

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 points in this direction but leaves room for a unified treatment and broader applicability (Hagbin, 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 $\mathbf{X} = [X_1 \ X_2 \ \dots \ X_p] \in \mathbb{R}^{n \times M}$, where $M = \sum_{i=1}^p m_i$:

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

We estimate a rank-one structure with penalties:

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

where $\Omega = \text{diag}(\Omega_1, \dots, \Omega_p)$ 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 $S(\alpha) = (I + \alpha\Omega)^{-1}$. 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: $\text{GCV}(\alpha) = \frac{\|(I - S(\alpha))(\mathbf{X}^\top u)\|_M^2}{(1 - \frac{1}{M} \text{tr } S(\alpha))^2}$.

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:

$$\min_{u,v} \|\mathbf{X} - uv^\top\|_F^2 + \sum_{j=1}^J \mathcal{P}_j^{[\theta]}(u, v) \quad (3)$$

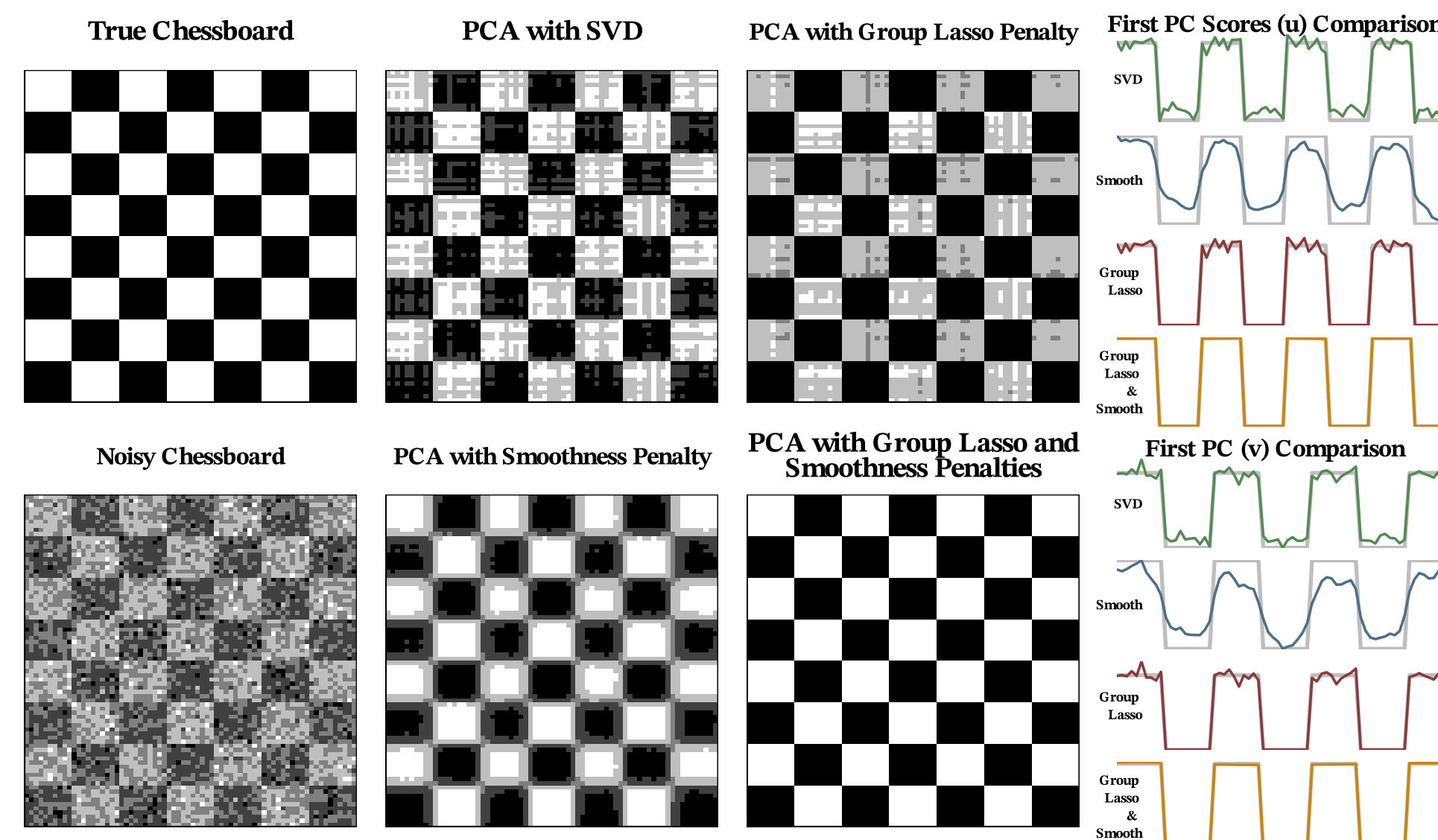
- where J is the number of penalty components, and θ is the vector of all tuning parameters. The composite penalty $\sum_{j=1}^J \mathcal{P}_j^{(\theta)}(u, v)$ lets us mix regularizers, e.g., **smoothness** with $\theta = (\alpha_u, \alpha_v)$ and **sparsity** with $\theta = (\gamma_u, \gamma_v)$ (controlling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

