Regularized Estimation of Spatial Patterns

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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** occuring

Flood

Drought

Climate Change

increases the odds of **extreme weather events** occuring

affects **human health** and **quality of life**

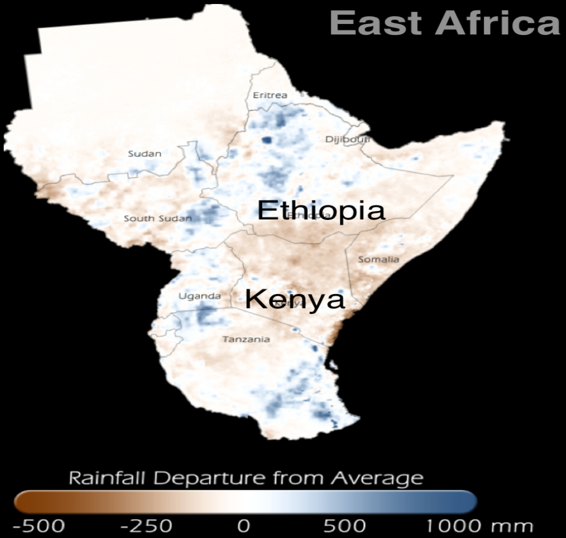
Drought in the East Africa

2011

10,000

People have died after the worst drought in 60 years.

Rainfall Anomalies



Climate Change

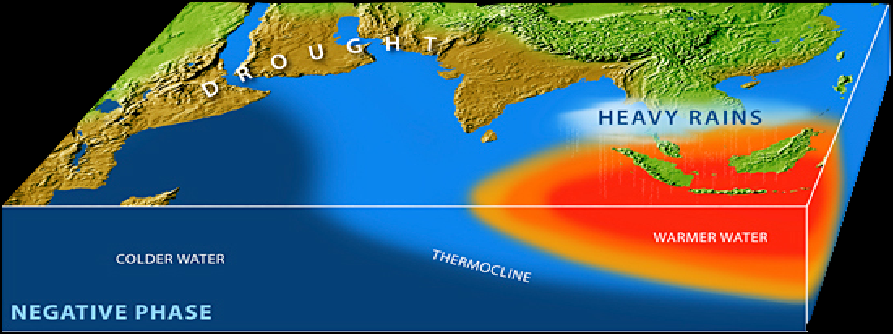
are associated with atmospheric dynamics.

Atmospheric dynamics

can be studied through spatial patterns.

Spatial pattern

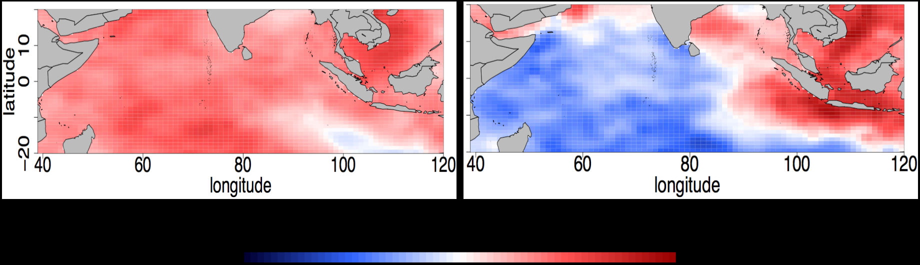
Sea surface temperature vs. Rainfalls



Dominant spatial patterns

Indian Ocean sea surface temperature anomalies

Basin-wide mode East-west dipole mode



Related to El Ninõ Southern Oscillation (ENSO), (Deser, 2009)

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Background

- Spatial processes of interest:

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

  - $D \subset \mathbb{R}^d$
  - mean zero
  - common covariance function: $C_\eta(\boldsymbol{s}^*, \boldsymbol{s}) = \mathrm{cov}(\eta_i(\boldsymbol{s}^*), \eta_i(\boldsymbol{s}))$
  - $\eta_1(\cdot), \ldots, \eta_n(\cdot)$: uncorrelated

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- Data at locations $\boldsymbol{s}_1, \ldots, \boldsymbol{s}_p \in D$,

$$Y_i(\boldsymbol{s}_j) = \eta_i(\boldsymbol{s}_j) + \epsilon_{ij}; i = 1, \ldots, n,\ j = 1, \ldots, p$$

  - $\epsilon_{ij} \sim (0, \sigma^2)$: white noise
  - ϵ_{ij} and $\eta_i(\boldsymbol{s}_j)$ are uncorrelated for any i, j

Targets

1. Detect the dominant spatial patterns (modes) of $\eta_1(\cdot), \ldots, \eta_n(\cdot)$
   - 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 $\{\eta_i(\boldsymbol{s}); \boldsymbol{s} \in D\}$

Rank-K spatial model

- Data:

$$Y_i(\boldsymbol{s}_j) = \eta_i(\boldsymbol{s}_j) \qquad\qquad + \epsilon_{ij}; \quad i = 1, \ldots, n, \quad j = 1 \ldots, p$$

Rank-K spatial model

- Data:

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

  - $(\xi_{i1}, \dots, \xi_{iK})' \sim (\mathbf{0}, \boldsymbol{\Lambda})$; $\boldsymbol{\Lambda}_{K \times K}$ is positive-definite
  - $\varphi_1(\cdot) \dots, \varphi_K(\cdot)$: K unknown orthonormal functions
  - ξ_{ik} uncorrelated with ϵ_{ij}

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Goal

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

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- Standard approach: principal component analysis (PCA)

Principal Component Analysis

- p-dimensional data vector:

$$\boldsymbol{Y}_i = (Y_i(\boldsymbol{s}_1), \ldots, Y_i(\boldsymbol{s}_p))' \sim (\boldsymbol{0}, \boldsymbol{\Sigma})$$

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

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- Spectral decomposition: $\boldsymbol{\Sigma}$
  - eigenvalues: $\lambda_1 \geq \cdots \geq \lambda_p$
  - eigenvectors: $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_p$

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  - eigenvectors: $\phi_1, \ldots, \phi_p$
- Dominant patterns: $\phi_1, \ldots, \phi_K$ (with $\lambda_1, \ldots, \lambda_K$ large)

Principal Component Analysis

- Data matrix: $\boldsymbol{Y}_{n\times p} = (\boldsymbol{Y}_1, \ldots, \boldsymbol{Y}_n)'$
- Sample covariance matrix: $\boldsymbol{S} = \boldsymbol{Y}'\boldsymbol{Y}/n$
- Spectral decomposition: $\boldsymbol{S}$
  - sample eigenvalues: $\tilde{\lambda}_1 \geq \cdots \geq \tilde{\lambda}_p$
  - sample eigenvectors: $\tilde{\phi}_1, \ldots, \tilde{\phi}_p$
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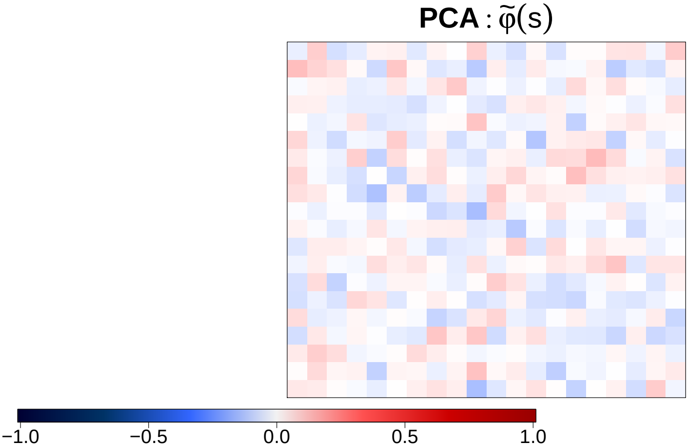
- Problems:
  - high estimation variability: n is small or p is large
    $\rightarrow$ unstable and noisy patterns
    $\rightarrow$ weak physical interpretation
  - without spatial structure of ϕ

Example:



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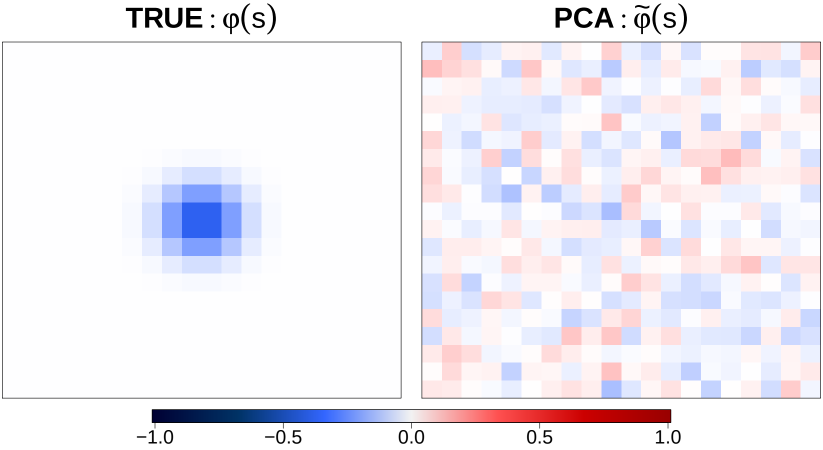

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retain the orthogonal constraint of ϕ_k

Quick review

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

PCA (alternative version)

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

$$\tilde{\boldsymbol{\Phi}} = \underset{\boldsymbol{\Phi}:\boldsymbol{\Phi}'\boldsymbol{\Phi}=\boldsymbol{I}_K}{\arg\min} \|\boldsymbol{Y} - \boldsymbol{Y}\boldsymbol{\Phi}\boldsymbol{\Phi}'\|_F^2$$

  - $\boldsymbol{\Phi}_{p\times K} = (\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_K)$ with $\phi_{jk} = \varphi_j(\boldsymbol{s}_k)$
  - $\|M\|_F^2 = \sum_{i=1}^{n}\sum_{j=1}^{p} m_{ij}^2$

