Regularized Multivariate Two-way Functional Principal Component Analysis

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BE THE DIFFERENCE.

Outline

Introduction

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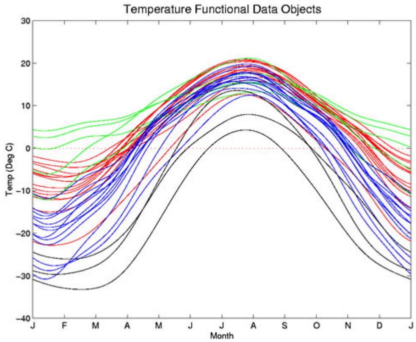

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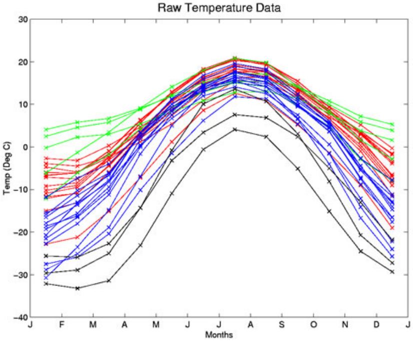
- In practice, these data are often recorded at discrete time points or grid locations, even though they originate from continuous processes in areas like engineering, finance, environmental science, and healthcare.



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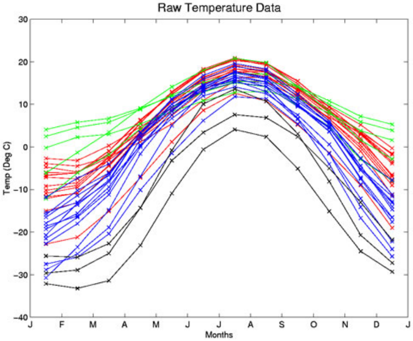
- In practice, these data are often recorded at discrete time points or grid locations, even though they originate from continuous processes in areas like engineering, finance, environmental science, and healthcare.
- **Functional Data Analysis (FDA)** is a statistical framework that treats these observations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



Functional Principal Component Analysis

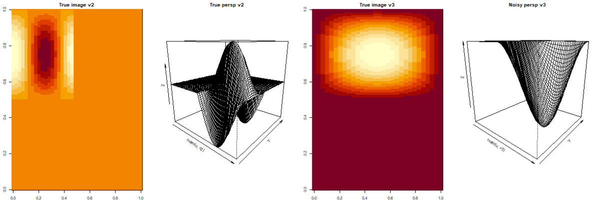
- **Functional PCA (FPCA):** An extension of classical PCA for dimension reduction and uncovering hidden patterns in functional data; it identifies orthogonal functions that capture the main sources of variation, preserving the most important information. [Ramsay and Silverman, 2005].

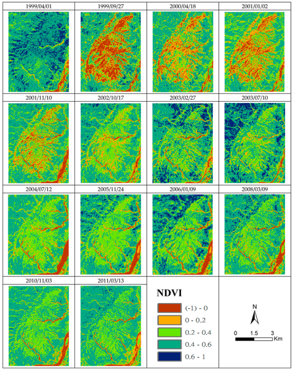
- **Extensions of FPCA:**
  - Smoothed FPCA: Adds roughness penalties [Silverman, 1996, Huang et al., 2008].
  - Sparse FPCA: Enforces sparsity for interpretability [Shen and Huang, 2008, Nie and Cao, 2020].
  - Multivariate FPCA (MFPCA) [Silverman, 1996, Happ and Greven, 2018].
  - Regularized MFPCA: Penalties improve estimation & interpretability [Haghbin et al., 2025].

- **Impact:** More adaptable, robust, and applicable across different problems.

Two-way Functional Principal Component Analysis

- **Two-way functional data:** Two-way functional data consist of a data matrix whose row and column domains are both structured. Observations vary along these two domains (e.g., time $\times$ frequency), with applications in climate science, neuroscience, etc.





Two-way Functional Principal Component Analysis

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- **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:** Extract the key functional directions that explain the main structure of the data using a low-rank representation. For functional data $X \in \mathbb{R}^{n\times m}$ contains n discretized functional observations (rows correspond to subjects) and m columns or 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:**

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

- **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]:

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

  - $X \in \mathbb{R}^{n \times m}$: discretized functional data.
  - $u \in \mathbb{R}^n$: scores.
  - $v \in \mathbb{R}^m$: 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. In particular, for $X = udv^\top$, v is the first principal component and $u = ud$ gives the associated scores.

