Regularized Multivariate Two-way Functional Principal Component Analysis

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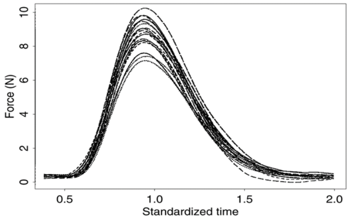
BE THE DIFFERENCE.

Outline

1. Introduction & Background
2. A SVD Approach for Regularized Multivariate FPCA
3. Two-way Regularized Multivariate FPCA
4. Conclusion & Future Work

Introduction

- **Functional data** are observations that change continuously over a domain (like time, space, or wavelength) and are often visualized as curves, trajectories, or functions rather than isolated points.



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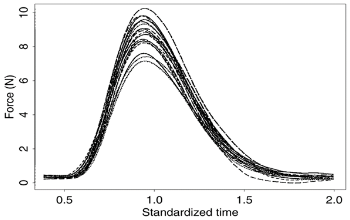
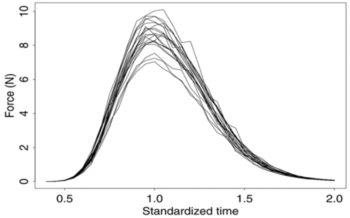
- In practice, these data are often recorded at discrete time points or grid locations, even though they originate from continuous processes in areas like engineering, finance, environmental science, and healthcare.





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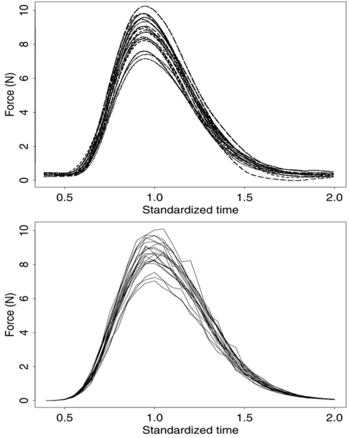
- In practice, these data are often recorded at discrete time points or grid locations, even though they originate from continuous processes in areas like engineering, finance, environmental science, and healthcare.
- **Functional Data Analysis (FDA)** is a statistical framework that treats these observations as realizations of smooth underlying functions, allowing for more accurate modeling and interpretation of continuous processes.

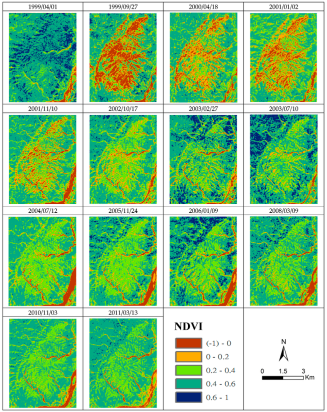


Functional Principal Component Analysis

- **Functional PCA (FPCA):** An extension of classical PCA for dimension reduction and uncovering hidden patterns in functional data; it identifies orthogonal functions that capture the main sources of variation, preserving the most important information. [Ramsay and Silverman, 2005].
- **Extensions of FPCA:**
  - Smoothed FPCA: Adds roughness penalties for smoothness [Silverman, 1996, Huang et al., 2008].
  - Sparse FPCA: Enforces sparsity for interpretability [Shen and Huang, 2008, Nie and Cao, 2020].
  - Multivariate FPCA (MFPCA): Extends FPCA to multivariate functions [Silverman, 1996, Happ and Greven, 2018].
  - Regularized MFPCA: Penalties improve estimation & interpretability [Haghbin et al., 2025].
- **Impact:** More adaptable, robust, and applicable across diverse scientific and business problems.

Two-way Functional Principal Component Analysis

- **Two-way functional data:** Observations vary along two domains (e.g., time $\times$ space, time $\times$ frequency), with applications in climate, neuroscience, finance, public health, and marketing.



Two-way Functional Principal Component Analysis

- **Two-way functional data:** Observations vary along two domains (e.g., time $\times$ space, time $\times$ frequency), with applications in climate, neuroscience, finance, public health, and marketing.
- **Extension of FPCA:** Huang [Jianhua Z. Huang and Buja, 2009] applied regularization to both left and right singular vectors in SVD.
- **Practical challenges:**
  - Data observed on discrete grids (minutes, hours, days).
  - Issues: measurement noise, irregular sampling, missing data, loss of smoothness.
- **Proposed framework:**
  - Unified FPCA for two-way multivariate functional data.
  - Smoothness penalties preserve functional structure.
  - Sparsity penalties enhance interpretability.
  - Effective for dimension reduction in complex datasets.

Foundations of FPCA through Minimizing Reconstruction Error

- **Goal:** Identify functional directions that maximize variance (low-rank approximation of functional data). For functional data $X \in \mathbb{R}^{n \times m}$ contains the discretized functional observations (rows correspond to subjects, columns to grid points), $v \in \mathbb{R}^m$ represents the estimated principal component (function), and $u \in \mathbb{R}^n$ denotes the associated principal component scores.
- **Reconstruction problem:**

$$\min_{u,v} \|X - uv^\top\|_F^2 = \mathrm{tr}\{(X - uv^\top)(X - uv^\top)^\top\},$$

- **Optimization steps:**

$$\text{Fix } v: \; u = \frac{Xv}{v^\top v} \qquad \text{and} \qquad \text{Fix } u: \; v = \frac{X^\top u}{u^\top u}$$

Extensions of FPCA via Regularization

- **Goal:** Balance **variance explanation**, **smoothness**, and **interpretability**.
- Reformulate FPCA as a **penalized low-rank approximation** problem:

$$\min_{u,v} \|X - uv^\top\|_F^2 + \mathcal{P}(u, v)$$

- Two directions:
  - **Smooth FPCA:** adds roughness penalty on functions.
  - **Sparse FPCA:** adds sparsity penalty on loadings.
- **Algorithms:** Based on iterative **power method** and **thresholding** updates.

Smooth Functional PCA

- Problem setup [Huang et al., 2008]:

$$\min_{u,v} \|X - uv^\top\|_F^2 + \alpha\, u^\top u\, v^\top \Omega v$$

  - $X \in \mathbb{R}^{n \times p}$: discretized functional data.
  - $u \in \mathbb{R}^n$: scores.
  - $v \in \mathbb{R}^p$: loading function.
  - Ω: roughness penalty matrix (e.g., integrated squared 2nd derivative).
  - α: tuning parameter

- A power algorithm is defined to compute the PCs while incorporating smoothness penalty.

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- Consider the SVD of X as $X = UDV^\top$, where U and V have orthonormal columns and D is diagonal with ordered singular values. In particular, for $X = udv^\top$, v is the first principal component and $u = ud$ gives the associated scores. With these representations, the power algorithm (described below) converges quickly, typically in only a few iterations.

Power Algorithm

Algorithm: Penalized Power Iteration

1. Initialize v.
2. Repeat until convergence:
   1. $u \leftarrow Xv$
   2. $v \leftarrow (I + \alpha\Omega)^{-1} X^\top u$
   3. $v \leftarrow \dfrac{v}{\|v\|}$
3. Update $X \leftarrow X - \sigma\, uv^\top$ and proceed to next component.

- For notational convenience, we define $S(\alpha) = (I + \alpha\Omega)^{-1} \in \mathbb{R}^{m\times m}$, which simplifies expressions involving regularization. The penalty matrix Ω is set up so that larger values of the quadratic form $v^\top \Omega v$ mean rougher functions. This means that it penalizes functions that change quickly between time points.

