Spatial Correlation Estimation for Sparsely Observed Functional Data

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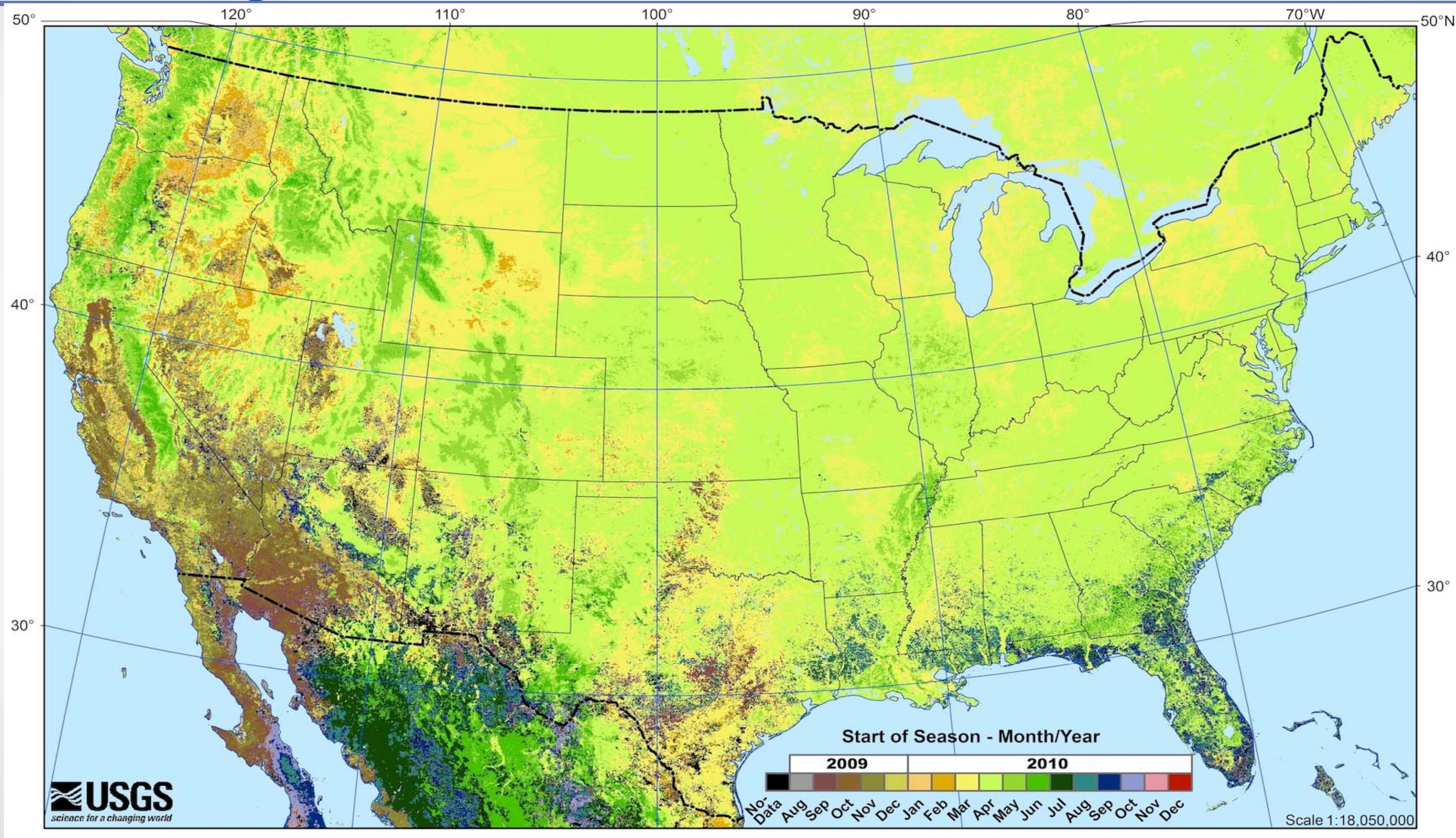
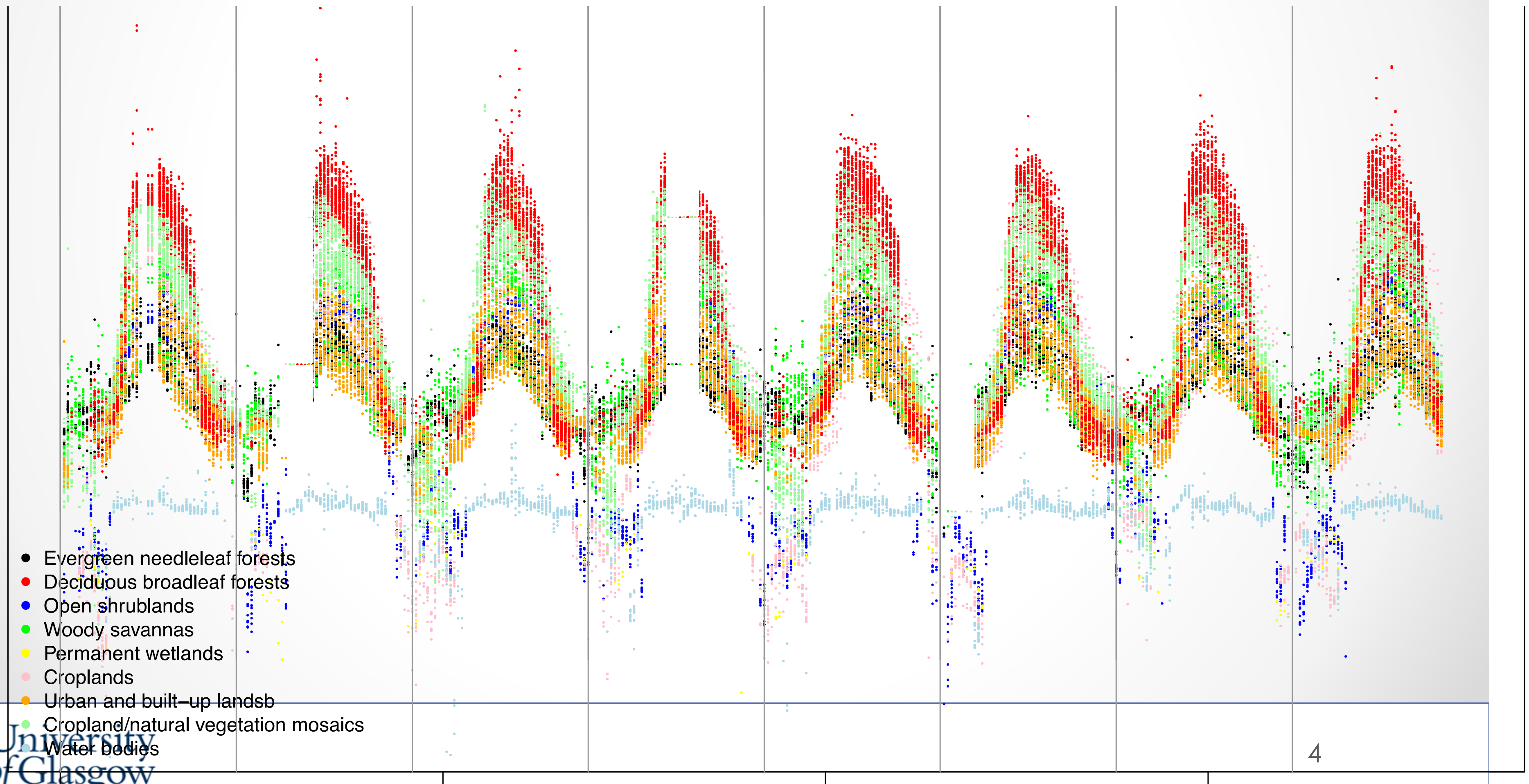
Outline

