Regularized Multivariate Functional Principal Component Analysis

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(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.

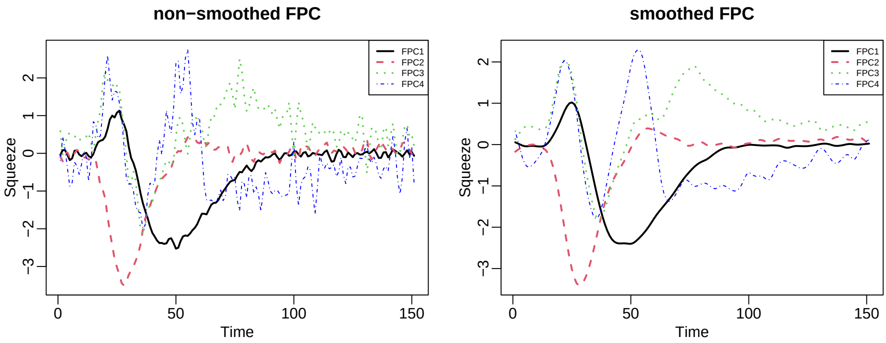
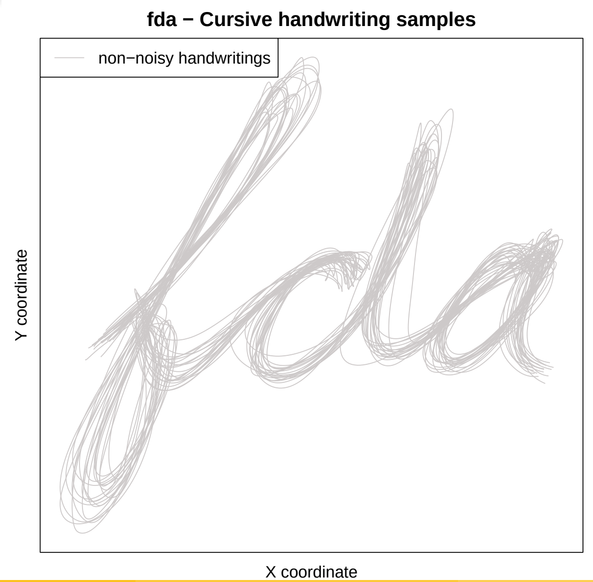


Figure: Estimated first four principal components for the pinch force data.
Left: non-smoothed FPCs.
Right: smoothed FPCs

Motivating Example: Cursive Handwriting



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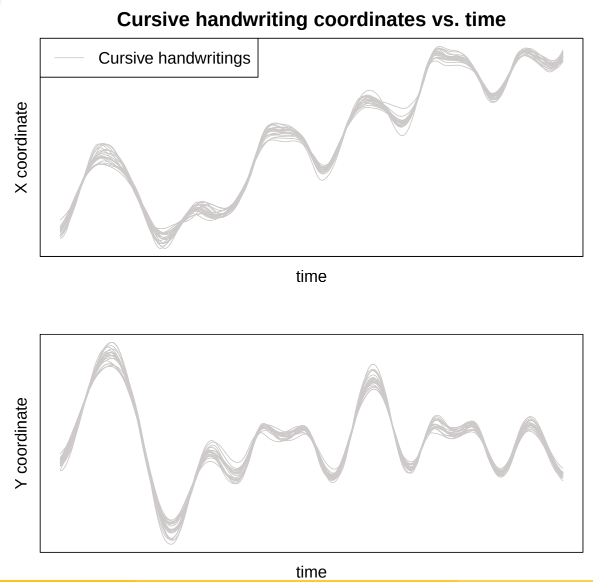

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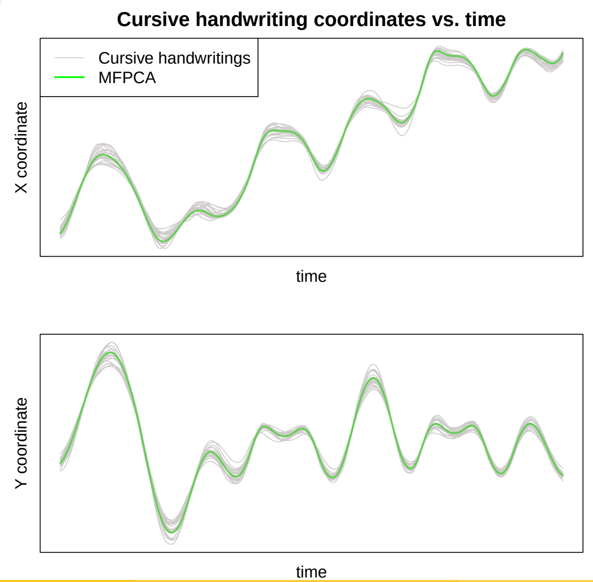

