Sparse & Functional Principal Components Analysis

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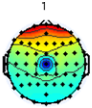
Structured Big-Data

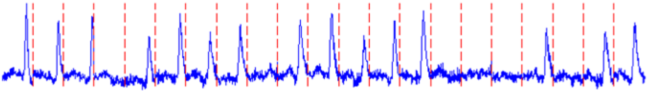
Structured Data = Data associated with locations.

- Time Series, Longitudinal & Spatial Data.
- Image data & Network Data.
- Tree Data.
- *Object-Oriented Data*

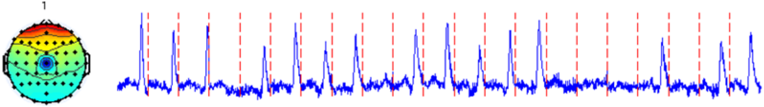
Examples of Massive Structured Data:

- Neuroimaging and Neural Recordings: MRI, fMRI, EEG, MEG, PET, DTI, direct neuronal recordings (spike trains), optigenetics.





Structured Big-Data



Data matrix, $\mathbf{X}_{L \times T}$, of L brain locations by T time points.

Goal: Unsupervised analysis of brain activation patterns and temporal neural activation patterns.

Principal Components Analysis:

- Exploratory Data Analysis.
- Pattern Recognition.
- Dimension Reduction.
- Data Visualization.

Review: PCA Models

1. Covariance: Leading eigenspace of Gaussian covariance.
   - Model: $\mathbf{X} \sim N(0, \mathbf{I} \otimes \mathbf{\Sigma}_{p \times p})$ and estimate leading eigenspace of $\mathbf{\Sigma}$.
   - Empirical Optimization Problem:

$$\underset{\mathbf{v}_k}{\text{maximize}} \quad \mathbf{v}_k^T \mathbf{X}^T \mathbf{X} \mathbf{v}_k \quad \text{subject to} \quad \mathbf{v}_k^T \mathbf{v}_k = 1 \ \& \ \mathbf{v}_k^T \mathbf{v}_j = 0 \ \forall \ k > j.$$

2. Matrix Factorization: Low-rank mean structure.
   - Model: $\mathbf{X} = \mathbf{M} + \mathbf{E}$ for mean matrix $\mathbf{M}$ that is low-rank and $\mathbf{E}$ iid additive noise.
   - Empirical Optimization Problem:

$$\underset{\mathbf{U},\mathbf{D},\mathbf{V}}{\text{minimize}} \ || \mathbf{X} - \mathbf{U} \mathbf{D} \mathbf{V}^T ||_F^2 \ \text{subject to} \ \mathbf{U}^T \mathbf{U} = \mathbf{I} \ \& \ \mathbf{V}^T \mathbf{V} = \mathbf{I}.$$

Solution: Singular Value Decomposition (SVD).

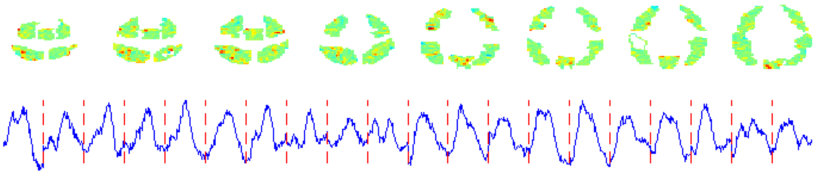
Review: Regularized PCA

Big-Data settings, regularize the leading eigenvalues leading to . . .

1. Functional PCA.
   - Encourage PC factors to be smooth with respect to known data structure. (Rice & Silverman, 1991; Silverman, 1996; Ramsay, 2006; Huang et al., 2008).
   - Leads to consistent PC estimates. (Silverman, 1996)
2. Sparse PCA.
   - Automatic feature / variable selection. (Jollieffe et al., 2003; Zou et al., 2006; d'Aspermont et al., 2007; Shen & Huang, 2008)
   - Leads to consistent PC estimates. (Johnstone & Lu, 2009; Amini & Wainwright, 2009; Shen et al., 2012, Vu & Lei, 2013)

Why Sparse & Functional PCA?

1. Applied Motivation (Neuroimaging):



2. Improved signal recovery, feature selection, interpretation, data visualization.
3. Question: Is there a general mathematical framework for regularization in the context of PCA?

Why Sparse & Functional PCA?

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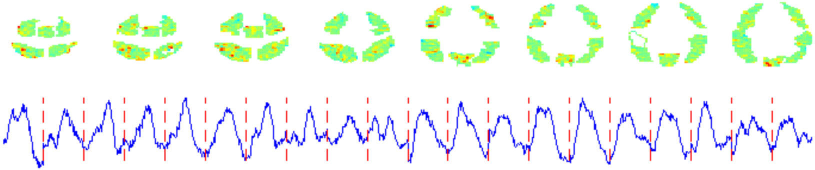


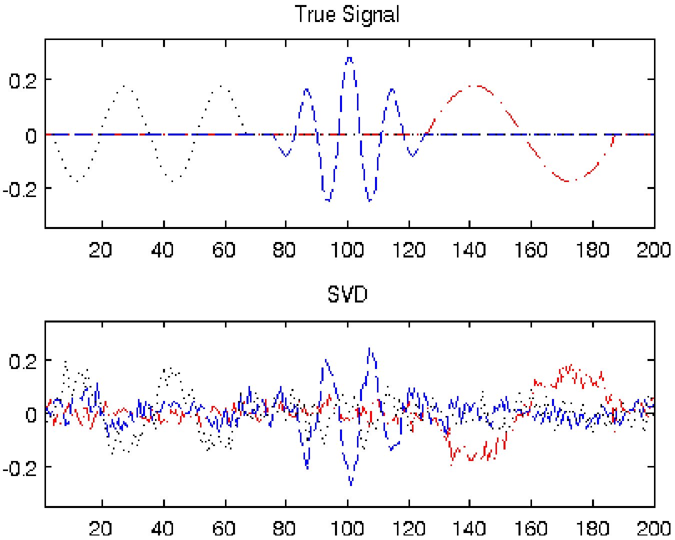
Objectives

(i) Formulate a (good) optimization framework to achieve SFPCA.