- Context and Background
- Moment Based Method
- Likelihood Based Method Method
- Curve Reconstruction Results
- Future Work

``Gap Filling" for missing remote sensing observation



Multi year remote sensing data

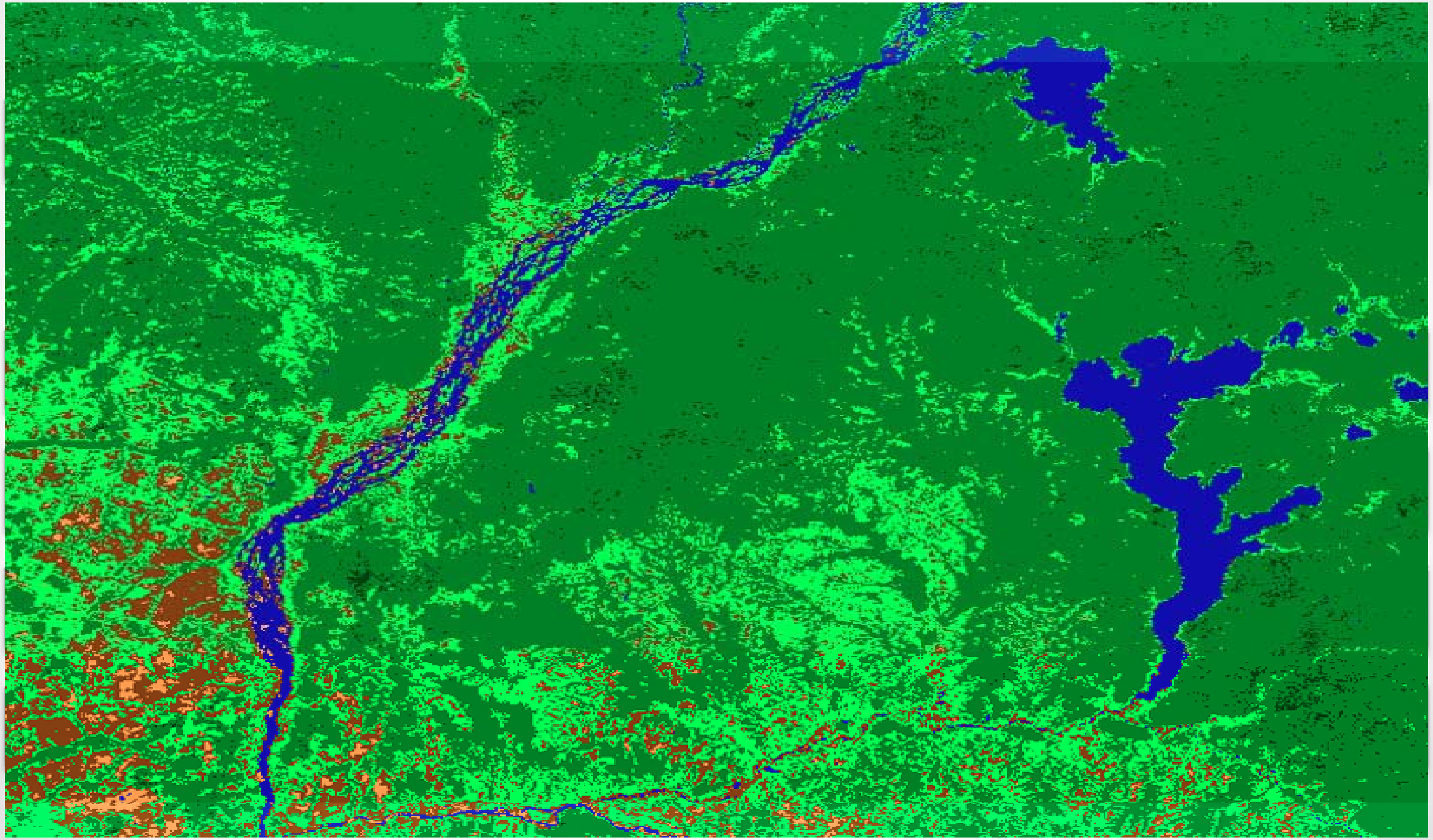


``Gap Filling" for missing remote sensing observation

- Longitudinal remote sensing data are collected for studying various climate ecosystem phenomenon
- Often a lot of observations are missing due to various reasons
    - Cloud Cover
    - Aerosol Content
    - Change of instrument
    - Fire
    - Snow

- Geoscientists would love to fill those gaps for applying "standard statistical techniques."

