

Regularized Estimation of Spatial Patterns

Wen-Ting Wang

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Joint work with [Hsin-Cheng Huang](#) @ Academia Sinica

Outline

1 Principal Component Analysis

Background

Proposed Method: Spatial PCA

2 Maximum Covariance Analysis

Background

Proposed Method: Spatial MCA

3 Numerical Examples

4 Summary

Climate Change

Climate Change

increases the odds of extreme weather events occurring

Flood



Drought



Climate Change

increases the odds of extreme weather events occurring
affects human health and quality of life

Drought in the East Africa

2011

10,000

People have been killed
by the worst drought in 60 years.

Climate Change

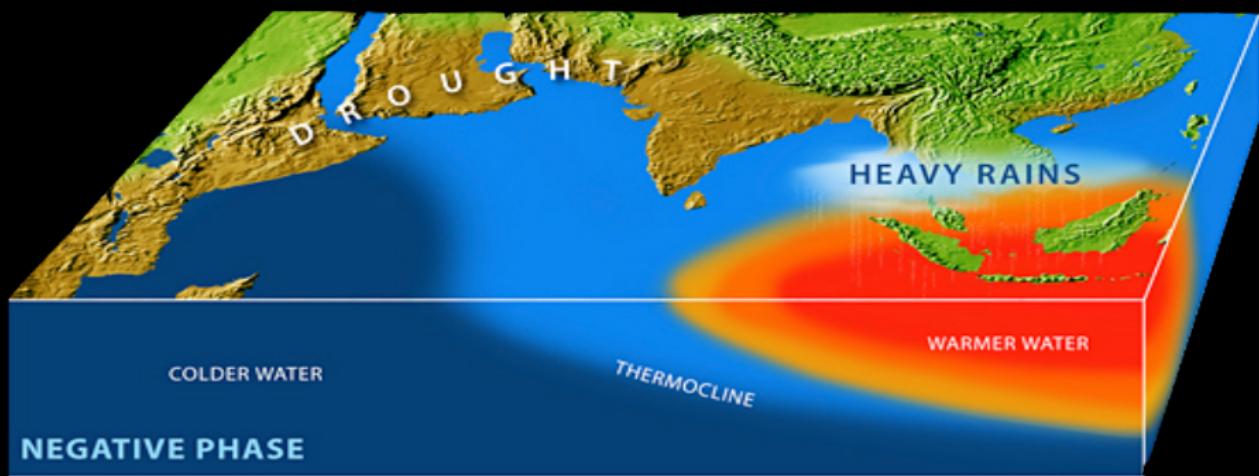
are associated with atmospheric dynamics.

Atmospheric dynamics

can be studied through spatial patterns.

Spatial Pattern

Sea surface temperature vs. Rainfall



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Background

- Spatial processes of interest:

$$\{\eta_i(\mathbf{s}); \mathbf{s} \in D\}; i = 1, \dots, n$$

- $D \subset \mathbb{R}^d$
- mean zero
- common covariance function: $C_\eta(\mathbf{s}^*, \mathbf{s}) = \text{cov}(\eta_i(\mathbf{s}^*), \eta_i(\mathbf{s}))$
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 - common covariance function: $C_\eta(\mathbf{s}^*, \mathbf{s}) = \text{cov}(\eta_i(\mathbf{s}^*), \eta_i(\mathbf{s}))$
 - $\eta_1(\cdot), \dots, \eta_n(\cdot)$: uncorrelated
 - Data at locations $\mathbf{s}_1, \dots, \mathbf{s}_p \in D$,
- $$Y_i(\mathbf{s}_j) = \eta_i(\mathbf{s}_j) + \epsilon_{ij}; i = 1, \dots, n, j = 1, \dots, p$$
- $\epsilon_{ij} \sim (0, \sigma^2)$: white noise
 - ϵ_{ij} and $\eta_i(\mathbf{s}_j)$ are uncorrelated for any i, j

Targets

- ① Detect the dominant spatial patterns (modes) of $\eta_1(\cdot), \dots, \eta_n(\cdot)$
 - interpret the **variability of spatial data** physically

- ② Estimate spatial covariance function $C_\eta(\cdot, \cdot)$
 - no specific assumption (e.g., parametric form or stationarity)
 - **spatial prediction** (kriging) of $\{\eta_i(s); s \in D\}$

Rank- K Spatial Model

- Data:

$$Y_i(s_j) = \eta_i(s_j) + \epsilon_{ij}; \quad i = 1, \dots, n, \quad j = 1, \dots, p$$

Rank- K Spatial Model

- Data:

$$Y_i(\mathbf{s}_j) = \sum_{k=1}^K \xi_{ik} \varphi_k(\mathbf{s}_j) + \epsilon_{ij}; \quad i = 1, \dots, n, \quad j = 1, \dots, p$$

- $(\xi_{i1}, \dots, \xi_{iK})' \sim (\mathbf{0}, \boldsymbol{\Lambda})$; $\boldsymbol{\Lambda}_{K \times K}$ is positive-definite
- $\varphi_1(\cdot), \dots, \varphi_K(\cdot)$: K unknown orthonormal functions
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- Spatial covariance function:

$$C_\eta(\mathbf{s}^*, \mathbf{s}) = \sum_{k=1}^K \sum_{k'=1}^K \lambda_{kk'} \varphi_k(\mathbf{s}^*) \varphi_{k'}(\mathbf{s})$$

- $\lambda_{kk'}$: (k, k') entry of $\boldsymbol{\Lambda}$

Goal

- Find $\varphi_1(\cdot), \dots, \varphi_K(\cdot)$ to represent the dominant patterns.

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- Standard approach: principal component analysis (PCA)

Principal Component Analysis

- p -dimensional data vector:

$$\mathbf{Y}_i = (Y_i(s_1), \dots, Y_i(s_p))' \sim (\mathbf{0}, \Sigma)$$

- Idea: find $\phi \in \mathbb{R}^p$ with $\phi'\phi = 1$, which maximizes $\text{Var}(\phi'\mathbf{Y}_i)$

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 - eigenvalues: $\lambda_1 \geq \dots \geq \lambda_p$
 - eigenvectors: ϕ_1, \dots, ϕ_p
- Dominant patterns: ϕ_1, \dots, ϕ_K (with $\lambda_1, \dots, \lambda_K$ large)

Principal Component Analysis

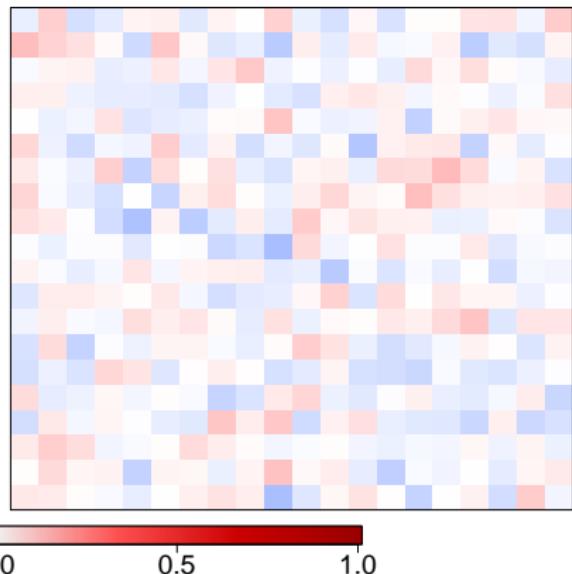
- Data matrix: $\mathbf{Y}_{n \times p} = (\mathbf{Y}_1, \dots, \mathbf{Y}_n)'$
- Sample covariance matrix: $\mathbf{S} = \mathbf{Y}'\mathbf{Y}/n$
- Spectral decomposition: \mathbf{S}
 - sample eigenvalues: $\tilde{\lambda}_1 \geq \dots \geq \tilde{\lambda}_p$
 - sample eigenvectors: $\tilde{\phi}_1, \dots, \tilde{\phi}_p$
- $\tilde{\phi}_1, \dots, \tilde{\phi}_K$ are estimates of ϕ_1, \dots, ϕ_K

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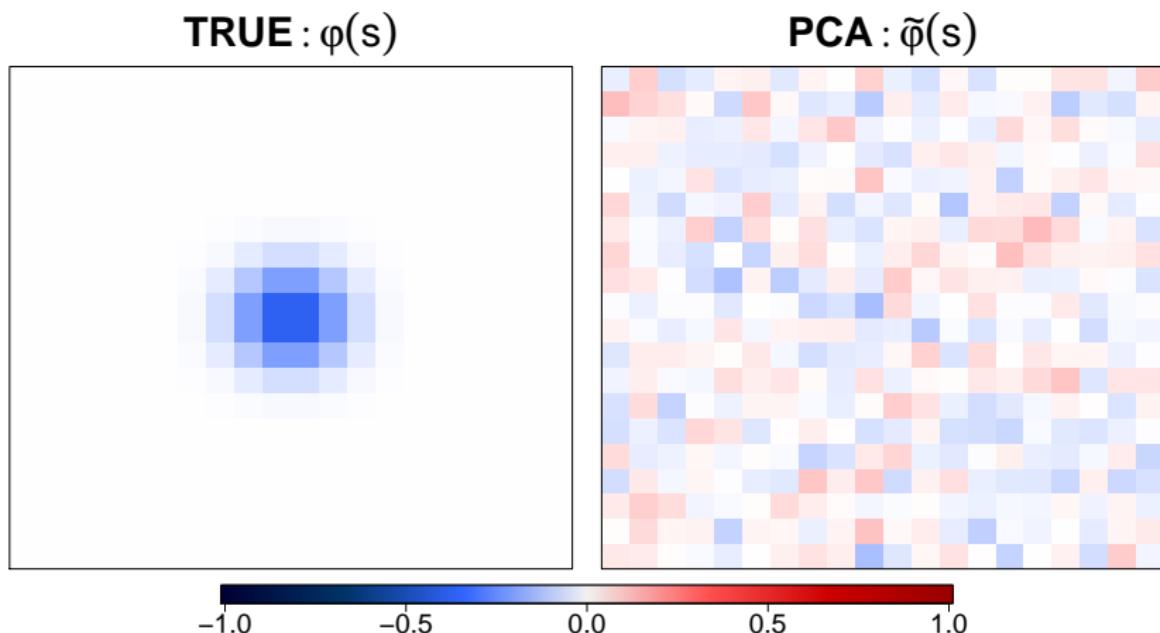
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- Problems:
 - high estimation variability: n is small or p is large
 - unstable and noisy patterns
 - weak physical interpretation
 - without spatial structure of ϕ