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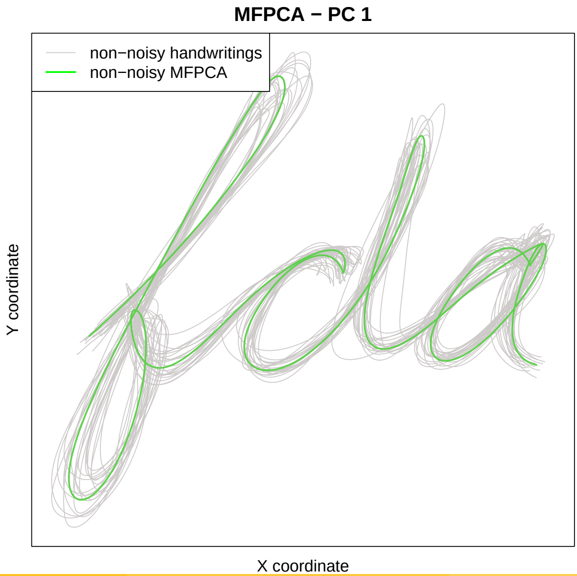

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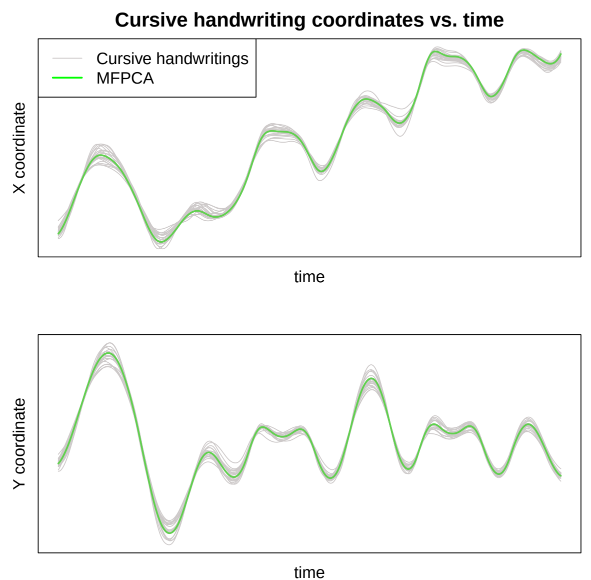

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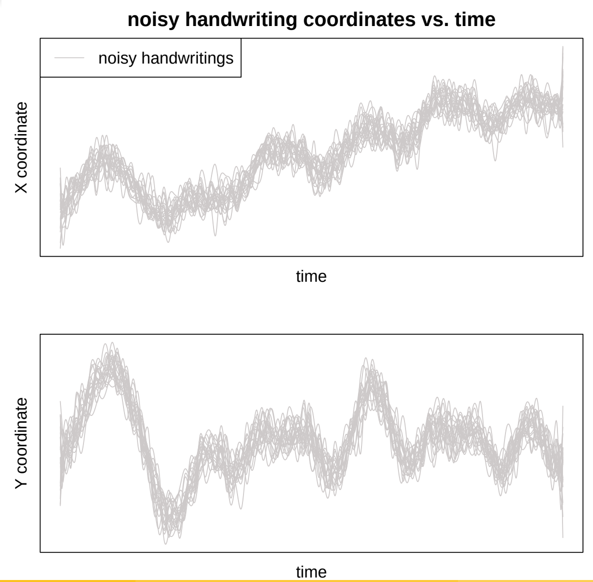

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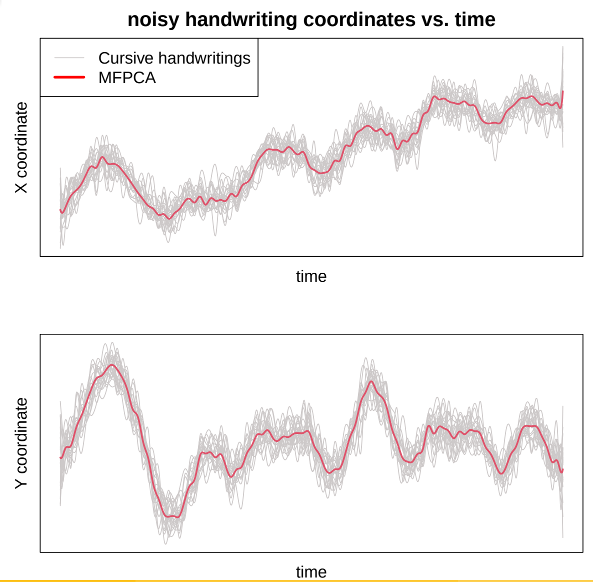