(ii) Develop a scalable algorithm to fit SFPCA.

(iii) Carefully study the properties of the model and algorithm from an optimization perspective.

Preview


True Signal
0.2
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-0.2
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60
80
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120
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160
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SVD
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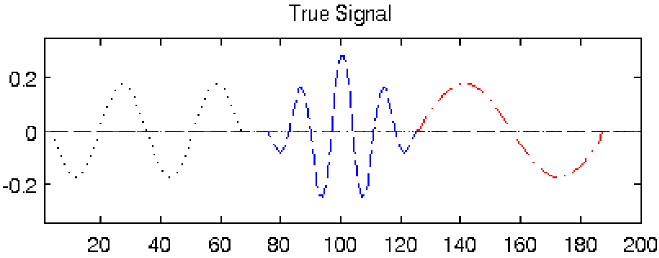

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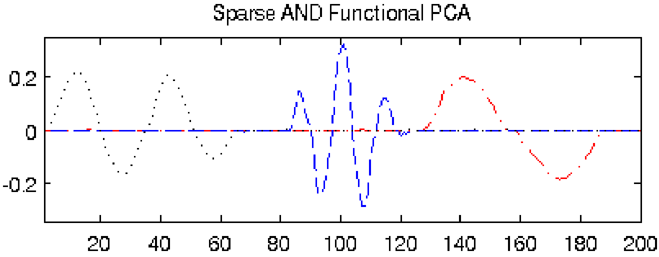

Sparse AND Functional PCA
0.2
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200

Setup

Matrix Factorization: Low-Rank Mean Model.

$$\mathbf{X}_{n \times p} = \sum_{k=1}^{K} d_k \, \mathbf{u}_k \, \mathbf{v}_k^T + \epsilon$$

- Assume data, $\mathbf{X}$, previously centered.
- PC Factors $\mathbf{v}$ and/or $\mathbf{u}$ are sparse and/or smooth.
- ϵ is iid noise; d_k is fixed, but unknown.
- Rows and / or columns of $\mathbf{X}$ arise from discretized curves or other features associated with locations.

Functional PCA & Two-Way FPCA

Encouraging smoothness:

- Continuous functions: 2^{nd} derivatives quantify curvature.
- Penalty: $\int f''(t) f''(t) dt$. Penalizes average squared curvature.
- Discrete extension: Squared second differences between adjacent variables.
- Discrete extension in matrix form:

$$\beta^T \mathbf{\Omega} \beta = \sum (\beta_{j+1} - 2\beta_j + \beta_{j-1})^2$$

  $\mathbf{\Omega}_{p \times p} \succ 0$ is the second differences matrix.

- Other possible choices $\mathbf{\Omega}$ that encourages smoothness. (Ramsay 2006).

Functional PCA & Two-Way FPCA

Functional PCA

$$\underset{\mathbf{v}}{\text{maximize}} \quad \mathbf{v}^T \mathbf{X}^T \mathbf{X} \mathbf{v} \quad \text{subject to} \quad \mathbf{v}^T (\mathbf{I} + \alpha_{\mathbf{v}} \boldsymbol{\Omega}_{\mathbf{v}}) \mathbf{v} = 1.$$

Silverman (1996)

Equivalent to:

- Regression Approach: (Huang et al., 2008)

$$\hat{\mathbf{u}} = \text{argmin}_{\mathbf{u}} \left\{ || \mathbf{X} \hat{\mathbf{v}} - \mathbf{u} ||_2^2 \right\}.$$
$$\hat{\mathbf{v}} = \text{argmin}_{\mathbf{v}} \left\{ || \mathbf{X}^T \hat{\mathbf{u}} - \mathbf{v} ||_2^2 + \alpha \, \mathbf{v}^T \boldsymbol{\Omega} \, \mathbf{v} \right\}.$$

- Half-Smoothing.

Functional PCA & Two-Way FPCA

Two-Way Functional PCA

$$\underset{\mathbf{u},\mathbf{v}}{\text{maximize}} \quad \mathbf{u}^T \mathbf{X} \mathbf{v} - \frac{1}{2} \mathbf{u}^T (\mathbf{I} + \alpha_{\mathbf{u}} \boldsymbol{\Omega}_{\mathbf{u}}) \mathbf{u} \, \mathbf{v}^T (\mathbf{I} + \alpha_{\mathbf{v}} \boldsymbol{\Omega}_{\mathbf{v}}) \mathbf{v} .$$

Huang et al. (2009)

- Equivalent to two-way half-smoothing.
- Related to two-way ℓ_2 penalized regression.

Sparse PCA & Two-Way SPCA

Sparse PCA via Penalized Regression

$$\hat{\mathbf{u}} = \operatorname{argmin}_{\mathbf{u}} \left\{ || \mathbf{X} \hat{\mathbf{v}} - \mathbf{u} ||_2^2 \right\}.$$

$$\hat{\mathbf{v}} = \operatorname{argmin}_{\mathbf{v}} \left\{ || \mathbf{X}^T \hat{\mathbf{u}} - \mathbf{v} ||_2^2 + \lambda || \mathbf{v} ||_1 \right\}.$$

Shen & Huang (2008).

Other SPCA approaches:

- Semi-definite programming.
- Covariance thresholding.

Sparse PCA & Two-Way SPCA

Two-Way Sparse PCA

$$\begin{aligned} \underset{\mathbf{u},\mathbf{v}}{\text{maximize}} \quad & \mathbf{u}^T \mathbf{X} \mathbf{v} - \lambda_{\mathbf{u}} || \mathbf{u} ||_1 - \lambda_{\mathbf{v}} || \mathbf{v} ||_1 \\ \text{subject to} \quad & \mathbf{u}^T \mathbf{u} \leq 1 \;\&\; \mathbf{v}^T \mathbf{v} \leq 1. \end{aligned}$$

Allen et al. (2011); Lagrangian of Witten et al. (2009); Related to Lee et al. (2010).

- SPCA of Shen & Huang (2008) a special case.
- Related to two-way penalized regression.

