Regularized Multivariate Two-way Functional Principal Component Analysis

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I. Background

- **Functional data are ubiquitous.**
  Modern sensors yield curves, images, and surfaces observed over time/space. Functional PCA (FPCA) summarizes such data with a few principal functions for interpretation and modeling (Ramsay & Silverman, 2005).
- **Extensions exist but are isolated.**
  - *Smoothed FPCA*: roughness penalties produce smoother, less noisy components (Huang, Shen, & Buja, 2008; Silverman, 1996).
  - *Sparse FPCA*: sparsity zeros out unimportant regions, improving interpretability (Nie & Cao, 2020; Shen & Huang, 2008).
  - *Multivariate FPCA (MFPCA)*: captures shared variation across multiple functional variables (Happ & Greven, 2018).
  - *Two-way functional data* (e.g., time × space): require structure in *both* domains.
- **Limitations.**
  Classical FPCA is noise-sensitive and can yield rough, dense patterns; many methods address *either* smoothness *or* sparsity, or are limited to univariate data.
- **Motivation.**
  Develop a regularized FPCA framework that (i) handles **multivariate** and **two-way** functional structures, (ii) imposes **smoothness** (noise reduction) and **sparsity** (feature selection) *simultaneously* on scores and loadings, and (iii) yields low-rank, interpretable, and stable components. Recent work (e.g., ReMFPCA) points in this direction but leaves room for a unified treatment and broader applicability (Haghbin, Zhao, & Maadooliat, 2025).

II. Methodology

1) *Multivariate FPCA Formulation:* Concatenate p functional variables into $\mathbf{X} \in \mathbb{R}^{n\times M}$, where $M = \sum_{i=1}^{p} m_i$.
We estimate a rank-one structure with penalties:

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

where $\boldsymbol{\Omega} = \mathrm{diag}(\Omega_1, \ldots, \Omega_p)$ encodes **roughness** and $p_\gamma(\cdot)$ induces **sparsity** (soft, hard, or SCAD) (Huang et al., 2008; Nie & Cao, 2020; Shen & Huang, 2008).

2) *Sequential Power Algorithm:* Let $S(\alpha) = (I + \alpha\boldsymbol{\Omega})^{-1}$. Iterate:

1. **Initialize:** v via rank-one SVD of $\mathbf{X}$.
2. **Repeat:**
   - $u \leftarrow \mathbf{X}v$
   - $v \leftarrow S(\alpha)\, h_\gamma(\mathbf{X}^\top u)$
   - $v \leftarrow v / \| v \|$

