

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 \times 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 (Hagbin, 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:

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

where $\mathbf{\Omega} = \text{diag}(\Omega_1, \dots, \Omega_p)$ 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 $S(\alpha) = (I + \alpha \mathbf{\Omega})^{-1}$. Iterate:

1. **Initialize**: v via rank-one SVD of \mathbf{X} .
2. **Repeat**:
 - $u \leftarrow \mathbf{X}v$
 - $v \leftarrow S(\alpha) h_\gamma(\mathbf{X}^\top u)$
 - $v \leftarrow v / \|v\|$
3. **Deflate**: $\mathbf{X} \leftarrow \mathbf{X} - \sigma uv^\top$ to extract additional components.

Tuning:

Choose γ by K -fold cross-validation.

Choose α by generalized cross-validation (GCV):

$$\text{GCV}(\alpha) = \frac{\| (I - S(\alpha))(\mathbf{X}^\top u) \|^2 / M}{(1 - \frac{1}{M} \text{tr } S(\alpha))^2}. \quad (2)$$

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:**

$$\min_{u,v} \| \mathbf{X} - uv^\top \|_F^2 + \sum_j^J \mathcal{P}_j^{(\theta)}(u, v) \quad (3)$$

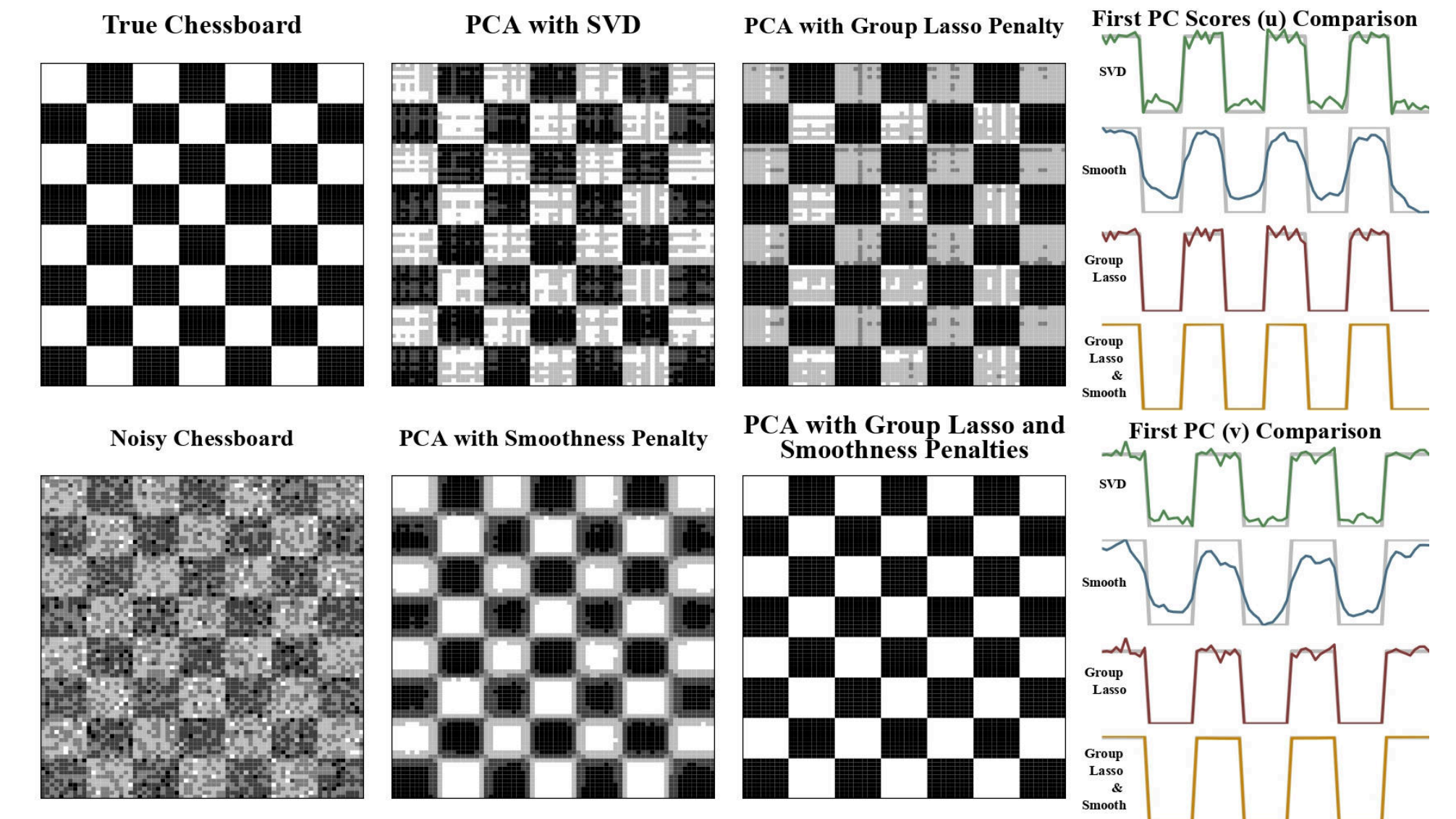
- where J is the number of penalty components, and θ is the vector of all tuning parameters. The composite penalty $\sum_{j=1}^J \mathcal{P}_j^{(\theta)}(u, v)$ lets us mix regularizers, e.g., smoothness with $\theta = (\alpha_u, \alpha_v)$ and sparsity with $\theta = (\gamma_u, \gamma_v)$ (controlling 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:**

- $\alpha_u, \alpha_v \rightarrow$ control **smoothness** of scores and loadings.
- $\gamma_u, \gamma_v \rightarrow$ control **sparsity** of scores and loadings.
- **Strategy (Conditional Tuning):**
 1. Initialize with no penalties.
 2. Use **cross-validation (CV)** to tune sparsity parameters.
 3. Use **generalized cross-validation (GCV)** to tune smoothness parameters.
 4. Alternate steps 2–3 until convergence for an optimal balance of smoothness and sparsity.



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:**
 - Hybrid data integration: joint analysis of scalar, functional, and imaging data.
 - Advanced models: kernel FPCA and neural-network-based nonlinear extensions.
 - Applications: neuroimaging, personalized medicine, and environmental monitoring.

V. REFERENCES

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