Example:

PCA : $\tilde{\varphi}(s)$



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retain the orthogonal constraint of ϕ_k

Quick Recap

- Data $\mathbf{Y}_i = (Y_i(\mathbf{s}_1), \dots, Y_i(\mathbf{s}_p))'$; $i = 1, \dots, n$
 - $Y_i(\mathbf{s}_j) = \sum_{k=1}^K \xi_{ik} \varphi_k(\mathbf{s}_j) + \epsilon_{ij}; \quad j = 1 \dots, p$
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 - $(\xi_{i1}, \dots, \xi_{iK})' \sim (\mathbf{0}, \boldsymbol{\Lambda})$; $\boldsymbol{\Lambda}_{K \times K} \succ \mathbf{0}$
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- $\lambda_{kk'}$: (k, k') entry of $\boldsymbol{\Lambda}$
- Unknown parameters: $\varphi_1(\cdot), \dots, \varphi_K(\cdot)$, $\boldsymbol{\Lambda}$, σ^2

PCA (alternative version)

- Data matrix: $\mathbf{Y}_{n \times p} = (\mathbf{Y}_1, \dots, \mathbf{Y}_n)'$
- PCA :

$$\tilde{\Phi} = \underset{\Phi: \Phi' \Phi = I_K}{\arg \min} \| \mathbf{Y} - \mathbf{Y} \Phi \Phi' \|_F^2$$

- $\Phi_{p \times K} = (\phi_1, \dots, \phi_K)$ with $\phi_{jk} = \varphi_j(\mathbf{s}_k)$
- $\| M \|_F^2 = \sum_{i=1}^n \sum_{j=1}^p m_{ij}^2$

Regularized PCA

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- $\Phi_{p \times K} = (\phi_1, \dots, \phi_K)$ with $\phi_{jk} = \varphi_j(s_k)$
- Objective function

$$\|\mathbf{Y} - \mathbf{Y}\Phi\Phi'\|_F^2$$

subject to $\Phi'\Phi = I_K$

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- Objective function

$$\|\mathbf{Y} - \mathbf{Y}\Phi\Phi'\|_F^2 + \tau_1 \sum_{k=1}^K J(\varphi_k) + \tau_2 \sum_{k=1}^K \sum_{j=1}^p |\varphi_k(s_j)|$$

subject to $\Phi'\Phi = I_K$

- $J(\varphi_k) = \sum_{z_1+\dots+z_d=2} \int_{R^d} \left(\frac{\partial^2 \varphi_k(\mathbf{s})}{\partial x_1^{z_1} \dots \partial x_d^{z_d}} \right)^2 d\mathbf{s}$
- $\mathbf{s} = (x_1, \dots, x_d)'$

- τ_1 : smoothness parameter
- τ_2 : sparseness parameter

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Spatial PCA (SpatPCA)

- $J(\varphi_k) = \phi'_k \Omega \phi_k$
 - $\Omega_{p \times p}$: determined only by s_1, \dots, s_p
 - Ref: Green and Silverman (1994)

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- Proposal: SpatPCA

$$\hat{\Phi} = \underset{\Phi: \Phi' \Phi = I_K}{\arg \min} \left\{ \|Y - Y\Phi\Phi'\|_F^2 + \tau_1 \sum_{k=1}^K \phi'_k \Omega \phi_k + \tau_2 \sum_{k=1}^K \sum_{j=1}^p |\phi_{jk}| \right\}$$

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- As $\tau_1 = \tau_2 = 0$, $\hat{\phi}_k$ is the k -th eigenvector of S .

SpatPCA: $\hat{\varphi}_1(\cdot), \dots, \hat{\varphi}_K(\cdot)$

- $(\hat{\varphi}_1(\cdot), \dots, \hat{\varphi}_K(\cdot))$ minimizes

$$\|\mathbf{Y} - \mathbf{Y}\Phi\Phi'\|_F^2 + \tau_1 \sum_{k=1}^K J(\varphi_k) + \tau_2 \sum_{k=1}^K \sum_{j=1}^p |\varphi_k(s_j)|,$$

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- $\hat{\varphi}_k(\cdot)$: smoothing spline based on $\hat{\phi}_k$

$$\hat{\varphi}_k(\mathbf{s}) = \sum_{i=1}^p a_i g(\|\mathbf{s} - \mathbf{s}_i\|) + b_0 + \sum_{j=1}^d b_j x_j$$

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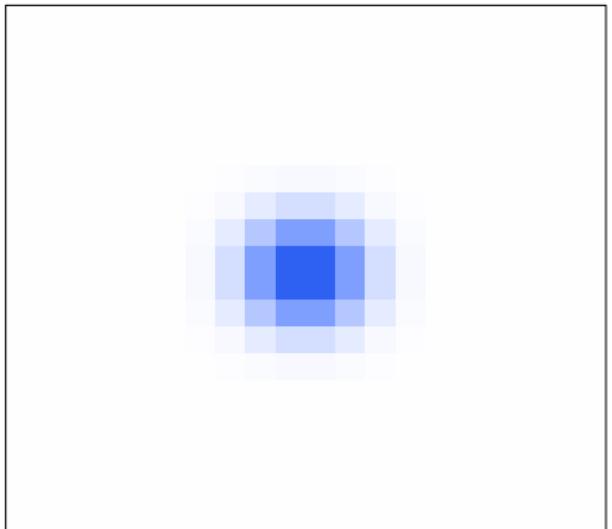
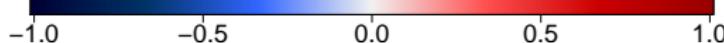
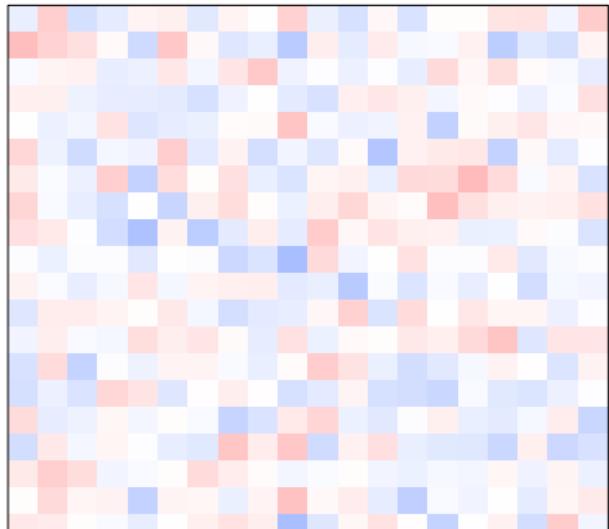
- $\mathbf{s} = (x_1, \dots, x_d)'$
- $g(r) = \begin{cases} \frac{1}{16\pi} r^2 \log r; & \text{if } d = 2, \\ \frac{\Gamma(d/2 - 2)}{16\pi^{d/2}} r^{4-d}; & \text{if } d = 1, 3, \end{cases}$

- $\mathbf{a} = (a_1, \dots, a_p)'$ and $\mathbf{b} = (b_0, b_1, \dots, b_d)'$ depend on $\hat{\phi}_k$

Why considering two penalties?

Proposed Method: Spatial PCA

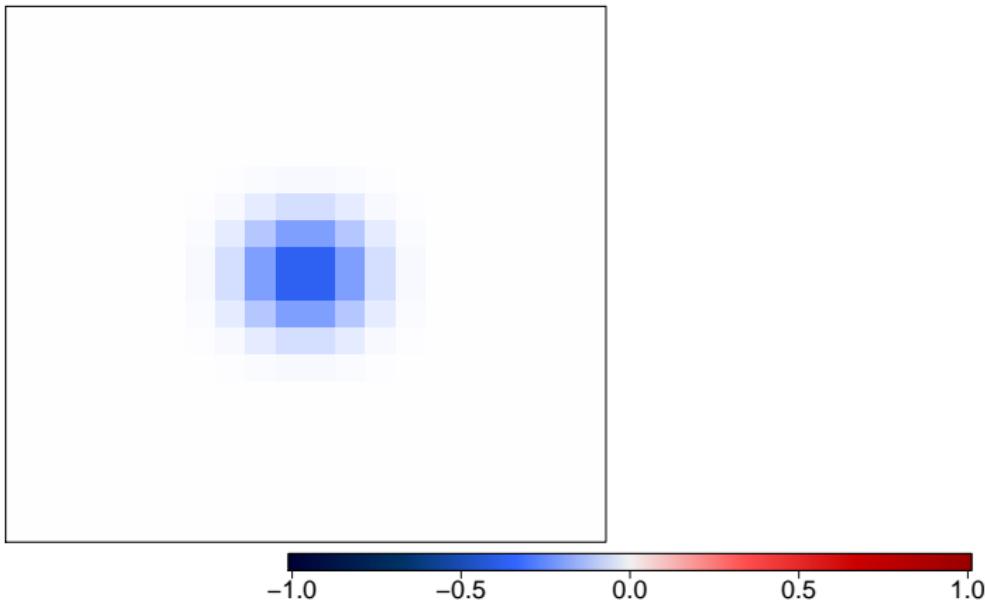
2D Example

TRUE : $\varphi(s)$ **PCA : $\tilde{\varphi}(s)$** 

Proposed Method: Spatial PCA

Case 1: $\hat{\varphi}(\cdot)$ as $\tau_2 = 0$ (only smoothness)