Two-Way Regularized PCA

Alternating Penalized Regressions

$$\hat{\mathbf{u}} = \operatorname{argmin}_{\mathbf{u}} \left\{ || \mathbf{X} \hat{\mathbf{v}} - \mathbf{u} ||_2^2 + \lambda_{\mathbf{u}} P_{\mathbf{u}}(\mathbf{u}) \right\}.$$

$$\hat{\mathbf{v}} = \operatorname{argmin}_{\mathbf{v}} \left\{ || \mathbf{X}^T \hat{\mathbf{u}} - \mathbf{v} ||_2^2 + \lambda_{\mathbf{v}} P_{\mathbf{v}}(\mathbf{v}) \right\}.$$

Questions:

1. Are sparse AND smoothing ℓ_2 penalties permitted?
2. What penalty types lead to convergent solutions?
3. What optimization problem is this class of algorithms solving?

We consider ...

Objective

Flexible combinations of smoothness and / or sparsity on the row and / or column PC factors.

Four Penalties:

- Row Sparsity: $\lambda_{\mathbf{u}} P_{\mathbf{u}}(\mathbf{u})$, for example $\lambda_{\mathbf{u}} || \, \mathbf{u} \, ||_1$.
- Row Smoothness: $\alpha_{\mathbf{u}} \, \mathbf{u}^T \, \boldsymbol{\Omega}_{\mathbf{u}} \, \mathbf{u}$; $\quad \boldsymbol{\Omega}_{\mathbf{u}}^{(n \times n)} \succ 0$.
- Column Sparsity: $\lambda_{\mathbf{v}} P_{\mathbf{v}}(\mathbf{v})$ for example $\lambda_{\mathbf{v}} || \, \mathbf{v} \, ||_1$.
- Column Smoothness: $\alpha_{\mathbf{v}} \, \mathbf{v}^T \, \boldsymbol{\Omega}_{\mathbf{v}} \, \mathbf{v}$; $\quad \boldsymbol{\Omega}_{\mathbf{v}}^{(p \times p)} \succ 0$.

Approach: Iteratively solve for the best rank-one solution in a greedy manner.

Formulating an Optimization Problem

We want . . .

1. To generalize existing methods for PCA, SPCA, FPCA, and two-way SPCA and FPCA.
   - These should all be special cases when regularization parameters are active.
2. Desirable numerical properties:
   - Identifiable PC factors.
   - Non-degenerate and Well-scaled solution and PC factors
   - Balanced regularization (NO regularization masking).
     - Regularization Masking: $\exists$ a $\lambda, \alpha > 0$ where the solution does not depend on both λ and α.
3. A computationally tractable algorithm in big-data settings.

Optimization Approaches: Natural Extensions?

Question:

1. Why not add ℓ_1 and smoothing ℓ_2 penalties to the Frobenius-norm loss of the SVD problem?

$$\underset{\mathbf{u}(:\mathbf{u}^T\mathbf{u}\leq 1),\mathbf{v}(:\mathbf{v}^T\mathbf{v}\leq 1)}{\text{minimize}} ||\mathbf{X} - (d)\,\mathbf{u}\,\mathbf{v}^T\,||_F^T + \lambda_{\mathbf{u}}||\,\mathbf{u}\,||_1 + \lambda_{\mathbf{v}}||\,\mathbf{v}\,||_1 + \alpha_{\mathbf{u}}\,\mathbf{u}^T\,\boldsymbol{\Omega}_{\mathbf{u}}\,\mathbf{u} + \alpha_{\mathbf{v}}\,\mathbf{v}^T\,\boldsymbol{\Omega}_{\mathbf{v}}\,\mathbf{v}\,.$$

   Unidentifiable, degenerate, does not generalize.

2. Why not add ℓ_1 penalties to the two-way FPCA optimization problem of Huang et al. (2009)?

$$\underset{\mathbf{u}(:\mathbf{u}^T\mathbf{u}\leq 1),\mathbf{v}(:\mathbf{v}^T\mathbf{v}\leq 1)}{\text{maximize}} \mathbf{u}^T\,\mathbf{X}\,\mathbf{v} - \frac{1}{2}\,\mathbf{u}^T(\mathbf{I} + \alpha_{\mathbf{u}}\,\boldsymbol{\Omega}_{\mathbf{u}})\,\mathbf{u}\,\mathbf{v}^T(\mathbf{I} + \alpha_{\mathbf{v}}\,\boldsymbol{\Omega}_{\mathbf{v}})\,\mathbf{v} - \lambda_{\mathbf{u}}||\,\mathbf{u}\,||_1 - \lambda_{\mathbf{v}}||\,\mathbf{v}\,||_1$$

3. Why not add smoothing ℓ_2 penalties to the two-way SPCA problem of Witten et al. (2009)?

$$\underset{\mathbf{u}(:\mathbf{u}^T\mathbf{u}\leq 1),\mathbf{v}(:\mathbf{v}^T\mathbf{v}\leq 1)}{\text{maximize}} \quad \mathbf{u}^T\,\mathbf{X}\,\mathbf{v} - \lambda_{\mathbf{u}}||\,\mathbf{u}\,||_1 - \lambda_{\mathbf{v}}||\,\mathbf{v}\,||_1 - \alpha_{\mathbf{u}}\,\mathbf{u}^T\,\boldsymbol{\Omega}_{\mathbf{u}}\,\mathbf{u} - \alpha_{\mathbf{v}}\,\mathbf{v}^T\,\boldsymbol{\Omega}_{\mathbf{v}}\,\mathbf{v}\,.$$

   Regularization masking, computationally challenging.

Assumptions on Penalties

A1 $\mathbf{\Omega_u} \succeq 0$ & $\mathbf{\Omega_v} \succeq 0$.

A2 $P()$'s are positive, homogeneous of order one, i.e. $P(cx) = cP(x) \; \forall \; c > 0$.

- Sparse penalties: ℓ_1-norm, SCAD, MC+, etc.
- Structured sparse: group lasso, fused lasso, generalized lasso, etc.

A3 If $P()$'s non-convex, then $P()$ can be decomposed into the difference of two convex functions, $P(x) = P_1(x) - P_2(x)$ for $P_1()$ and $P_2()$ convex.

- Includes common non-convex penalties such as SCAD, MC+, log-concave, etc.