Properties of remotely sensed ecosystem data



Background and Context

Model for independent curves

$$Y_i(t) = \sum_{k=1}^{K} \gamma_{ik} \phi_k(t) + \varepsilon_i(t)$$

where eigen-scores γ_{ik} are independent across i.

- However, in real world, many applications have correlated $Y_i(t)$ across i.
  - ❖ example: spatial-temporal data, online auction data, time course gene expression data.
- Most existing work treat them as i.i.d.
- Asymptotic property holds for mild correlation.

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Previous Research

- Yao,Muller and Wang 2004 outlined the **moment based** methods to estimate covariance surface and eigenstructure of the random process assuming i.i.d. curves.

    - Also suggested reconstructing curve trajectories ("gap filling") using expected principal component scores.

Question: How to estimate eigenstructure and reconstructing trajectories assuming correlated curves?

Concurrent Research

- "Reduced Rank Mixed Effects Models for Spatially Correlated Hierarchical Functional Data" JASA 2010, Zhou et al.
  - Mentioned by Maurice Berk during his multilevel talk.

- Principal components analysis for sparsely observed correlated functional data using a kernel smoothing approach, Electron. J. Statist. Volume 5 (2011). Paul and Peng

- Some that I have missed …

Our Model for correlate data

2. Our Model:

$$Y_i(t) = \sum_{k=1}^{K} \gamma_{ik}\phi_k(t) + \varepsilon_i(t)$$

where

$$\operatorname{cov}(\gamma_{ip}, \gamma_{jq}) = \begin{cases} 0, & p \neq q \\ \rho^{|i-j|}\lambda_k, & p = q = k \end{cases}$$

more general model:

$$\operatorname{cov}(\gamma_{ip}, \gamma_{jq}) = \begin{cases} 0, & p \neq q \\ matern(d(i,j), \alpha_k, \beta_k)\lambda_k, & p = q = k \end{cases}$$

Goal: estimating ρ or more generally α_k and β_k

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Estimation of Parameters

Moment Based Method

- local linear smoothing of the covariance surface $\sum_0$ and
- lag-d cross-covariance surface $\sum_d$ where d = 1,2,...D,
- take ratios of eigenvalues as covariance estimates and fit matern or other parametric models.

Likelihood based method

- Marginal likelihood is hard to optimize.
- Turn to joint likelihood of Y and and treat as random effects.
- Use EM(expectation maximization) to solve the optimal parameters ρ, α_k and β_k

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Moment based method

- Covariance Model

$$\text{cov}(Y_i, Y_j) = \Phi \, \text{cov}(\gamma_i, \gamma_j)\Phi' + \sigma^2 \text{I}$$

$$= \Phi \, diag(\text{cov}(\gamma_{i1}, \gamma_{j1}), \text{cov}(\gamma_{i2}, \gamma_{j2}), \ldots, \text{cov}(\gamma_{iK}, \gamma_{jK}))\Phi' + \sigma^2 \text{I}$$

- Smooth covariance to get estimate of $\sum_0 = \text{cov}(Y_i, Y_i)$
  - raw covariance $G_i(T_{is}, T_{it}) = (Y_{is} - \mu(T_{is}))(Y_{it} - \mu(T_{it}))$
  - Smooth $G_{ij}(T_{is}, T_{jt})$ using local linear smoother and get

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Moment based method

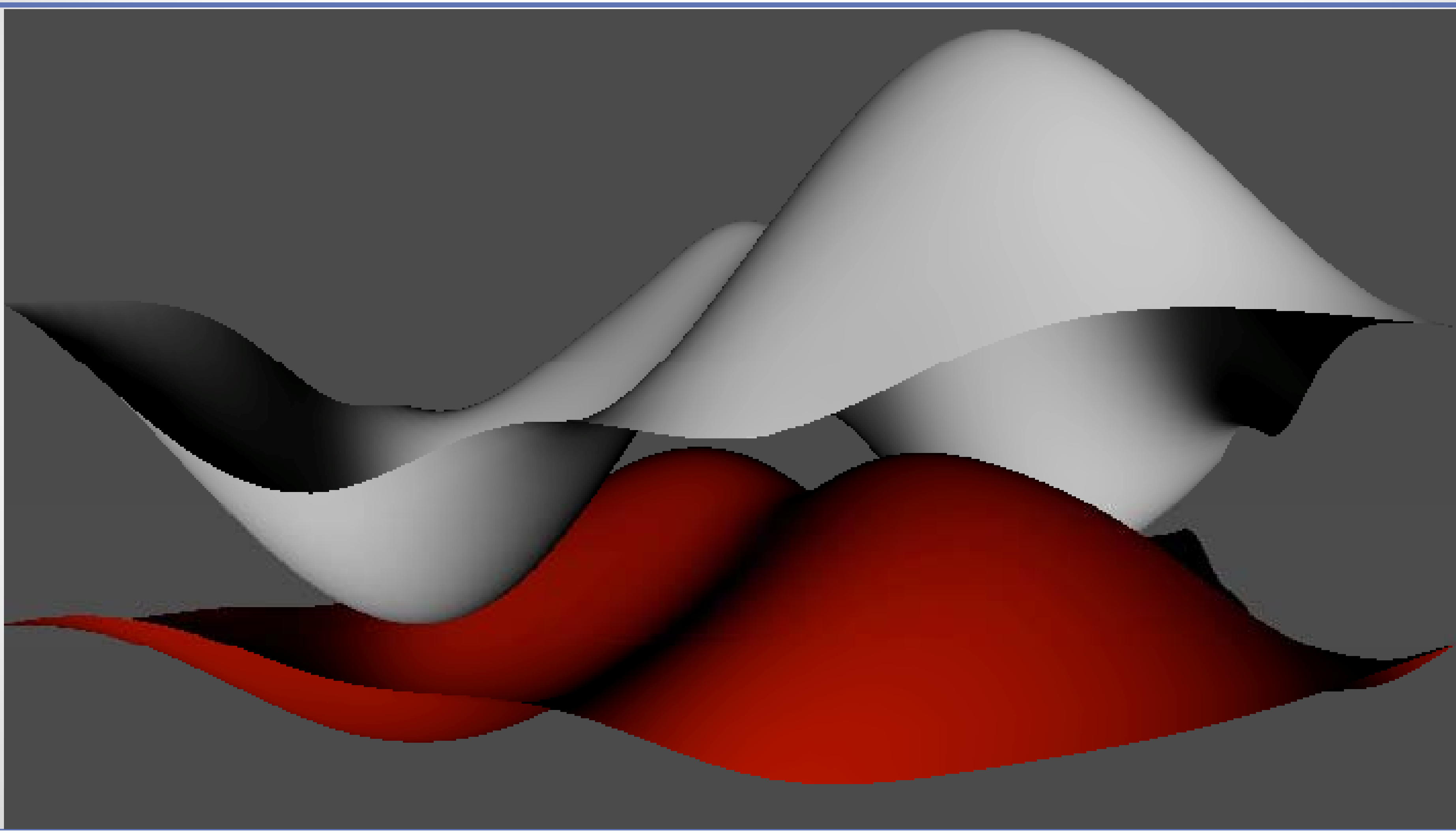
- Smooth lag-d covariance to get estimate of $\Sigma_{d(i,j)} = \text{cov}(Y_i, Y_j)$