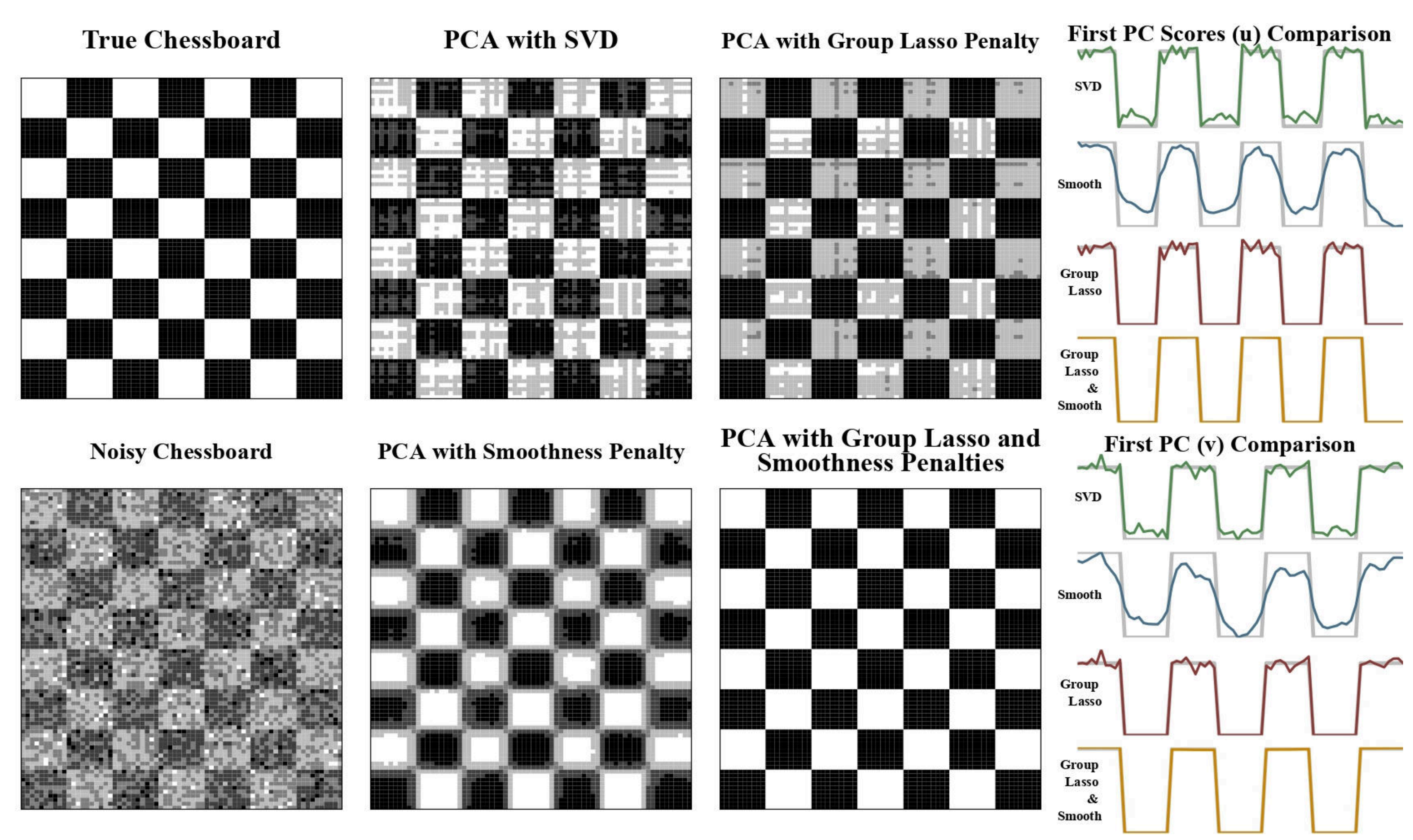
Tuning:
Choose γ by K-fold cross-validation.
Choose α by generalized cross-validation (GCV): $\mathrm{GCV}(\alpha) = \frac{\|(I-S(\alpha))(\mathbf{X}^\top u)\|^2/M}{(1-\frac{1}{M}\,\mathrm{tr}\, S(\alpha))^2}$.

III. 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. Classical FPCA focuses on one domain and penalizes only one set of components, often ignoring structure in the second direction.
- **Framework & Penalty:**

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

- where 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 $\theta = (\alpha_u, \alpha_v)$ and sparsity with $\theta = (\gamma_u, \gamma_v)$ (controlling sparsity), and can include other structures as needed.
- **Sequential Power Algorithm:**
  1. Initialize u, v using rank-one SVD of $\mathbf{X}$.
  2. Update u with smoothing and sparsity transformations:
     $u \leftarrow S_u^{[\alpha_u]} h_u^{[\gamma_u]}(\mathbf{X}v)$
  3. Update v similarly:
     $v \leftarrow S_v^{[\alpha_v]} h_v^{[\gamma_v]}(\mathbf{X}^\top u)$
  4. Normalize v and deflate $\mathbf{X}$ to extract further components.
- **Tuning:**
  - $\alpha_u, \alpha_v \longrightarrow$ control **smoothness** of scores and loadings.
  - $\gamma_u, \gamma_v \longrightarrow$ control **sparsity** of scores and loadings.
  - Conditional tuning alternates CV for sparsity and GCV for smoothness to achieve an optimal balance.



IV. Conclusion & Future Work

- **Comprehensive Framework:** ReMPCA extends PCA to curves, images, and functional data, combining smoothness (denoising, interpretability) and sparsity (feature selection) for structured, low-rank components.
- **Methodology:** Penalized SVD with roughness and sparsity penalties applies regularization to both scores (u) and loadings (v), tuned via GCV and CV.
- **Results:** Two-way regularization improves reconstruction and interpretability, outperforming one-way methods across simulated and real datasets.
- **Software:** Implemented in the ReMPCA R package with automated tuning, diagnostics, and visualization tools.
- **Future Work:** Extend to hybrid scalar–functional–image data, nonlinear kernels, and applications in neuroimaging, medicine, and environmental science.