SFPCA Optimization Problem

Rank-one Sparse & Functional PCA the solution to:

$$\begin{aligned} \underset{\mathbf{u},\mathbf{v}}{\text{maximize}} \quad & \mathbf{u}^T \mathbf{X} \mathbf{v} - \lambda_{\mathbf{u}} P_{\mathbf{u}}(\mathbf{u}) - \lambda_{\mathbf{v}} P_{\mathbf{v}}(\mathbf{v}) \\ \text{subject to} \quad & \mathbf{u}^T (\mathbf{I} + \alpha_{\mathbf{u}} \boldsymbol{\Omega}_{\mathbf{u}}) \mathbf{u} \leq 1 \ \& \ \mathbf{v}^T (\mathbf{I} + \alpha_{\mathbf{v}} \boldsymbol{\Omega}_{\mathbf{v}}) \mathbf{v} \leq 1. \end{aligned}$$

- Penalty Parameters: $\lambda_{\mathbf{u}}, \lambda_{\mathbf{v}}, \alpha_{\mathbf{u}}, \alpha_{\mathbf{v}} \geq 0$.

Relationship to Other PCA Approaches

Theorem

(i) If $\lambda_{\mathbf{u}}, \lambda_{\mathbf{v}}, \alpha_{\mathbf{u}}, \alpha_{\mathbf{v}} = 0$, then equivalent to PCA / the SVD of $\mathbf{X}$.

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(iii) If $\alpha_{\mathbf{u}}, \alpha_{\mathbf{v}} = 0$, then equivalent to a special case of the two-way Sparse PCA (Allen et al., 2011), which is the Lagrangian of (Witten et al., 2009) and closely related to that (Lee et al., 2010).

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(iv) If $\lambda_{\mathbf{u}}, \lambda_{\mathbf{v}}, \alpha_{\mathbf{u}} = 0$, then equivalent to the Functional PCA solution of (Silverman, 1996) and (Huang et al., 2008).

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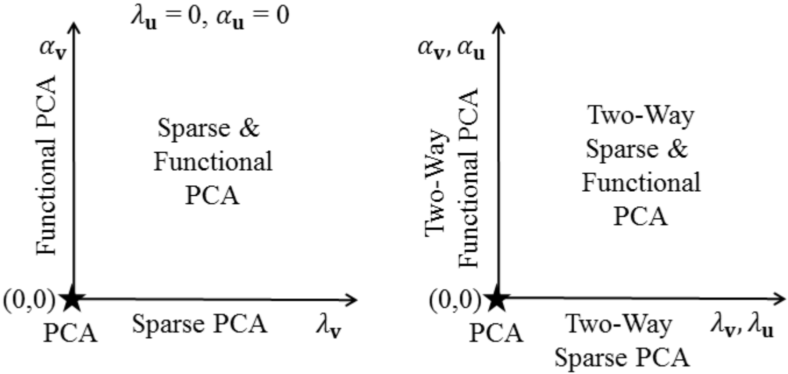
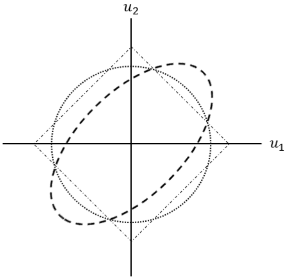


Desirable Numerical Properties

Theorem

1. Identifiable ($\mathbf{u}$ and $\mathbf{v}$) up to a sign change.
2. Balanced regularization (no *regularization masking*):
   - $\exists$ a $\lambda_{\mathbf{u}}^{max}$ s.t. $\mathbf{u}^* = 0$.
   - $(\mathbf{u}^*, \mathbf{v}^*)$ depend on all non-zero regularization parameters.
3. Well-scaled and non-degenerate.
   - Either $\mathbf{u}^{*,T}(\mathbf{I} + \alpha_{\mathbf{u}} \boldsymbol{\Omega}_{\mathbf{u}})\, \mathbf{u}^* = 1$ and $\mathbf{v}^{*,T}(\mathbf{I} + \alpha_{\mathbf{v}} \boldsymbol{\Omega}_{\mathbf{v}})\, \mathbf{v}^* = 1$,
   - Or $\mathbf{u}^* = 0$ and $\mathbf{v}^* = 0$.



SFPCA Optimization Problem

Rank-one Sparse & Functional PCA the solution to:

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$$\text{subject to} \quad \mathbf{u}^T (\mathbf{I} + \alpha_{\mathbf{u}} \boldsymbol{\Omega}_{\mathbf{u}}) \mathbf{u} \leq 1 \ \& \ \mathbf{v}^T (\mathbf{I} + \alpha_{\mathbf{v}} \boldsymbol{\Omega}_{\mathbf{v}}) \mathbf{v} \leq 1.$$

- Non-convex, non-differentiable, QCQP.
- $P()$ convex $\Longrightarrow$ bi-convex.
  - Convex in $\mathbf{v}$ with $\mathbf{u}$ fixed as well as the converse.

Idea: Alternating optimization.

Relationship to Penalized Regression

Theorem

The solution to the SFPCA problem with respect to $\mathbf{u}$ is given by:

$$\hat{\mathbf{u}} = \text{argmin}_{\mathbf{u}} \left\{ \frac{1}{2} || \mathbf{X} \mathbf{v} - \mathbf{u} ||_2^2 + \lambda_{\mathbf{u}} P_{\mathbf{u}}(\mathbf{u}) + \frac{\alpha_{\mathbf{u}}}{2} \mathbf{u}^T \boldsymbol{\Omega}_u \mathbf{u} \right\}$$

$$\mathbf{u}^* = \begin{cases} \hat{\mathbf{u}} / ||\hat{\mathbf{u}}||_{\mathbf{I} + \alpha_{\mathbf{u}} \boldsymbol{\Omega}_{\mathbf{u}}} & ||\hat{\mathbf{u}}||_{\mathbf{I} + \alpha_{\mathbf{u}} \boldsymbol{\Omega}_{\mathbf{u}}} > 0 \\ 0 & \text{otherwise.} \end{cases}$$

- Analogous to re-scaled Elastic Net problem! (Zou & Hastie, 2005).
- Result holds because of A2, order-one penalties.