  where $d(i,j) = d$

  - raw covariance $G_{ij}(T_{is}, T_{jt}) = (Y_{is} - \mu(T_{is}))(Y_{jt} - \mu(T_{jt}))$

  - Smooth $G_{ij}(T_{is}, T_{jt})$ using local linear smoother and get $\hat{\Sigma}_{d(i,j)}$

Moment based method



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Moment based method

How to use the lagged covariance surfaces

Calculate Eigenvalue ratio

eigenvalues of $\hat{\Sigma}_0$: $\pi_{0,k}, k = 1, 2 \ldots K$

eigenvalues of $\hat{\Sigma}_d$: $\pi_{d,k}, k = 1, 2 \ldots K$

For given k, we have $\hat{cor}_d(\gamma_{ik}, \gamma_{jk}) = \dfrac{\pi_{d,k}}{\pi_{0,k}}$ for d = 1,2,…D

These $\dfrac{\pi_{d,k}}{\pi_{0,k}}$ can be used to fit model parameters

Simulation Results for moment based method

Simulation scheme

- 3 eigenfunctions, 100 curves, 10 time points.
- AR(1) type spatial correlation(parameter is ρ) =0.2, 0.4, 0.6, 0.8.
- noise standard deviation σ = 0.05, 0.2, 0.5, 1.
- Results for estimation of ρ eigenfunction 1 to 3 with moment based method