Power Algorithm

Algorithm: Penalized Power Iteration

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

- For notational convenience, we define smoothness matrix $S(\alpha) = (I + \alpha\Omega)^{-1} \in \mathbb{R}^{m \times m}$, which simplifies expressions involving regularization. The roughness 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.

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

Sparse Functional PCA

- *Standard FPCA faces several key challenges:*
  - FPCs are typically dense, formed as linear combinations of all grid points $\rightarrow$ hard to interpret.
  - Dense components often capture noise, leading to unstable and less reliable results.
  - All grid points contribute, there is no feature selection $\rightarrow$ so uninformative regions are included.
  - In many real-world applications, parts of the data are structurally zero. Also, when $m \gg n$, the data matrix becomes rank-deficient $\rightarrow$ further complicating estimation.

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- **Sparsity** directly addresses these issues:
  - It highlights the most relevant features, making components more interpretable.
  - It filters noise and uninformative variation, producing more stable and robust PCs.
  - It acts as a feature selector, shrinking most coefficients to zero, focusing on informative regions.
  - It is useful in high-dimensional or sparse settings, improving estimation and revealing essential structure.

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- Sparse FPCA with $p_\gamma(v)$ as sparsity penalty term [Shen and Huang, 2008]:

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

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 $X \approx duv^\top$, and set $u \leftarrow du$.
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 γ controlling number of non-zero loadings in v ($0 =$ dense, $m =$ 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 $X^1, \ldots, X^K$.
2. For each sparse tuning parameter $j \in \{0, 1, \ldots, m\}$ (level of sparsity), do the following:
   1. For $k = 1, \ldots, K$, 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 $j_0 = \arg\min\{CV(j)\}$.

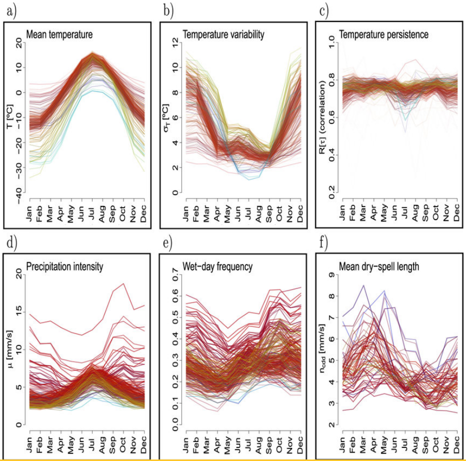
Overview of Existing Approaches

- **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.

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

Regularized MFPCA

- **Context**
  - Univariate FDA → **Multivariate FDA** → joint modes of variation across functions



Regularized MFPCA

- **Context**
  - Univariate FDA $\rightarrow$ **Multivariate FDA** $\rightarrow$ joint modes of variation across functions
- **Challenges**
  - Discretization & irregular grids $\rightarrow$ noise, missing data
  - High dimensionality and limited sample size $\rightarrow$ unstable eigenfunctions
  - 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**: $\mathbf{X} = \left[\, X_1 \; X_2 \; \cdots \; X_p \,\right]$

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

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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  A smoothness penalty is imposed on v.
- The block-diagonal penalty matrix is $\boldsymbol{\Omega} = \text{diag}(\Omega_1, \Omega_2, \ldots, \Omega_p)$, 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. $v \leftarrow S(\alpha)\mathbf{X}^\top u$
   3. $v \leftarrow v / \|v\|$
3. Update $\mathbf{X} \leftarrow \mathbf{X} - \sigma u v^\top$ to extract the next PC.

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

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

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

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 Sparse MFPCA

1. Initialization: Compute rank-one SVD of $\boldsymbol{X}$, $\boldsymbol{X} \approx duv^\top$, and set $u \leftarrow du$.
2. Iterate until convergence:
   1. Update left singular vector: $u \leftarrow \boldsymbol{X}v$
   2. Update right singular vector: $v \leftarrow \boldsymbol{h}_{\boldsymbol{\gamma}} \boldsymbol{X}^\top u$
   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. $v \leftarrow \boldsymbol{S}(\alpha)\boldsymbol{h}(\gamma_{\boldsymbol{v}})\boldsymbol{X}^\top u$
   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 $n = m = 101$, $t_j \in [-1, 1]$

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- **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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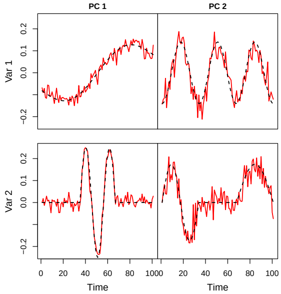