Tunning Smoothness Parameters

- To select the optimal tuning parameters α efficiently, one can use a traditional Cross-Validation (CV) criterion and a computationally efficient closed-form Generalized Cross-Validation (GCV) criterion:

$$\mathrm{CV}(\alpha) = \frac{1}{m} \sum_{j=1}^{m} \frac{\left[\{(I - S(\alpha))(X^T u)\}_{jj}\right]^2}{(1 - \{S(\alpha)\}_{jj})^2},$$

where $\{\cdot\}_{jj}$ denotes the j-th diagonal element.

$$\mathrm{GCV}(\alpha) = \frac{1}{m} \frac{\|(I - S(\alpha))(X^T u)\|^2}{\left(1 - \frac{1}{m}\mathrm{tr}\{S(\alpha)\}\right)^2}.$$

Sparse Functional PCA

- *Standard FPCA loadings are dense, involving linear combinations of all grid points → hard to interpret.*
  Sparsity highlights only the most relevant features, thereby enhancing interpretability.
- *Dense loadings capture noise → unstable components.*
  Sparsity filters out uninformative variation, yielding more robust principal components, reducing dimensionality, and facilitating interpretation.
- *All grid points contribute equally → no feature selection.*
  Sparsity acts as an inherent feature selector, directing attention to key time points, with most entries reduced to zero while only a few contribute meaningfully to the structure.
- Sparse FPCA formulation [Shen and Huang, 2008]:

$$\min_{u,v} \|X - uv^\top\|_F^2 + p_\gamma(v) \tag{1}$$

where $p_\gamma(v)$ is a sparsity-inducing penalty.

Sparsity penalties

- **Soft-thresholding (Lasso):**

$$p_\gamma^{\text{soft}}(|\theta|) = 2\gamma|\theta|, \xrightarrow[\text{minimizer}]{} h_\gamma^{\text{soft}}(y) = \text{sign}(y)(|y|-\gamma)_+$$

- **Hard thresholding:**

$$p_\gamma^{\text{hard}}(|\theta|) = \gamma^2 I(|\theta| \neq 0), \xrightarrow[\text{minimizer}]{} h_\gamma^{\text{hard}}(y) = I(|y| > \gamma)\, y$$

- **SCAD penalty:**

$$p_\gamma^{\text{SCAD}}(|\theta|) = \begin{cases} 2\gamma|\theta|, & |\theta| \leq \gamma, \\ \dfrac{\theta^2 - 2a\gamma|\theta| + \gamma^2}{a-1}, & \gamma < |\theta| \leq a\gamma, \\ \dfrac{(a+1)\gamma^2}{2}, & |\theta| > a\gamma, \end{cases} \xrightarrow[\text{minimizer}]{} h_\gamma^{\text{SCAD}}(y) = \begin{cases} \text{sign}(y)(|y|-\gamma)_+, & |y| \leq 2\gamma, \\ \dfrac{(a-1)y - \text{sign}(y)a\gamma}{a-2}, & 2\gamma < |y| \leq a\gamma, \\ y, & |y| > a\gamma, \end{cases}$$

where $a = 3.7$ (Fan and Li [2001]).

sFPCA-rSVD Algorithm

To implement the sPCA-rSVD algorithm discussed above, we use the following iterative procedure to minimize the objective function defined in Equation (1).

Algorithm: sFPCA-rSVD

1. Initialization: Compute the best rank-one approximation of X using singular value decomposition (SVD), where $X \approx suv^\top$, and set $u \leftarrow su$.
2. Iterate until convergence:
    1. Update Left Singular Vector: $u \leftarrow Xv$
    2. Update Right Singular Vector: $v \leftarrow h_\gamma X^\top u$
    3. Normalize Right Singular Vector: $v \leftarrow \dfrac{v}{\|v\|}$

Cross-Validation for Sparsity Selection

- **Sparsity parameter**: Tuning parameter controlling number of non-zero loadings in v ($0 =$ dense, $p =$ full sparsity).

Algorithm: K-fold CV Tuning Parameter Selection - Degree of sparsity

1. Randomly group the rows of side-by-side data matrix X into K roughly equal-sized groups, denoted as $X^1, ..., X^K$.
2. For each sparse tuning parameter $j \in \{0, 1, ..., p\}$ (level of sparsity), do the following:
   1. For $k = 1, ..., K$, let X^{-k} be the data matrix X leaving out X^k. Apply Algorithm sFPCA-rSVD on X^{-k} and derive the FPC scores $u^{-k}(j)$. Then project X^k onto $u^{-k}(j)$ to obtain $v^k(j)$.
   2. Calculate the K-fold CV scores defined as: (N is the number of grid points in X^k)

$$CV_j = \sum_{k=1}^{K} \frac{\|X^k - u^{-k}(j)v^k(j)\|^2}{N}$$

3. Select the degree of sparsity as $j_0 = \arg\min\{CV(j)\}$.

Overview of Existing Approaches

- **Smooth FPCA:**
  - Pros: Produces smooth eigenfunctions.
  - Algorithm: Penalized power iteration.
  - Tuning: α (smoothness) via GCV.
- **Sparse FPCA:**
  - Pros: Feature selection $\rightarrow$ interpretable.
  - Algorithm: sFPCA-rSVD algorithm.
  - Tuning: γ (sparsity) via CV.
- **Combined Approaches:** Smooth + Sparse together.

$$\min_{u,v} \|X - uv^\top\|_F^2 + \alpha v^\top \Omega v + p_\gamma(v)$$

- Trade-off: **Variance explained vs Interpretability vs Smoothness**.

Regularized MFPCA

- **Context**
  - Univariate FDA $\rightarrow$ **Multivariate FDA** (e.g., simultaneously recorded EEG channels, growth patterns of multiple anatomical measures.)
  - MFPCA $\rightarrow$ **joint modes of variation** across functions
- **Challenges**
  - Discretization & irregular grids $\rightarrow$ noise, missing data
  - High dimensionality and limited sample size $\rightarrow$ unstable eigenfunctions (sensitive to small fluctuations in the data)
  - Cross-function correlation $\rightarrow$ requires enforcing smoothness both within and across functions
- **Proposed Solution: Penalized SVD**
  - **Smoothness penalties**: roughness on derivatives
  - **Sparsity penalties**: Soft, hard, or SCAD
  - **Block-diagonal roughness matrix** for cross-function structure
- **Impact**
  - Produces **smooth, sparse, interpretable** joint modes
  - More stable & applicable to high-dimensional multivariate FDA

Methodology: Multivariate Functional Data Framework

- A multivariate functional dataset is formed by **concatenating p functional data matrices**.
    - Each variable: $X_i \in \mathbb{R}^{n\times m_i}$ where n: number of observations and m_i: grid points

- **Rank-one approximation** (per variable):

$$X_i \approx u_i v_i^\top, \quad u_i \in \mathbb{R}^n,\ v_i \in \mathbb{R}^{m_i}$$

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- **Full data matrix**: $\mathbf{X} = [X_1 \quad X_2 \quad \cdots \quad X_p] \in \mathbb{R}^{n \times \sum_{i=1}^{p} m_i}$

$$\boldsymbol{X} = \begin{bmatrix} x_{11}(t_{11}) & \cdots & x_{11}(t_{1,m_1}) & \cdots & x_{1p}(t_{p1}) & \cdots & x_{1p}(t_{p,m_p}) \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{n1}(t_{11}) & \cdots & x_{n1}(t_{1,m_1}) & \cdots & x_{np}(t_{p1}) & \cdots & x_{np}(t_{p,m_p}) \end{bmatrix}.$$

Penalized Smooth MFPCA

- Standard FPCA loadings may be noisy; smoothness penalties (via block-diagonal Ω_i) improve structure and interpretability.
- Let $\boldsymbol{X} \in \mathbb{R}^{n \times M}$ denote multivariate functional data, where $M = \sum_{i=1}^{p} m_i$.
  Its best rank-one approximation is $\boldsymbol{X} \approx uv^\top$,
  with $u \in \mathbb{R}^n$ (score vector) and $v = [v_1, v_2, \ldots, v_p]^\top \in \mathbb{R}^M$ (loading vector).
  A smoothness penalty is imposed on v.

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- The block-diagonal penalty matrix is $\boldsymbol{\Omega} = \mathrm{diag}(\Omega_1, \Omega_2, \ldots, \Omega_p)$, where each $\Omega_i \in \mathbb{R}^{m_i \times m_i}$ is a univariate roughness penalty matrix.

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- The penalized reconstruction error is

$$\min_{u,v} \|\boldsymbol{X} - uv^\top\|_F^2 + \boldsymbol{\alpha}^\top (v^\top \boldsymbol{\Omega} v),$$

where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_p)^\top$ controls smoothness.