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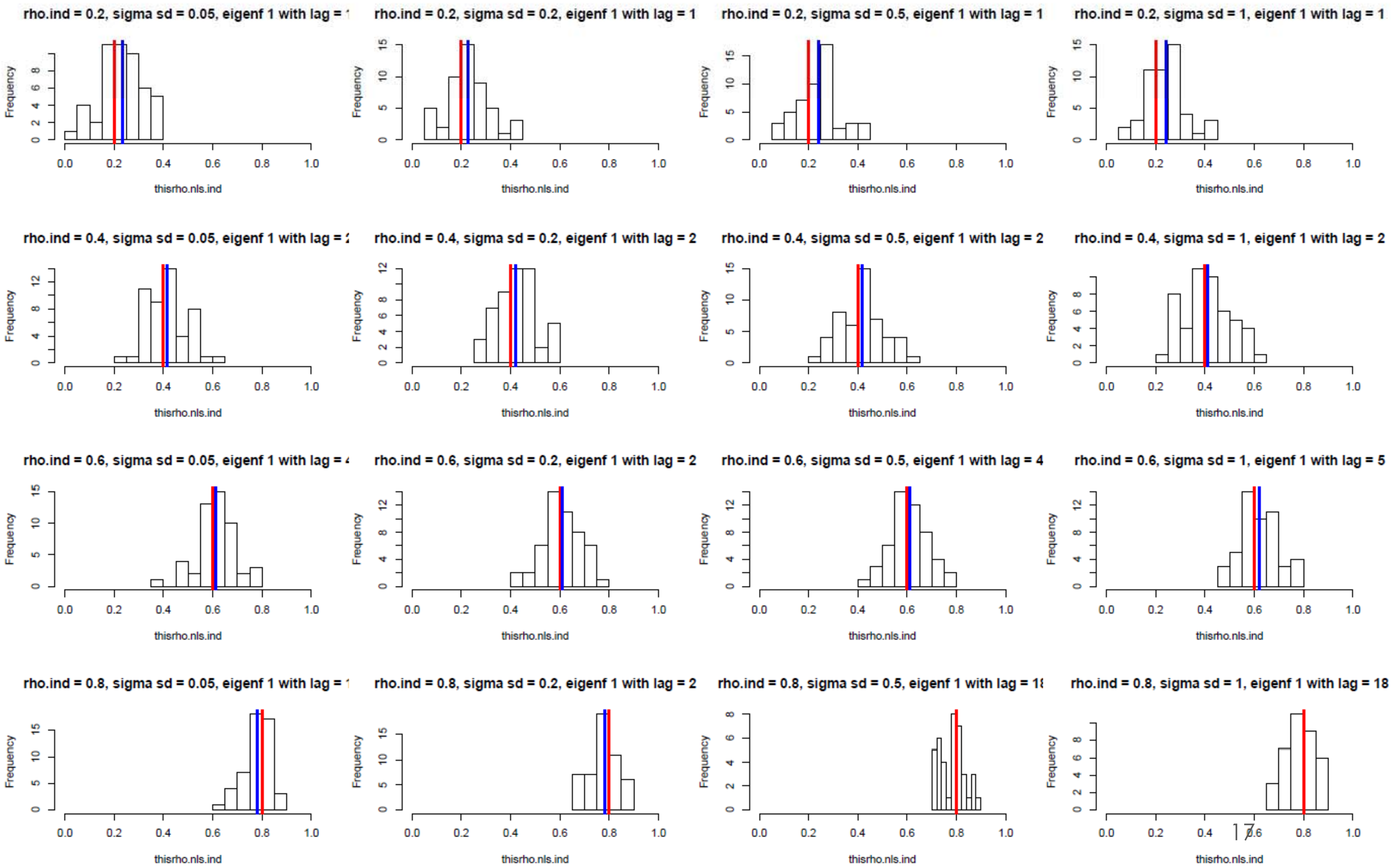
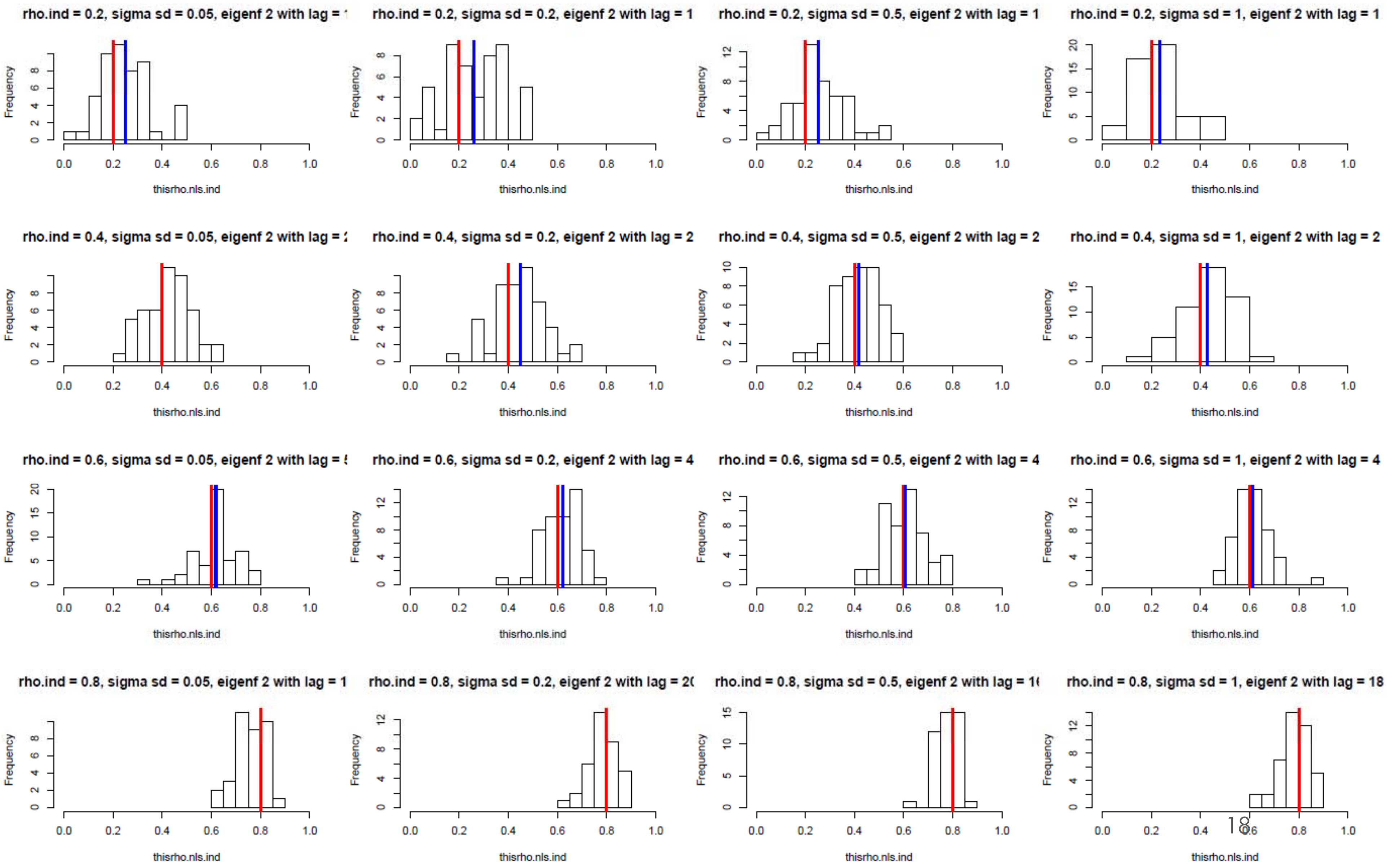
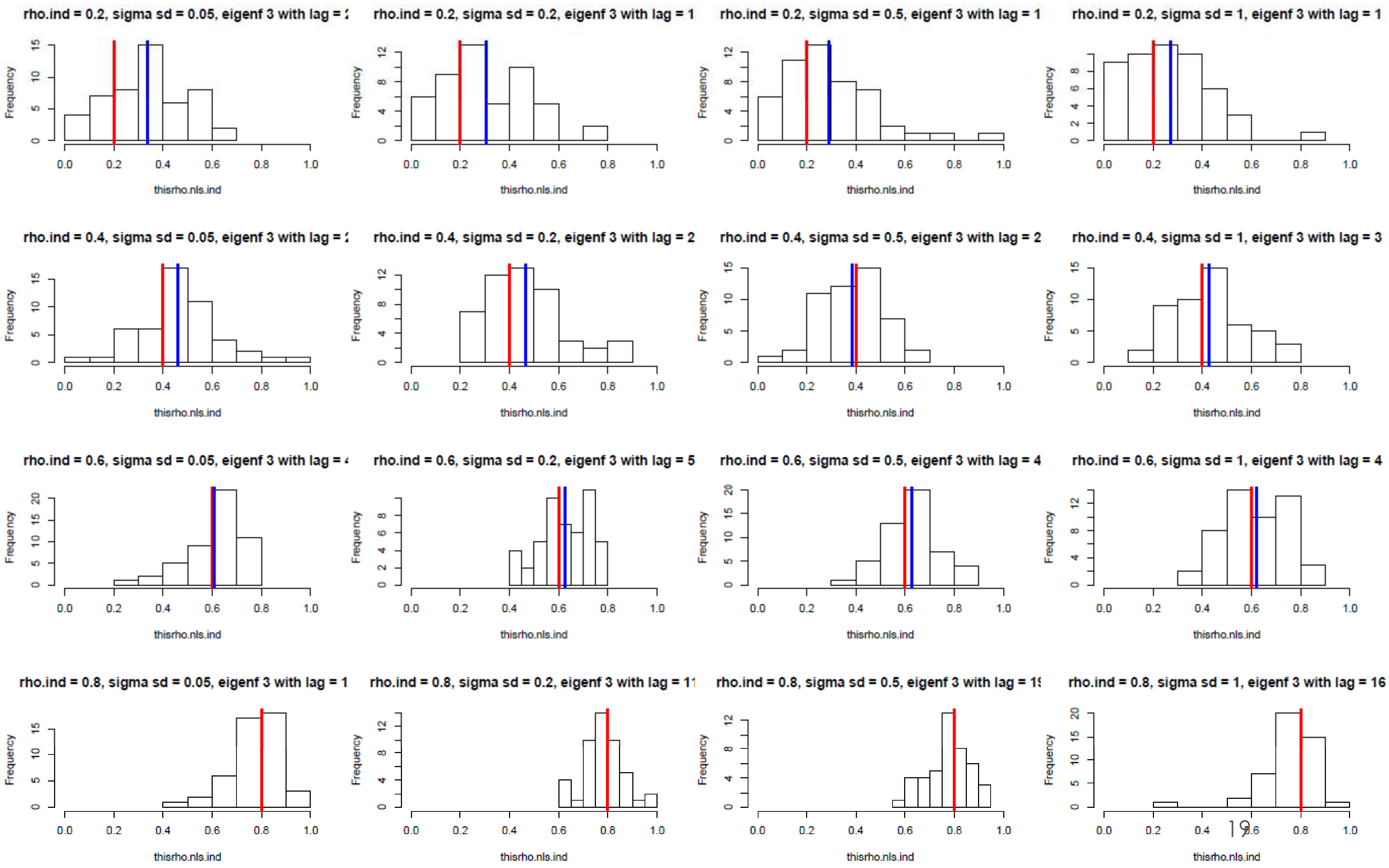
Simulation Results: Ratio of first eigen values



