Regularized Multivariate Two-way Functional Principal Component Analysis

KLINGLER College of Arts & Sciences
MARQUETTE UNIVERSITY
Mathematical and Statistical Sciences

Mobina Pourmoshir, Dr. Mehdi Maadooliat
Marquette University
Department of Mathematical and Statistical Sciences

I. Background

- **Functional data are ubiquitous.**
  Modern sensors yield curves, images, and surfaces observed over time or 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 works point in this direction but leaves room for a unified framework and wider applicability (Haghbin, Zhao, & Maadooliat, 2025).

II. Methodology

1) ***Multivariate FPCA:*** Concatenate p functional variables, where the i-th variable is observed on m_i grid points, into $\mathbf{X} = \begin{bmatrix} X_1 & X_2 & \cdots & X_p \end{bmatrix} \in \mathbb{R}^{n \times M}$, where $M = \sum_{i=1}^{p} m_i$:

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

We estimate a rank-one structure with penalties:

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

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

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

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

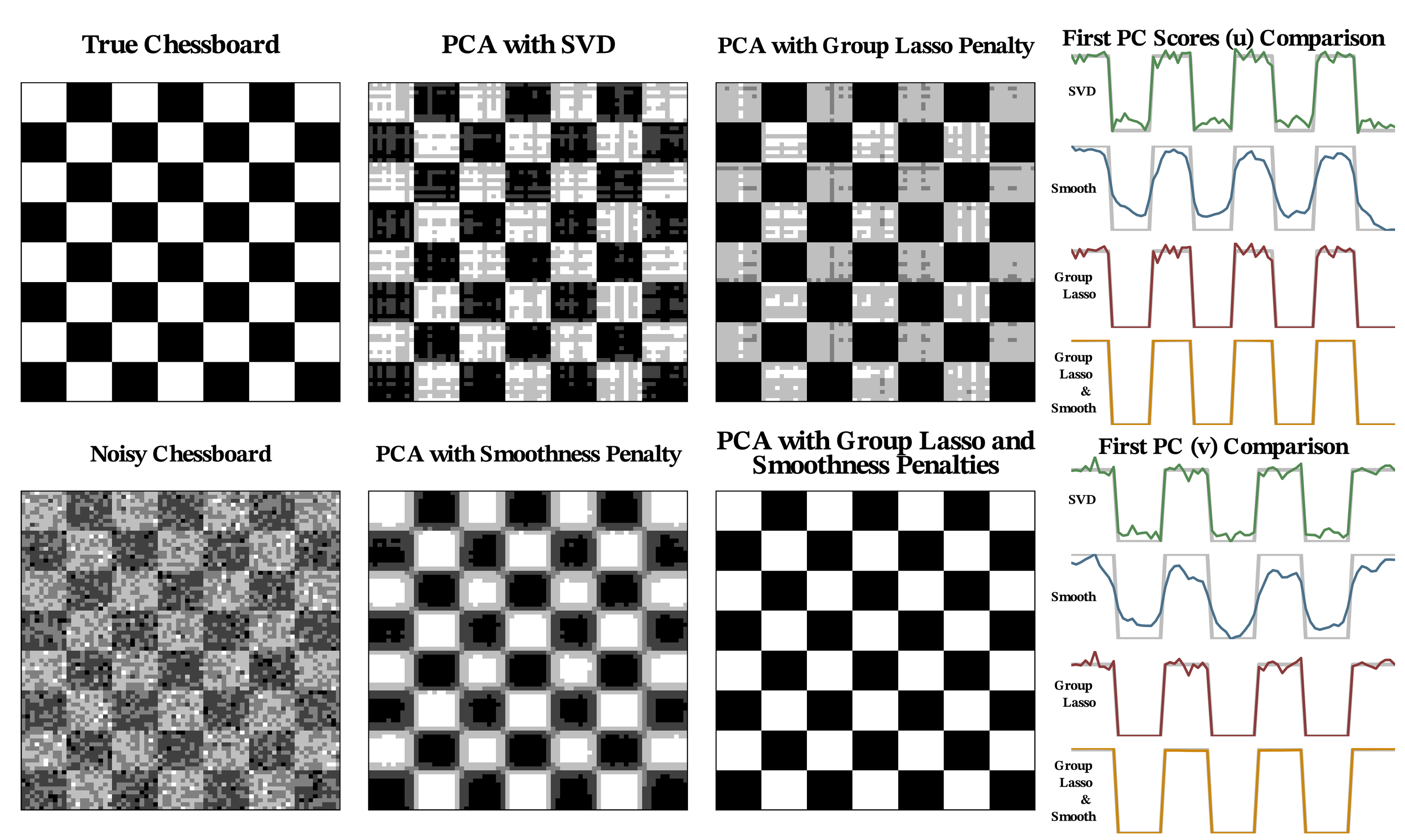
Tuning:
Choose $\boldsymbol{\gamma}$ (Degree of sparsity) by K-fold cross-validation.
Choose $\boldsymbol{\alpha}$ by generalized cross-validation: $\mathrm{GCV}(\boldsymbol{\alpha}) = \frac{\|(I - \boldsymbol{S}(\boldsymbol{\alpha}))(\boldsymbol{X}^\top u)\|^2 / M}{\left(1 - \frac{1}{M}\,\mathrm{tr}\, \boldsymbol{S}(\boldsymbol{\alpha})\right)^2}$.