Regularized PCA

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- $\boldsymbol{\Phi}_{p\times K} = (\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_K)$ with $\phi_{jk} = \varphi_j(\boldsymbol{s}_k)$
- Objective function

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

subject to $\boldsymbol{\Phi}'\boldsymbol{\Phi} = \boldsymbol{I}_K$

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- Objective function

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

subject to $\boldsymbol{\Phi}'\boldsymbol{\Phi} = \boldsymbol{I}_K$

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

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  - $\boldsymbol{s} = (x_1, \ldots, x_d)'$
- τ_1: smoothness parameter
- τ_2: sparseness parameter

Spatial PCA (SpatPCA)

- $J(\varphi_k) = \phi_k' \boldsymbol{\Omega} \phi_k$
  - $\boldsymbol{\Omega}_{p \times p}$: determined only by $\boldsymbol{s}_1, \ldots, \boldsymbol{s}_p$
  - Ref: Green and Silverman (1994)

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- Proposal: SpatPCA

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

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- Proposal: SpatPCA

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

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

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

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

  subject to $\boldsymbol{\Phi}'\boldsymbol{\Phi} = \boldsymbol{I}_K$
- $\hat{\varphi}_k(\cdot)$: smoothing spline based on $\hat{\boldsymbol{\phi}}_k$

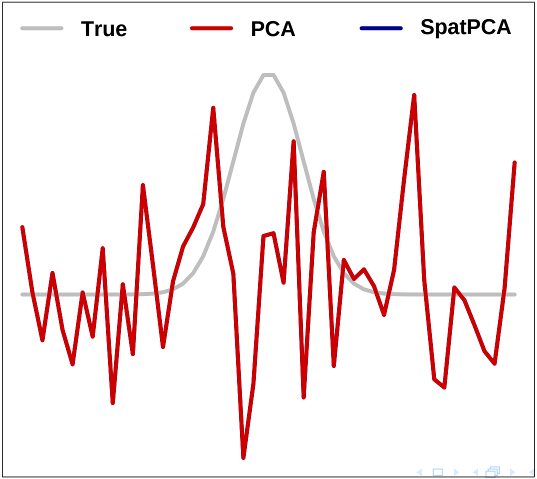
$$\hat{\varphi}_k(\boldsymbol{s}) = \sum_{i=1}^{p} a_i g(\|\boldsymbol{s} - \boldsymbol{s}_i\|) + b_0 + \sum_{j=1}^{d} b_j x_j$$

  - $\boldsymbol{s} = (x_1, \ldots, x_d)'$
  - $g(r) = \begin{cases} \dfrac{1}{16\pi} r^2 \log r; & \text{if } d = 2, \\ \dfrac{\Gamma(d/2-2)}{16\pi^{d/2}} r^{4-d}; & \text{if } d = 1, 3, \end{cases}$
  - $\boldsymbol{a} = (a_1, \ldots, a_p)'$ and $\boldsymbol{b} = (b_0, b_1, \ldots, b_d)'$ depend on $\hat{\boldsymbol{\phi}}_k$

Why considering two penalties?

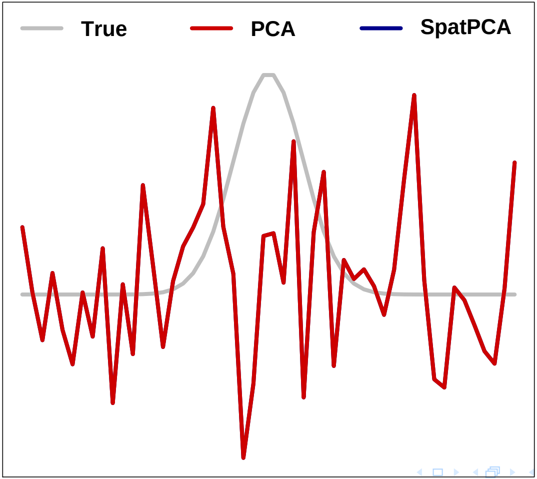
1D Example

$$\tau_1 = 0$$



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

$\tau_1 = 0$



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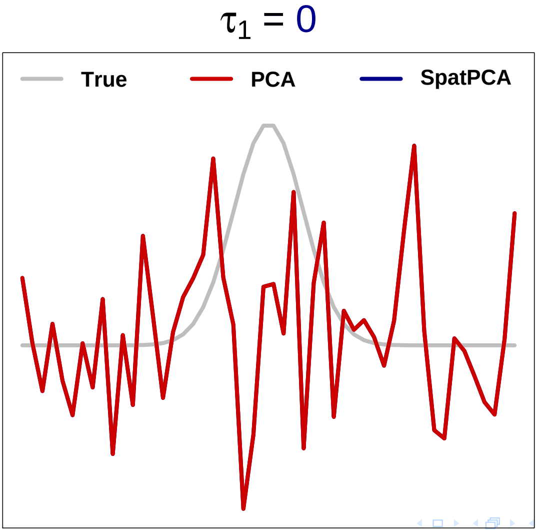
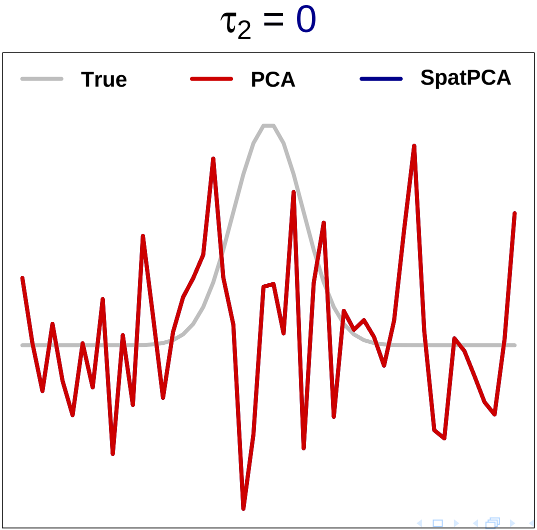


Case 2: $\hat{\varphi}(\cdot)$ as $\tau_1 = 0$ (only sparseness)



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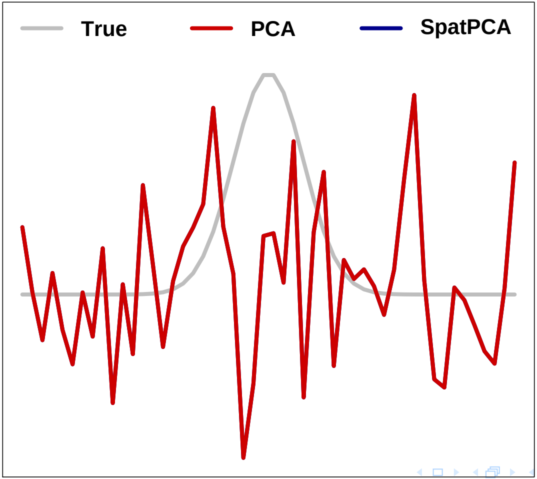
$\tau_2 = 0$



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

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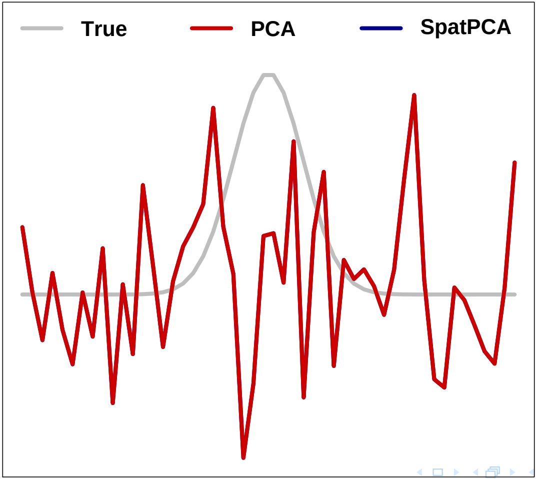

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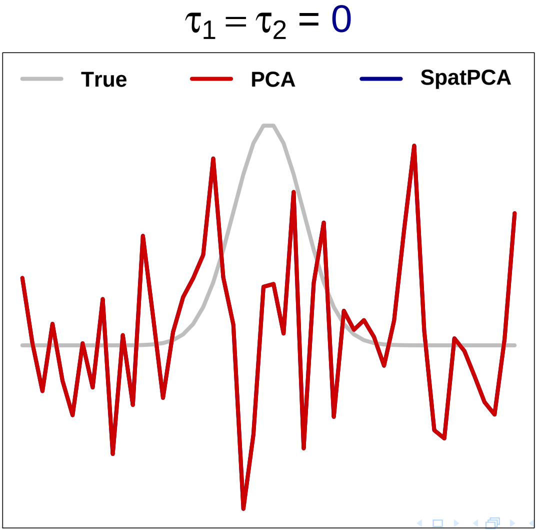
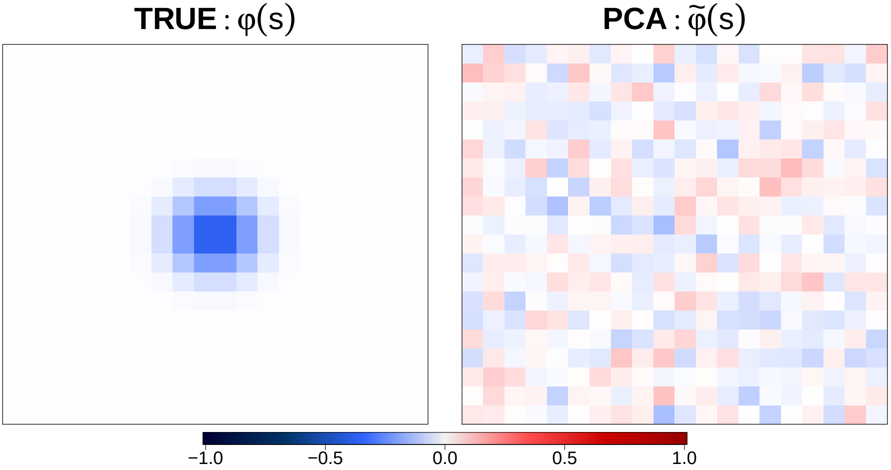