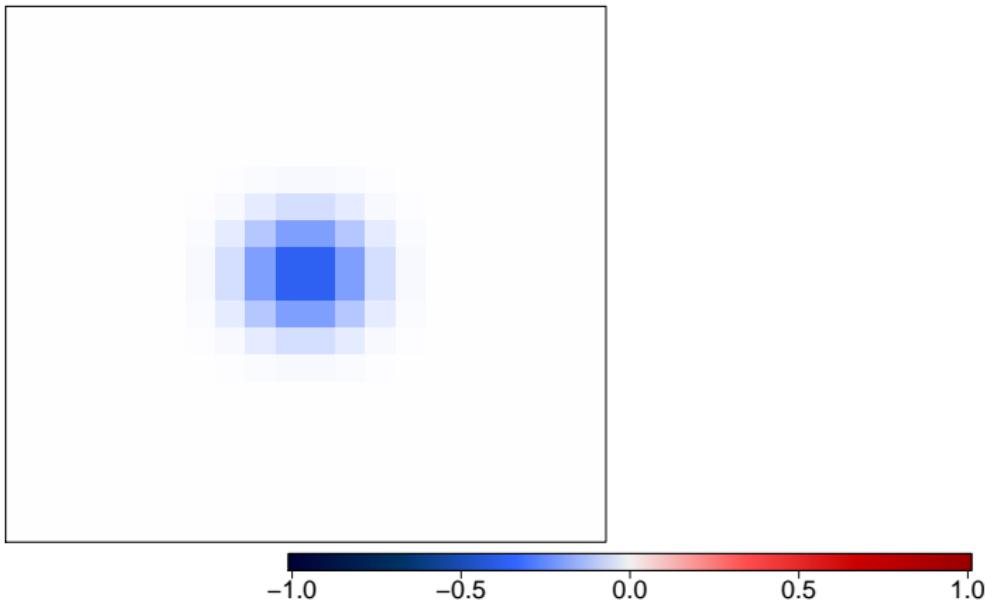
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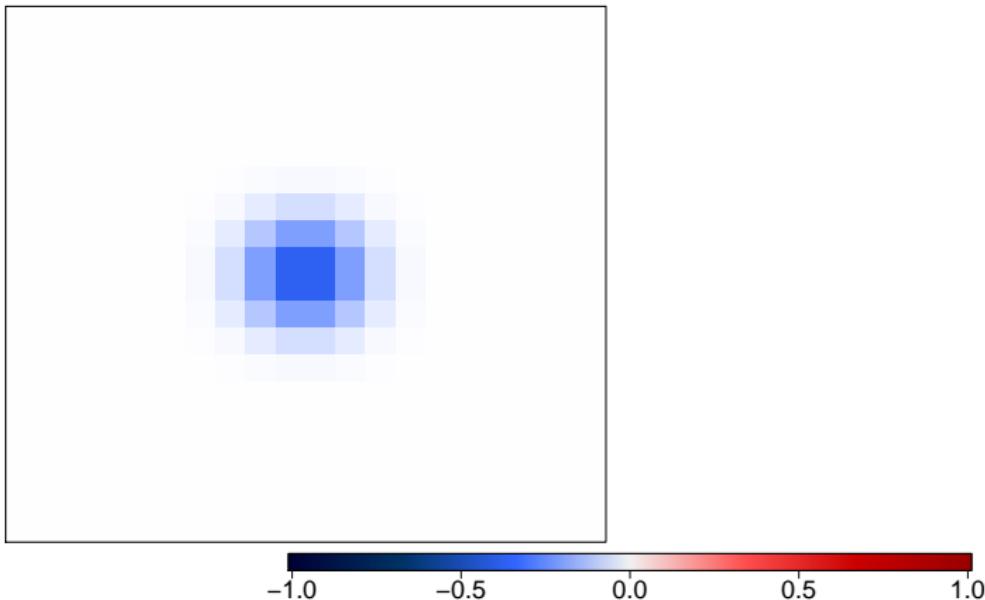
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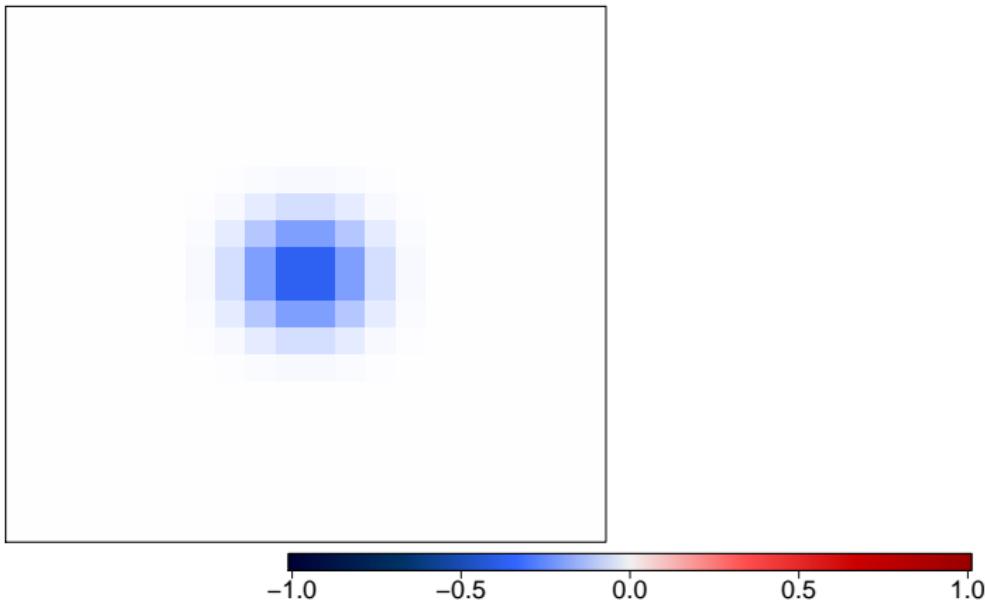
Case 2: $\hat{\varphi}(\cdot)$ as $\tau_1 = 0$ (only sparseness)

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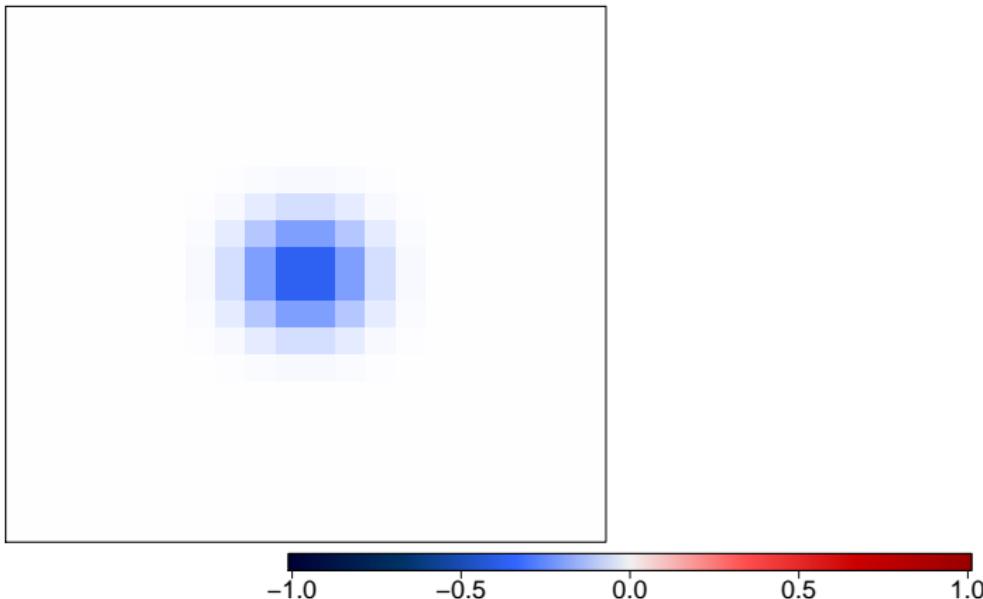
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Proposed Method: Spatial PCA

Case 3: $\hat{\varphi}(\cdot)$ as $\tau_1 = \tau_2$

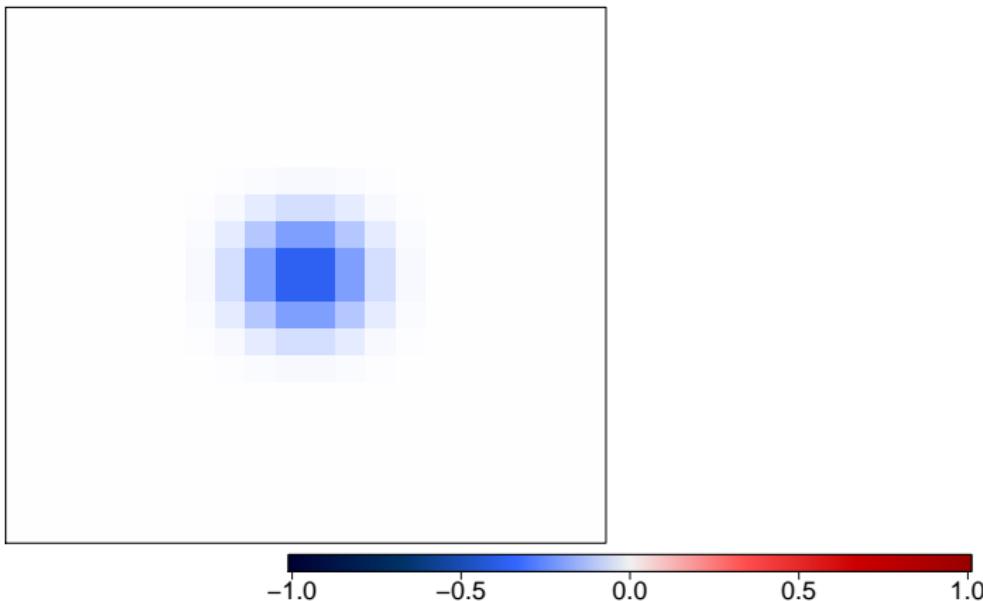
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Proposed Method: Spatial PCA

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Selection of (τ_1, τ_2)

- M -fold cross-validation:

$$\text{CV}(\tau_1, \tau_2) = \frac{1}{M} \sum_{m=1}^M \| \mathbf{Y}^{(m)} - \mathbf{Y}^{(m)} \hat{\Phi}_{\tau_1, \tau_2}^{(-m)} (\hat{\Phi}_{\tau_1, \tau_2}^{(-m)})' \|_F^2$$