Simulation Results: Ratio of 2nd eigen values



Simulation Results: Ratio of 3rd eigen values



Likelihood Method

- Spatial correlation introduced through random effects
- Random effects are zero mean and satisfy the following

$$\mathrm{cov}(\gamma_{ip}, \gamma_{jq}) = \begin{cases} 0, & p \neq q \\ \rho^{|i-j|}\lambda_k, & p = q = k \end{cases}$$

Then

$$\mathrm{cov}(\tilde{\gamma}) = \begin{pmatrix} 1 & \rho & \rho^2 & \cdots & \rho^{n-1} \\ \rho & 1 & \rho & \cdots & \rho^{n-2} \\ \rho^2 & \rho & 1 & \cdots & \rho^{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho^{n-1} & \rho^{n-2} & \rho^{n-3} & \cdots & 1 \end{pmatrix} \otimes \Lambda$$

where

$$\Lambda = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_K \end{pmatrix}$$

Likelihood Method

We express the eigenfunctions $\{\phi_k(t)\}_{k=1}^K$ by basis expansion. Let $\{\mathbf{B}_i\}_{i=1}^n$ be the evaluation matrix of basis and $\mathbf{\Theta}$ be the coefficient matrix of $\{\phi_k(t)\}_{k=1}^K$ on basis functions. Then $\mathbf{\Phi}_i = \mathbf{B}_i\mathbf{\Theta}$ Hence, the full model is expressed as

$$\begin{pmatrix} \mathbf{Y}_1 \\ \vdots \\ \mathbf{Y}_n \end{pmatrix} = \begin{pmatrix} \mathbf{B}_1\mathbf{\Theta} & & \\ & \ddots & \\ & & \mathbf{B}_n\mathbf{\Theta} \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \vdots \\ \gamma_n \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{B}_1 & & \\ & \ddots & \\ & & \mathbf{B}_n \end{pmatrix} \begin{pmatrix} \mathbf{\Theta} & & \\ & \ddots & \\ & & \mathbf{\Theta} \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \vdots \\ \gamma_n \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{pmatrix}$$

where

- $\mathbf{Y}_i \to n_i \times 1$ vector of observed values for curve i.
- $\boldsymbol{\epsilon}_i \to n_i \times 1$ vector of measurement errors for curve i.
- $\mathbf{\Phi}_i \to n_i \times K$ matrix of eigenfunction evaluation on curve i.
- $\gamma_i \to K \times 1$ vector of random effects of curve i
- $\mathbf{B}_i \to n_i \times P$ matrix of P basis functions evaluation.
- $\mathbf{\Theta} \to P \times K$ matrix of coefficient matrix of K eigenfunctions on P basis functions.