2D Example



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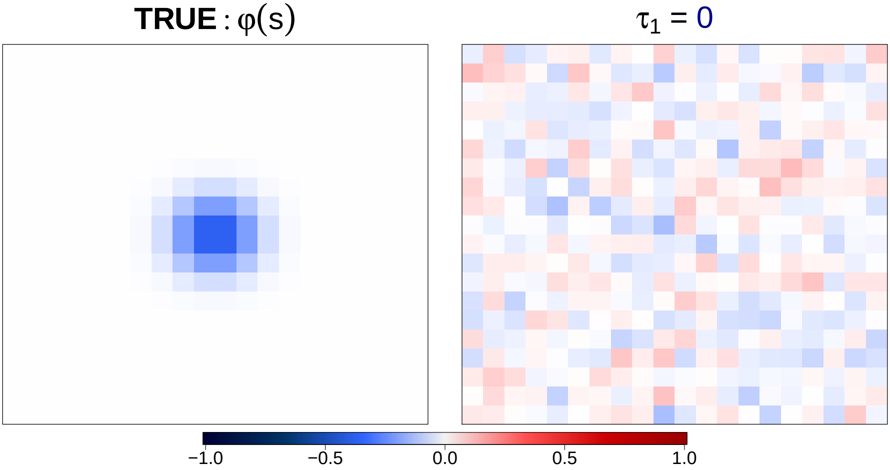

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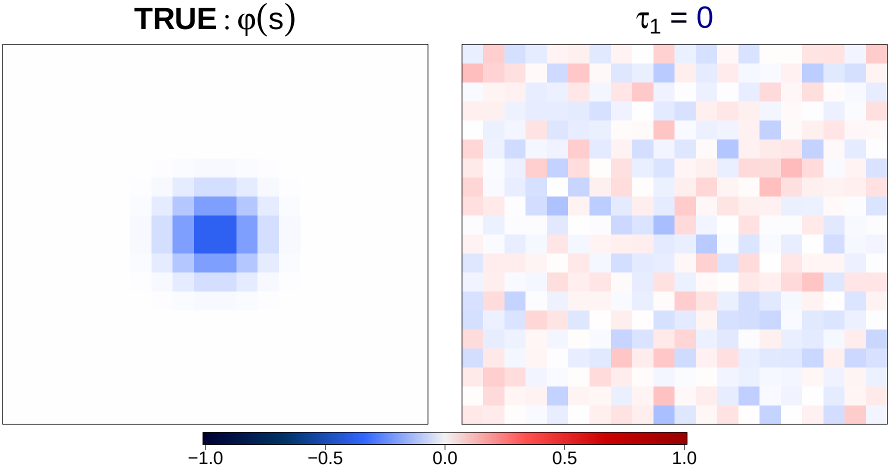

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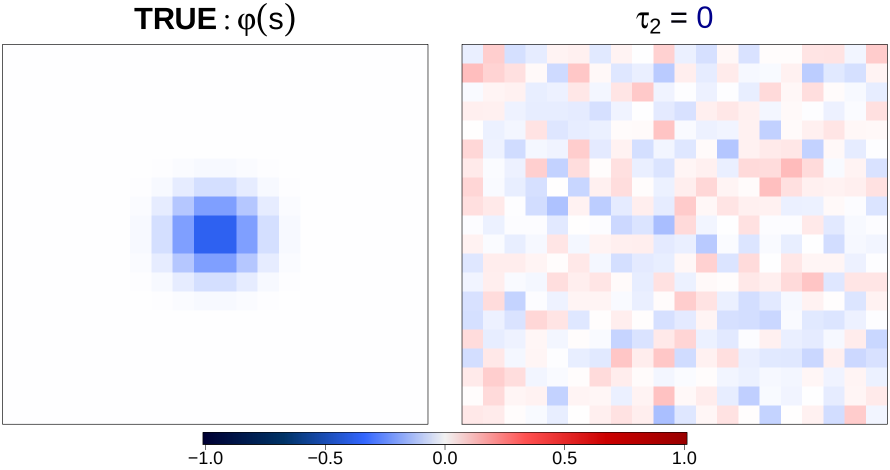

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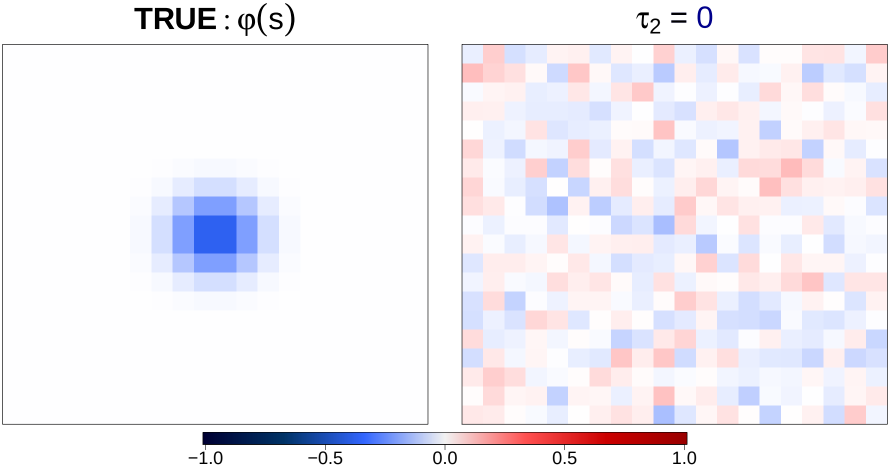

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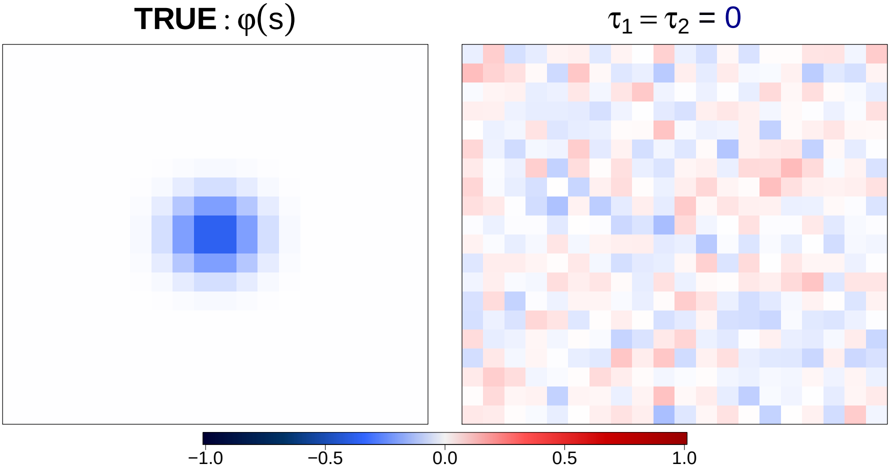

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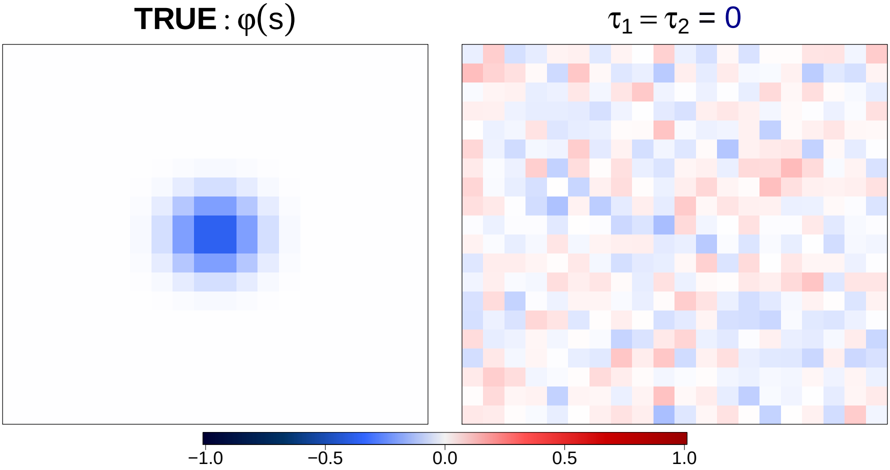

Selection of (τ_1, τ_2)

- M-fold cross-validation:

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

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

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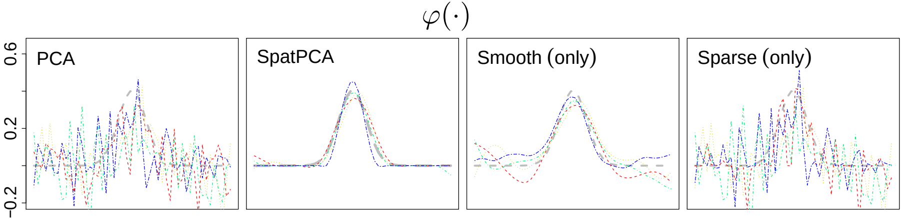
- Find τ_1 and τ_2 which minimize $\text{CV}(\tau_1, \tau_2)$