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- Partition $\{\mathbf{Y}_1, \dots, \mathbf{Y}_n\}$ into M parts with equal (or roughly) size
- $\mathbf{Y}^{(m)}$: the sub-matrix of \mathbf{Y} corresponding to the m -th part
- $\hat{\Phi}_{\tau_1, \tau_2}^{(-m)}$: the estimate of Φ for (τ_1, τ_2) based on $\mathbf{Y}^{(-m)}$
 - $\mathbf{Y}^{(-m)}$: remaining data, i.e., \mathbf{Y} excluding $\mathbf{Y}^{(m)}$

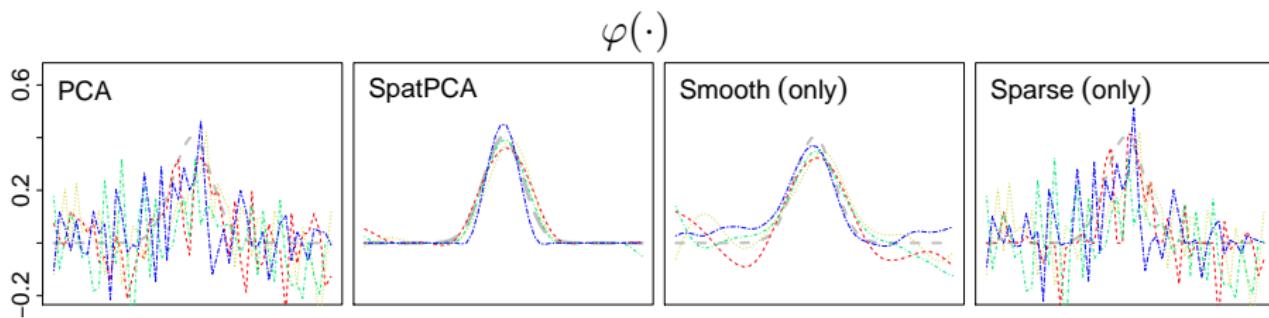
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- Find τ_1 and τ_2 which minimize $\text{CV}(\tau_1, \tau_2)$

Example (1D): Estimation of $\varphi(\cdot)$



- τ_1, τ_2 selected by 5-fold CV

Reconstruction of $\eta(\cdot)$

- What if we want to reconstruct the spatial process $\eta(\cdot)$
- Observe only at p locations

Reconstruction of $\eta(\cdot)$

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- Observe only at p locations
- Spatial best linear unbiased prediction of $\eta_i(s_0)$:

$$\hat{\eta}_i(s_0) = \mathbf{c}'(s_0) \boldsymbol{\Sigma}^{-1} \mathbf{Y}_i$$

- $\mathbf{c}(s_0) = (C_\eta(s_0, s_1), \dots, C_\eta(s_0, s_p))'$
- $\boldsymbol{\Sigma} = \text{var}(\mathbf{Y}_i) = \boldsymbol{\Phi} \boldsymbol{\Lambda} \boldsymbol{\Phi}' + \sigma^2 \mathbf{I}$
- $C_\eta(s^*, s) = \sum_{k=1}^K \sum_{k'=1}^K \lambda_{kk'} \varphi_k(s^*) \varphi_{k'}(s)$
- Ref: Cressie and Johannesson (2008)

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- Till now, σ^2 and $\boldsymbol{\Lambda}$ are unknown

Estimation of σ^2 and Λ

- Λ has $K(K + 1)/2$ unknown elements

Estimation of σ^2 and Λ

- Λ has $K(K + 1)/2$ unknown elements
- Apply the regularized method (Tzeng and Huang, 2015):

$$(\hat{\sigma}^2, \hat{\Lambda}) = \arg \min_{(\sigma^2, \Lambda) : \sigma^2 \geq 0, \Lambda \succeq 0} \left\{ \frac{1}{2} \|S - (\hat{\Phi} \Lambda \hat{\Phi}' + \sigma^2 I)\|_F^2 + \gamma \|\hat{\Phi} \Lambda \hat{\Phi}'\|_* \right\}$$

- 1st term : goodness of fit based on $\text{var}(Y_i) = \Phi \Lambda \Phi' + \sigma^2 I$
- $\hat{\Phi}$: given SpatPCA estimate
- $\gamma \geq 0$ (selected by M-fold CV)
- $\|M\|_* = \text{tr}((M'M)^{1/2})$

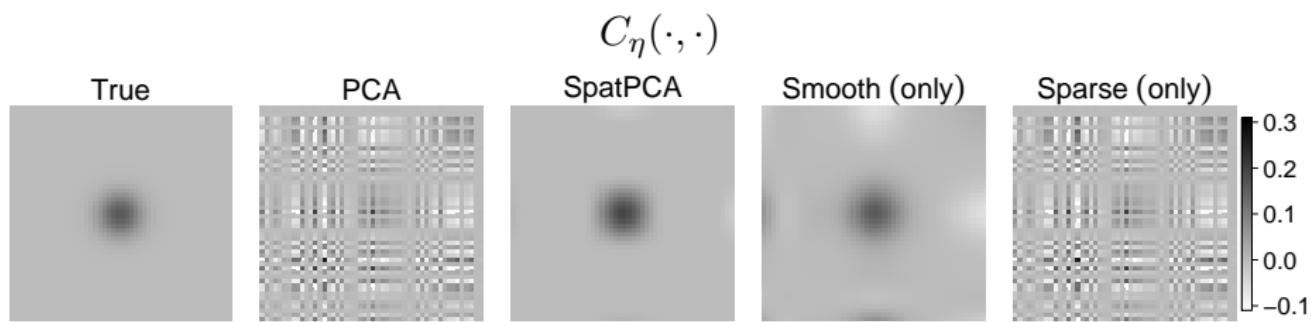
Estimation of σ^2 and Λ

- Λ has $K(K + 1)/2$ unknown elements
- Apply the regularized method (Tzeng and Huang, 2015):

$$(\hat{\sigma}^2, \hat{\Lambda}) = \arg \min_{(\sigma^2, \Lambda) : \sigma^2 \geq 0, \Lambda \succeq 0} \left\{ \frac{1}{2} \|S - (\hat{\Phi} \Lambda \hat{\Phi}') + \sigma^2 I\|_F^2 + \gamma \|\hat{\Phi} \Lambda \hat{\Phi}'\|_* \right\}$$

- 1st term : goodness of fit based on $\text{var}(Y_i) = \Phi \Lambda \Phi' + \sigma^2 I$
- $\hat{\Phi}$: given SpatPCA estimate
- $\gamma \geq 0$ (selected by M-fold CV)
- $\|M\|_* = \text{tr}((M'M)^{1/2})$
- Spatial prediction of $\eta_i(s_0)$: $\hat{\eta}_i(s_0) = \hat{c}'(s_0)(\hat{\Phi} \hat{\Lambda} \hat{\Phi}') + \hat{\sigma}^2 I^{-1} Y_i$
 - $\hat{c}(s_0) = (\hat{C}_\eta(s_0, s_1), \dots, \hat{C}_\eta(s_0, s_p))'$
 - $\hat{C}_\eta(s^*, s) = \sum_{k=1}^K \sum_{k'=1}^K \hat{\lambda}_{kk'} \hat{\varphi}_k(s^*) \hat{\varphi}_{k'}(s)$

Example (1D): Covariance Function Estimation



- γ selected by 5-fold CV

Outline

1 Principal Component Analysis

Background

Proposed Method: Spatial PCA

2 Maximum Covariance Analysis

Background

Proposed Method: Spatial MCA

3 Numerical Examples

4 Summary

How rainfalls in East Africa are affected by sea surface temperature in the Indian Ocean?

How rainfalls in East Africa are affected by sea surface temperature in the Indian Ocean?

- Analyze this problem via their coupled spatial patterns
- Ref: Omondi et al.,2013

Background

- Bivariate spatial processes:

$$\{(\eta_{1i}(\mathbf{s}_1), \eta_{2i}(\mathbf{s}_2)) : \mathbf{s}_1 \in D_1, \mathbf{s}_2 \in D_2\}; \quad i = 1, \dots, n$$

- $D_1, D_2 \subset \mathbb{R}^d$
- $\eta_{11}(\mathbf{s}_1), \dots, \eta_{1n}(\mathbf{s}_1)$: uncorrelated and mean zero
- $\eta_{21}(\mathbf{s}_2), \dots, \eta_{2n}(\mathbf{s}_2)$: uncorrelated and mean zero
- common spatial covariance function:
 - $C_{11}(\mathbf{s}_1, \mathbf{s}_1^*) = \text{cov}(\eta_{1i}(\mathbf{s}_1), \eta_{1i}(\mathbf{s}_1^*))$
 - $C_{22}(\mathbf{s}_2, \mathbf{s}_2^*) = \text{cov}(\eta_{2i}(\mathbf{s}_2), \eta_{2i}(\mathbf{s}_2^*))$
 - $C_{12}(\mathbf{s}_1, \mathbf{s}_2) = \text{cov}(\eta_{1i}(\mathbf{s}_1), \eta_{2i}(\mathbf{s}_2))$

Background

- Data at locations $s_{11}, \dots, s_{1p_1} \in D_1$ and $s_{21}, \dots, s_{2p_2} \in D_2$
 - $Y_{1i}(s_{1j}) = \eta_{1i}(s_{1j}) + \epsilon_{1ij}; j = 1, \dots, p_1$
 - $\epsilon_{1ij} \sim (0, \sigma_1^2)$
 - ϵ_{1ij} : uncorrelated with $\eta_1(\cdot)$
 - $Y_{2i}(s_{2j}) = \eta_{2i}(s_{2j}) + \epsilon_{2ij}; j = 1, \dots, p_2$
 - $\epsilon_{2ij} \sim (0, \sigma_2^2)$
 - ϵ_{2ij} : uncorrelated with $\eta_2(\cdot)$
 - $i = 1, \dots, n$

Targets

- Find dominant coupled patterns between $\eta_{1i}(\cdot)$ and $\eta_{2i}(\cdot)$
 - to study how variations of $\eta_{1i}(\cdot)$ affect $\eta_{2i}(\cdot)$