MFPCA Power Algorithm

Algorithm: Regularized Power Iteration for Smooth MFPCA

1. Initialize v.
2. Repeat until convergence:
   1. $u \leftarrow \mathbf{X}v$
   2. $v \leftarrow (I + \alpha\boldsymbol{\Omega})^{-1}\mathbf{X}^\top u$
   3. $v \leftarrow v/\|v\|$
3. Update $\mathbf{X} \leftarrow \mathbf{X} - \sigma uv^\top$ to extract the next PC.

- The smoothing operator is $\boldsymbol{S}(\boldsymbol{\alpha}) = (I + \alpha\boldsymbol{\Omega})^{-1} \in \mathbb{R}^{M\times M}$.

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- The smoothing operator is $\boldsymbol{S}(\alpha) = (I + \alpha\boldsymbol{\Omega})^{-1} \in \mathbb{R}^{M\times M}$.
- The smoothing parameter α is selected via generalized cross-validation (GCV), defined as

$$\mathrm{GCV}(\alpha) = \frac{1}{M}\frac{\|(I - \boldsymbol{S}(\alpha))(\mathbf{X}^T u)\|^2}{\left(1 - \frac{1}{M}\mathrm{tr}\{\mathbf{S}(\alpha)\}\right)^2}. \tag{2}$$

Penalized Sparse Multivariate FPCA

- **Goal:** Extend sparse FPCA to multivariate functional data, imposing **sparsity** (select important regions) and **smoothness** (reduce noise).
- **Sparsity penalties:** Soft, hard, or SCAD thresholding Shen and Huang [2008], Zhenhua Lin and Wang [2017], Nie and Cao [2020].

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- Sparsity parameters: $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_p)$, where γ_i ranges from 0 (no sparsity) to m_i for each variable.

Algorithm: Regularized Power Iteration for Smooth MFPCA

1. Initialization: Compute rank-one SVD of $\boldsymbol{X}$, $\boldsymbol{X} \approx suv^\top$, and set $u \leftarrow su$.
2. Iterate until convergence:
   1. Update left singular vector: $u \leftarrow \boldsymbol{X}v$
   2. Update right singular vector: $v \leftarrow \boldsymbol{h_\gamma} \boldsymbol{X}^\top u$
   3. Normalize right singular vector: $v \leftarrow \dfrac{v}{\|v\|}$

Smooth and Sparse Multivariate FPCA

- The combined implementation of smoothness and sparsity on the loading vector v in multivariate functional data is achieved by the following algorithm:

Algorithm: Regularized Power Iteration for Smooth MFPCA

1. Initialize unit vectors u and v using SVD of $\boldsymbol{X}$ (best rank-one approximation of $\boldsymbol{X}$)
2. Repeat till convergence
   1. $u \leftarrow \boldsymbol{X} v$
   2. $v \leftarrow \boldsymbol{S}(\alpha)\boldsymbol{h}(\gamma_v)\boldsymbol{X}^\top u$
   3. $v \leftarrow \frac{v}{\|v\|}$
3. Update $\boldsymbol{X} = \boldsymbol{X} - \sigma u v^\top$ and proceed to find the next principal component.

- Algorithm CV Tuning for Sparsity and equation (2) are used to tune the sparsity level via K-fold CV and the smoothing parameter via GCV, respectively.

Simulation: Estimation Performance

- **Data-generating process:** Two functional variables:

$$X_{ij}^{(1)} = u_{i1} v_{11}(t_j) + u_{i2} v_{12}(t_j) + \epsilon_{ij}^{(1)}, \quad X_{ij}^{(2)} = u_{i1} v_{21}(t_j) + u_{i2} v_{22}(t_j) + \epsilon_{ij}^{(2)},$$

  - where $u_{i1} \sim N(0, \sigma_1^2)$, $u_{i2} \sim N(0, \sigma_2^2)$, $\epsilon_{ij}^{(k)} \sim N(0, \sigma^2)$, and $n = m = 101$, $t_j \in [-1, 1]$
- **True functional PCs:**
  - Variable 1: $v_{11}(t) = \frac{t+\sin(\pi t)}{s_1}$, $v_{12}(t) = \frac{\cos(3\pi t)}{s_2}$
  - Variable 2:

$$v_{21}(t) = \begin{cases} \dfrac{\sin(3\pi t)}{s_3}, & t \in (-\frac{1}{3}, \frac{1}{3}), \\ 0, & \text{otherwise}, \end{cases} \qquad v_{22}(t) = \begin{cases} \dfrac{\sin(2\pi t)}{s_4}, & t \leq -\frac{1}{3}, \\ \dfrac{\sin(\pi t)}{s_4}, & t \geq \frac{1}{3}, \\ 0, & \text{otherwise}. \end{cases}$$

Here, s_1, s_2, s_3, s_4 are normalizing constants ensuring unit L^2 norm.

Simulation: Estimation Performance

Scenarios tested:

1. Unpenalized Multivariate SVD (baseline)
2. Smoothed Multivariate SVD (smoothness penalty)
3. Sparse Multivariate SVD (sparsity penalty)
4. Sparse + Smoothed Multivariate SVD (combined regularization)

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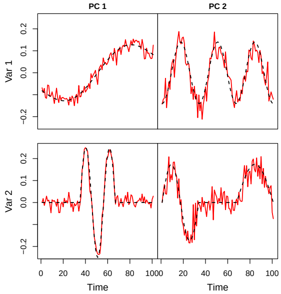

(a) MFPCA

Simulation: Estimation Performance

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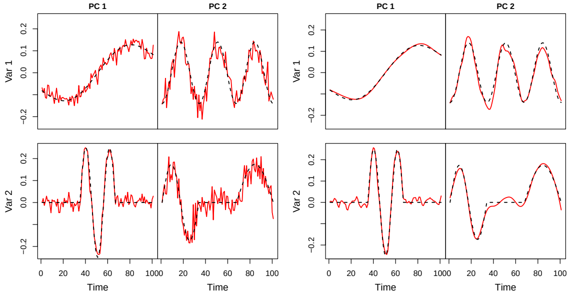

(a) MFPCA (b) Smoothed MFPCA

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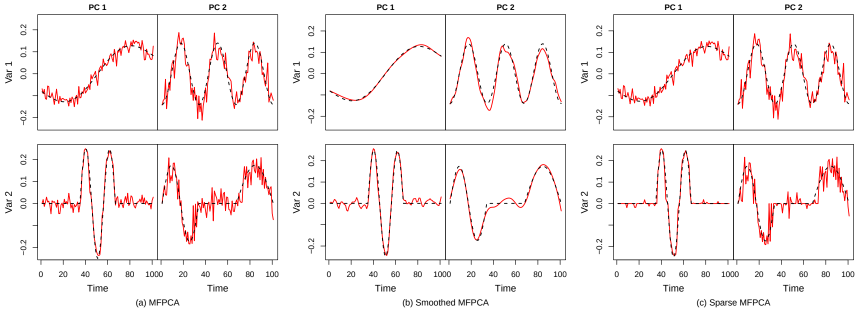

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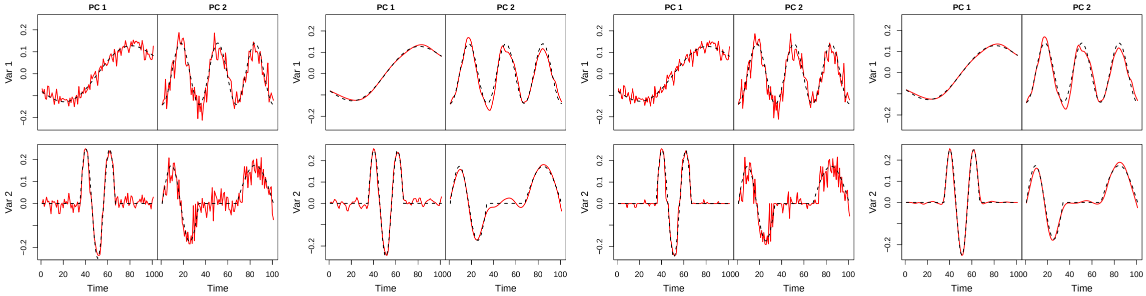