Example (1D): 5-fold CV



Reconstruction of $\eta(\cdot)$

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  - $\boldsymbol{c}(\boldsymbol{s}_0) = (C_\eta(\boldsymbol{s}_0, \boldsymbol{s}_1), \ldots, C_\eta(\boldsymbol{s}_0, \boldsymbol{s}_p))'$
  - $\boldsymbol{\Sigma} = \text{var}(\boldsymbol{Y}_i) = \boldsymbol{\Phi\Lambda\Phi}' + \sigma^2\boldsymbol{I}$
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  - 1st term : goodness of fit based on var$(\boldsymbol{Y}_i) = \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}' + \sigma^2 \boldsymbol{I}$
  - $\hat{\mathbf{\Phi}}$: given SpatPCA estimate
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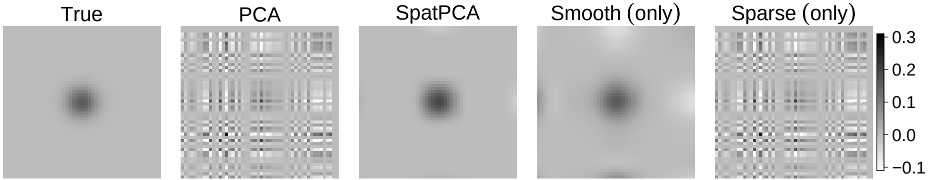
  - $\|\boldsymbol{M}\|_* = \text{tr}((\boldsymbol{M}'\boldsymbol{M})^{1/2})$
- Spatial prediction of $\eta_i(\boldsymbol{s}_0)$: $\hat{\eta}_i(\boldsymbol{s}_0) = \hat{\boldsymbol{c}}'(\boldsymbol{s}_0)(\hat{\boldsymbol{\Phi}}\hat{\boldsymbol{\Lambda}}\hat{\boldsymbol{\Phi}}' + \hat{\sigma}^2 \boldsymbol{I})^{-1} \boldsymbol{Y}_i$
  - $\hat{\boldsymbol{c}}(\boldsymbol{s}_0) = (\hat{C}_\eta(\boldsymbol{s}_0, \boldsymbol{s}_1), \ldots, \hat{C}_\eta(\boldsymbol{s}_0, \boldsymbol{s}_p))'$
  - $\hat{C}_\eta(\boldsymbol{s}^*, \boldsymbol{s}) = \sum_{k=1}^K \sum_{k'=1}^K \hat{\lambda}_{kk'} \hat{\varphi}_k(\boldsymbol{s}^*) \hat{\varphi}_{k'}(\boldsymbol{s})$

Solution of (σ^2, Λ)

- $$(\hat{\sigma}^2, \hat{\boldsymbol{\Lambda}}) = \underset{(\sigma^2, \boldsymbol{\Lambda}): \sigma^2 \geq 0,\, \boldsymbol{\Lambda} \succeq \mathbf{0}}{\arg\min} \left\{ \frac{1}{2} \left\| \boldsymbol{S} - (\hat{\boldsymbol{\Phi}} \boldsymbol{\Lambda} \hat{\boldsymbol{\Phi}}' + \sigma^2 \boldsymbol{I}) \right\|_F^2 + \gamma \| \hat{\boldsymbol{\Phi}} \boldsymbol{\Lambda} \hat{\boldsymbol{\Phi}}' \|_* \right\}$$
- Closed-form solutions:
  - $\hat{\boldsymbol{\Lambda}} = \hat{\boldsymbol{V}} \text{diag}(\hat{\lambda}_1^*, \ldots, \hat{\lambda}_K^*) \hat{\boldsymbol{V}}'$
  - $$\hat{\sigma}^2 = \begin{cases} \dfrac{1}{p - \hat{L}} \left(\text{tr}(\boldsymbol{S}) - \displaystyle\sum_{k=1}^{\hat{L}} (\hat{d}_k - \gamma) \right); & \text{if } \hat{d}_1 > \gamma, \\ \dfrac{1}{p} (\text{tr}(\boldsymbol{S}))\,; & \text{if } \hat{d}_1 \leq \gamma\,, \end{cases}$$
    - $\hat{\boldsymbol{V}} \text{diag}(\hat{d}_1, \ldots, \hat{d}_K) \hat{\boldsymbol{V}}'$: eigen-decomposition of $\hat{\boldsymbol{\Phi}}' \boldsymbol{S} \hat{\boldsymbol{\Phi}}$ with $\hat{d}_1 \geq \cdots \geq \hat{d}_K$
    - $\hat{L} = \max \left\{ L : \hat{d}_L - \gamma > \frac{1}{p-L} \left(\text{tr}(\boldsymbol{S}) - \sum_{k=1}^{L} (\hat{d}_k - \gamma) \right), L = 1, \ldots, K \right\}$
    - $\hat{\lambda}_k^* = \max(\hat{d}_k - \hat{\sigma}^2 - \gamma, 0);\ k = 1, \ldots, K$

Example (1D)

$$C_\eta(\cdot,\cdot)$$



Outline

1. Principal Component Analysis
   - Background
   - Proposed method: Spatial PCA
2. **Maximum Covariance Analysis**
   - Background
   - Proposed method: Spatial MCA
3. Numerical Examples
4. Summary

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

How precipitations 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:

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

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

Background

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

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),

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

  - nonnegative singular values: $d_1 \geq d_2 \geq \cdots$
  - $\{u_k(\cdot)\}$ and $\{v_k(\cdot)\}$: sets of orthonormal basis functions
  - similar to the Karhunen-Loéve expansion

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- Assume $d_{K+1} = 0$.
- $(u_1(\cdot), v_1(\cdot)), \ldots, (u_K(\cdot), v_K(\cdot))$: K dominant coupled patterns

Goal

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

Goal

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

Bivariate data vector

- $$\begin{pmatrix} \boldsymbol{Y}_{1i} \\ \boldsymbol{Y}_{2i} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\eta}_{1i} \\ \boldsymbol{\eta}_{2i} \end{pmatrix} + \begin{pmatrix} \boldsymbol{\epsilon}_{1i} \\ \boldsymbol{\epsilon}_{2i} \end{pmatrix}; i = 1, \ldots, n$$
  - $$\begin{pmatrix} \boldsymbol{Y}_{1i} \\ \boldsymbol{Y}_{2i} \end{pmatrix} = \begin{pmatrix} (Y_{1i}(\boldsymbol{s}_{11}), \ldots, Y_{1i}(\boldsymbol{s}_{1p_1}))' \\ (Y_{2i}(\boldsymbol{s}_{21}), \ldots, Y_{2i}(\boldsymbol{s}_{2p_2}))' \end{pmatrix}$$
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  - $$\begin{pmatrix} \boldsymbol{\epsilon}_{1i} \\ \boldsymbol{\epsilon}_{2i} \end{pmatrix} = \begin{pmatrix} (\epsilon_{1i1}, \ldots, \epsilon_{1ip_1})' \\ (\epsilon_{2i1}, \ldots, \epsilon_{2ip_2})' \end{pmatrix}$$
- Assume $p_1 \geq p_2$

Maximum covariance analysis (MCA)

- Bivariate data vector

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

  - $\boldsymbol{\Sigma}_{12} = \text{cov}(\boldsymbol{Y}_{1i}, \boldsymbol{Y}_{2i}) = \text{cov}(\boldsymbol{\eta}_{1i}, \boldsymbol{\eta}_{2i})$
- Idea: find $\boldsymbol{u} \in \mathcal{R}^{p_1}$ and $\boldsymbol{v} \in \mathcal{R}^{p_2}$, with $\|\boldsymbol{u}\|_2 = \|\boldsymbol{v}\|_2 = 1$, which maximize

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

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

Sample maximum covariance analysis

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

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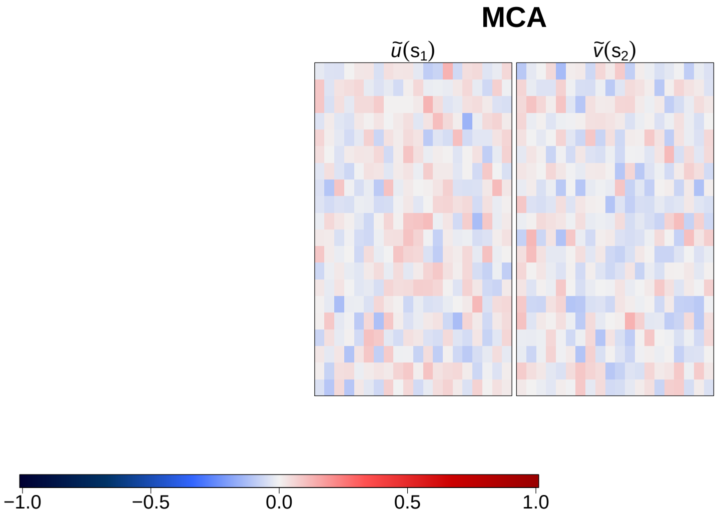
- $(\tilde{\boldsymbol{u}}_1, \tilde{\boldsymbol{v}}_1), \ldots, (\tilde{\boldsymbol{u}}_K, \tilde{\boldsymbol{v}}_K)$: estimates of $(\boldsymbol{u}_1, \boldsymbol{v}_1), \ldots, (\boldsymbol{u}_K, \boldsymbol{v}_K)$
- Problem:
  - high estimation variability: n small, p_1 or p_2 large
    - noisy patterns $\rightarrow$ low interpretation
  - without a spatial structure of $(\boldsymbol{u}, \boldsymbol{v})$

Example:



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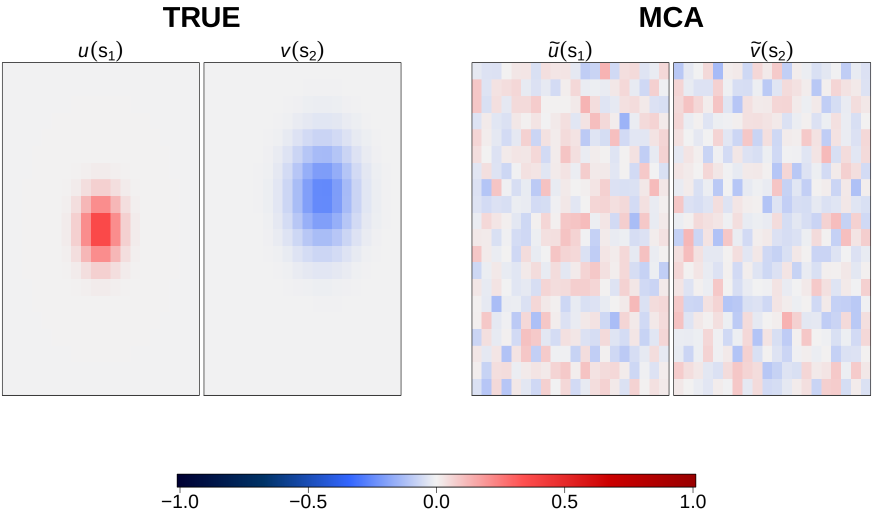

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retain that orthogonal constraints for $(\boldsymbol{u}, \boldsymbol{v})$.