(a) MFPCA

Simulation: Estimation Performance

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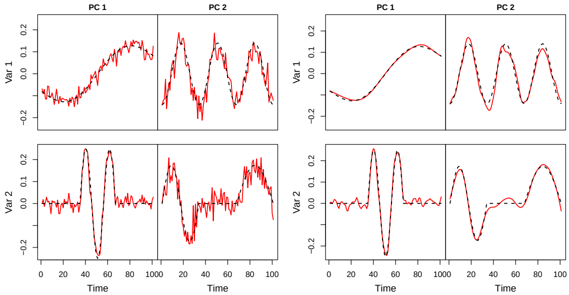

(a) MFPCA (b) Smoothed MFPCA

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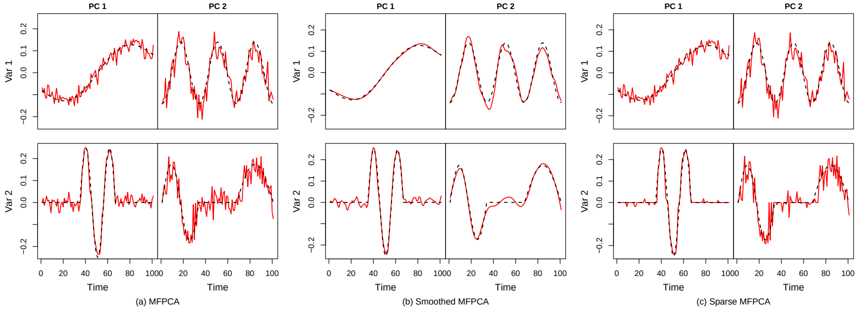

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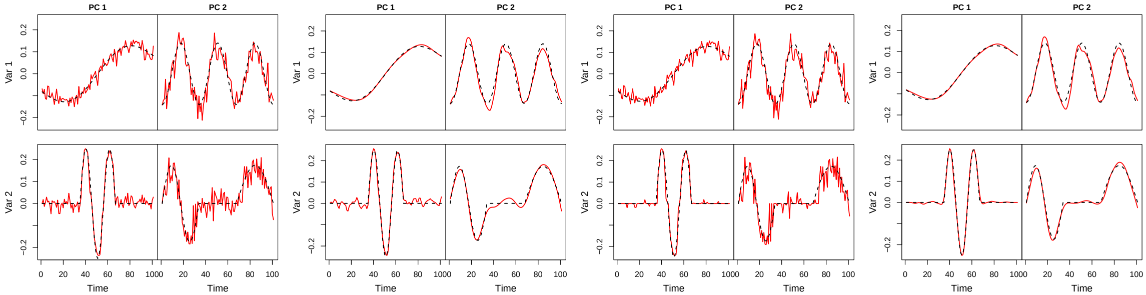


(a) MFPCA (b) Smoothed MFPCA (c) Sparse MFPCA (d) Smoothed and Sparse MFPCA

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:

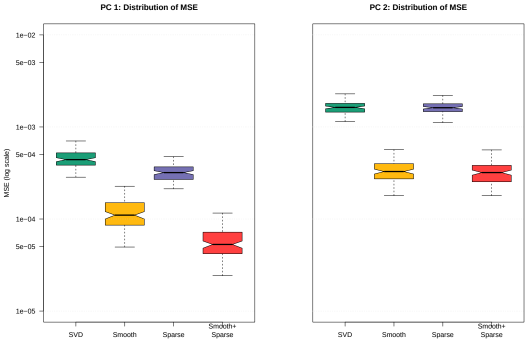
$$\overline{\mathrm{MSE}}_{k\ell} = \frac{1}{R}\sum_{r=1}^{R}\mathrm{MSE}_{k\ell}^{(r)}$$

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**

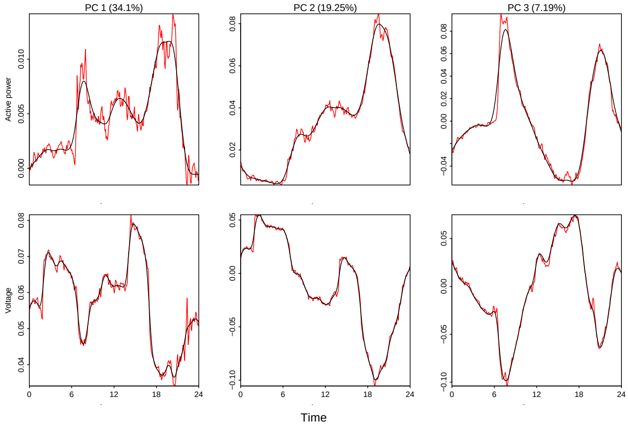
PC2: Quartiles and Mean log10(MSE)

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.