Relationship to Penalized Regression

$$\underset{\mathbf{u}}{\text{minimize}} \quad \frac{1}{2} || \mathbf{X} \, \mathbf{v} - \mathbf{u} \, ||_2^2 + \lambda_{\mathbf{u}} P_{\mathbf{u}}(\mathbf{u}) + \frac{\alpha_{\mathbf{u}}}{2} \, \mathbf{u}^T \, \mathbf{\Omega}_u \, \mathbf{u}$$

- Can be solved by (accelerated) proximal gradient descent.
- Geometric convergence, $O(k \log k)$, for convex penalties.
- A3, difference of convex, ensures convergence for non-convex penalties.
- Closed form proximal operator for many penalties: $\text{prox}_P(\mathbf{y}, \lambda) = \text{argmin}_{\mathbf{x}} \{ \frac{1}{2} ||\mathbf{x} - \mathbf{y}||_2^2 + \lambda P(\mathbf{x}) \}$.
  - Some form of thresholding (i.e. soft-thresholding for ℓ_1 penalty).

SFPCA Algorithm

Rank-One Algorithm

1. Initialize $\mathbf{u}$ and $\mathbf{v}$ to that of the rank-1 SVD of $\mathbf{X}$. Set $\mathbf{S_u} = \mathbf{I} + \alpha_\mathbf{u} \mathbf{\Omega_u}$ and $L_\mathbf{u} = \lambda_{max}(\mathbf{S_u})$; set $\mathbf{S_v} = \mathbf{I} + \alpha_\mathbf{v} \mathbf{\Omega_v}$ and $L_\mathbf{v} = \lambda_{max}(\mathbf{S_v})$.
2. Repeat until convergence:
    1. Estimate $\hat{\mathbf{u}}$. Repeat until convergence:
    $\mathbf{u}^{(t+1)} = \text{prox}_{P_\mathbf{u}} \left(\mathbf{u}^{(t)} + \frac{1}{L}(\mathbf{X}\,\mathbf{v}^* - \mathbf{S_u}\,\mathbf{u}^{(t)}), \frac{\lambda_\mathbf{u}}{L_\mathbf{u}} \right)$.
    2. Set $\mathbf{u}^* = \begin{cases} \hat{\mathbf{u}}/\|\hat{\mathbf{u}}\|_{\mathbf{S_u}} & \|\hat{\mathbf{u}}\|_{\mathbf{S_u}} > 0 \\ 0 & \text{otherwise.} \end{cases}$
    3. Estimate $\hat{\mathbf{v}}$. Repeat until convergence:
    $\mathbf{v}^{(t+1)} = \text{prox}_{P_\mathbf{v}} \left(\mathbf{v}^{(t)} + \frac{1}{L}(\mathbf{X}^T\,\mathbf{u}^* - \mathbf{S_v}\,\mathbf{v}^{(t)}), \frac{\lambda_\mathbf{v}}{L_\mathbf{v}} \right)$.
    4. Set $\mathbf{v}^* = \begin{cases} \hat{\mathbf{v}}/\|\hat{\mathbf{v}}\|_{\mathbf{S_v}} & \|\hat{\mathbf{v}}\|_{\mathbf{S_v}} > 0 \\ 0 & \text{otherwise.} \end{cases}$
3. Return $\mathbf{u} = \mathbf{u}^* / \|\,\mathbf{u}^*\,\|_2$, $\mathbf{v} = \mathbf{v}^* / \|\,\mathbf{v}^*\,\|_2$, and $d = \mathbf{u}^T\,\mathbf{X}\,\mathbf{v}$.

Convergence

Theorem: Convergence of rank-one SFPCA.

For $P_{\mathbf{u}}$ and $P_{\mathbf{v}}$ convex,

- The SFPCA Algorithm convergences to a stationary point of the SFPCA problem.
- The solution is unique given an initial starting point.

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For $P_{\mathbf{u}}$ and $P_{\mathbf{v}}$ convex,

- The SFPCA Algorithm convergences to a stationary point of the SFPCA problem.
- The solution is unique given an initial starting point.

- Multi-rank solutions can be computed in a greedy manner (power method).
- Several deflation schemes available (Mackey, 2009).
- Subtraction deflation most common:
  - Fit rank-one SFPCA to $\mathbf{X}$ to estimate 1st PC factors.
  - Subtract rank one fit, $\mathbf{X} - d_1 \, \mathbf{u}_1 \, \mathbf{v}_1^T$, and apply SFPCA to estimate 2nd PC factors.

Extensions: Non-Negativity Constraints

$$\begin{aligned} \underset{\mathbf{u},\mathbf{v}}{\text{maximize}} \quad & \mathbf{u}^T \mathbf{X} \mathbf{v} - \lambda_{\mathbf{u}} P_{\mathbf{u}}(\mathbf{u}) - \lambda_{\mathbf{v}} P_{\mathbf{v}}(\mathbf{v}) \\ \text{subject to} \quad & \mathbf{u}^T (\mathbf{I} + \alpha_{\mathbf{u}} \boldsymbol{\Omega}_{\mathbf{u}}) \mathbf{u} \leq 1 \ \& \ \mathbf{v}^T (\mathbf{I} + \alpha_{\mathbf{v}} \boldsymbol{\Omega}_{\mathbf{v}}) \mathbf{v} \leq 1, \\ & \mathbf{u} \geq 0 \ \& \ \mathbf{v} \geq 0. \end{aligned}$$

Corollary

Replace $\text{prox}_P()$ with the *positive proximal operator*, $\text{prox}_P^+(\mathbf{y}, \lambda) = \text{argmin}_{\mathbf{x}:\mathbf{x}\geq 0}\{\frac{1}{2}||\mathbf{x} - \mathbf{y}||_2^2 + \lambda P(\mathbf{x})\}$.

- Same convergence guarantees hold.

Selecting Regularization Parameters

- Cross-validation (CV), Generalized CV, BIC, etc.
- Nested vs. Grid search.

Ideas:

- Select $\alpha_{\mathbf{u}}$ and $\lambda_{\mathbf{u}}$ together.
- Exploit connection to Elastic Net to compute degrees of freedom for BIC.

Example for ℓ_1 penalty:

- Let $\mathcal{A}(\mathbf{u})$ be the active set of $\mathbf{u}$.