Quick review

- Data: $\boldsymbol{Y}_{1i} = (Y_{1i}(\boldsymbol{s}_{11}), \ldots, Y_{1i}(\boldsymbol{s}_{1p_1}))'$, $\boldsymbol{Y}_{2i} = (Y_{2i}(\boldsymbol{s}_{21}), \ldots, Y_{2i}(\boldsymbol{s}_{p_2}))'$; $i = 1, \ldots, n$
  - $Y_{1i}(\boldsymbol{s}_{1j}) = \eta_{1i}(\boldsymbol{s}_{1j}) + \epsilon_{1ij}$; $j = 1, \ldots, p_1$
    - $\epsilon_{1ij} \sim (0, \sigma_1^2)$
    - ϵ_{1ij}: uncorrelated with $\eta_1(\cdot)$
  - $Y_{2i}(\boldsymbol{s}_{2j}) = \eta_{2i}(\boldsymbol{s}_{2j}) + \epsilon_{2ij}$; $j = 1, \ldots, p_2$
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- Spatial cross-covariance function:

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

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

MCA (alternative version)

- Sample cross-covariance matrix: $\boldsymbol{S}_{12} = \boldsymbol{Y}_1'\boldsymbol{Y}_2/n$
- MCA: perform SVD of $\boldsymbol{S}_{12}$

- Alternative method:

$$(\tilde{\boldsymbol{U}}, \tilde{\boldsymbol{V}}) = \operatorname*{arg\,max}_{\boldsymbol{U},\boldsymbol{V}} \operatorname{tr}(\boldsymbol{U}'\boldsymbol{S}_{12}\boldsymbol{V}),$$

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

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

Regularized MCA

- Sample cross-covariance matrix: $\boldsymbol{S}_{12} = \boldsymbol{X}'\boldsymbol{Y}/n$
- $\boldsymbol{U}_{p_1 \times K} = (\boldsymbol{u}_1, \ldots, \boldsymbol{u}_K)$ with $u_{jk} = u_k(\boldsymbol{s}_{1j})$
- $\boldsymbol{V}_{p_2 \times K} = (\boldsymbol{v}_1, \ldots, \boldsymbol{v}_K)$ with $v_{jk} = v_k(\boldsymbol{s}_{2j})$
- Objective function:

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

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

Regularized MCA

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- $\boldsymbol{V}_{p_2 \times K} = (\boldsymbol{v}_1, \ldots, \boldsymbol{v}_K)$ with $v_{jk} = v_k(\boldsymbol{s}_{2j})$
- Objective function:

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

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

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- $\boldsymbol{V}_{p_2 \times K} = (\boldsymbol{v}_1, \ldots, \boldsymbol{v}_K)$ with $v_{jk} = v_k(\boldsymbol{s}_{2j})$

- Objective function:

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

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

  - $J(u_k(\cdot)) = \sum_{z_1 + \cdots + z_d = 2} \int_{R^d} \left(\frac{\partial^2 u_k(\boldsymbol{s})}{\partial x_1^{z_1} \ldots \partial x_d^{z_d}} \right)^2 d\boldsymbol{s}$
    - $\boldsymbol{s} = (x_1, \ldots, x_d)'$
  - τ_{1u}, τ_{1v}: smoothness parameter
  - τ_{2u}, τ_{2v}: sparseness parameter

Spatial MCA (SpatMCA)

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

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  - Green and Silverman (1994)

- SpatMCA: $(\hat{\boldsymbol{U}},\hat{\boldsymbol{V}})$ maximizes:

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

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

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

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

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

- $(\hat{u}_1(\cdot), \hat{v}_1(\cdot)), \ldots, (\hat{u}_K(\cdot), \hat{v}_K(\cdot))$ maximizes
$$\mathrm{tr}(\boldsymbol{U}'\boldsymbol{S}_{12}\boldsymbol{V}) - \sum_{k=1}^{K}\left\{\tau_{1u}J(u_k)+\tau_{2u}\sum_{j=1}^{p_1}|u_k(\boldsymbol{s}_{1j})| + \tau_{1v}J(v_k)+\tau_{2v}\sum_{j=1}^{p_2}|v_k(\boldsymbol{s}_{2j})|\right\},$$
subject to $\boldsymbol{U}'\boldsymbol{U} = \boldsymbol{V}'\boldsymbol{V} = \boldsymbol{I}_K$

- $$\hat{u}_k(\boldsymbol{s}_1) = \sum_{i=1}^{p_1} a_{1i} g(\|\boldsymbol{s}_1 - \boldsymbol{s}_{1i}\|) + b_{10} + \sum_{j=1}^{d} b_{1j} x_{1j}$$
$$\hat{v}_k(\boldsymbol{s}_2) = \sum_{i=1}^{p_2} a_{2i} g(\|\boldsymbol{s}_2 - \boldsymbol{s}_{2i}\|) + b_{20} + \sum_{j=1}^{d} b_{2j} x_{2j}$$

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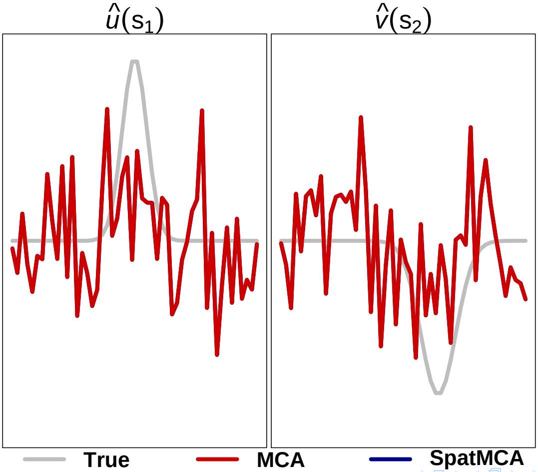
$$\hat{v}_k(\boldsymbol{s}_2) = \sum_{i=1}^{p_2} a_{2i}g(\|\boldsymbol{s}_2 - \boldsymbol{s}_{2i}\|) + b_{20} + \sum_{j=1}^{d} b_{2j}x_{2j}$$
  - $\boldsymbol{s}_1 = (x_{11}, \ldots, x_{1d})'$; $\boldsymbol{s}_2 = (x_{21}, \ldots, x_{2d})'$
  - $g(r) = \begin{cases} \frac{1}{16\pi} r^2 \log r; & \text{if } d = 2, \\ \frac{\Gamma(d/2-2)}{16\pi^{d/2}} r^{4-d}; & \text{if } d = 1, 3, \end{cases}$
  - $\boldsymbol{a}_1 = (a_{11}, \ldots, a_{1p_1})'$ and $\boldsymbol{b}_1 = (b_{10}, b_{11}, \ldots, b_{1d})'$ based on $\hat{\boldsymbol{u}}_k$
  - $\boldsymbol{a}_2 = (a_{21}, \ldots, a_{2p_2})'$ and $\boldsymbol{b}_2 = (b_{20}, b_{21}, \ldots, b_{2d})'$ based on $\hat{\boldsymbol{v}}_k$

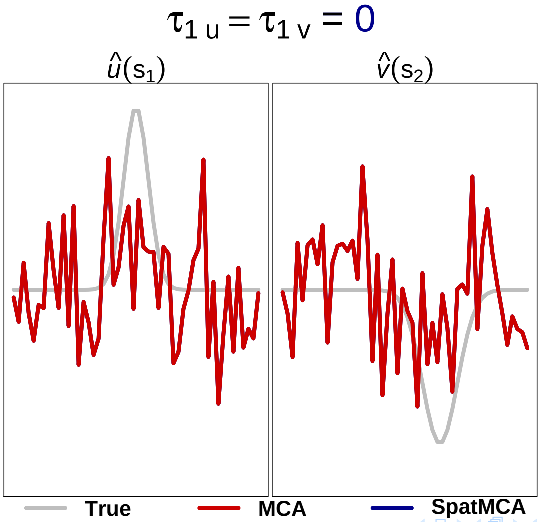
Why roughness and Lasso penalties?