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



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

Two-way Regularized MFPCA

- **Two-way functional data:** Two-way functional data consist of a data matrix whose row and column domains are both structured
- **Limitation of standard FPCA [Ramsay and Silverman, 2005]:**
  - Focuses on one domain (often time).
  - Penalties applied only to loadings $\rightarrow$ ignores structure in second domain.
  - Results may be rough or overly dense along the unpenalized axis.

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  - Penalties applied only to loadings $\rightarrow$ ignores structure in second domain.
  - Results may be rough or overly dense along the unpenalized axis.
- **Two-way FPCA [Jianhua Z. Huang and Buja, 2009]:**
  - Introduced **smoothness penalties** on both scores and loadings.
  - Produces coherent, interpretable *component surfaces* instead of jagged approximations.
- **Our contribution:**
  - Extend to **two-way multivariate functional data** (multiple functional variables).
  - Combine **smoothness** + **sparsity** **penalties** in both directions.
  - Result: Low-rank, interpretable, noise-robust PCs 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 [Jianhua Z. Huang and Buja, 2009]:

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

- **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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  - Sparsity $\rightarrow$ highlights key observations & time regions.
- **Novelty:** First framework to combine **both** in two-way functional data.

- 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. $v \leftarrow \boldsymbol{S}_v^{[\boldsymbol{\alpha}_v]}\, \boldsymbol{h}_v^{[\boldsymbol{\gamma}_v]}(\boldsymbol{X}^\top u)$
   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

- 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.
- **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 $\widehat{\mathrm{CV}}_j \le \widehat{\mathrm{CV}}_{j^\star} + \widehat{\mathrm{SE}}_{j^\star}$.

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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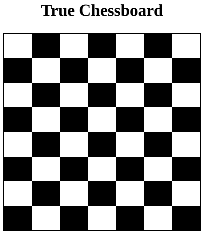
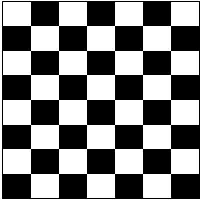
Chessboard

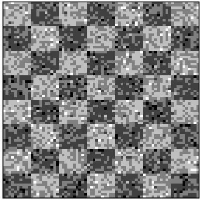


Chessboard

True Chessboard



Noisy Chessboard



Chessboard

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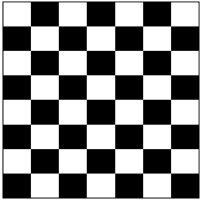
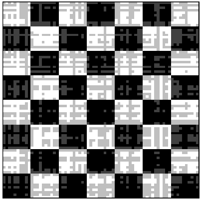
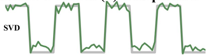