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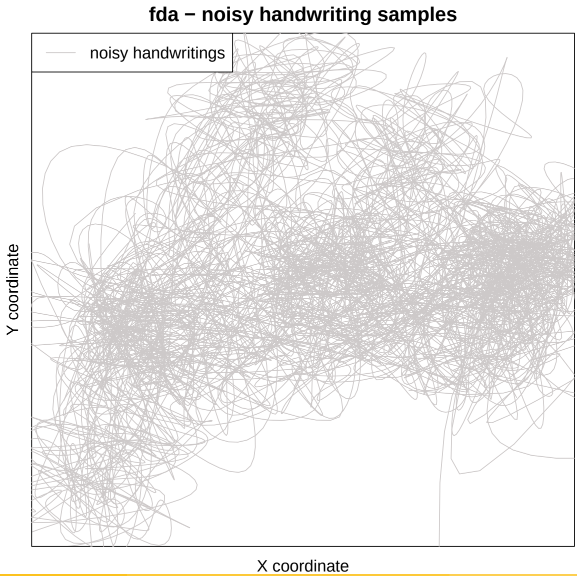

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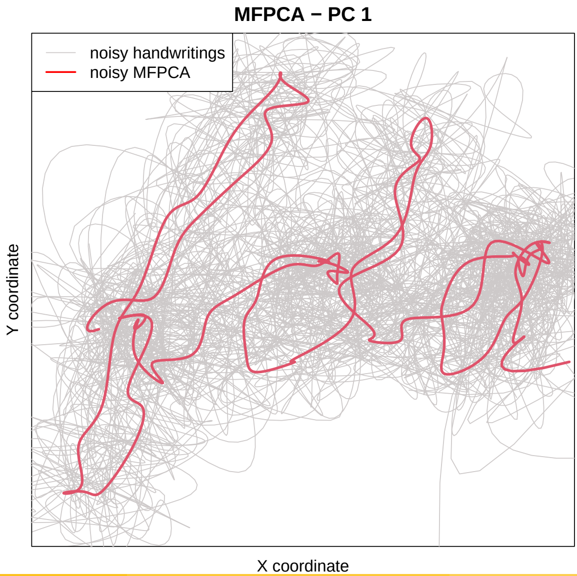

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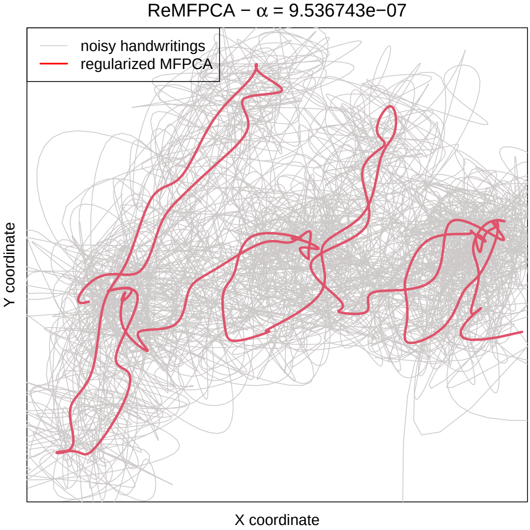

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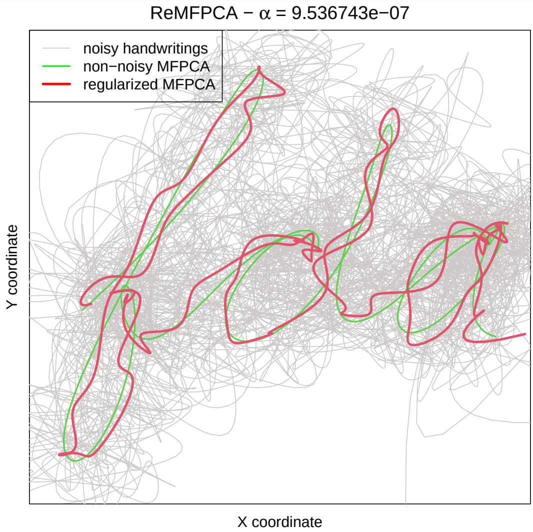

Literature Review

- 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).
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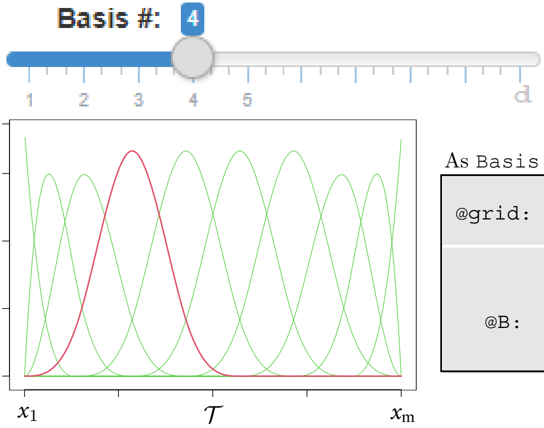
Representation of the functional data (FD) in ReMFPCA



As Basis object:

@grid:	vector	$(x_1, x_2, \ldots, x_{\mathrm{m}})$
@B:	matrix	$\begin{pmatrix} \mathbf{b_{11}} & \cdots & b_{\mathrm{d}1} \\ \vdots & \cdots & \vdots \\ \mathbf{b_{1m}} & \cdots & b_{\mathrm{dm}} \end{pmatrix}$