Rank- K Cross-Covariance Model

- $D_1, D_2 \subset \mathbb{R}^d$: continuous domain
- Azaïez and Belgacem (2015),

$$C_{12}(\mathbf{s}_1, \mathbf{s}_2) = \text{cov}(\eta_{1i}(\mathbf{s}_1), \eta_{2i}(\mathbf{s}_2)) = \sum_{k=1}^{\infty} d_k u_k(\mathbf{s}_1) v_k(\mathbf{s}_2)$$

- nonnegative singular values: $d_1 \geq d_2 \geq \dots$
- $\{u_k(\cdot)\}$ and $\{v_k(\cdot)\}$: sets of orthonormal basis functions
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- $\{u_k(\cdot)\}$ and $\{v_k(\cdot)\}$: sets of orthonormal basis functions
- similar to the Karhunen-Loéve expansion
- Assume $d_{K+1} = 0$.
- $(u_1(\cdot), v_1(\cdot)), \dots, (u_K(\cdot), v_K(\cdot))$: K dominant coupled patterns

Goal

- Find $(u_1(\cdot), v_1(\cdot)), \dots, (u_K(\cdot), v_K(\cdot))$ as K coupled patterns

Goal

- Find $(u_1(\cdot), v_1(\cdot)), \dots, (u_K(\cdot), v_K(\cdot))$ as K coupled patterns
- Common approach: maximum covariance analysis (MCA)

Bivariate Data Vector

- $$\begin{pmatrix} Y_{1i} \\ Y_{2i} \end{pmatrix} = \begin{pmatrix} \eta_{1i} \\ \eta_{2i} \end{pmatrix} + \begin{pmatrix} \epsilon_{1i} \\ \epsilon_{2i} \end{pmatrix}; i = 1, \dots, n$$
 - $$\begin{pmatrix} Y_{1i} \\ Y_{2i} \end{pmatrix} = \begin{pmatrix} (Y_{1i}(\mathbf{s}_{11}), \dots, Y_{1i}(\mathbf{s}_{1p_1}))' \\ (Y_{2i}(\mathbf{s}_{21}), \dots, Y_{2i}(\mathbf{s}_{2p_2}))' \end{pmatrix}$$
 - $$\begin{pmatrix} \eta_{1i} \\ \eta_{2i} \end{pmatrix} = \begin{pmatrix} (\eta_{1i}(\mathbf{s}_{11}), \dots, \eta_{1i}(\mathbf{s}_{1p_1}))' \\ (\eta_{2i}(\mathbf{s}_{21}), \dots, \eta_{2i}(\mathbf{s}_{2p_2}))' \end{pmatrix}$$
 - $$\begin{pmatrix} \epsilon_{1i} \\ \epsilon_{2i} \end{pmatrix} = \begin{pmatrix} (\epsilon_{1i1}, \dots, \epsilon_{1ip_1})' \\ (\epsilon_{2i1}, \dots, \epsilon_{2ip_2})' \end{pmatrix}$$
- **Assume** $p_1 \geq p_2$

Maximum Covariance Analysis (MCA)

- Bivariate data vector

$$\begin{pmatrix} \mathbf{Y}_{1i} \\ \mathbf{Y}_{2i} \end{pmatrix} \stackrel{i.i.d.}{\sim} \left(\begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{pmatrix} \right)$$

– $\boldsymbol{\Sigma}_{12} = \text{cov}(\mathbf{Y}_{1i}, \mathbf{Y}_{2i}) = \text{cov}(\boldsymbol{\eta}_{1i}, \boldsymbol{\eta}_{2i})$

- Idea: find $\mathbf{u} \in \mathcal{R}^{p_1}$ and $\mathbf{v} \in \mathcal{R}^{p_2}$, with $\|\mathbf{u}\|_2 = \|\mathbf{v}\|_2 = 1$, which maximize

$$d = \text{cov}(\mathbf{u}' \mathbf{Y}_{1i}, \mathbf{v}' \mathbf{Y}_{2i}) = \mathbf{u}' \boldsymbol{\Sigma}_{12} \mathbf{v}$$

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- Singular value decomposition (SVD): $\boldsymbol{\Sigma}_{12} = \mathbf{U} \mathbf{D} \mathbf{V}'$
 - Singular values: $\mathbf{D}_{K \times K} = \text{diag}(d_1, \dots, d_K); d_1 \geq \dots \geq d_K > 0$
 - Left singular vectors: $\mathbf{U}_{p_1 \times K} = \{\mathbf{u}_1, \dots, \mathbf{u}_K\}$
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- Coupled pattern: $(\mathbf{u}_1, \mathbf{v}_1), \dots, (\mathbf{u}_K, \mathbf{v}_K)$

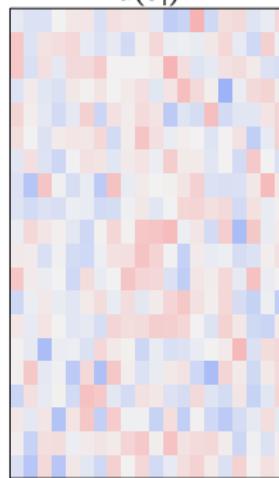
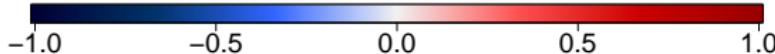
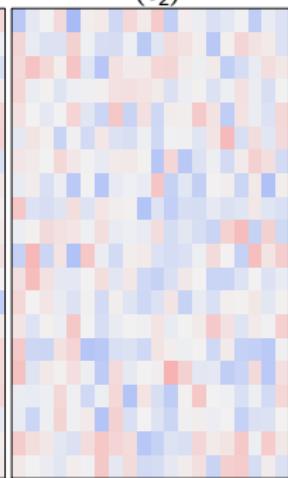
Sample Maximum Covariance Analysis

- Bivariate data matrix: $(\mathbf{Y}_1, \mathbf{Y}_2)$
 - $\mathbf{Y}_1 = (\mathbf{Y}_{11}, \dots, \mathbf{Y}_{1n})'$; $\mathbf{Y}_2 = (\mathbf{Y}_{21}, \dots, \mathbf{Y}_{2n})'$
- Sample cross-covariance matrix: $S_{12} = \mathbf{Y}_1' \mathbf{Y}_2 / n$
- Singular value decomposition (SVD): $S_{12} = \tilde{\mathbf{U}} \tilde{\mathbf{D}} \tilde{\mathbf{V}}'$
 - $\tilde{\mathbf{D}}_{p_2 \times p_2} = \text{diag}(\tilde{d}_1 \dots \tilde{d}_{p_2})$; $\tilde{d}_1 \geq \dots \geq \tilde{d}_{p_2} \geq 0$
 - $\tilde{\mathbf{U}}_{p_1 \times p_2} = \{\tilde{\mathbf{u}}_1, \dots, \tilde{\mathbf{u}}_{p_2}\}$
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- $(\tilde{\mathbf{u}}_1, \tilde{\mathbf{v}}_1), \dots, (\tilde{\mathbf{u}}_K, \tilde{\mathbf{v}}_K)$: estimates of $(\mathbf{u}_1, \mathbf{v}_1), \dots, (\mathbf{u}_K, \mathbf{v}_K)$

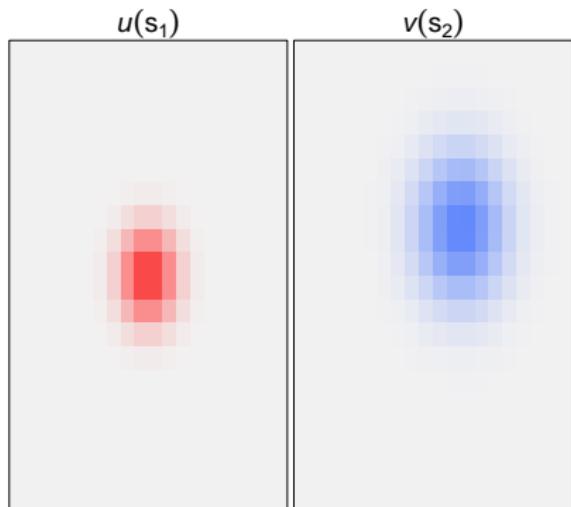
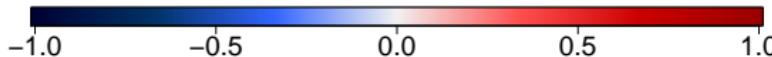
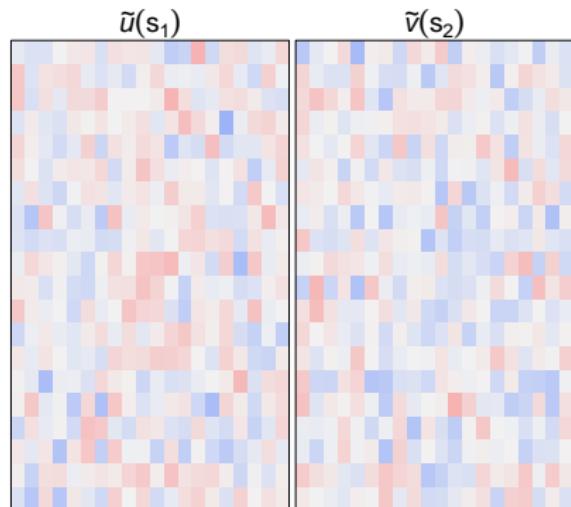
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- Problem:
 - high estimation variability: n small, p_1 or p_2 large
 - noisy patterns → low interpretation
 - without a spatial structure of (\mathbf{u}, \mathbf{v})

Example:

MCA $\tilde{u}(s_1)$  $\tilde{v}(s_2)$ 

Example:

TRUE**MCA**

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retain that orthogonal constraints for (u, v) .