(a) MFPCA (b) Smoothed MFPCA (c) Sparse MFPCA (d) Smoothed and Sparse MFPCA

Simulation: Estimation Performance

Accuracy measures:

1. Variable-wise MSE:

$$\mathrm{MSE}_{k\ell} = \frac{1}{m} \sum_{j=1}^{m} (\hat{v}_{k\ell}(t_j) - v_{k\ell}(t_j))^2$$

2. Replication-averaged MSE:

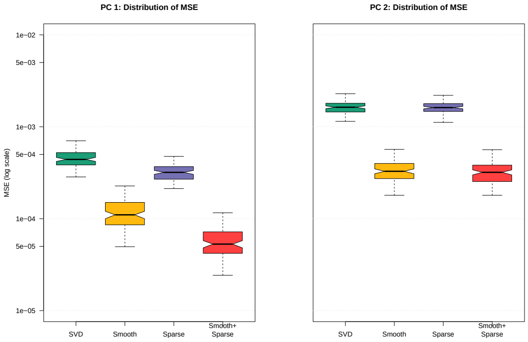
$$\overline{\mathrm{MSE}}_{k\ell} = \frac{1}{R} \sum_{r=1}^{R} \mathrm{MSE}_{k\ell}^{(r)}$$

3. Multivariate MSE:

$$\mathrm{MSE}_{\ell}^{(\mathrm{multi})} = \frac{1}{m} \sum_{j=1}^{m} \sum_{k=1}^{2} (\hat{v}_{k\ell}(t_j) - v_{k\ell}(t_j))^2$$

Simulation: Estimation Performance

- **Performance across four methods (SVD, Smooth, Sparse, Smooth+Sparse):**
  - Smoothness and/or sparsity **reduce MSE** compared to unregularized SVD.
  - **Smooth+Sparse** yields lowest error and most stable estimates.
  - Smooth estimator performs consistently well; sparsity alone less effective (esp. for PC2).
  - Joint regularization achieves best **bias–variance tradeoff**.



PC1: Quartiles and Mean log10(MSE)

Method	Q1	Median	Mean	Q3
SVD	-3.41	-3.35	-3.34	-3.28
Smooth	-4.07	-3.96	-3.92	-3.82
Sparse	-3.57	-3.50	-3.49	-3.43
Smooth+Sparse	**-4.38**	**-4.28**	**-4.22**	**-4.14**

PC2: Quartiles and Mean log10(MSE)

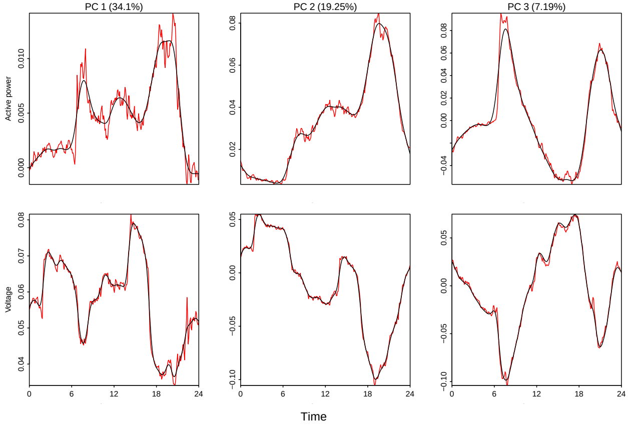
Method	Q1	Median	Mean	Q3
SVD	-2.84	-2.79	-2.79	-2.75
Smooth	-3.56	-3.48	-3.47	-3.40
Sparse	-2.83	-2.79	-2.79	-2.75
Smooth+Sparse	**-3.59**	**-3.50**	**-3.49**	**-3.42**

Application: Household Power Consumption

- **Dataset:** Bivariate functional data including active power and voltage consumption [Hebrail and Berard, 2012] for one household between December 2006 and November 2010.
- **Scaling:** To equalize the contribution of each variable in the multivariate analysis, we rescale them following [Happ and Greven, 2018].

$$\tilde{X}_j(t_i) = \hat{w}_j^{1/2} X_j(t_i),$$

$$\hat{w}_j = \left(\frac{1}{m} \sum_{i=1}^{m} \widehat{\mathrm{Var}}(X_j(t_i)) \right)^{-1}.$$



First 3 PCs: MFPCA (red) vs ReMFPCA (black)

Regularization reduces noise while preserving the dominant daily consumption patterns, enhancing interpretability without losing key structure.

Two-way Regularized MFPCA

- **Two-way functional data:** Each observation is a *matrix of curves*, with smooth variation across **two domains** (e.g., time $\times$ space in air quality, time $\times$ channels in EEG).

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- **Our contribution:**
  - Extend to **multivariate functional data** (multiple functional variables).
  - Combine **smoothness** + **sparsity** **penalties** in both directions.
  - Result: Low-rank, interpretable, noise-robust principal components for high-dimensional applications.

Two-way Smoothed MFPCA: Setup & Penalty

- Two-way multivariate functional data: $\boldsymbol{X} \in \mathbb{R}^{n \times M}, \quad M = \sum_{i=1}^{p} m_i$.
- Roughness matrices: $\boldsymbol{\Omega}_u \in \mathbb{R}^{n \times n}$, $\boldsymbol{\Omega}_v \in \mathbb{R}^{M \times M}$ (symmetric, non-negative definite).
- Smoothers: $\boldsymbol{S}_u(\alpha_u) = (I + \alpha_u \boldsymbol{\Omega}_u)^{-1}, \qquad \boldsymbol{S}_v(\boldsymbol{\alpha}_v) = (I + \boldsymbol{\alpha}_v \boldsymbol{\Omega}_v)^{-1}$.

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- Penalized rank-one reconstruction:

$$\min_{u,v} \|\boldsymbol{X} - uv^\top\|_F^2 + \mathcal{P}(u, v)$$

- Penalty [Jianhua Z. Huang and Buja, 2009]:
  $\mathcal{P}(u, v; \alpha_u, \boldsymbol{\alpha}_v) = u^\top(\alpha_u \boldsymbol{\Omega}_u)u \, \|v\|^2 + \|u\|^2 \, v^\top(\boldsymbol{\alpha}_v \boldsymbol{\Omega}_v)v + u^\top(\alpha_u \boldsymbol{\Omega}_u)u \; v^\top(\boldsymbol{\alpha}_v \boldsymbol{\Omega}_v)v$.
- Multivariate v: $\boldsymbol{\Omega}_v = \mathrm{diag}(\Omega_1, \ldots, \Omega_p)$.

Two-way Smoothed MFPCA: Conditional GCV

- Minimizers:

$$u = \frac{\boldsymbol{S}_u(\alpha_u)\boldsymbol{X}v}{v^\top(I+\boldsymbol{\alpha}_v\boldsymbol{\Omega}_v)\,v} = \frac{\boldsymbol{S}_u(\alpha_u)}{1+\boldsymbol{\alpha}_v\boldsymbol{R}_v(v)}\,\frac{\boldsymbol{X}v}{\|v\|^2}, \qquad v = \frac{\boldsymbol{S}_v(\boldsymbol{\alpha}_v)\boldsymbol{X}^\top u}{u^\top(I+\alpha_u\boldsymbol{\Omega}_u)\,u} = \frac{\boldsymbol{S}_v(\boldsymbol{\alpha}_v)}{1+\alpha_u\boldsymbol{R}_u(u)}\,\frac{\boldsymbol{X}^\top u}{\|u\|^2}.$$

- Rayleigh quotients: $\boldsymbol{R}_u(u) = \frac{u^\top\boldsymbol{\Omega}_u u}{\|u\|^2}, \qquad \boldsymbol{R}_v(v) = \frac{v^\top\boldsymbol{\Omega}_v v}{\|v\|^2}.$