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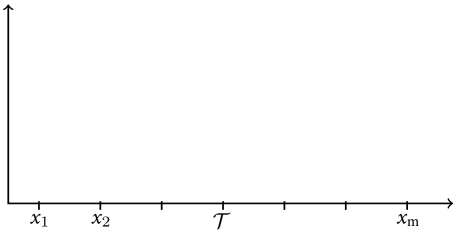

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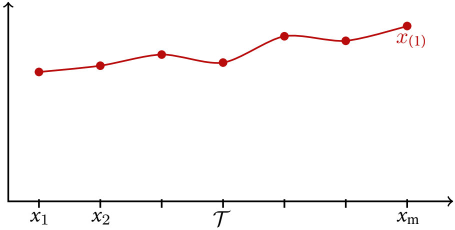

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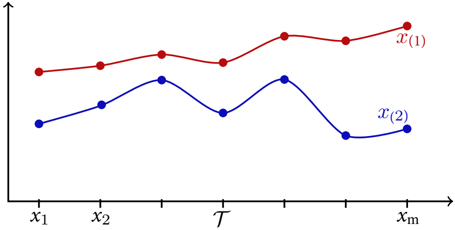

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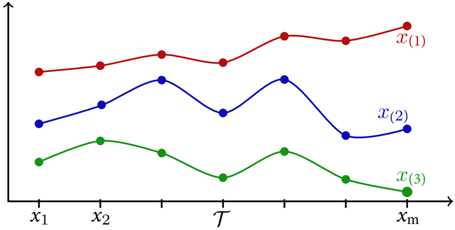

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`@C:`	`matrix`	$\begin{pmatrix} c_{11} & c_{21} & c_{31} & \dots \\ \vdots & \vdots & \vdots & \vdots \\ c_{1d} & c_{2d} & c_{3d} & \dots \end{pmatrix}$

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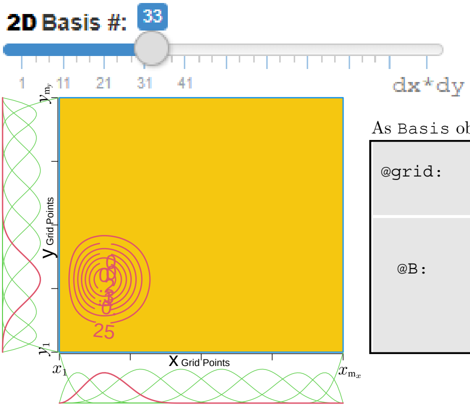

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`@B:`	`matrix`	$\begin{pmatrix} b_{11} & \ldots & b_{dx,1} & \ldots & b_{đ1} \\ \vdots & \ldots & \vdots & \ldots & \vdots \\ b_{1\tilde{m}} & \ldots & b_{dx,\tilde{m}} & \ldots & b_{đ\tilde{m}} \end{pmatrix}$ $đ = d_x * d_y$

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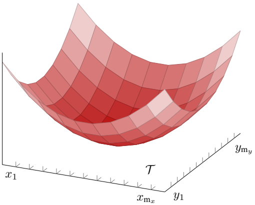

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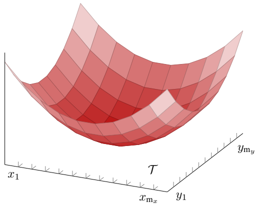

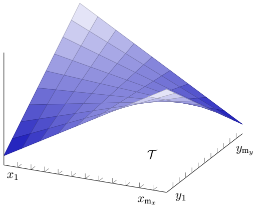

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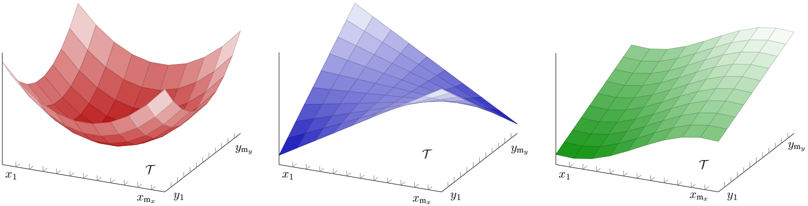

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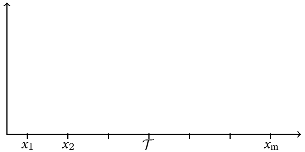
- How about Multivariate Functional Data (MFD) observed over different dimensional domains?