Quick Recap

- **Data:** $\mathbf{Y}_{1i} = (Y_{1i}(\mathbf{s}_{11}), \dots, Y_{1i}(\mathbf{s}_{1p_1}))'$, $\mathbf{Y}_{2i} = (Y_{2i}(\mathbf{s}_{21}), \dots, Y_{2i}(\mathbf{s}_{p_2}))'$; $i = 1, \dots, n$
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 - ϵ_{2ij} : **uncorrelated with** $\eta_2(\cdot)$

Quick Recap

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- **Spatial cross-covariance function:**

$$C_{12}(\mathbf{s}_1, \mathbf{s}_2) = \text{cov}(\eta_{1i}(\mathbf{s}_1), \eta_{2i}(\mathbf{s}_2)) = \sum_{k=1}^K d_k u_k(\mathbf{s}_1) v_k(\mathbf{s}_2)$$

- $d_1 \geq \dots \geq d_K \geq 0$
- $u_1(\cdot), \dots, u_K(\cdot)$: K unknown orthonormal functions
- $v_1(\cdot), \dots, v_K(\cdot)$: K unknown orthonormal functions

MCA (alternative version)

- Sample cross-covariance matrix: $S_{12} = \mathbf{Y}_1' \mathbf{Y}_2 / n$
- MCA: perform SVD of S_{12}
- Alternative method:

$$(\tilde{\mathbf{U}}, \tilde{\mathbf{V}}) = \arg \max_{\mathbf{U}, \mathbf{V}} \text{tr}(\mathbf{U}' S_{12} \mathbf{V}),$$

subject to $\mathbf{U}' \mathbf{U} = \mathbf{V}' \mathbf{V} = \mathbf{I}_K$

- $\mathbf{U}_{p_1 \times K} = (\mathbf{u}_1, \dots, \mathbf{u}_K)$ with $u_{jk} = u_k(s_{1j})$
- $\mathbf{V}_{p_2 \times K} = (\mathbf{v}_1, \dots, \mathbf{v}_K)$ with $v_{jk} = v_k(s_{2j})$

Regularized MCA

- Sample cross-covariance matrix: $S_{12} = \mathbf{X}'\mathbf{Y}/n$
- $\mathbf{U}_{p_1 \times K} = (\mathbf{u}_1, \dots, \mathbf{u}_K)$ with $u_{jk} = u_k(s_{1j})$
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- Objective function:

$$\text{tr}(\mathbf{U}'\mathbf{S}_{12}\mathbf{V})$$

subject to $\mathbf{U}'\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{I}_K$

Regularized MCA

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$$\text{tr}(\mathbf{U}'\mathbf{S}_{12}\mathbf{V}) - \sum_{k=1}^K \left\{ \tau_{1u} J(u_k) + \tau_{2u} \sum_{j=1}^{p_1} |u_k(s_{1j})| + \tau_{1v} J(v_k) + \tau_{2v} \sum_{j=1}^{p_2} |v_k(s_{2j})| \right\}$$

subject to $\mathbf{U}'\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{I}_K$

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subject to $\mathbf{U}'\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{I}_K$

— $J(u_k(\cdot)) = \sum_{z_1+\dots+z_d=2} \int_{R^d} \left(\frac{\partial^2 u_k(\mathbf{s})}{\partial x_1^{z_1} \dots \partial x_d^{z_d}} \right)^2 d\mathbf{s}$

• $\mathbf{s} = (x_1, \dots, x_d)'$

— τ_{1u}, τ_{1v} : smoothness parameter

— τ_{2u}, τ_{2v} : sparseness parameter

Spatial MCA (SpatMCA)

- $J(u_k(\cdot)) = \mathbf{u}'_k \boldsymbol{\Omega}_1 \mathbf{u}_k, J(v_k(\cdot)) = \mathbf{v}'_k \boldsymbol{\Omega}_2 \mathbf{v}_k$
 - $\boldsymbol{\Omega}_1 \succ \mathbf{0}$: determined only by s_{11}, \dots, s_{1p_1}
 - $\boldsymbol{\Omega}_2 \succ \mathbf{0}$: determined only by s_{21}, \dots, s_{2p_2}
 - Green and Silverman (1994)

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 - Green and Silverman (1994)
- SpatMCA: $(\hat{\mathbf{U}}, \hat{\mathbf{V}})$ maximizes:

$$\text{tr}(\mathbf{U}' \mathbf{S}_{12} \mathbf{V}) - \sum_{k=1}^K \left\{ \tau_{1u} \mathbf{u}'_k \boldsymbol{\Omega}_1 \mathbf{u}_k + \tau_{2u} \sum_{j=1}^{p_1} |u_{jk}| + \tau_{1v} \mathbf{v}'_k \boldsymbol{\Omega}_2 \mathbf{v}_k + \tau_{2v} \sum_{j=1}^{p_2} |v_{jk}| \right\}$$

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subject to $\mathbf{U}' \mathbf{U} = \mathbf{V}' \mathbf{V} = \mathbf{I}_K$

- As $\tau_{1u} = \tau_{1v} = \tau_{2u} = \tau_{2v} = 0$, $(\hat{\mathbf{U}}, \hat{\mathbf{V}}) = (\tilde{\mathbf{U}}, \tilde{\mathbf{V}})$ (sample MCA)

Proposed Method: Spatial MCA

SpatMCA: $(\hat{u}_1(\cdot), \hat{v}_1(\cdot)), \dots, (\hat{u}_K(\cdot), \hat{v}_K(\cdot))$

- $(\hat{u}_1(\cdot), \hat{v}_1(\cdot)), \dots, (\hat{u}_K(\cdot), \hat{v}_K(\cdot))$ maximizes

$$\text{tr}(\mathbf{U}' \mathbf{S}_{12} \mathbf{V}) - \sum_{k=1}^K \left\{ \tau_{1u} J(u_k) + \tau_{2u} \sum_{j=1}^{p_1} |u_k(s_{1j})| + \tau_{1v} J(v_k) + \tau_{2v} \sum_{j=1}^{p_2} |v_k(s_{2j})| \right\},$$

subject to $\mathbf{U}' \mathbf{U} = \mathbf{V}' \mathbf{V} = \mathbf{I}_K$

- $\hat{u}_k(s_1) = \sum_{i=1}^{p_1} a_{1i} g(\|s_1 - s_{1i}\|) + b_{10} + \sum_{j=1}^d b_{1j} x_{1j}$
 $\hat{v}_k(s_2) = \sum_{i=1}^{p_2} a_{2i} g(\|s_2 - s_{2i}\|) + b_{20} + \sum_{j=1}^d b_{2j} x_{2j}$

SpatMCA: $(\hat{u}_1(\cdot), \hat{v}_1(\cdot)), \dots, (\hat{u}_K(\cdot), \hat{v}_K(\cdot))$

- $(\hat{u}_1(\cdot), \hat{v}_1(\cdot)), \dots, (\hat{u}_K(\cdot), \hat{v}_K(\cdot))$ maximizes

$$\text{tr}(\mathbf{U}' \mathbf{S}_{12} \mathbf{V}) - \sum_{k=1}^K \left\{ \tau_{1u} J(u_k) + \tau_{2u} \sum_{j=1}^{p_1} |u_k(s_{1j})| + \tau_{1v} J(v_k) + \tau_{2v} \sum_{j=1}^{p_2} |v_k(s_{2j})| \right\},$$

subject to $\mathbf{U}' \mathbf{U} = \mathbf{V}' \mathbf{V} = \mathbf{I}_K$

- $\hat{u}_k(\mathbf{s}_1) = \sum_{i=1}^{p_1} a_{1i} g(\|\mathbf{s}_1 - \mathbf{s}_{1i}\|) + b_{10} + \sum_{j=1}^d b_{1j} x_{1j}$

$$\hat{v}_k(\mathbf{s}_2) = \sum_{i=1}^{p_2} a_{2i} g(\|\mathbf{s}_2 - \mathbf{s}_{2i}\|) + b_{20} + \sum_{j=1}^d b_{2j} x_{2j}$$

– $\mathbf{s}_1 = (x_{11}, \dots, x_{1d})'$; $\mathbf{s}_2 = (x_{21}, \dots, x_{2d})'$

$$g(r) = \begin{cases} \frac{1}{16\pi} r^2 \log r; & \text{if } d = 2, \\ \frac{\Gamma(d/2 - 2)}{16\pi^{d/2}} r^{4-d}; & \text{if } d = 1, 3, \end{cases}$$

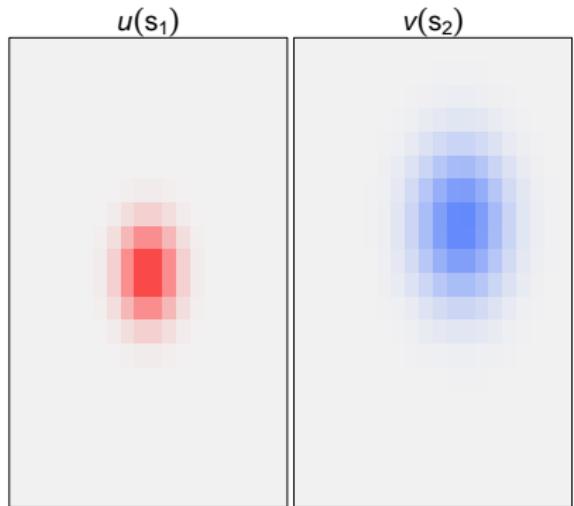
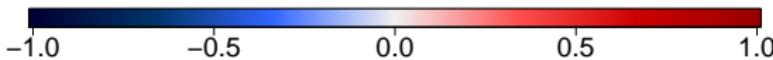
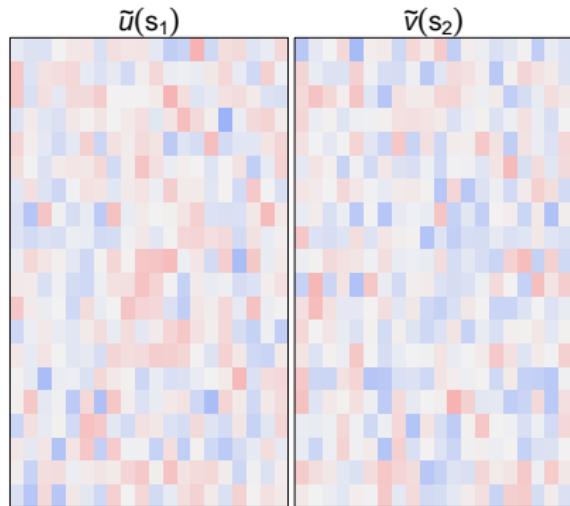
– $\mathbf{a}_1 = (a_{11}, \dots, a_{1p_1})'$ and $\mathbf{b}_1 = (b_{10}, b_{11}, \dots, b_{1d})'$ based on $\hat{\mathbf{u}}_k$

– $\mathbf{a}_2 = (a_{21}, \dots, a_{2p_2})'$ and $\mathbf{b}_2 = (b_{20}, b_{21}, \dots, b_{2d})'$ based on $\hat{\mathbf{v}}_k$

Why **roughness** and **Lasso** penalties?

