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- We developed ReMFPCA based on regularized functional SVD approach.
- An efficient power algorithm is proposed with two flexible choices:
 - Simultaneous power method: Jointly estimates all FPCs with a common smoothing parameter (FPCs will have the α -orthogonality in Sobolev space).
 - Sequential power method: Estimating each FPC sequentially, where different smoothing parameters are allowed for each FPC (we will lose the α -orthogonal property).
- A closed form GCV is derived from the regularized functional SVD approach, where it can significantly improve computational efficiency.
 - Proposed GCV criteria can be embedded within the power algorithm.

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Questions?

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