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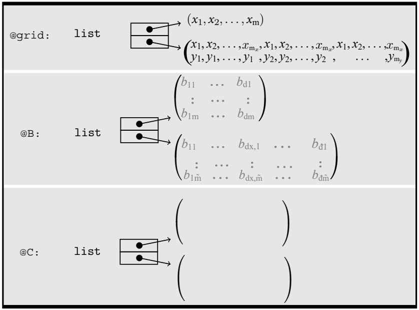

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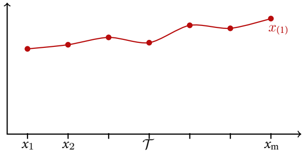

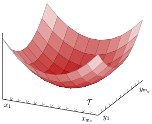

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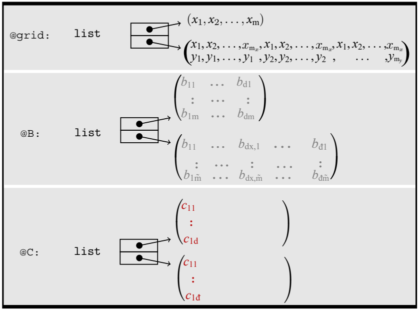

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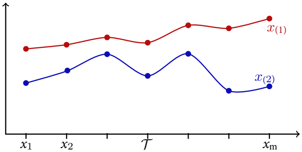

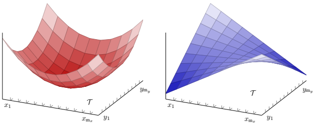

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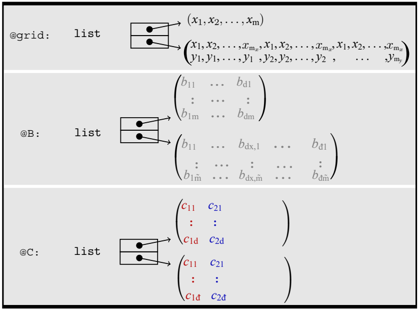

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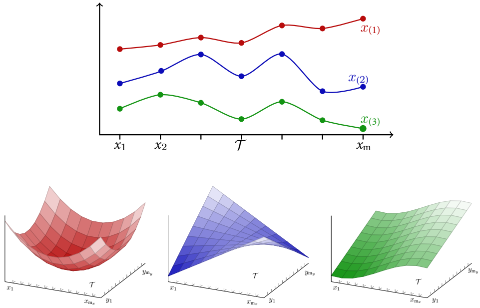

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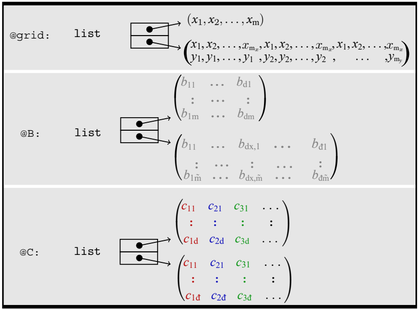

Regularized MFPCA

- 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
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Preliminary Notations

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

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

- The Sobolev space W_j^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

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

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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 $\mathbb{W}^2 := W_1^2 \times \cdots \times W_p^2$.
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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

$$\boldsymbol{\mathcal{X}} = \sum_{i=1}^{m} \sqrt{\lambda_i}\, \boldsymbol{v}_i \otimes \boldsymbol{\varphi}_i, \tag{1}$$

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:

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

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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 $\mathbb{H}^{\boldsymbol{d}} := H_1^{d_1} \times \cdots \times H_p^{d_p}$.
- The minimization problem given in (2) becomes

$$\min_{\underset{\sim}{\boldsymbol{b}},\boldsymbol{v}} \|\underset{\sim}{\boldsymbol{B}} - \boldsymbol{v}\underset{\sim}{\boldsymbol{b}}^\top\|_F^2 + \boldsymbol{v}^\top \boldsymbol{v}\underset{\sim}{\boldsymbol{b}}^\top \boldsymbol{\Omega_\alpha} \underset{\sim}{\boldsymbol{b}}, \quad (3)$$

where $\underset{\sim}{\boldsymbol{B}} = \boldsymbol{B}\boldsymbol{G}^{\frac{1}{2}}$, $\underset{\sim}{\boldsymbol{b}} = \boldsymbol{G}^{\frac{1}{2}}\boldsymbol{b}$, $\boldsymbol{\Omega_\alpha} = \boldsymbol{G}^{-\frac{1}{2}}\boldsymbol{D_\alpha}\boldsymbol{G}^{-\frac{1}{2}}$, and

- $\boldsymbol{B}$ is the matrix associated to the projection coefficients of $\boldsymbol{\mathcal{X}}$ on $\mathbb{H}^{\boldsymbol{d}}$,
- $\boldsymbol{b}$ is the vector corresponding to the projection coefficients of φ on $\mathbb{H}^{\boldsymbol{d}}$,
- $\boldsymbol{G} := \text{diag}\,\{\boldsymbol{G}_1, \cdots, \boldsymbol{G}_p\}$, where $\boldsymbol{G}_j = \left[\langle v_j^l, v_j^k\rangle_{H_j}\right]_{l,k=1}^{d_j}$,
- $\boldsymbol{D_\alpha} := \text{diag}\{\alpha_1\boldsymbol{D}_1, \cdots, \alpha_p\boldsymbol{D}_p\}$, where $\boldsymbol{D}_j = \left[\langle v_j^{l\prime\prime}, v_j^{k\prime\prime}\rangle_{H_j}\right]_{l,k=1}^{d_j}$.