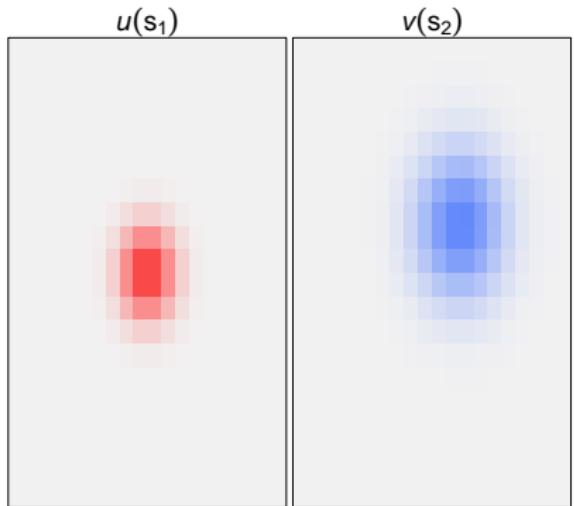
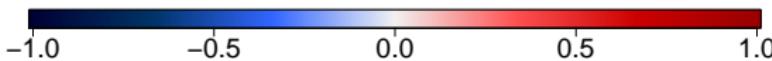
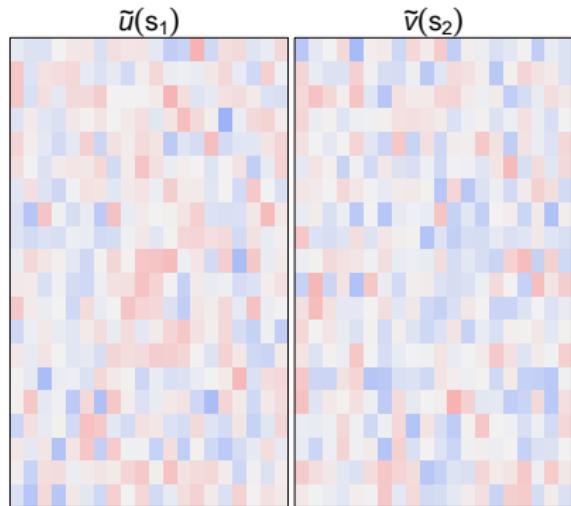
Proposed Method: Spatial MCA

2D Example

TRUE**MCA**

Proposed Method: Spatial MCA

2D Example

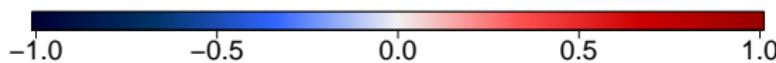
TRUE**MCA**

Case 1: $\tau_{2u} = \tau_{2v} = 0$ (only smoothness)

TRUE

$u(s_1)$

$v(s_2)$

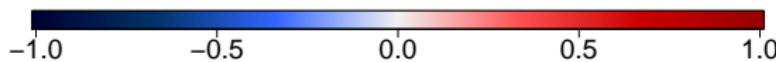


Case 1: $\tau_{2u} = \tau_{2v} = 0$ (only smoothness)

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$v(s_2)$

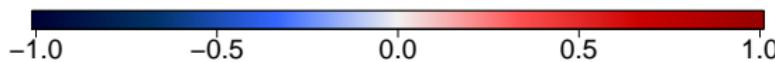
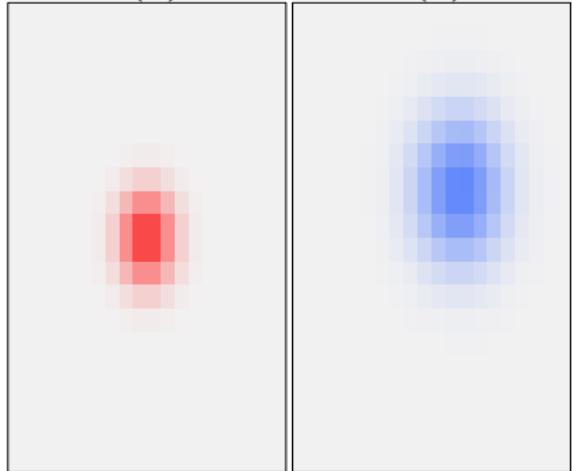


Case 2: $\tau_{1u} = \tau_{1v} = 0$ (only sparseness)

TRUE

$u(s_1)$

$v(s_2)$

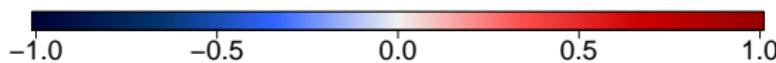
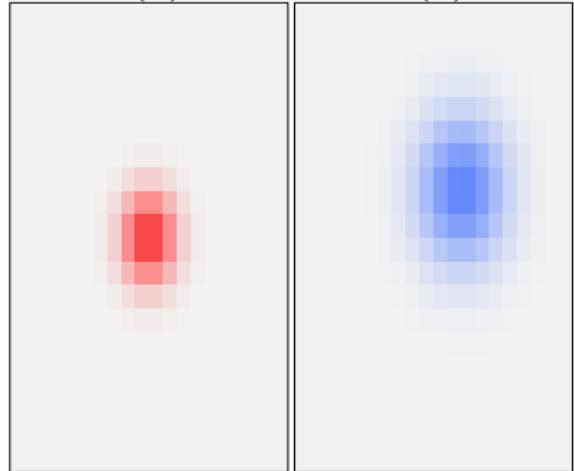


Case 2: $\tau_{1u} = \tau_{1v} = 0$ (only sparseness)

TRUE

$u(s_1)$

$v(s_2)$



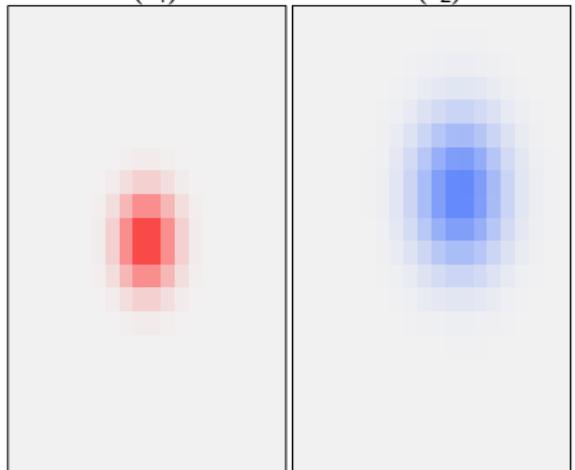
Case 3: $\tau_{1u} = \tau_{1v} = \tau_{2u} = \tau_{2v}$

kr

TRUE

$u(s_1)$

$v(s_2)$

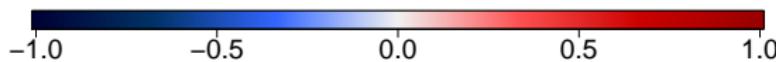
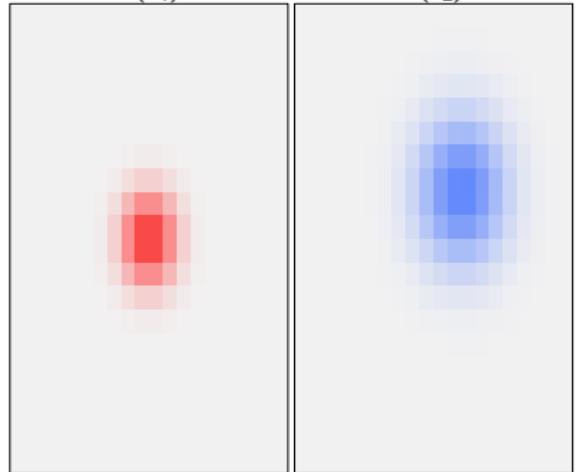


Case 3: $\tau_{1u} = \tau_{1v} = \tau_{2u} = \tau_{2v}$

TRUE

$u(s_1)$

$v(s_2)$



Estimation of D

Given the SpatMCA estimate $(\hat{\mathbf{U}}, \hat{\mathbf{V}})$,

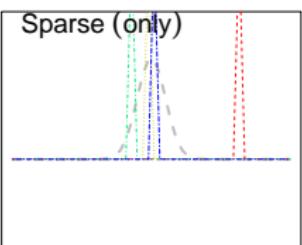
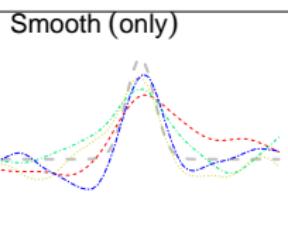
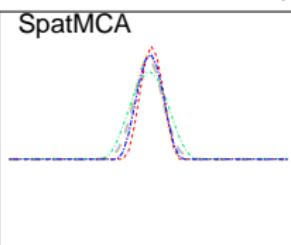
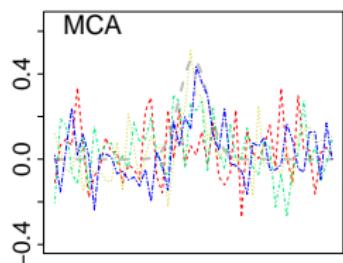
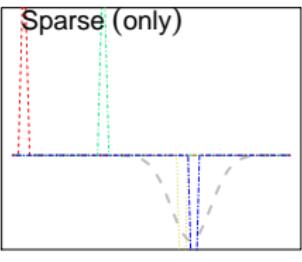
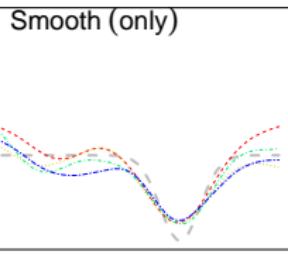
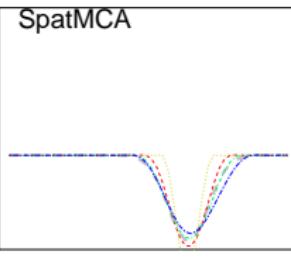
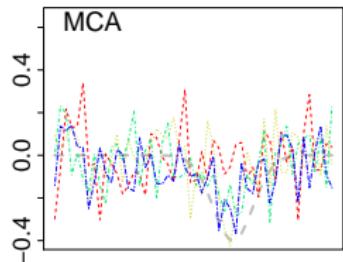
$$\hat{\mathbf{D}} = \arg \min_{d_1, \dots, d_K \geq 0} \|S_{12} - \hat{\mathbf{U}}\hat{\mathbf{D}}\hat{\mathbf{V}}'\|_F^2 = \text{diag}(\hat{d}_1, \dots, \hat{d}_K)$$