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- Conditional GCV criteria:

$$\mathrm{GCV}_u(\alpha_u;\boldsymbol{\alpha}_v) = \frac{\frac{1}{n}\left\|\left(I-\frac{\boldsymbol{S}_u(\alpha_u)}{1+\boldsymbol{\alpha}_v\boldsymbol{R}_v(v)}\right)\frac{\boldsymbol{X}v}{\|v\|^2}\right\|^2}{\left(1-\frac{1}{n}\,\mathrm{tr}\left(\frac{\boldsymbol{S}_u(\alpha_u)}{1+\boldsymbol{\alpha}_v\boldsymbol{R}_v(v)}\right)\right)^2}, \qquad \mathrm{GCV}_v(\boldsymbol{\alpha}_v;\alpha_u) = \frac{\frac{1}{m}\left\|\left(I-\frac{\boldsymbol{S}_v(\boldsymbol{\alpha}_v)}{1+\alpha_u\boldsymbol{R}_u(u)}\right)\frac{\boldsymbol{X}^\top u}{\|u\|^2}\right\|^2}{\left(1-\frac{1}{m}\,\mathrm{tr}\left(\frac{\boldsymbol{S}_v(\boldsymbol{\alpha}_v)}{1+\alpha_u\boldsymbol{R}_u(u)}\right)\right)^2}.$$

- **Optimization:** Alternate updates of u and v using GCV until convergence $\rightarrow$ two-way regularized components.

Two-way Smooth + Sparse MFPCA

- **Goal:** Extract components that are **low-rank, smooth, and sparse**.
  - Smoothness $\rightarrow$ coherent variation across subjects & functions.
  - Sparsity $\rightarrow$ highlights key observations & time regions.
- **Novelty:** First framework to combine **both** in two-way functional data.

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- Data matrix $\boldsymbol{X}$: seek u, v solving:

$$\min_{u,v} \|\boldsymbol{X} - uv^\top\|_F^2 + \sum_{j}^{J} \mathcal{P}_j^{[\theta]}(u, v)$$

- J is the number of penalty components, and θ is the vector of all tuning parameters.
- The composite penalty $\sum_{j=1}^{J} \mathcal{P}_j^{(\theta)}(u, v)$ lets us mix regularizers, e.g., smoothness with $\theta = (\alpha_u, \boldsymbol{\alpha}_v)$ and sparsity with $\theta = (\gamma_u, \boldsymbol{\gamma}_v)$ (controlling sparsity), and can include other structures as needed.

Sequential Power Algorithm

Algorithm: Two-way Smooth + Sparse MFPCA (Sequential Power)

1. Initialization: Rank-one SVD of $\boldsymbol{X}$: $\boldsymbol{X} \approx s\, u^{(0)} v^{(0)\top}$; set $u \leftarrow s\, u^{(0)}$, $v \leftarrow v^{(0)}$.
2. Repeat until convergence:
   1. $u \leftarrow \boldsymbol{S}_u^{[\alpha_u]}\, \boldsymbol{h}_u^{[\gamma_u]}(\boldsymbol{X}\, v)$
   2. $v \leftarrow \boldsymbol{S}_v^{[\alpha_v]}\, \boldsymbol{h}_v^{[\gamma_v]}(\boldsymbol{X}^\top u)$
   3. $v \leftarrow v / \|v\|$
3. $\boldsymbol{X} \leftarrow \boldsymbol{X} - \sigma\, u\, v^\top$ to extract the next component.

- Smoothness parameters are selected with conditional GCV, while sparsity parameters are chosen via cross-validation (CV).

Selection of Regularization Parameters

- Four sets of tuning parameters:
  - α_u: smoothness of u, γ_u: sparsity of u
  - $\boldsymbol{\alpha}_v$: smoothness of v, $\boldsymbol{\gamma}_v$: sparsity of v
- **Challenge:** Ordering of tuning (smoothness vs. sparsity) affects convergence and solutions.

Selection of Regularization Parameters

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- **Challenge:** Ordering of tuning (smoothness vs. sparsity) affects convergence and solutions.
- **Strategy: Conditional tuning**
  1. Initialize all penalties at 0.
  2. Tune γ_u via K-fold CV.
  3. Sequentially tune $\gamma_{v,i}$ using Algorithm:Two-way Smooth + Sparse MFPCA.
  4. With sparsity fixed, tune α_u by GCV.
  5. Tune $\alpha_{v,i}$ using two-way GCV.
  6. Iterate steps 2–5 until stable.
- This alternating scheme **isolates sparsity vs. smoothness** while ensuring accuracy + interpretability.

K-Fold CV algorithm for Sparsity

K-Fold CV (Row Sparsity)

1. Split $\boldsymbol{X} \in \mathbb{R}^{n\times M}$ into K column groups $\{\boldsymbol{X}^{(1)}, \dots, \boldsymbol{X}^{(K)}\}$.
2. For each γ_j and $k = 1, \dots, K$:
    1. Train on $\boldsymbol{X}^{(-k)}$, estimate $u_j^{(-k)}$.
    2. Validate: $v_j^{(k)} = \boldsymbol{X}^{(k)\top} u_j^{(-k)}$.
    3. Fold error:

$$\mathrm{Err}_j^{(k)} = \frac{1}{\tilde{M}} \|\boldsymbol{X}^{(k)} - u_j^{(-k)} (v_j^{(k)})^\top\|_F^2.$$

3. CV score: $\widehat{\mathrm{CV}}_j = \frac{1}{K} \sum_k \mathrm{Err}_j^{(k)}$.
4. Select $j_0 = \arg\min_j \widehat{\mathrm{CV}}_j$.

K-Fold CV + 1-SE Rule

1. Use same folds to collect $\mathrm{Err}_j^{(k)}$.
2. Compute mean $\widehat{\mathrm{CV}}_j$ and SE $\widehat{\mathrm{SE}}_j$:

$$\widehat{\mathrm{SE}}_j = \sqrt{\frac{1}{K(K-1)} \sum_k (\mathrm{Err}_j^{(k)} - \widehat{\mathrm{CV}}_j)^2}.$$

3. Let $j^\star = \arg\min_j \widehat{\mathrm{CV}}_j$.
4. Choose sparsest j_0 with $\widehat{\mathrm{CV}}_j \leq \widehat{\mathrm{CV}}_{j^\star} + \widehat{\mathrm{SE}}_{j^\star}$.

K-Fold CV algorithm for Sparsity

K-Fold CV (Column Sparsity)

1. Split $\boldsymbol{X} \in \mathbb{R}^{n \times M}$ into K row groups $\{\boldsymbol{X}^{(1)}, \ldots, \boldsymbol{X}^{(K)}\}$.
2. For each γ_j and $k = 1, \ldots, K$:
   1. Train on $\boldsymbol{X}^{(-k)}$, estimate $v_j^{(-k)}$.
   2. Validate: $u_j^{(k)} = \boldsymbol{X}^{(k)} v_j^{(-k)}$.
   3. Fold error:
   $$\mathrm{Err}_j^{(k)} = \frac{1}{\tilde{n}} \|\boldsymbol{X}^{(k)} - u_j^{(k)} (v_j^{(-k)})^\top\|_F^2.$$
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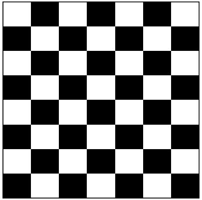
Chessboard

True Chessboard



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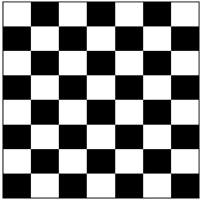
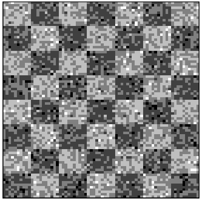


Noisy Chessboard



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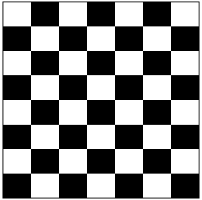
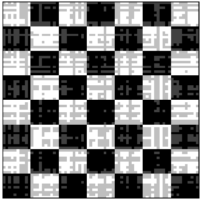
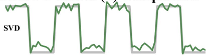