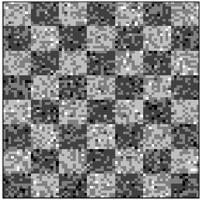
PCA with SVD



First PC Scores (u) Comparison

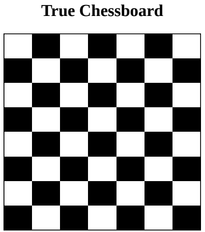


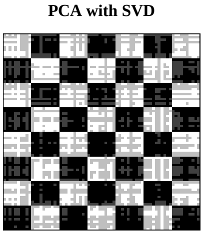
Noisy Chessboard

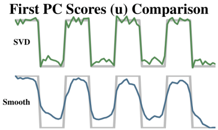


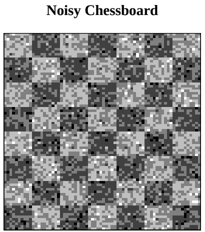
First PC (v) Comparison

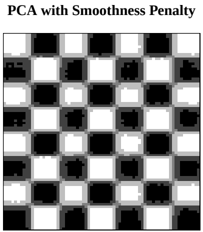
Chessboard

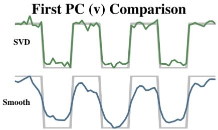

True Chessboard


PCA with SVD

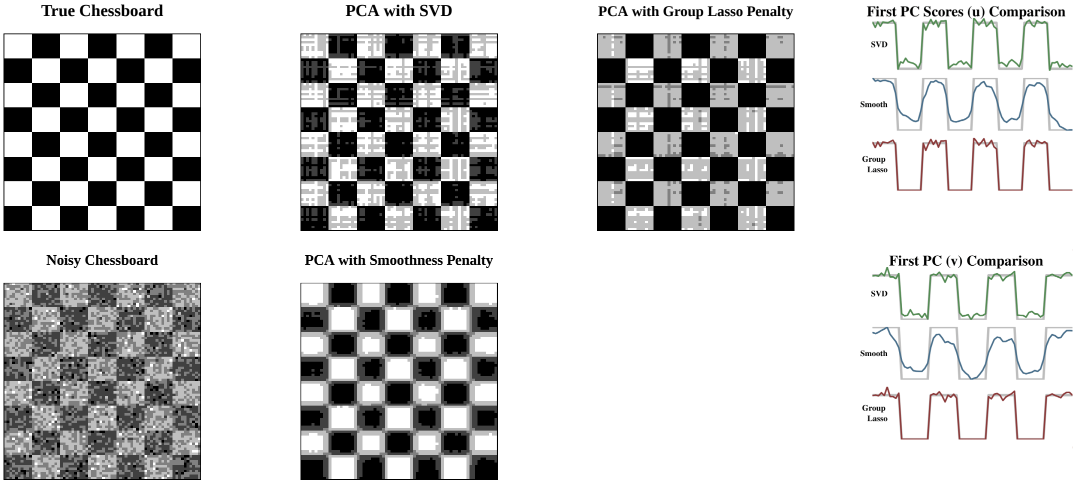

First PC Scores (u) Comparison
SVD
Smooth


Noisy Chessboard


PCA with Smoothness Penalty


First PC (v) Comparison
SVD
Smooth

Chessboard


True Chessboard
PCA with SVD
PCA with Group Lasso Penalty
First PC Scores (u) Comparison
SVD
Smooth
Group Lasso
Noisy Chessboard
PCA with Smoothness Penalty
First PC (v) Comparison
SVD
Smooth
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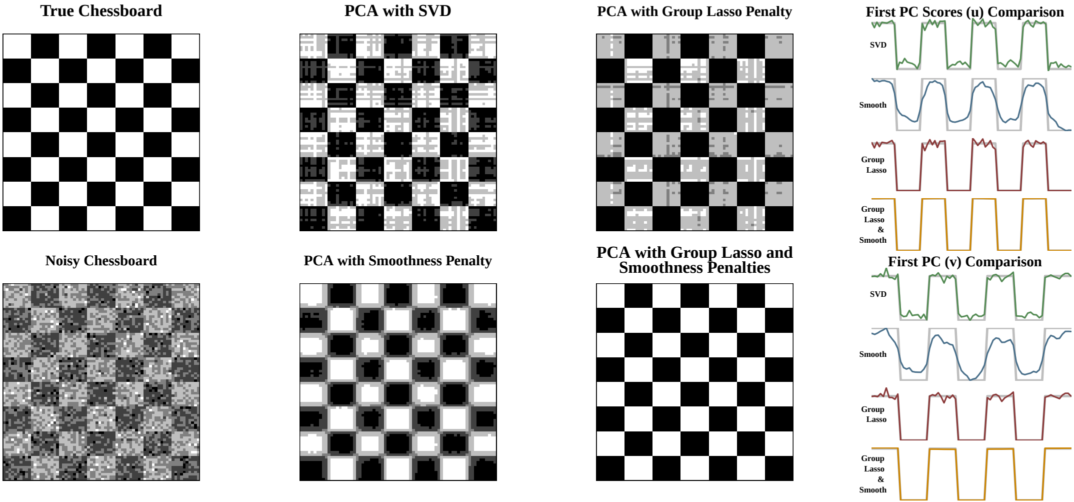
Chessboard


True Chessboard
PCA with SVD
PCA with Group Lasso Penalty
First PC Scores (u) Comparison
SVD
Smooth
Group Lasso
Group Lasso & Smooth
Noisy Chessboard
PCA with Smoothness Penalty
PCA with Group Lasso and Smoothness Penalties
First PC (v) Comparison
SVD
Smooth
Group Lasso
Group Lasso & Smooth

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

$$u_1(s) = \begin{cases} \sin(\pi s), & s > 0, \\ 0, & \text{otherwise}, \end{cases} \qquad u_2(s) = \sin(2\pi s), \quad s \in [-1, 1].$$