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- $\boldsymbol{b}$ is the vector corresponding to the projection coefficients of $\boldsymbol{\varphi}$ on $\mathbb{H}^{\boldsymbol{d}}$,
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Implementation Strategy: Power algorithm

- To optimize (3), one may use the following iterative power algorithm:
  1. Initialize $\boldsymbol{b}$.
  2. Repeat until convergence:
     a. $\boldsymbol{v} \leftarrow \boldsymbol{BGb}$,
     b. $\boldsymbol{b} \leftarrow \mathrm{S}_\alpha^2 \boldsymbol{G} \boldsymbol{B}^\top \boldsymbol{v}$,
     c. normalize $\boldsymbol{b}$.

  Here $\mathrm{S}_\alpha = (\boldsymbol{G} + \boldsymbol{D}_\alpha)^{-\frac{1}{2}}$ is referred to a half-smoothing matrix.

- For a fixed $\boldsymbol{v}$, the penalized SVD in (3) becomes a penalized regression problem:

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

where

$$\bar{\boldsymbol{y}} := \left[\underset{\sim}{\boldsymbol{B}}_{.1}^\top, \underset{\sim}{\boldsymbol{B}}_{.2}^\top, \ldots, \underset{\sim}{\boldsymbol{B}}_{.d}^\top\right]^\top \in \mathbb{R}^{nd}, \quad \bar{\boldsymbol{X}} := \begin{bmatrix} \boldsymbol{v} & & \\ & \ddots & \\ & & \boldsymbol{v} \end{bmatrix} \in \mathbb{R}^{nd \times d}.$$

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

$$\|\bar{y} - \bar{X}\underset{\sim}{b}\|^2 + \underset{\sim}{b}^\top(v^\top v\Omega_\alpha)\underset{\sim}{b}, \quad (4)$$

where

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Tuning parameters selection based on GCV

The GCV criteria can be simply nested within the power algorithm

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

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

a) $\boldsymbol{v} \leftarrow \boldsymbol{BGb}$

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

c) Normalize b

Simply nest GCV selection of $\boldsymbol{\alpha}$ inside step (b)

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.
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  - Losing the α-orthogonality property in Sobolev space.

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Simulation setup

- Let $\mathbf{X}(\boldsymbol{t})$ be a bivariate functional observation. We define a bivariate orthonormal basis system $\boldsymbol{\psi}_m(\boldsymbol{t})$, where

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

We adopt the following functional data generating model:

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

- The goal is to examine scenarios where varying levels of noise are added to each $\boldsymbol{\psi}_m(\boldsymbol{t})$, where $\tilde{\boldsymbol{\psi}}_m(\boldsymbol{t}) = \boldsymbol{\psi}_m(\boldsymbol{t}) + \boldsymbol{\epsilon}_m(\boldsymbol{t})$.

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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:

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

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

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

where $\hat{x}_i = \sum_{m=1}^{J} \langle y_i, \hat{\psi}_m \rangle_{\mathbb{H}} \hat{\psi}_m$.

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Comparison result (for different trend patterns in eigenvalues)