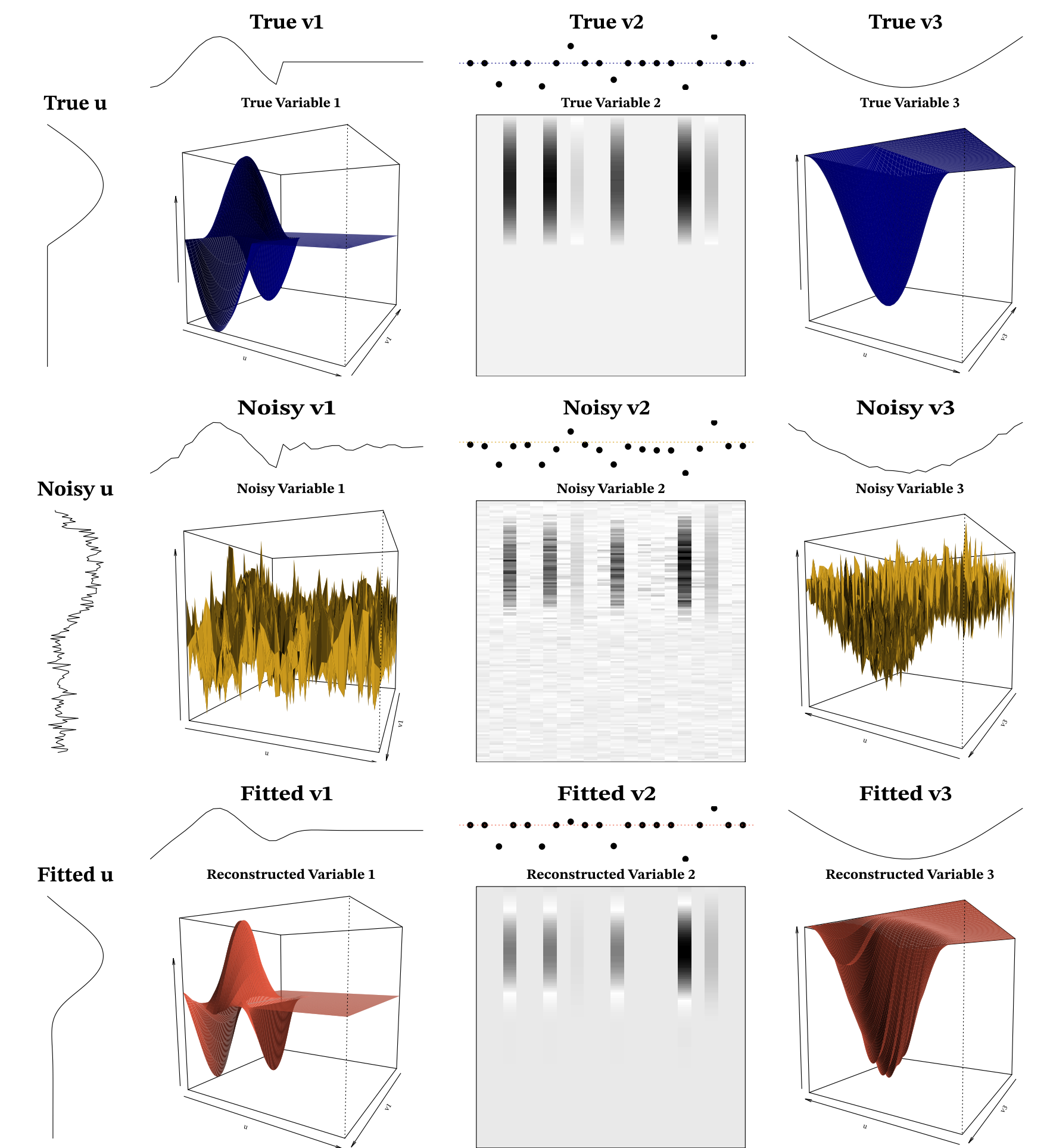
• Tuning parameters:

- ▶ $\alpha_u, \alpha_v \rightarrow$ **smoothness** of u and v .
- ▶ $\gamma_u, \gamma_v \rightarrow$ **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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