PCA with SVD



First PC Scores (u) Comparison



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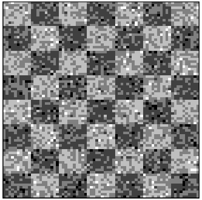
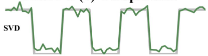


First PC (v) Comparison



Chessboard

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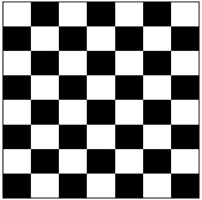

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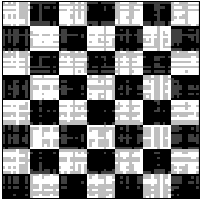

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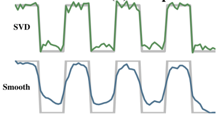

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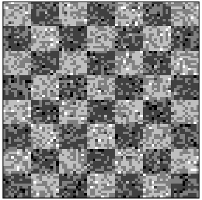
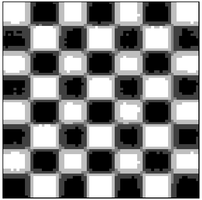
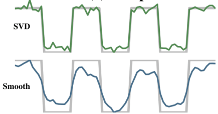


PCA with Smoothness Penalty



First PC (v) Comparison



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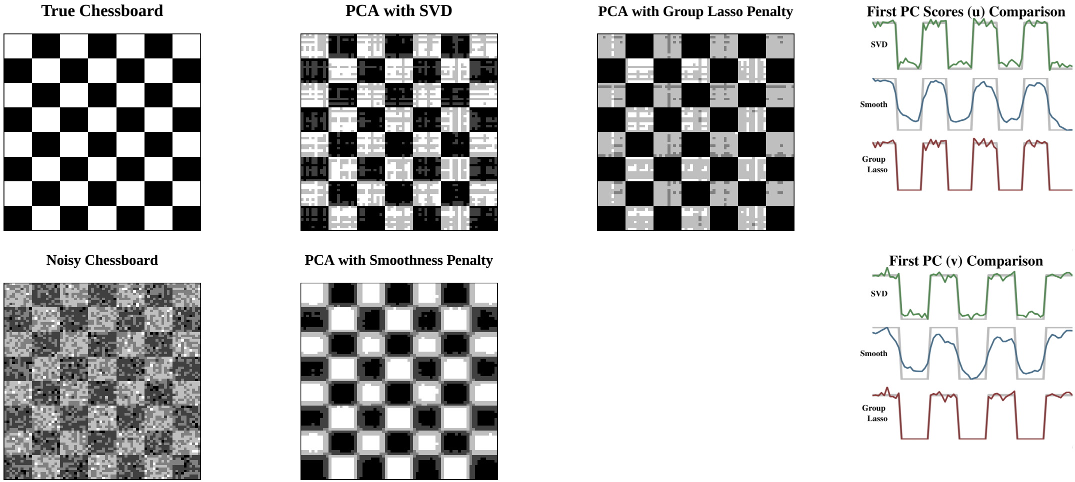
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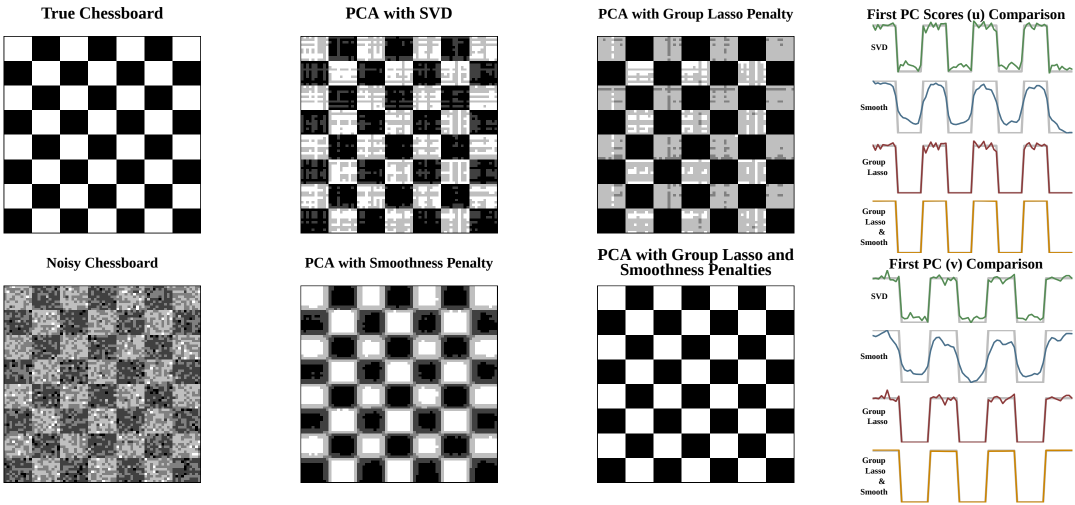
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Variance Explained: Classical vs Regularized FPCA

- **Classical FPCA:** Loadings v_j orthonormal; scores $u_j = Xv_j$ uncorrelated. Variance explained by first J PCs:

$$\sum_{j=1}^{J} \|u_j\|^2 = \mathrm{trace}(V_J^\top X^\top X\, V_J), \qquad V_J = [v_1, \ldots, v_J].$$

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- **Issue under regularization:** smoothness/sparsity break orthogonality $\rightarrow$ scores become correlated $\rightarrow$ naive sum $\sum \|u_j\|^2$ **double-counts** variance (cf. Huang et al., 2008).

Subspace-Projection Definition of Explained Variance

- Normalize loadings and stack:

$$V_J = [v_1, \ldots, v_J], \qquad v_j \leftarrow \frac{v_j}{\|v_j\|}.$$

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where H_J is a a symmetric idempotent matrix. $(H_J^2 = H_J,\ H_J^\top = H_J)$

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- Projected data and explained variance:

$$X_J = XH_J, \qquad \mathrm{V}_{\text{tot}} = \mathrm{tr}(X^\top X), \qquad \mathcal{V}_J = \|X_J\|_F^2 = \mathrm{tr}(H_J X^\top X H_J).$$

PVE, Incremental PVE, and Properties

- Incremental variance:

$$\Delta\mathcal{V}_j = \mathcal{V}_j - \mathcal{V}_{j-1}, \qquad \mathcal{V}_0 = 0.$$

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- **Proportion of variance explained (PVE):**

$$\mathrm{PVE}(J) = \frac{\mathcal{V}_J}{\mathsf{V}_{\mathsf{tot}}}, \qquad \mathrm{pve}_j = \frac{\Delta\mathcal{V}_j}{\mathsf{V}_{\mathsf{tot}}} = \mathrm{PVE}(j) - \mathrm{PVE}(j-1).$$

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- **Key properties:**
  - No double-counting (works with correlated scores).
  - Reduces to classical PCA when $V_J^\top V_J = I_J$.
  - Monotone in J ($\mathcal{V}_J$ increases).
  - $\Delta\mathcal{V}_j$ = unique variance added by component j.