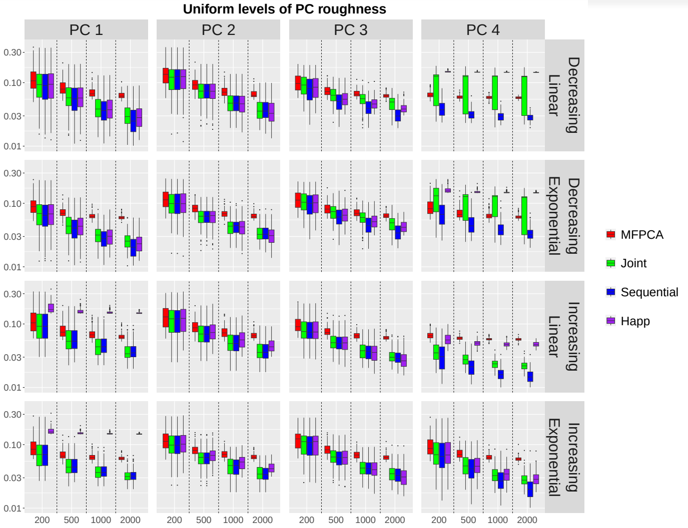

Figure: $Err(\hat{\psi}_m)$

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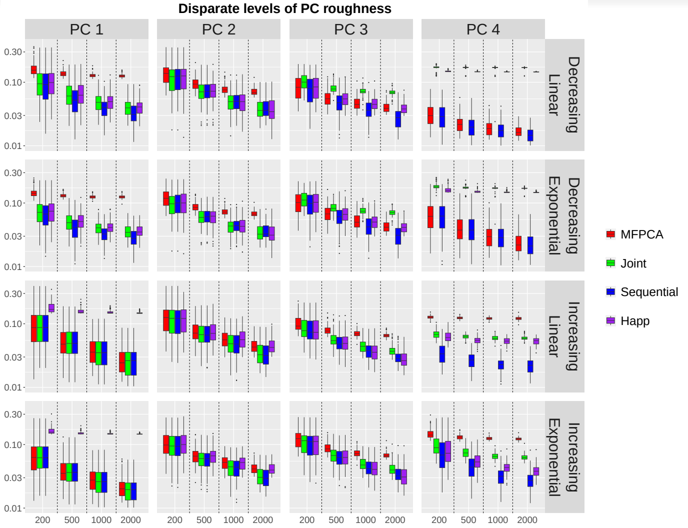

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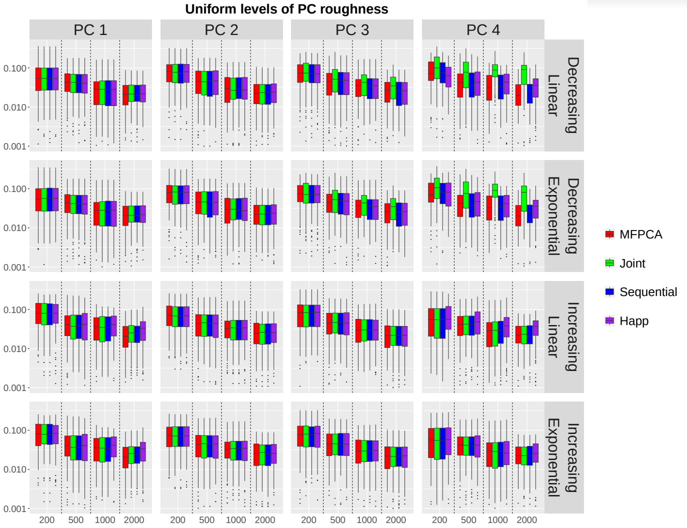

Figure: $Err(\hat{\lambda}_m)$

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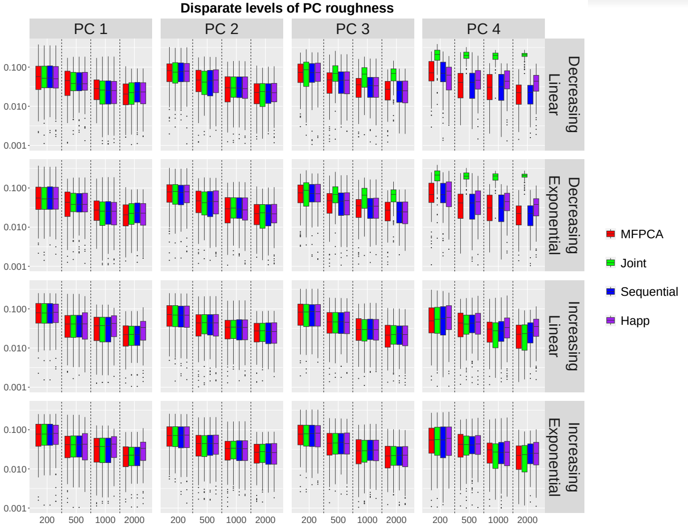

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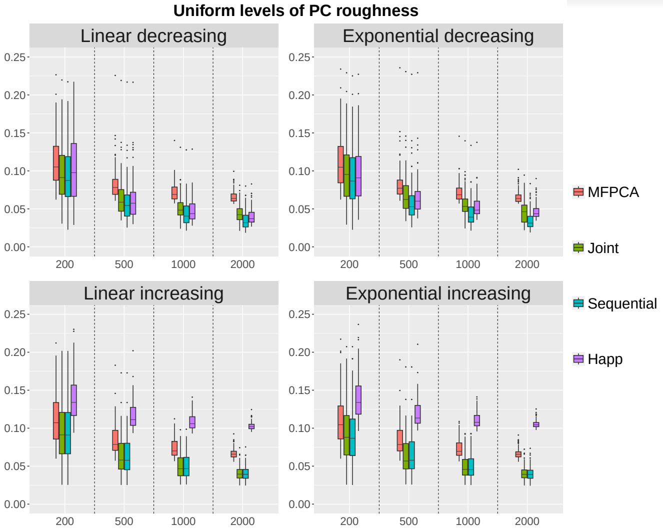