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- **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:

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

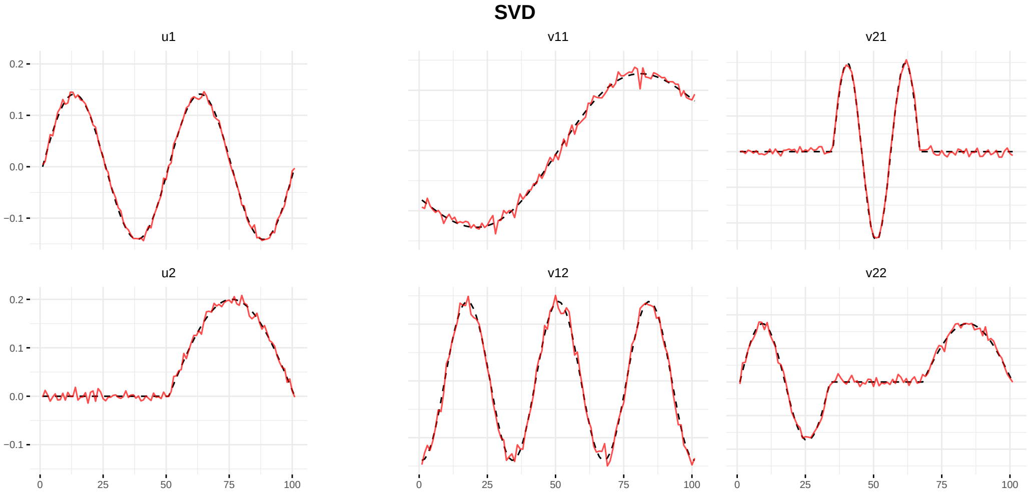
- **Relative ISE (R_ISE):** ratio vs best method

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

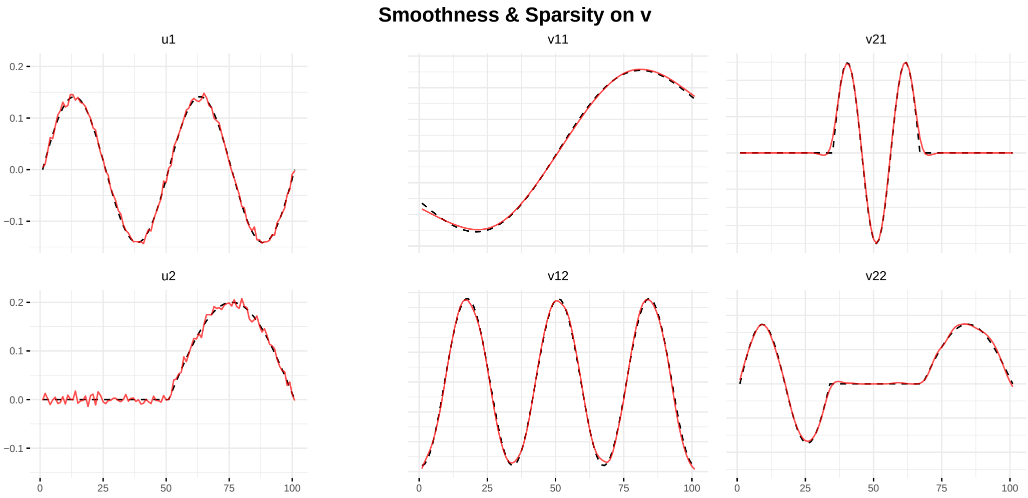
- **Monte Carlo averages:**

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

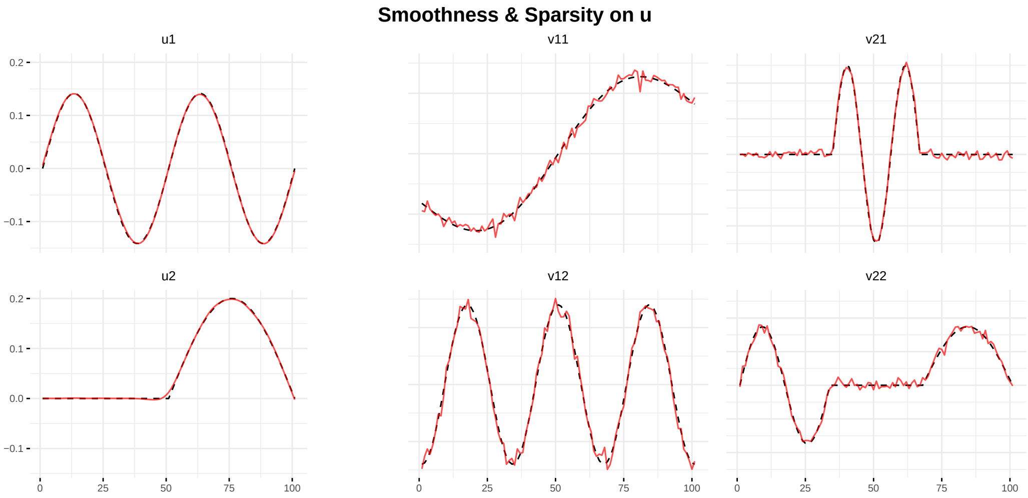
Simulation Results (SVD)