1D Example

$$\tau_{1\,u} = \tau_{1\,v} = 0$$



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



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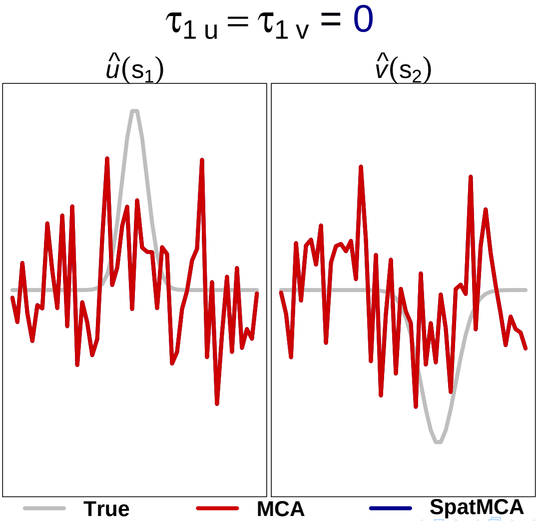
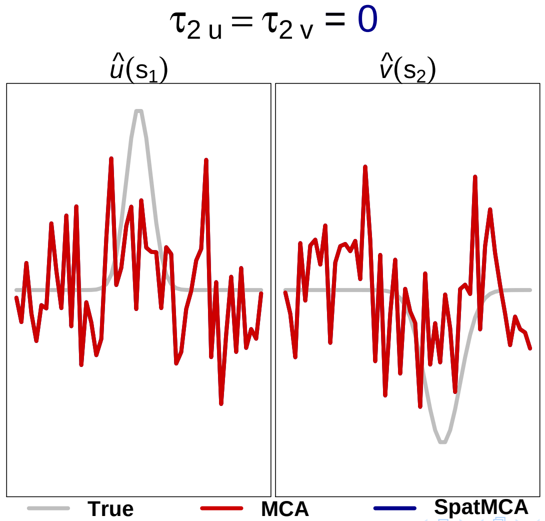


Case 2: $\tau_{1u} = \tau_{1v} = 0$ (only sparseness)



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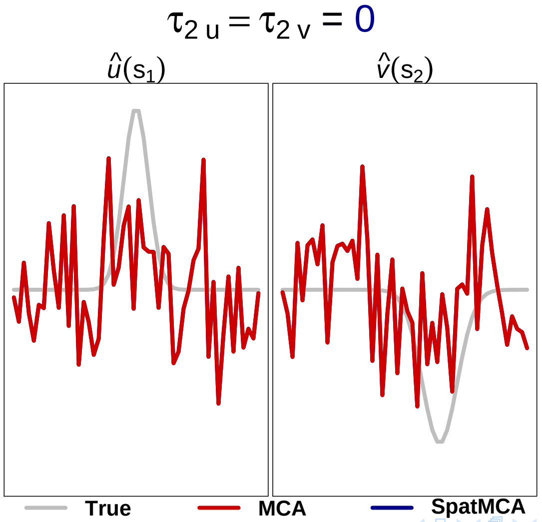
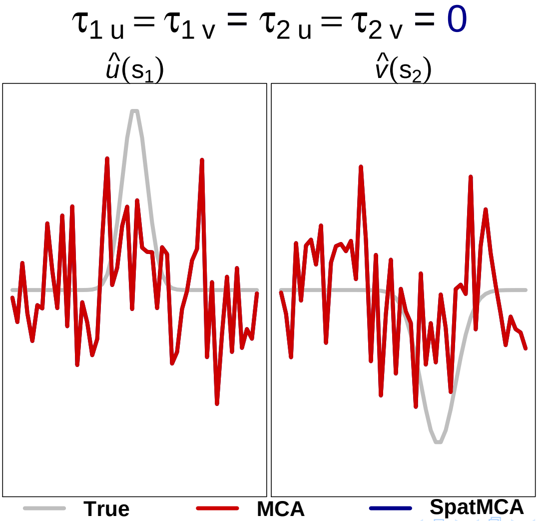


Case 3: $\tau_{1u} = \tau_{1v} = \tau_{2u} = \tau_{2v}$



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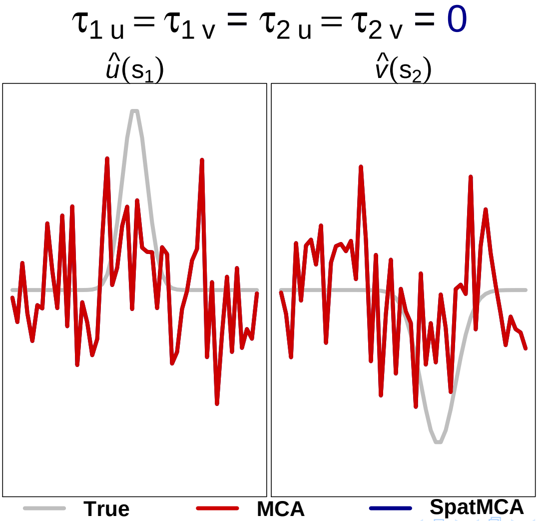
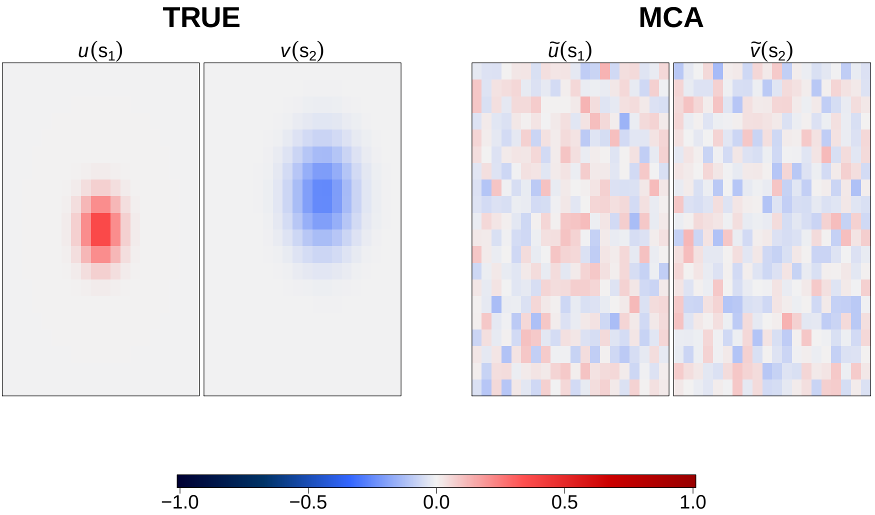


2D Example



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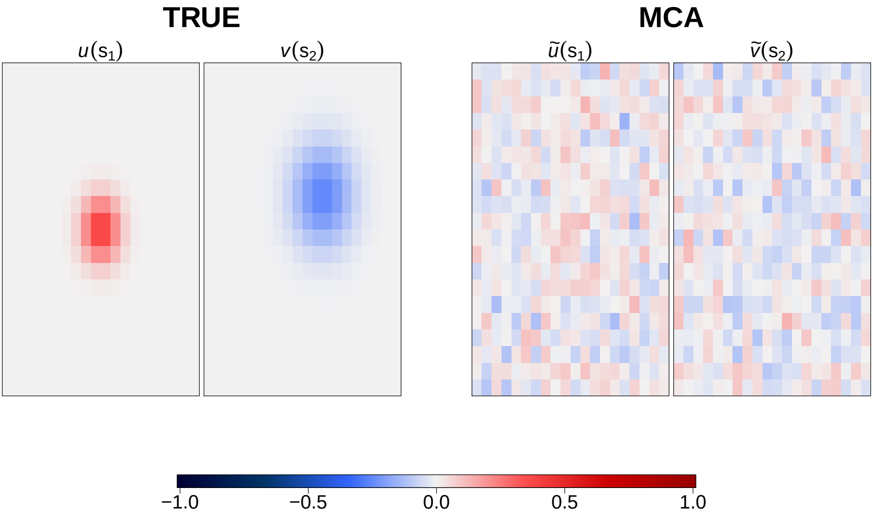

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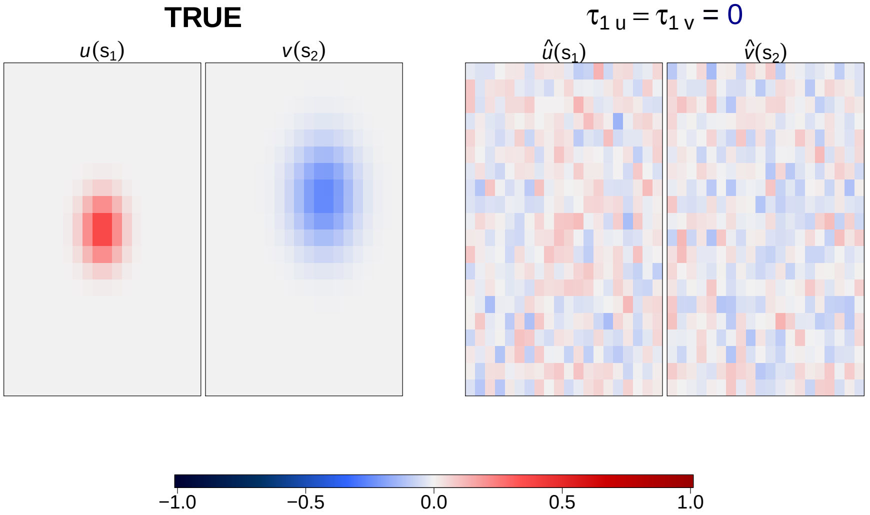

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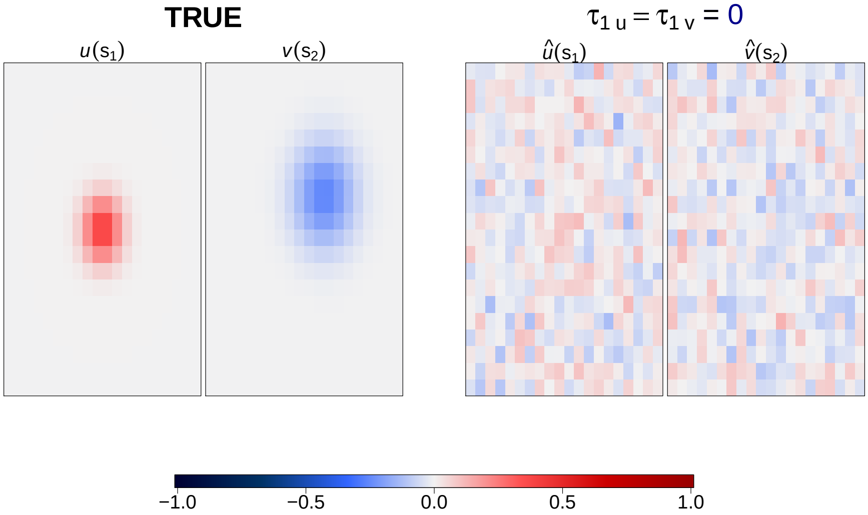