Figure: MRAE

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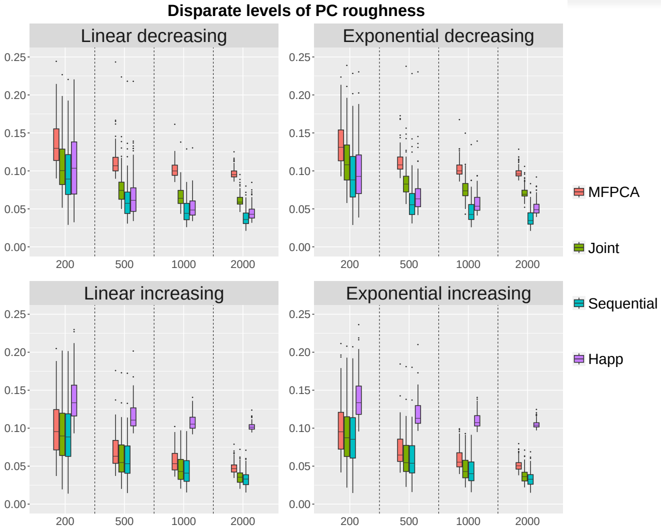
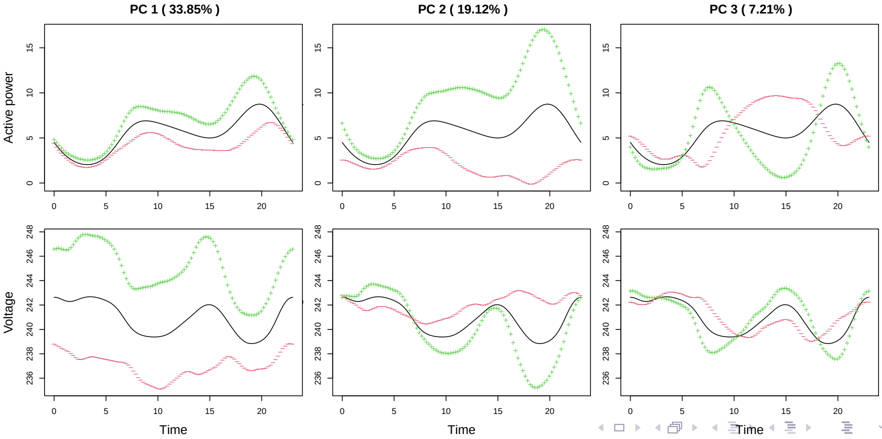


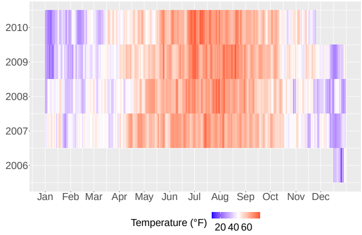
Figure: MRAE

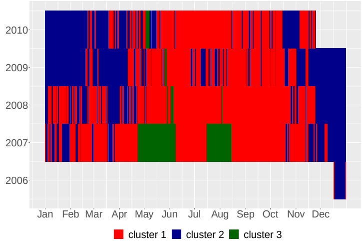
Household electric power consumption data

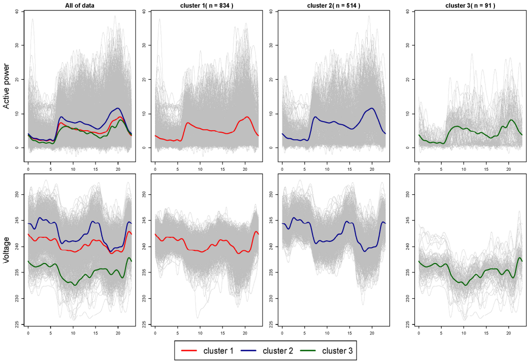
- Consider a bivariate functional data that include active power and voltage consumption of one household in Sceaux (7km of Paris, France) between December 2006 and November 2010.



Interpretation of PC scores: FPC1







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

Interpretation of PC scores: FPC3

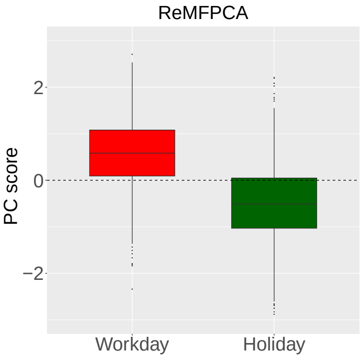


Figure: Boxplot of PC3 scores

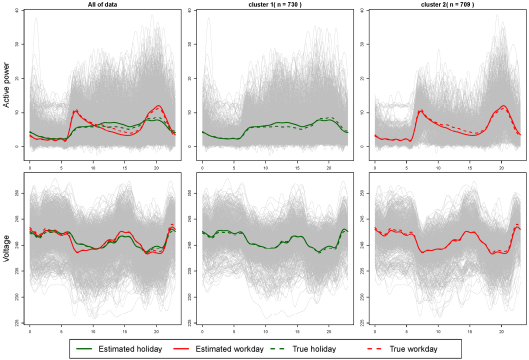


Figure: Clustering details on original data.

Conclusion

- 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.

Thank you!

- Collaborators
  - Yue Zhao, Ph.D. Candidate, Marquette University
  - Hossein Haghbin, Assistant Professor, Persian Gulf University

Questions?

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