The compact format becomes,

$$\tilde{\mathbf{Y}} = \tilde{\mathbf{B}}\tilde{\mathbf{\Theta}}\tilde{\gamma} + \tilde{\epsilon}$$

Likelihood Steps

Model:

$$\tilde{\mathbf{Y}} \sim \mathcal{N}(\mathbf{0}, \tilde{\mathbf{B}}\tilde{\mathbf{\Theta}}\mathbf{\Gamma}\tilde{\mathbf{\Theta}}'\tilde{\mathbf{B}}' + \sigma^2\mathbf{I})$$

Marginal Likelihood

$$L(\tilde{\mathbf{Y}}) = (2\pi)^{-N/2}|\tilde{\mathbf{B}}\tilde{\mathbf{\Theta}}\mathbf{\Gamma}\tilde{\mathbf{\Theta}}'\tilde{\mathbf{B}}' + \sigma^2\mathbf{I}|^{-1/2}\exp(-\frac{1}{2}\tilde{\mathbf{Y}}'(\tilde{\mathbf{B}}\tilde{\mathbf{\Theta}}\mathbf{\Gamma}\tilde{\mathbf{\Theta}}'\tilde{\mathbf{B}}' + \sigma^2\mathbf{I})^{-1}\tilde{\mathbf{Y}})$$

- Direct maximizing of this likelihood over $\varrho, \sigma^2, \Lambda$ and Θ is a difficult non-convex optimization problem.
- Solution: EM procedure by treating random effects as missing data and focus on the joint log likelihood

Joint log likelihood

$$\begin{aligned}\mathcal{L}(\tilde{\mathbf{Y}}, \tilde{\gamma}) &= C - N\log\sigma - \frac{1}{2\sigma^2}\sum_{i=1}(\mathbf{Y}_i - \mathbf{B}_i\mathbf{\Theta}\boldsymbol{\gamma}_i)'(\mathbf{Y}_i - \mathbf{B}_i\mathbf{\Theta}\boldsymbol{\gamma}_i) \\ &\quad -\frac{1}{2}\left(K\log D(\rho) + n\sum_{k=1}^{K}\log\lambda_k + \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{K} g_{ij}(\rho)\lambda_k^{-1}\gamma_{ik}\gamma_{jk}\right)\end{aligned}$$

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EM Step

E-Step:

It is easy to show that $\mathbb{E}(\mathcal{L}(\mathbf{Y}, \tilde{\gamma})|\mathbf{Y}, \boldsymbol{\Delta})$ depends on $\boldsymbol{\gamma}_i$ only through $\{\widehat{\gamma}_i = \mathbb{E}(\boldsymbol{\gamma}_i|\mathbf{Y}, \boldsymbol{\Delta})\}_{i=1}^n$, $\{\widehat{\gamma_{ik}\gamma_{jk}} = \mathbb{E}(\gamma_{ik}\gamma_{jk}|\tilde{\mathbf{Y}}, \boldsymbol{\Delta})\}_{k=1,i\neq j=1}^{K,n}$ and $\{\widehat{\boldsymbol{\gamma}_i\boldsymbol{\gamma}_i'} = \mathbb{E}(\boldsymbol{\gamma}_i\boldsymbol{\gamma}_i'|\tilde{\mathbf{Y}}, \boldsymbol{\Delta})\}_{i=1}^n$. Note that for each i, $\widehat{\boldsymbol{\gamma}_i\boldsymbol{\gamma}_i'} = \widehat{\gamma}_i\widehat{\gamma}_i{}' + \mathbb{V}(\boldsymbol{\gamma}_i|\tilde{\mathbf{Y}}, \boldsymbol{\Delta})$

M-Step

M-step is to maximize $\mathbb{E}(\mathcal{L}(\tilde{\mathbf{Y}}, \tilde{\gamma})|\tilde{\mathbf{Y}}, \boldsymbol{\Delta})$ over $\boldsymbol{\Lambda}$, $\boldsymbol{\Theta}$, σ^2 and ρ.

- Note that Λ and ϱ are separated from Θ and σ^2
- optimization over these parameters one at a time and do it iteratively.

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Simulation Results for moment based method

Simulation scheme

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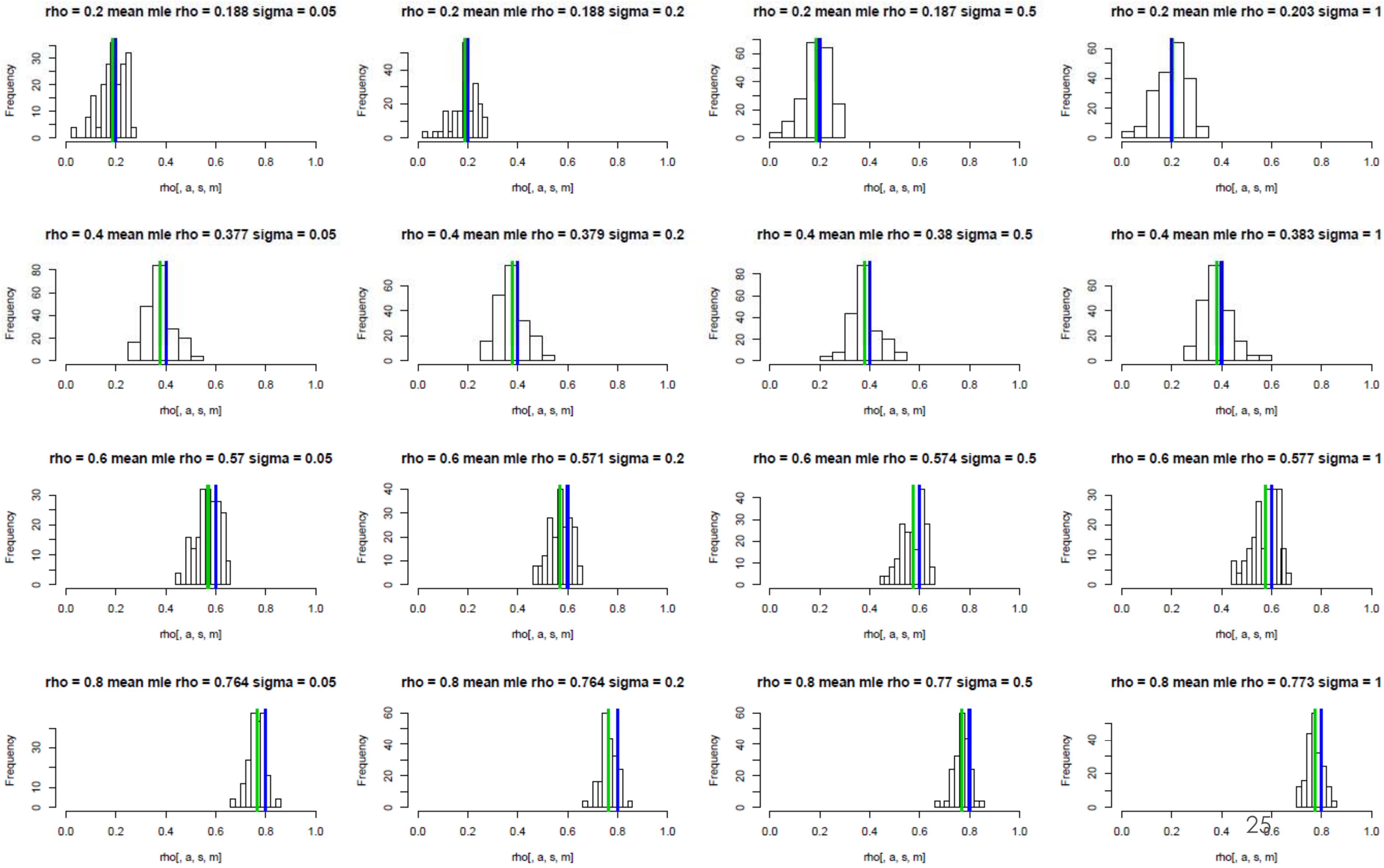
- AR(1) type spatial correlation(parameter is ϱ) =0.2, 0.4, 0.6, 0.8.
- noise standard deviation σ = 0.05, 0.2, 0.5, 1.
- Results for estimation of ϱ eigenfunction 1 to 3 with moment based method