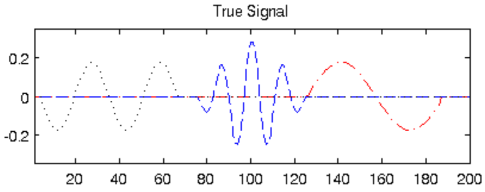
$$\hat{df}(\alpha_{\mathbf{u}}, \lambda_{\mathbf{u}}) = \mathrm{trace}\left[\left(\mathbf{I}_{\mathcal{A}(\mathbf{u})} - \frac{\alpha_{\mathbf{u}}}{2} \boldsymbol{\Omega}_{\mathbf{u}}(\mathcal{A}(\mathbf{u}), \mathcal{A}(\mathbf{u})) \right)^{-1} \right].$$

Simulation I

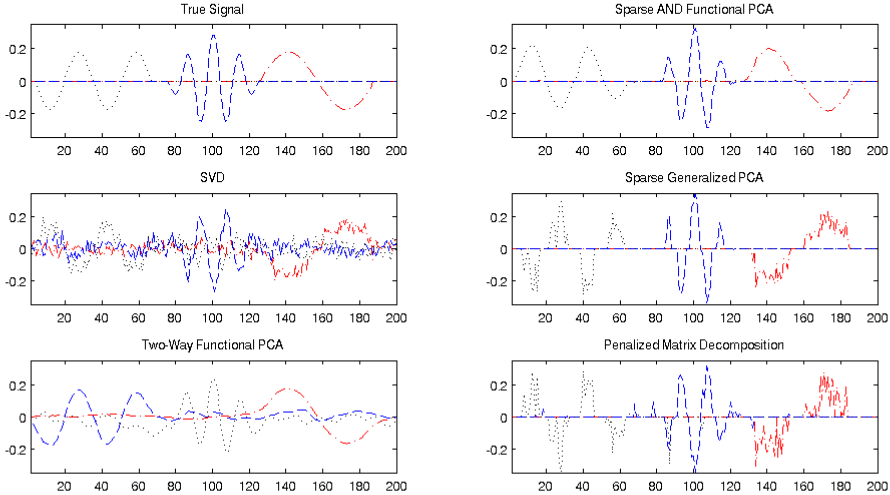
Setup: Rank-3 Model with sparse & smooth right factors.

$$\mathbf{X}_{n \times p} = \sum_{k=1}^{K} d_k \, \mathbf{u}_k \, \mathbf{v}_k^T + \epsilon$$

- $\epsilon_{ij} \overset{iid}{\sim} N(0, 1)$.
- $\mathbf{u}_k$ random orthonormal vectors of length n;
  $D = \mathrm{diag}([n/4, n/5, n/6]^T)$.
- $\mathbf{v}_k$ fixed signal vectors of length $p = 200$:



Simulation I



Simulation I

Table: $n = 100$ Results.

		TWFPCA	SSVD	PMD	SGPCA	SFPCA
$\mathbf{v}_1$	TP	-	0.897	0.568	0.768	**0.935**
	FP	-	0.323	0.001	0.006	**0.052**
	r$\angle$	**0.153**	0.625	2.220	0.726	0.189
$\mathbf{v}_2$	TP	-	0.783	0.657	0.445	**0.713**
	FP	-	0.320	0.106	0.002	**0.047**
	r$\angle$	5.980	0.549	0.597	0.829	**0.438**
$\mathbf{v}_3$	TP	-	0.771	0.514	0.499	**0.883**
	FP	-	0.316	0.066	0.004	**0.054**
	r$\angle$	3.660	0.855	1.270	1.010	**0.468**
	rSE	0.668	0.760	1.000	0.737	**0.450**

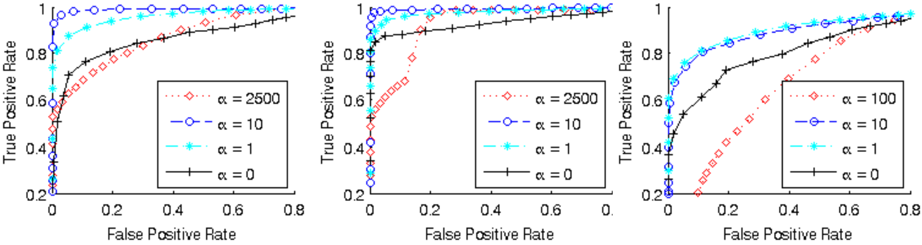
Simulation I

Table: $n = 300$ Results.

		TWFPCA	SSVD	PMD	SGPCA	SFPCA
$\mathbf{v}_1$	TP	-	0.973	0.509	0.921	**0.987**
	FP	-	0.322	0.000	0.005	**0.068**
	r$\angle$	0.768	0.487	15.700	0.553	**0.152**
$\mathbf{v}_2$	TP	-	0.919	0.773	0.839	**0.967**
	FP	-	0.319	0.000	0.038	**0.048**
	r$\angle$	52.300	0.428	1.310	0.488	**0.320**
$\mathbf{v}_3$	TP	-	0.943	0.530	0.849	**0.972**
	FP	-	0.314	0.000	0.015	**0.060**
	r$\angle$	33.100	0.545	5.940	0.631	**0.131**
	rSE	1.170	0.790	3.380	0.809	**0.655**

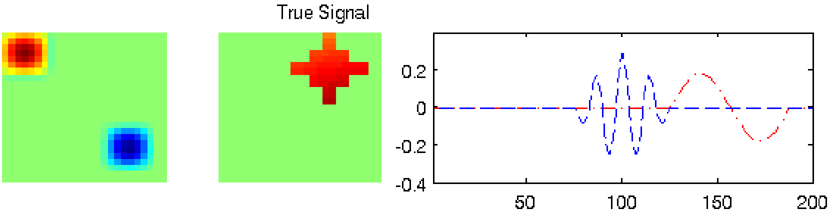
Simulation I

SFPCA also improves feature selection . . .