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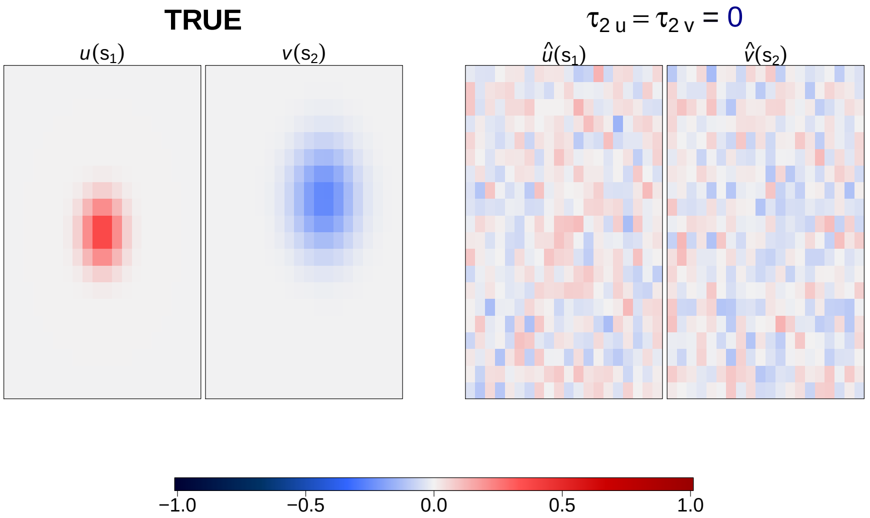

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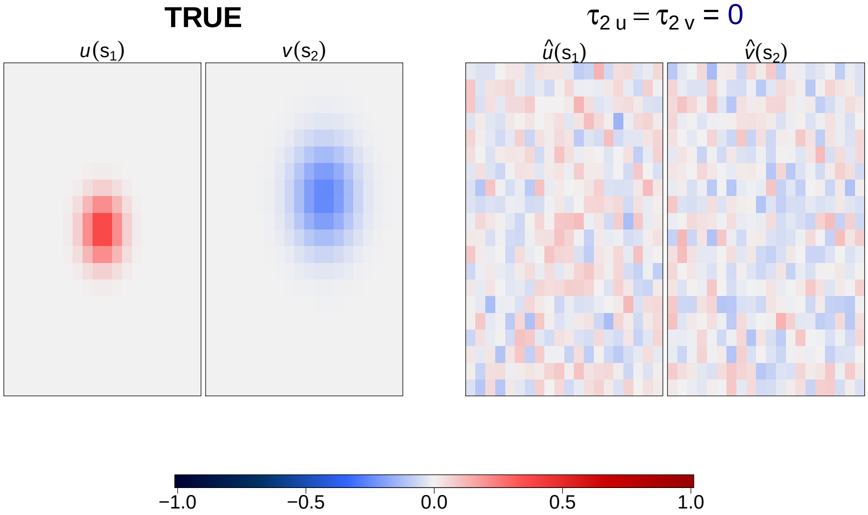

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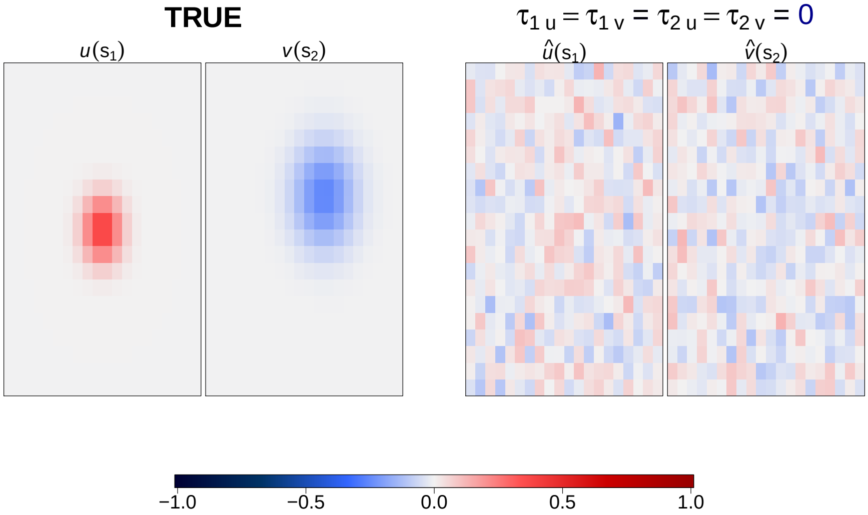

Estimation of D

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

$$\hat{\boldsymbol{D}} = \underset{d_1,\dots,d_K \geq 0}{\arg\min} \|\boldsymbol{S}_{12} - \hat{\boldsymbol{U}}\boldsymbol{D}\hat{\boldsymbol{V}}'\|_F^2 = \mathrm{diag}(\hat{d}_1, \dots, \hat{d}_K)$$

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

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

- The proposed CV criterion is

$$\mathrm{CV}(\tau_{1u}, \tau_{2u}, \tau_{1v}, \tau_{2v}) = \frac{1}{M}\sum_{m=1}^{M} \|\boldsymbol{S}_{12}^{(m)} - \hat{\boldsymbol{U}}^{(-m)}_{\tau_{1u},\tau_{2u}} \hat{\boldsymbol{D}}^{(-m)}_{\tau_{1u},\tau_{2u},\tau_{1v},\tau_{2v}} (\hat{\boldsymbol{V}}^{(-m)}_{\tau_{1v},\tau_{2v}})'\|_F^2$$

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  - Partition $\{(\boldsymbol{Y}_{11}, \boldsymbol{Y}_{21}), \dots, (\boldsymbol{Y}_{1n}, \boldsymbol{Y}_{2n})\}$ into M parts with equal size n_M
  - $\boldsymbol{S}_{12}^{(m)} = (\boldsymbol{Y}_1^{(m)})'\boldsymbol{Y}_2^{(m)}/n_M$ based on the m-th part data $(\boldsymbol{Y}_1^{(m)}, \boldsymbol{Y}_2^{(m)})$
  - $\hat{\boldsymbol{U}}_{\tau_1,\tau_2}^{(-m)}, \hat{\boldsymbol{V}}_{\tau_1,\tau_2}^{(-m)}, \hat{\boldsymbol{D}}_{\tau_{1u},\tau_{2u},\tau_{1v},\tau_{2v}}^{(-m)}$: based on $(\boldsymbol{Y}_1^{(-m)}, \boldsymbol{Y}_2^{(-m)})$
    - $(\boldsymbol{Y}_1^{(-m)}, \boldsymbol{Y}_2^{(-m)})$: remaining data, i.e., $\boldsymbol{Y}_1, \boldsymbol{Y}_2$ excluding $(\boldsymbol{Y}_1^{(m)}, \boldsymbol{Y}_2^{(m)})$

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

- High computation cost to select $\{\tau_{1u}, \tau_{2u}, \tau_{1v}, \tau_{2v}\}$ simultaneously

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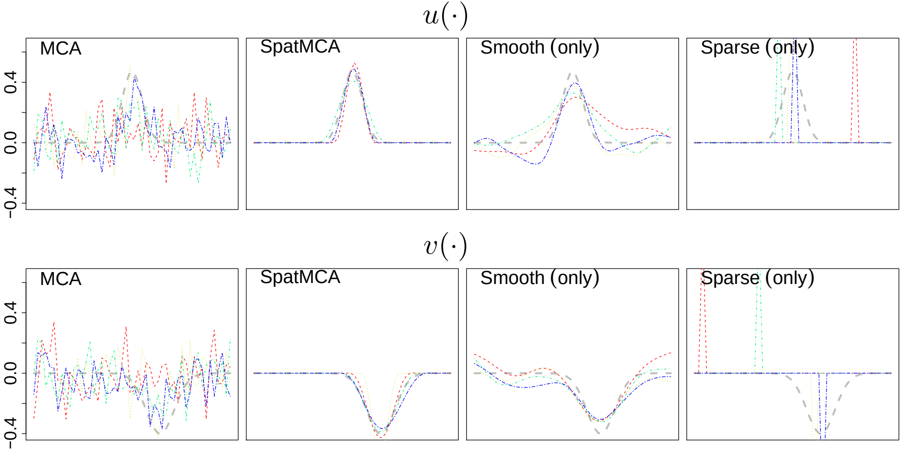
- High computation cost to select $\{\tau_{1u}, \tau_{2u}, \tau_{1v}, \tau_{2v}\}$ simultaneously
- Two-step procedure:
  1. Select smoothness parameters τ_{1u} and τ_{1v}:

$$(\hat{\tau}_{1u}, \hat{\tau}_{1v}) = \underset{\{\tau_{1u}, \tau_{1v}\} \subset [0,\infty)^2}{\arg\min} \mathrm{CV}(\tau_{1u}, 0, \tau_{1v}, 0),$$

  2. Select sparseness parameters τ_{2u} and τ_{2v}:

$$(\hat{\tau}_{2u}, \hat{\tau}_{2v}) = \underset{\{\tau_{2u}, \tau_{2v}\} \subset [0,\infty)^2}{\arg\min} \mathrm{CV}(\hat{\tau}_{1u}, \tau_{2u}, \hat{\tau}_{1v}, \tau_{2v}).$$