Simulation: Two-way Functional Data

- **Data-generating process:**
$$X_{ij}^{(1)} = u_{i1}v_{11}(t_j) + u_{i2}v_{12}(t_j) + \epsilon_{ij}^{(1)}, \quad X_{ij}^{(2)} = u_{i1}v_{21}(t_j) + u_{i2}v_{22}(t_j) + \epsilon_{ij}^{(2)},$$
- **Latent scores:** generated as smooth functions
$$u_1(s) = \begin{cases} \sin(\pi s), & s > 0, \\ 0, & \text{otherwise}, \end{cases} \qquad u_2(s) = \sin(2\pi s), \quad s \in [-1, 1].$$
- **Functional PCs:**
  - Variable 1: $v_{11}(t) = \frac{t+\sin(\pi t)}{s_1}, \qquad v_{12}(t) = \frac{\cos(3\pi t)}{s_2}$
  - Variable 2:
$$v_{21}(t) = \begin{cases} \dfrac{\sin(3\pi t)}{s_3}, & t \in (-\frac{1}{3}, \frac{1}{3}), \\ 0, & \text{otherwise}, \end{cases} \qquad v_{22}(t) = \begin{cases} \dfrac{\sin(2\pi t)}{s_4}, & t \leq -\frac{1}{3}, \\ \dfrac{\sin(\pi t)}{s_4}, & t \geq \frac{1}{3}, \\ 0, & \text{otherwise}. \end{cases}$$

Evaluation Metrics

- **Integrated Squared Error (ISE):**
  For replicate r and component u_1:

$$\mathrm{ISE}_r^{(u_1,\text{method})} = \frac{1}{m}\sum_{j=1}^{m}\left(u_1(t_j) - \widehat{u}_1^{(\text{method})}(t_j)\right)^2.$$

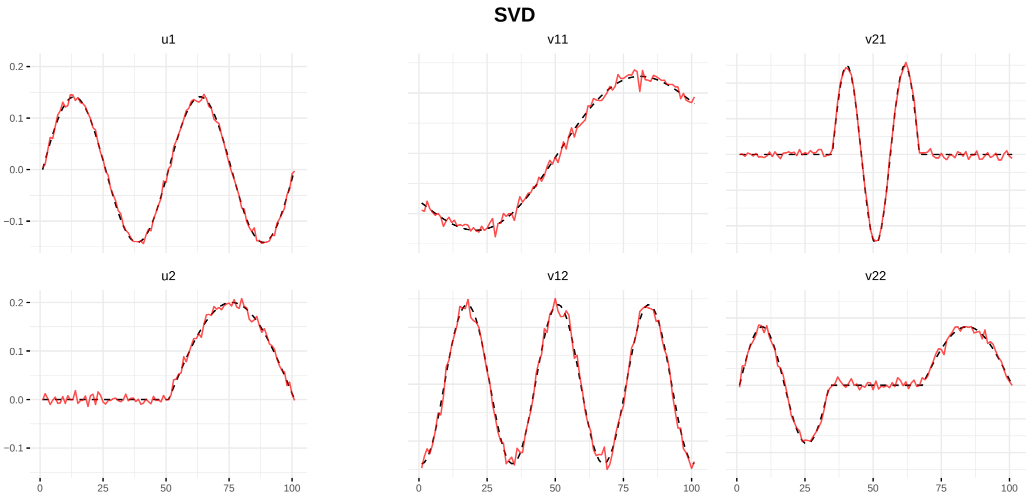
- **Relative ISE (R_ISE):** ratio vs best method

$$R_r^{(u_1,\text{method})} = \frac{\mathrm{ISE}_r^{(u_1,\text{method})}}{\mathrm{ISE}_r^{(u_1,\text{best})}}.$$

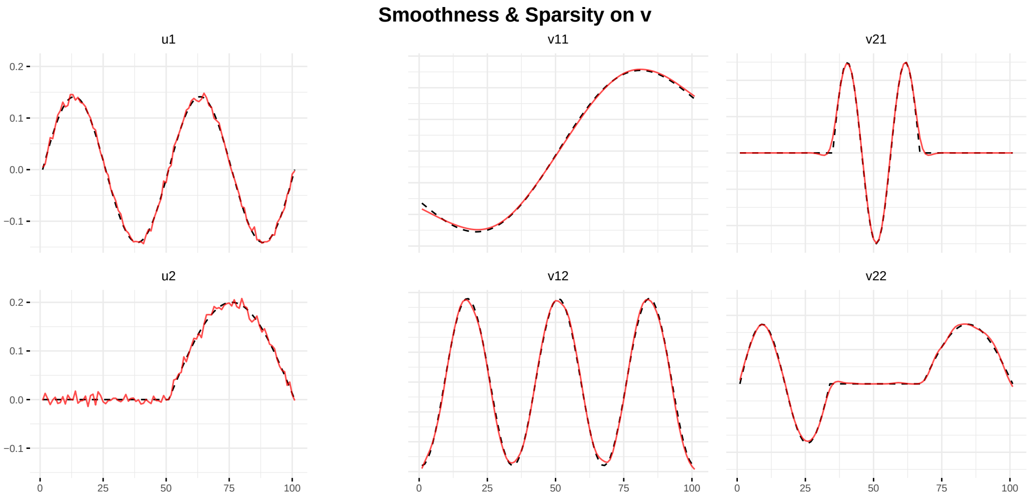
- **Monte Carlo averages:**

$$\overline{R}^{(u_1,\text{method})} = \frac{1}{N}\sum_{r=1}^{N} R_r^{(u_1,\text{method})}, \qquad \mathrm{SE}(\overline{R}) = \sqrt{\frac{1}{N(N-1)}\sum_{r=1}^{N}\left(R_r - \overline{R}\right)^2}.$$

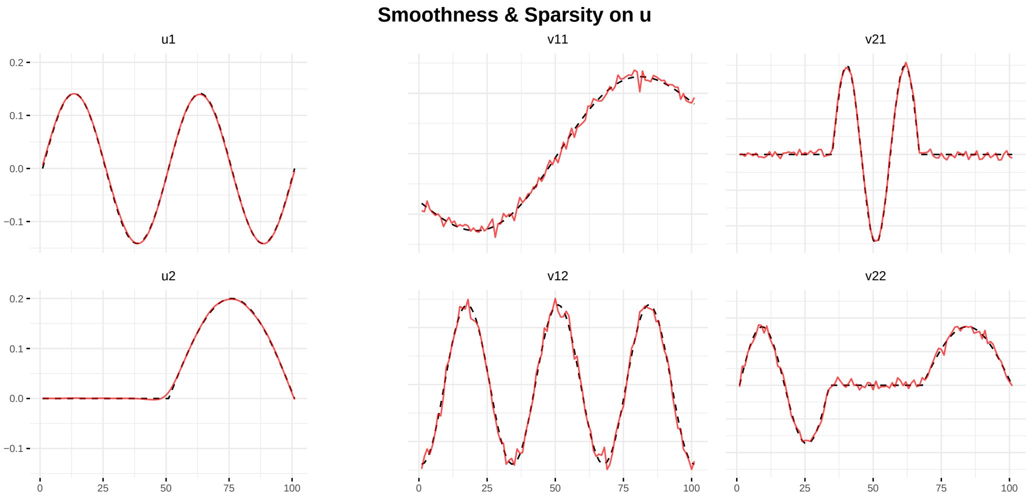
Simulation Results (SVD)



Simulation Results (Smoothness and Sparsity on v)

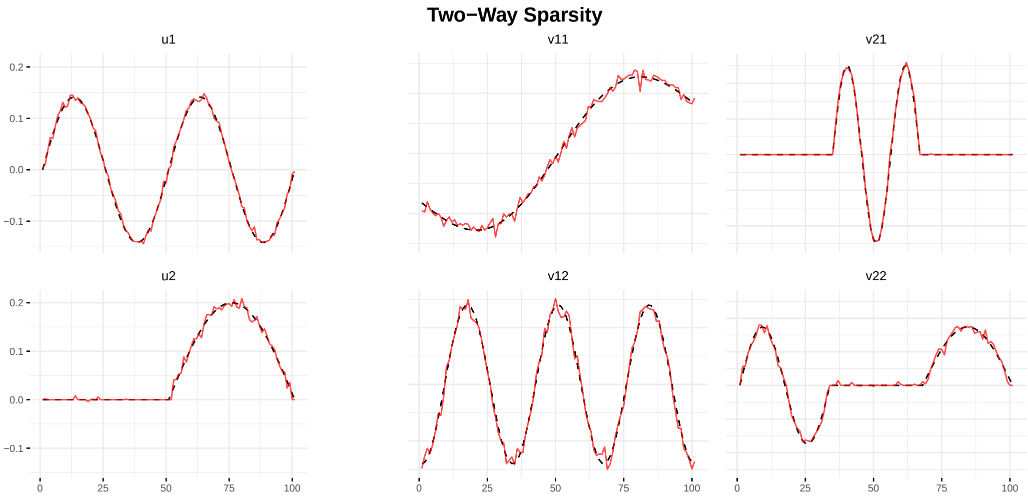


Simulation Results (Smoothness and Sparsity on u)