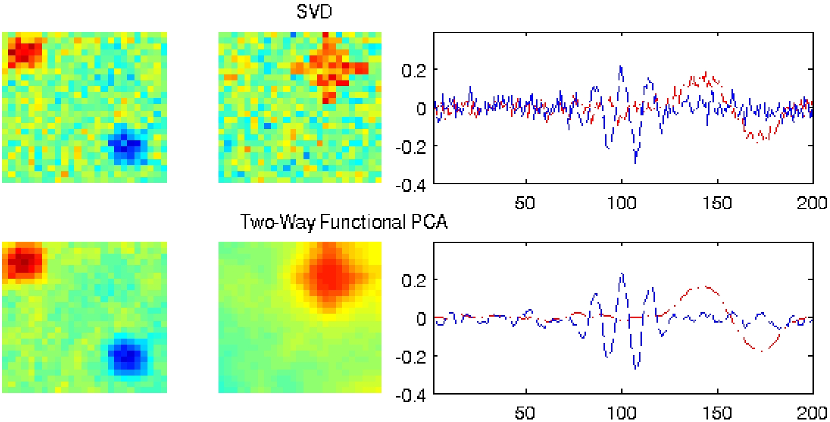


Simulation II

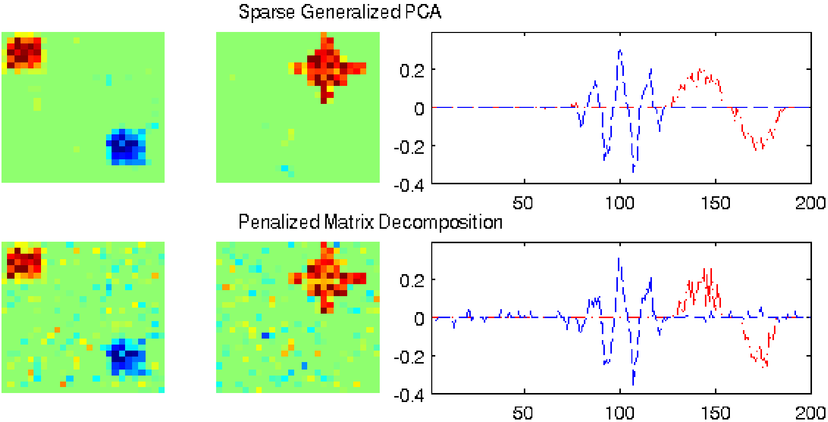
Setup: Rank-2 Model with sparse & smooth spatial (25×25 grid) and temporal (200-length vector) factors.



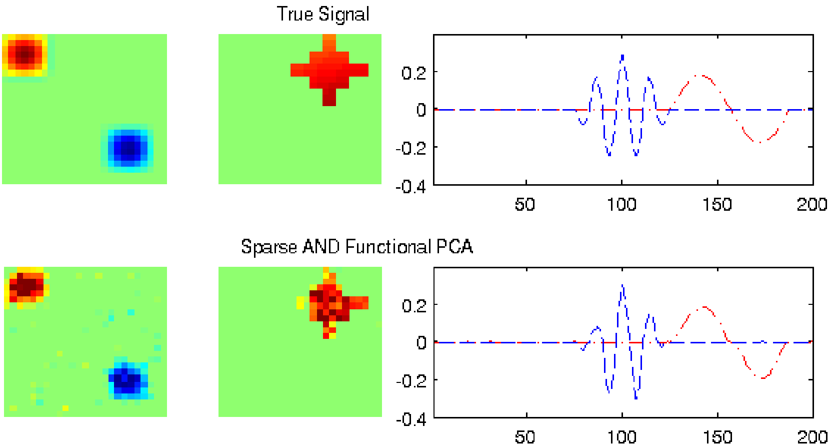
Simulation II



Simulation II



Simulation II



1. Motivation
2. Background & Challenges: Regularized PCA
3. Sparse & Functional PCA Model
4. Sparse & Functional PCA Algorithm
5. Simulation Studies
6. Case Study: EGG Data

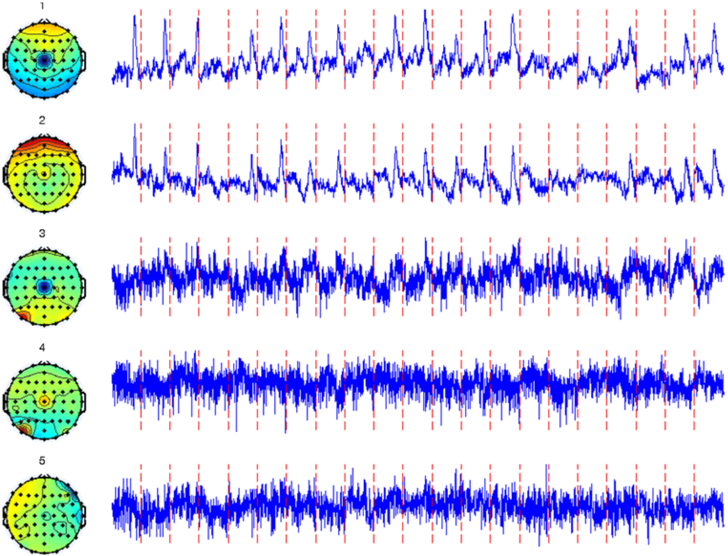
EEG Predisposition to Alcoholism

Data:

- EEG measures electrical signals in the active brain over time.
- Sampled from 64 channels at 256Hz.
- Consider 1^{st} alcoholic subject over epochs relating to non-matching image stimuli.
- Data matrix: 57×5376, channel location by epoch time points (21 epochs of 256 time points each).
- $\mathbf{\Omega_u}$ weighted squared second differences matrix using spherical distances between channel locations.
- $\mathbf{\Omega_v}$ squared second differences matrix between time points.