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:**

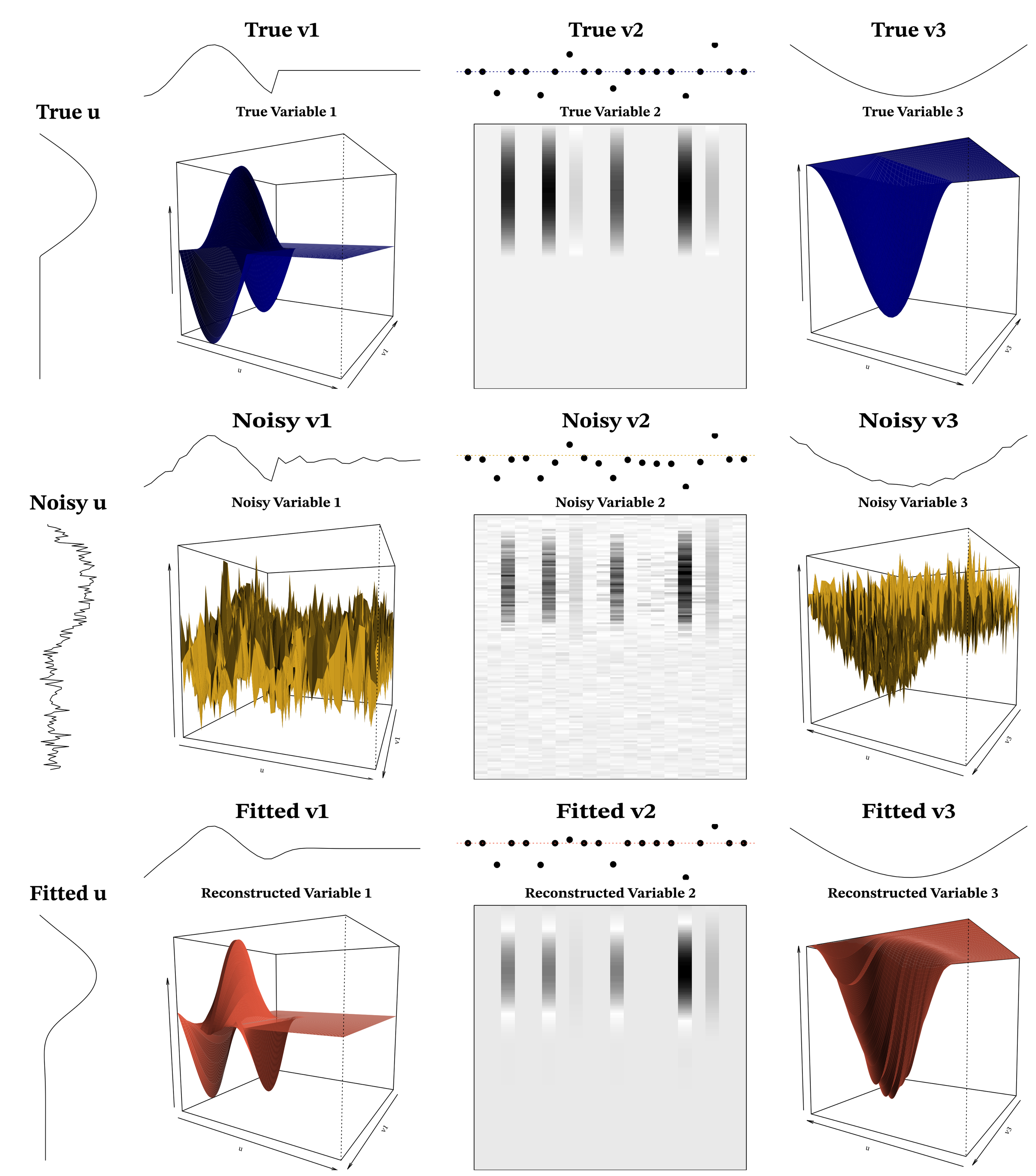
$$\min_{u,v} \| \boldsymbol{X} - uv^\top \|_F^2 + \sum_{j}^{J} \mathcal{P}_j^{[\theta]}(u, v) \tag{3}$$

- 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 $\theta = (\alpha_u, \boldsymbol{\alpha}_v)$ and sparsity with $\theta = (\gamma_u, \boldsymbol{\gamma}_v)$ (controlling sparsity), and can include other structures as needed.
- **Sequential Power Algorithm:**
  1. Initialize u, v using rank-one SVD of $\boldsymbol{X}$.
  2. Update u with smoothing and sparsity transformations:
     $u \leftarrow S_u^{[\alpha_u]} h_u^{[\gamma_u]}(\boldsymbol{X} v)$
  3. Update v similarly:
     $v \leftarrow \boldsymbol{S}_{\boldsymbol{v}}^{[\boldsymbol{\alpha}_v]} \boldsymbol{h}_{\boldsymbol{v}}^{[\gamma_v]}(\boldsymbol{X}^\top u)$
  4. Normalize v and deflate $\boldsymbol{X}$ to extract further components.
- **Tuning parameters:**
  - $\alpha_u, \boldsymbol{\alpha}_v \longrightarrow$ **smoothness** of u and v.
  - $\gamma_u, \boldsymbol{\gamma}_v \longrightarrow$ **sparsity** of u and v.
  - **Conditional tuning strategy:**
    1. Start with no penalties.
    2. Tune sparsity parameters via CV.
    3. Tune smoothness parameters via GCV.
    4. Alternate until convergence.



IV. Conclusion

- **Comprehensive Framework:** ReMPCA extends PCA to functional data, combining smoothness (denoising) and sparsity (feature selection) for structured, low-rank PCs.
- **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 tuning, and visualization tools.
- **Future Work:** Extend to hybrid scalar–functional–image data, nonlinear kernels, and applications in neuroimaging, medicine, and environmental science.



V. References

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