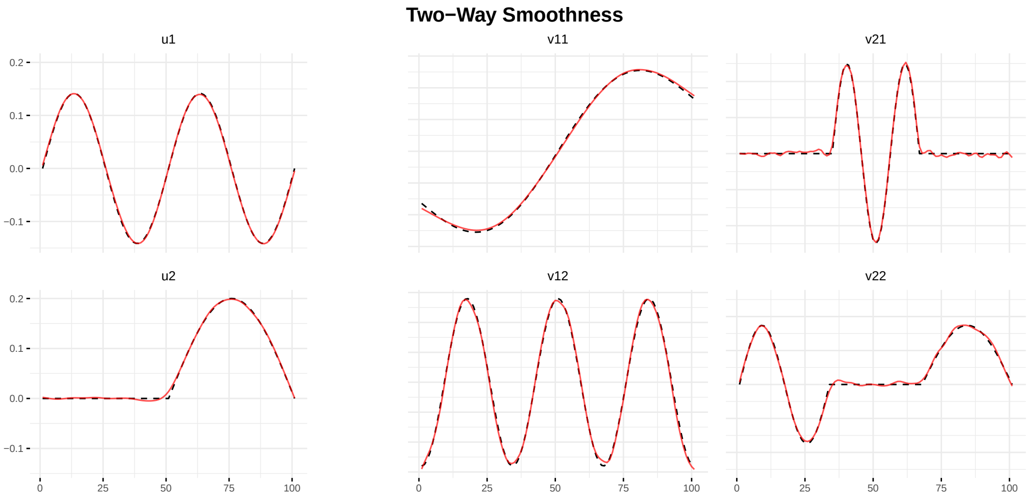
Simulation Results (Smoothness and Sparsity on v)



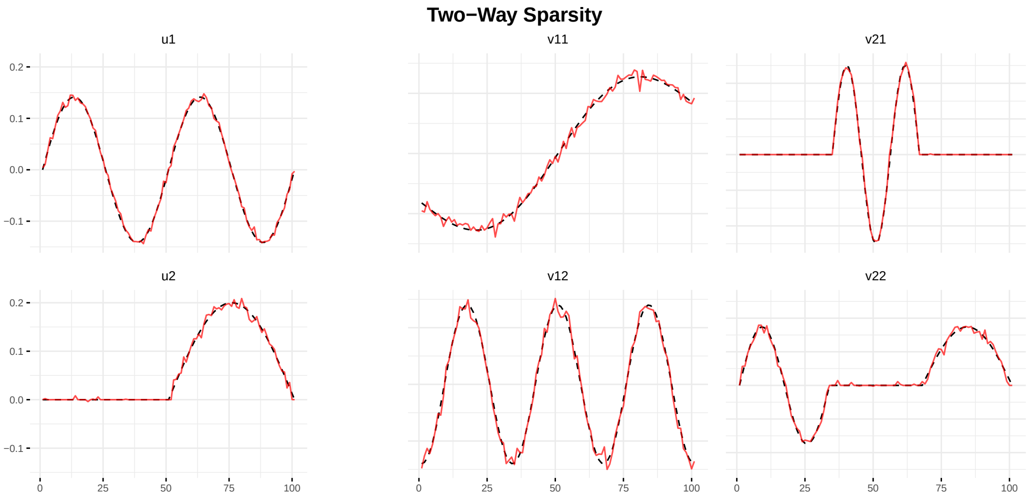
Simulation Results (Smoothness and Sparsity on u)