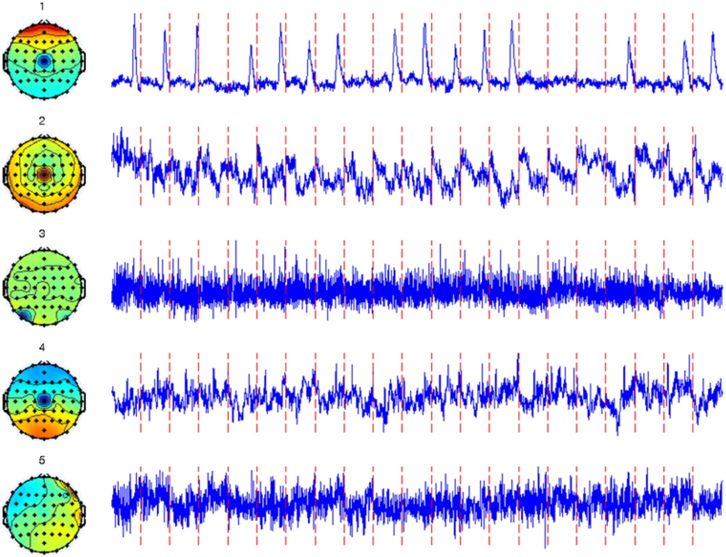
EEG Results

PCA Results:



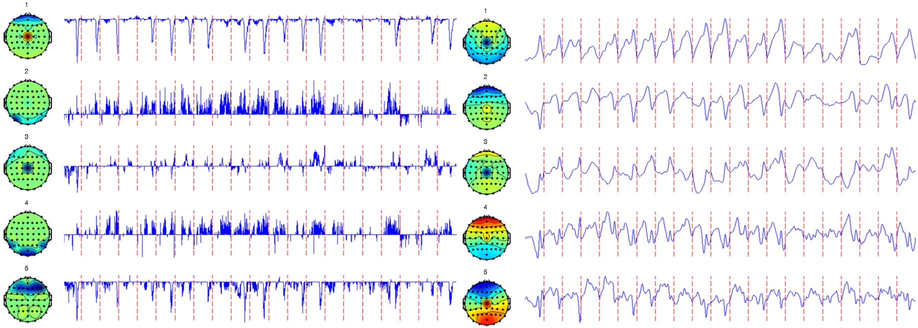
EEG Results

Independent Component Analysis (ICA) Results:



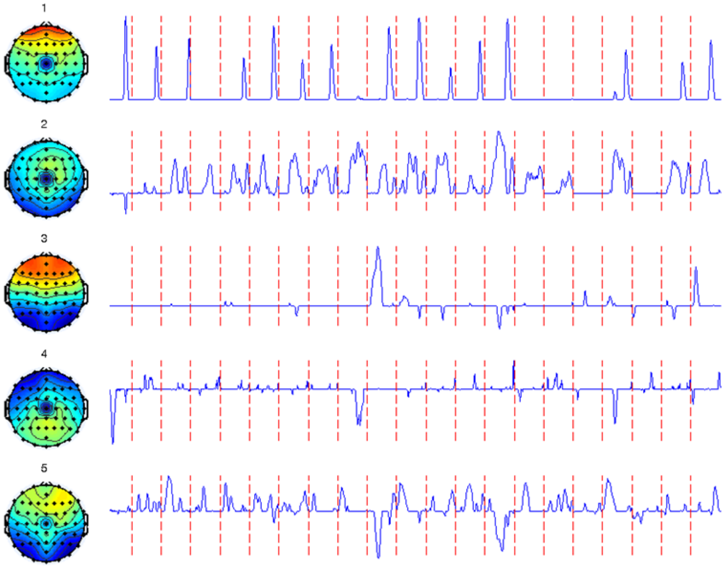
EEG Results

Penalized Matrix Decomposition & Two-Way FPCA Results:



EEG Results

Sparse & Functional PCA Results:



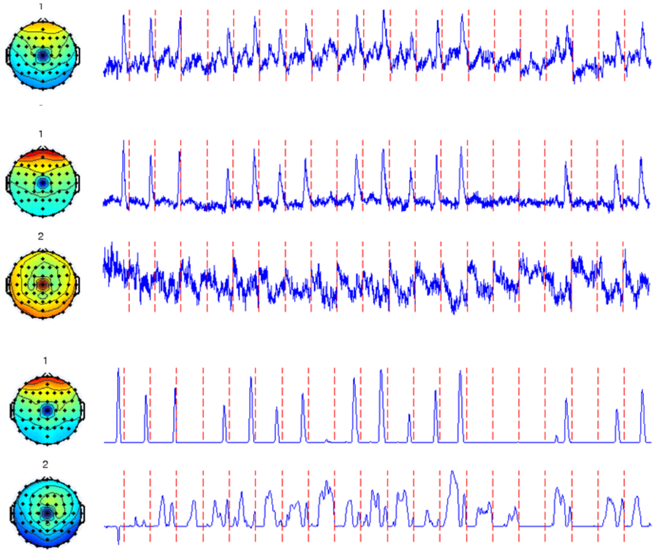
EEG Results

Comparison:

PCA:

ICA:

SFPCA:



EEG Results

SFPCA Notes:

- 3.28 seconds to converge. (Software entirely in Matlab).
- BIC selected $\lambda_{\mathbf{u}} = 0$ (spatial sparsity) for first 5 components.
- BIC selected $\alpha_{\mathbf{u}} = 10 - 12$, $\alpha_{\mathbf{v}} = 0.5 - 10$, and $\lambda_{\mathbf{v}} = 1 - 2.5$ for first 5 components.

Flexible, data-driven selection of appropriate amount of regularization.

Summary & Future Work

Summary

- SFPCA generalizes much of the existing literature on regularized PCA via alternating regressions.
- SFPCA has the flexibility to permit many types of regularization in a data-driven manner.
- SFPCA results in better signal recovery and more interpretable factors as well as improved feature selection.

Future Statistical Work:

- Statistical consistency, especially in high-dimensional settings.
- Extensions to other multivariate methods: CCA, PLS, LDA, Clustering, and etc.

The Bigger Picture: Modern Multivariate Analysis

Goal: Flexible, data-driven approaches for analyzing complex big-data.

Approach: Alternating penalized regressions framework and deflation for any eigenvalue or singular value problems.

Can mix and match any of the following:

- Generalizations that permit non-iid noise: Generalized PCA (Allen et al., 2013).
- Non-negativity constraints. (Today's talk; Zaas, ; Allen and Maletic-Savatic, 2011).
- Higher-order data and multi-way arrays. (Allen, 2012; Allen, 2013).
- Structured Signal: Sparsity and/or Smoothness. (Today's talk).

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Software available at:

`http://www.stat.rice.edu/~gallen/software.html`

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