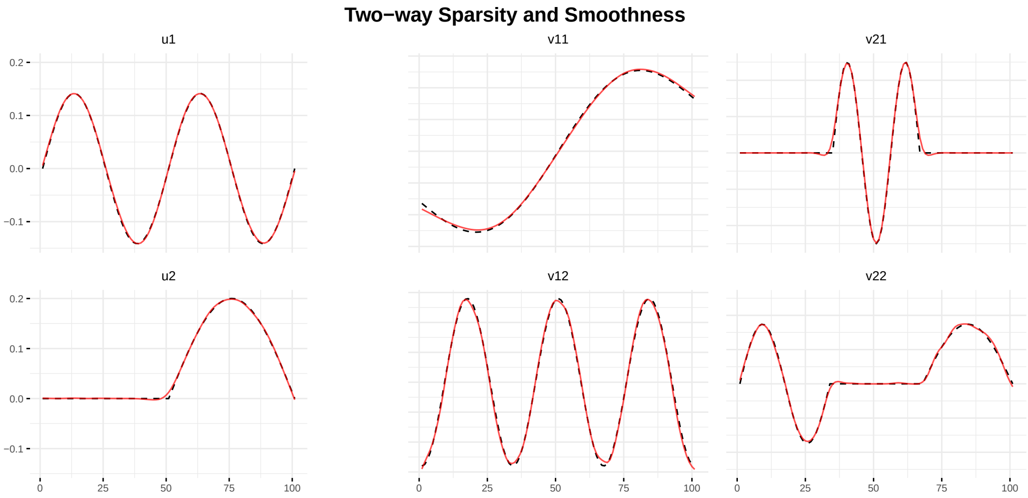


Simulation Results (Two-Way Smoothness)

Simulation Results (Two-Way Sparsity)



Simulation Results (Two-way Sparsity and Smoothness)



Simulation Results

Table 3: Mean ISE for each method and parameter

Method	u1	u2	v1	v2
SVD	0.3651	0.1587	0.00005	0.00010
Smooth+Sparse v	0.3651	0.1587	**0.00002**	**0.00002**
Smooth+Sparse u	**0.3650**	**0.1584**	0.00005	0.00010
Two-way Smoothness	**0.3650**	0.1585	**0.00002**	**0.00002**
Two-way Sparsity	0.3651	0.1586	0.00004	0.00009
Two-way Sm+Sp	**0.3650**	**0.1584**	**0.00002**	**0.00002**

Table 4: Mean Relative ISE for each method and parameter

Method	u1	u2	v1	v2
SVD	1.000	1.001	8.21	5.23
Two-way Sparsity	1.000	1.001	7.71	4.61
Smooth+Sparse v	1.000	1.001	1.05	**1.01**
Smooth+Sparse u	**1.000**	**1.000**	8.19	5.21
Two-way Smoothness	**1.000**	**1.000**	**1.00**	1.21

- Two-way Smooth+Sparse consistently yields the lowest errors across u and v.

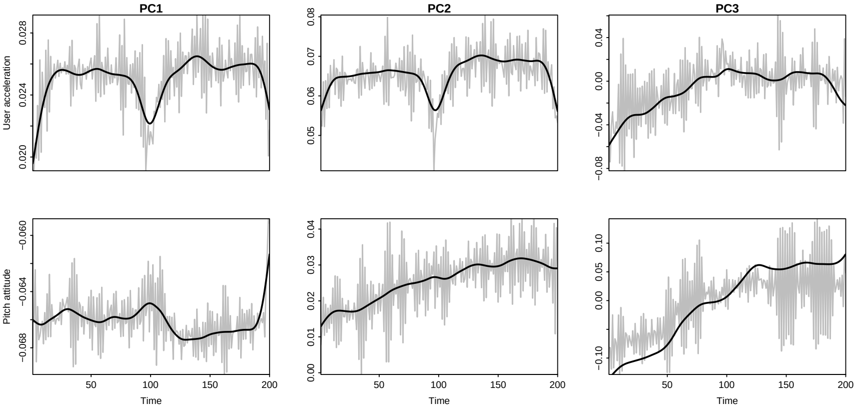
Application: Motion Sense Data

- **Dataset:** Acceleration and pitch from 24 people, 4 activities (jogging, walking, sitting, standing), about 2–3 min each.
- **Goal:** Compare SVD vs **two-way sparse + smooth ReMFPCA** on these multivariate functional signals.
- **Rescaling (Happ & Greven, 2018):** balance variables so each contributes equally.

$$\hat{w}_j = \left(\frac{1}{m} \sum_{i=1}^{m} \widehat{\mathrm{Var}}(X_j(t_i)) \right)^{-1}, \qquad \tilde{X}_j(t_i) = \hat{w}_j^{1/2} X_j(t_i).$$

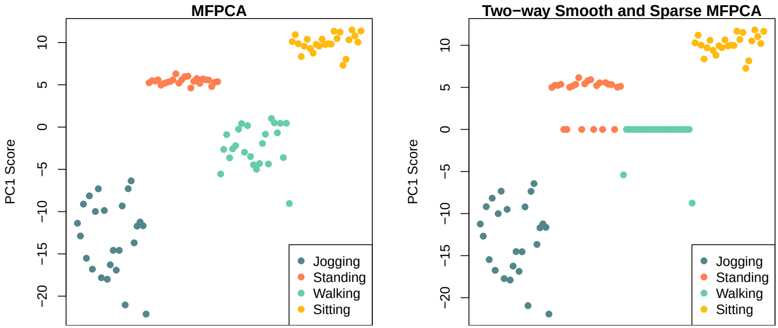
- **Penalties used:** smoothness + sparsity on loadings v; sparsity on scores u (treated as random effects).

Results: Functional PCs (SVD vs ReMFPCA)



- **SVD (gray):** noisy, high-frequency wiggles.
- **ReMFPCA (black):** smoother, more interpretable PCs capturing dominant structure.

Results: PC Scores and Interpretation



- Sparsity on scores: **PC1 scores for walking about 0** (partially standing too).
- Interpretation: walking contributes little to PC1; removing it **improves interpretability** without hurting fit.
- Takeaway: **Two-way smooth + sparse ReMFPCA** yields cleaner PCs and activity-informative scores.

Conclusion & Future Work

- **Unified FPCA Framework**
  - Combines **smoothness** (denoise, interpretability) + **sparsity** (variable selection).
  - Extends from **univariate** $\rightarrow$ **multivariate** $\rightarrow$ **two-way functional data**.
- **Methodology**
  - Penalized SVD with roughness + ℓ_1 penalties.
  - Two-way regularization: smoothness & sparsity on both **scores (*u*)** and **loadings (*v*)**.
  - Efficient parameter tuning: **conditional GCV** & **K-fold CV** (with 1-SE rule).
- **Results**
  - Simulations & applications (mortality, call-center, image data).
  - Outperforms one-way or single-penalty methods.
  - Produces **low-rank, denoised, interpretable components**.

Accessible Implementation: R Package & Future Work

- Implemented in **R package `ReMPCA` (GitHub)**
  - Univariate & multivariate FPCA with penalties.
  - Two-way MFPCA for matrix-valued functions.
  - Automated tuning (CV, GCV, 1-SE rule).
  - Diagnostic tools: variance explained, visualization, heatmaps.
  - Early support for **hybrid data (scalar + functional + image)**.
- **Hybrid Data Extensions**
  - Image–Functional Hybrid PCA $\rightarrow$ simultaneous dimension reduction.
  - Scalar–Functional Integration $\rightarrow$ joint low-dim space.
  - Nonlinear Extensions $\rightarrow$ kernel FPCA, neural nets.
- **Applications:**
  - Neuroimaging
  - Personalized medicine
  - Environmental monitoring

  Takeaway: Smooth + sparse + two-way FPCA offers a **theoretical foundation, practical algorithms, and open software** to enable next-generation functional data analysis.

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Thank you!

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