Regularized Multivariate Two-way Functional Principal Component Analysis

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BE THE DIFFERENCE.

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:

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

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

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

III. Two-way Extension

IV. References

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