Example (1D): 5-fold CV



Outline

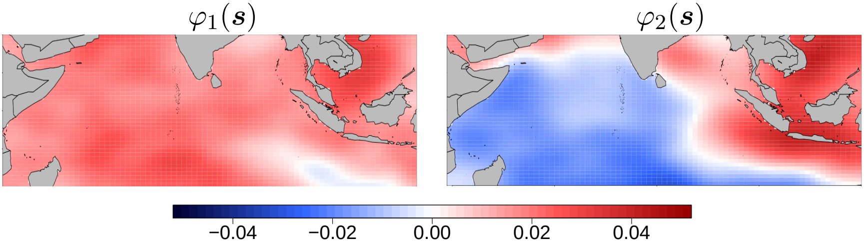
1. Principal Component Analysis
   - Background
   - Proposed method: Spatial PCA
2. Maximum Covariance Analysis
   - Background
   - Proposed method: Spatial MCA
3. **Numerical Examples**
4. Summary

Example: Artificial Sea Surface Temperature Data

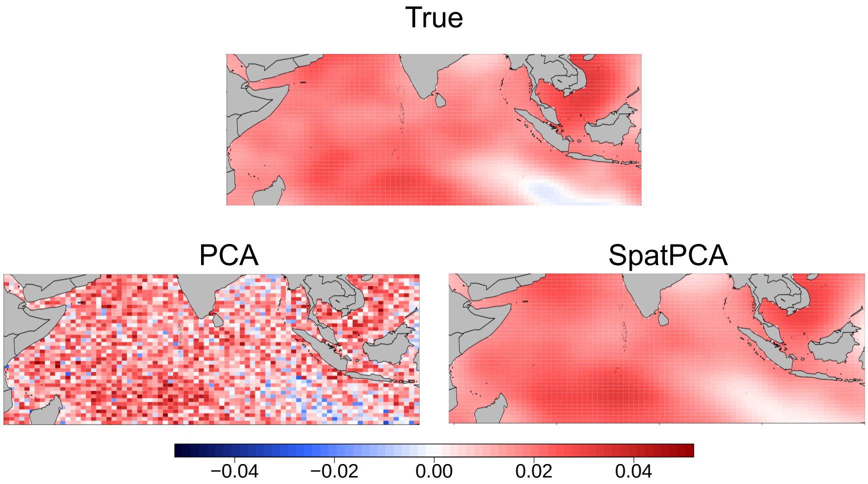
- Data settings:

$$Y_i(\boldsymbol{s}_j) = \xi_{i1}\varphi_1(\boldsymbol{s}_j) + \xi_{i2}\varphi_2(\boldsymbol{s}_j) + \epsilon_{ij};$$

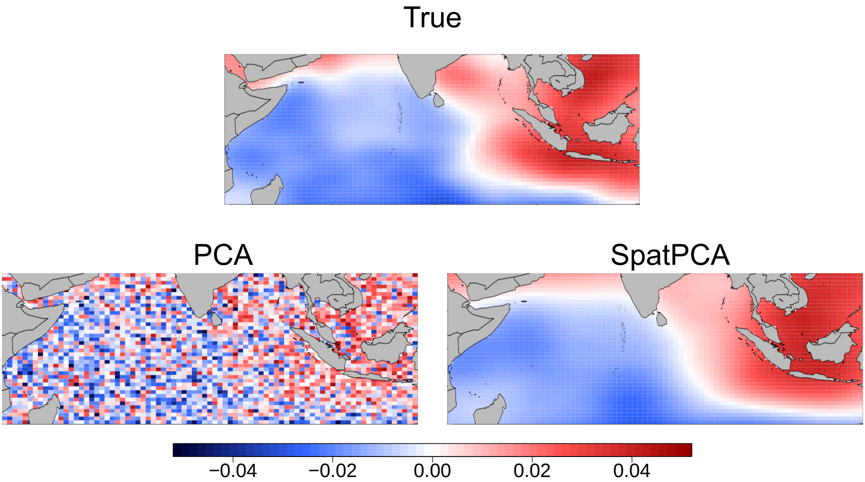
  - $j = 1, \ldots, p = 2,780$, $i = 1, \ldots, n = 60$
  - $\boldsymbol{s}_1, \ldots, \boldsymbol{s}_{2780}$: located in the Indian Ocean
  - $\xi_{i1} \sim N(0, 101.7)$, $\xi_{i2} \sim N(0, 17.1)$, cov$(\xi_{i1}, \xi_{i2}) = 0$
  - $\epsilon_{ij} \sim N(0, 1)$
  - Apply SpatPCA with (τ_1, τ_2) selected by 5-fold CV



Result I: $\varphi_1(s)$



Result I: $\varphi_2(s)$



Performance: PCA vs. SpatPCA

- Loss function: $\mathrm{Loss}(\hat{C}_\eta) = \sum_{i=1}^{p}\sum_{j=1}^{p}\left(\hat{C}_\eta(\boldsymbol{s}_i, \boldsymbol{s}_j) - C_\eta(\boldsymbol{s}_i, \boldsymbol{s}_j)\right)^2$
- 50 replications
  - γ: selected by 5-fold CV

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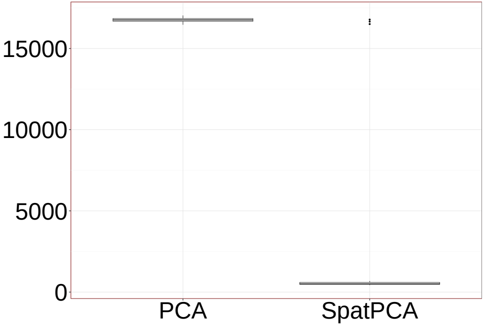
- Boxplot:



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: $p_1 = 3,591$
  - Precipitation:
    - 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

Real data analysis

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  - Sea surface temperature (SST):
    - Region: Indian Ocean (20°N and 30°S; 20°E and 120°E)
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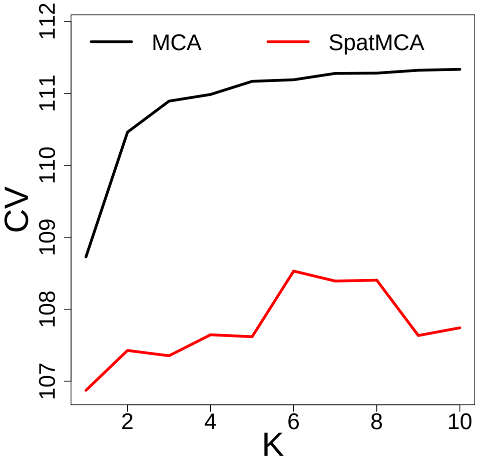
  - Precipitation:
    - Region: Eastern African (6°N and 12°S; 20°E and 42°E)
    - Number of grids: $p_2 = 255$
  - Time period (monthly): Jan. 2011- Dec. 2015 $\rightarrow n = 60$
  - Remove monthly mean
- Goal: find coupled patterns of the SST and precipitation data
- Reference: Omondi et al. (2013)

Real data analysis

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

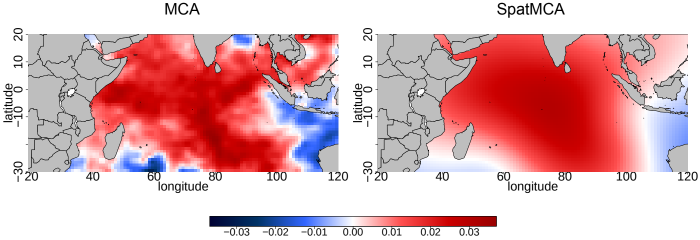
Result: CV vs. K



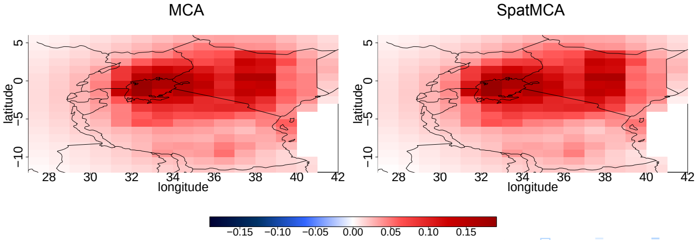
- $\hat{K} = 1$ for MCA and SpatMCA

Result: 1st coupled pattern

- SST

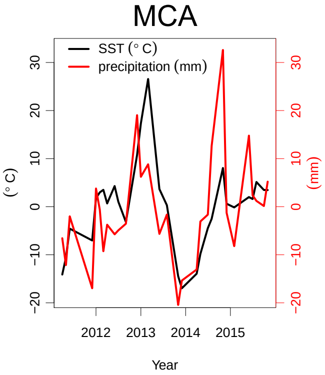


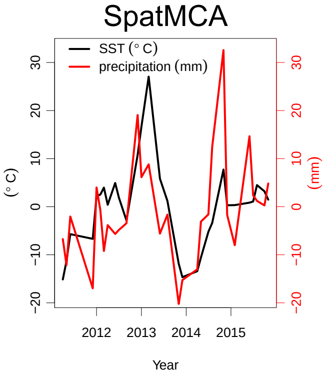
- Precipitation



Result: 1st maximum covariance variables

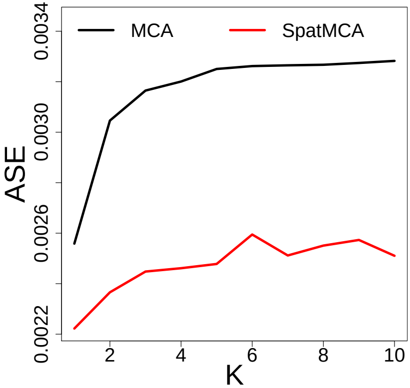
- 1st maximum covariance variables: $\{\hat{\boldsymbol{u}}_1' \boldsymbol{Y}_{1i}\}$; $\{\hat{\boldsymbol{v}}_1' \boldsymbol{Y}_{2i}\}$
- Pearson's correlation: 0.6 for MCA and SpatMCA





Result: average squared error (ASE)

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



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- with the roughness and Lasso penalties
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SpatPCA/ SpatMCA:

- high-dimensional structure $\rightarrow$ 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!