- $\hat{d}_k = \min(\hat{u}'_k S_{12} \hat{v}_k, 0)$

Selection of $(\tau_{1u}, \tau_{2u}, \tau_{1v}, \tau_{2v})$

- Similar to SpatPCA, $(\tau_{1u}, \tau_{2u}, \tau_{1v}, \tau_{2v})$ is selected by K-fold cross validation
 - CV criterion is based on rank-K approximation

Example (1D): 5-fold CV

 $u(\cdot)$  $v(\cdot)$ 

Outline

① Principal Component Analysis

Background

Proposed Method: Spatial PCA

② Maximum Covariance Analysis

Background

Proposed Method: Spatial MCA

③ Numerical Examples

④ Summary

Real data analysis

- Bivariate data:
 - Sea surface temperature (SST):
 - Region: Indian Ocean (20°N and 30°S ; 20°E and 120°E)
 - Number of grids: $p_1 = 3,591$
 - Rainfall:
 - Region: Eastern African (6°N and 12°S ; 20°E and 42°E)
 - Number of grids: $p_2 = 255$
 - Time period (monthly): Jan. 2011- Dec. 2015 $\rightarrow n = 60$
 - Remove monthly mean

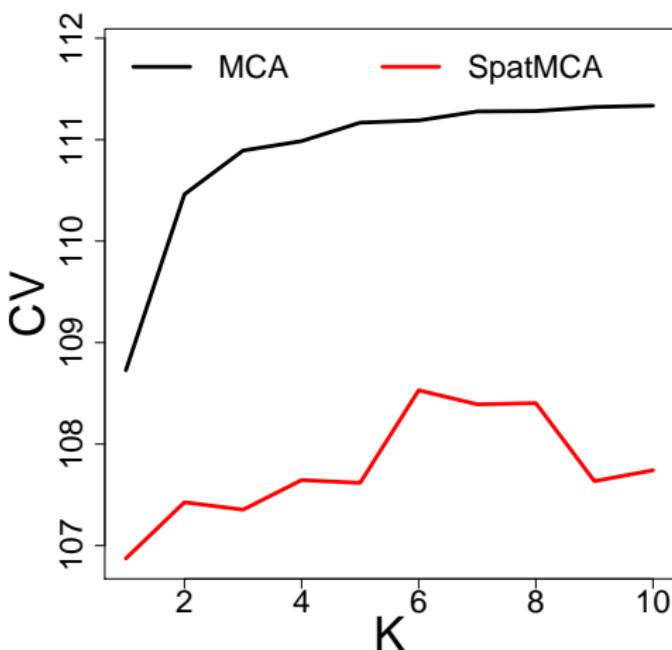
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 - Number of grids: $p_2 = 255$
 - Time period (monthly): Jan. 2011- Dec. 2015 $\rightarrow n = 60$
 - Remove monthly mean
- Goal: find coupled patterns of the **SST** and **rainfall** data
- Reference: Omondi et al. (2013)

Real data analysis

- Randomly decompose the data into two parts with 30 time points
 - Training data
 - Validation data
- SpatMCA: based on 5-fold CV

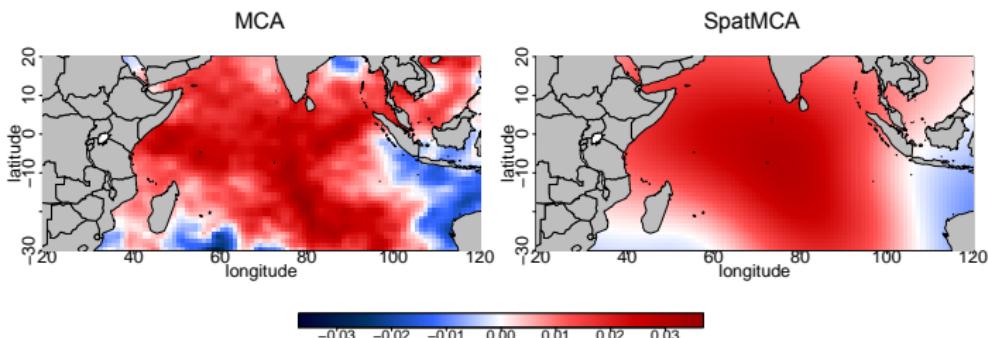
Result: CV vs. K



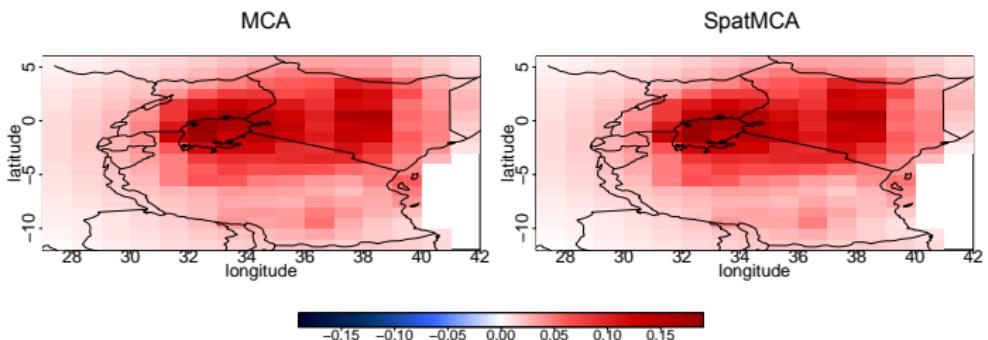
- $\hat{K} = 1$ for MCA and SpatMCA

Result: 1st coupled pattern

- SST

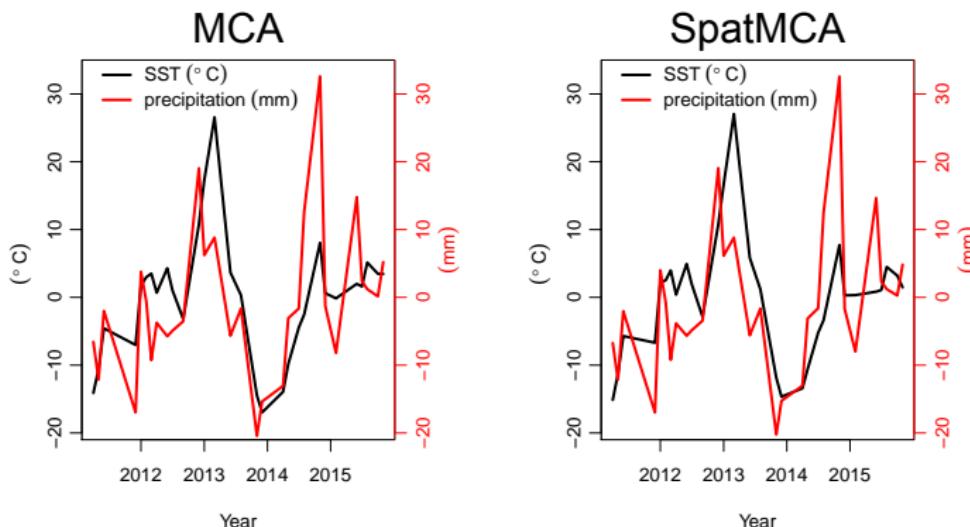


- Rainfall



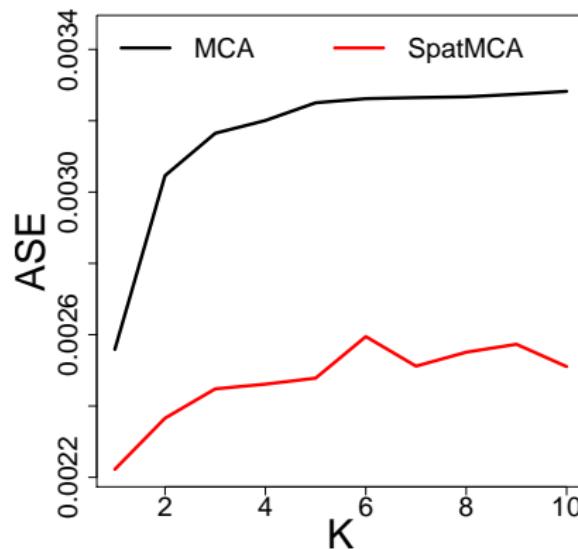
Result: 1st Maximum covariance Variables

- 1st maximum covariance variables: $\{\hat{u}'_1 Y_{1i}\}$; $\{\hat{v}'_1 Y_{2i}\}$
- Pearson's correlation: 0.6 for MCA and SpatMCA



Result: Average Squared Error (ASE)

- $\text{ASE} = \frac{1}{p_1 p_2} \|S_{12}^v - \hat{U}_K \hat{D}_K \hat{V}'_K\|_F^2$
 - S_{12}^v : sample cross-covariance matrix based on validation data
- Result:



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SpatPCA/ SpatMCA:

- high-dimensional structure → low-dimensional structure
- with the **roughness** and **Lasso** penalties
- enhance physical interpretation, e.g. **spatial localized patterns**

Summary

SpatPCA/ SpatMCA:

- high-dimensional structure → low-dimensional structure
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- non-stationary spatial covariance function (SpatPCA)
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Summary

SpatPCA/ SpatMCA:

- high-dimensional structure → low-dimensional structure
- with the **roughness** and **Lasso** penalties
- enhance physical interpretation, e.g. **spatial localized patterns**
- non-stationary spatial covariance function (SpatPCA)
- can cope with **irregular spaced** locations
- simple and efficient algorithm
- R CRAN packages: *SpatPCA*; *SpatMCA*

Thanks for your attention!