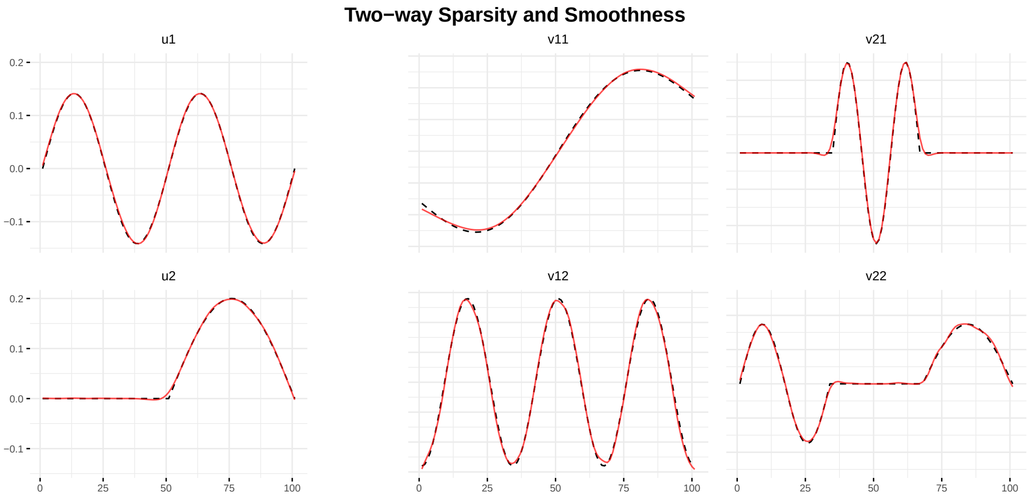
Simulation Results (Two-Way Smoothness)



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.

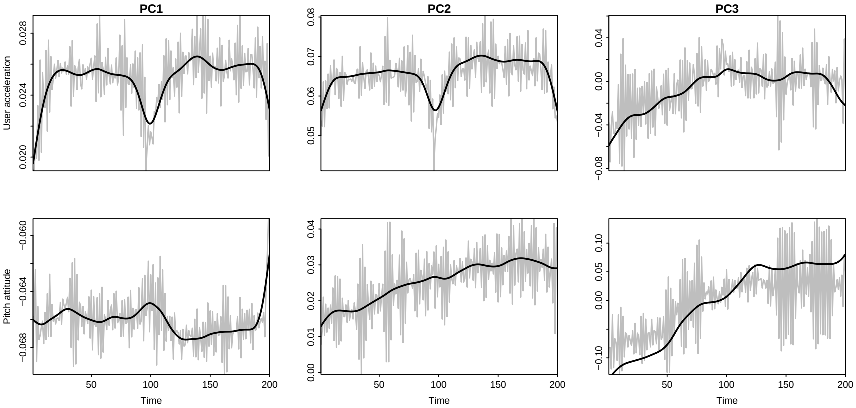
- **Goal:** Compare SVD vs **two-way sparse + smooth ReMFPCA** on these multivariate functional signals.

- **Rescaling [Happ and Greven, 2018]:** balance variables so each contributes equally.

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

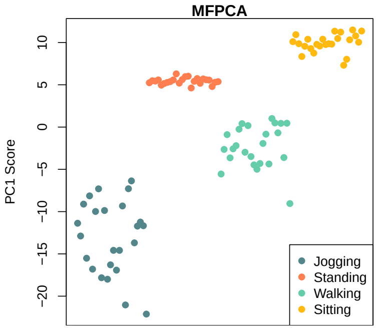
- **Penalties used:** smoothness + sparsity on loadings v; sparsity on scores u.

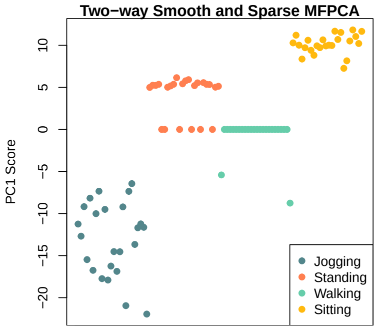
Results: Functional PCs (SVD vs ReMFPCA)



- **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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Appendix

Variance Explained: Classical vs Regularized FPCA

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

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

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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).

Appendix

Subspace-Projection Definition of Explained Variance

- Normalize loadings and stack:

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

Appendix

Subspace-Projection Definition of Explained Variance

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- Orthogonal projector matrix onto span $(v_1, \dots, v_J)$:

$$H_J = V_J \, (V_J^\top V_J)^{-1} V_J^\top,$$

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:

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

Appendix

PVE, Incremental PVE, and Properties

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

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

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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.