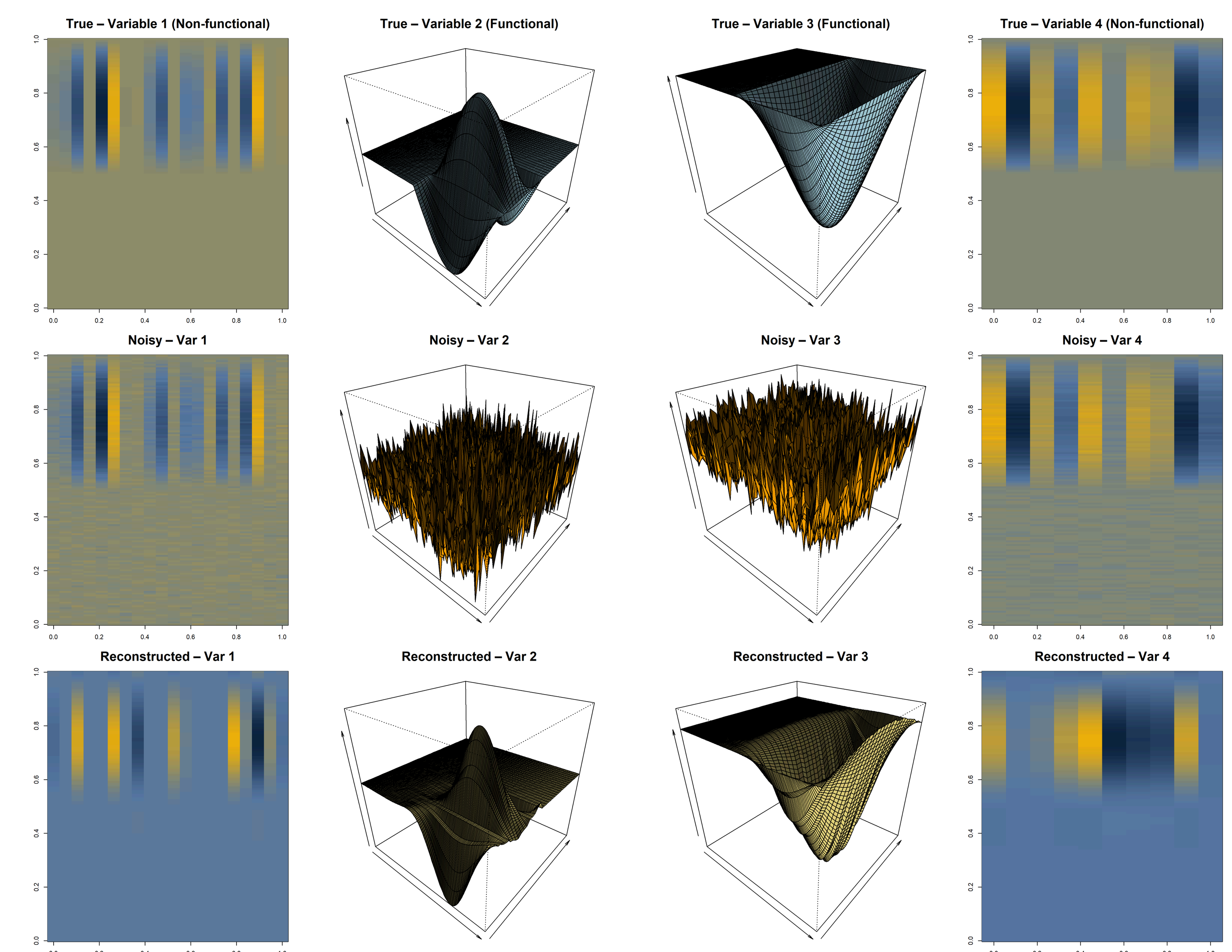


Figure 1: Hybrid data example

V. References

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