EM estimates of correlation parameter



Reconstruction Results

- Given the estimate of spatial correlation structure, we can compute the expected principal component scores γ_{ik}

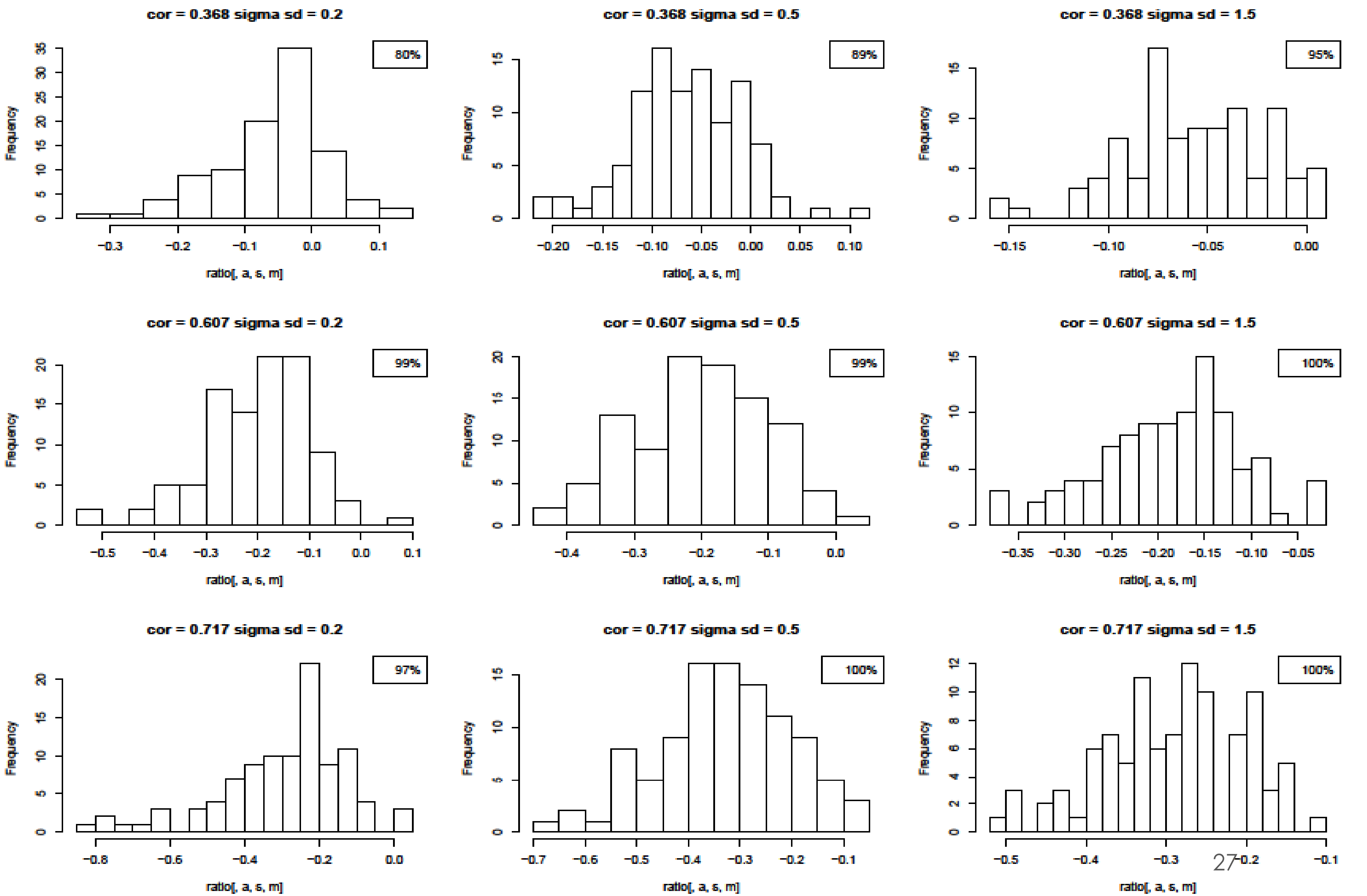
$$\hat{\hat{\gamma}}_{ik} = E(\gamma_{ik} \mid Y_1, Y_2, \ldots, Y_N)$$

- In the i.i.d curve case, the information set only include curve i,

$$\hat{\gamma}_{ik} = E(\gamma_{ik} \mid Y_i)$$

- For AR(1) correlated curves, curves were reconstructed using using $\hat{\gamma}_{ik}$ and $\hat{\hat{\gamma}}_{ik}$
- Performance measured by sum of squared errors over all curves.
- Negative log ratio suggest better performance

Histogram of log ratio of squared error



Future Work

Consistency

- For moment based estimates

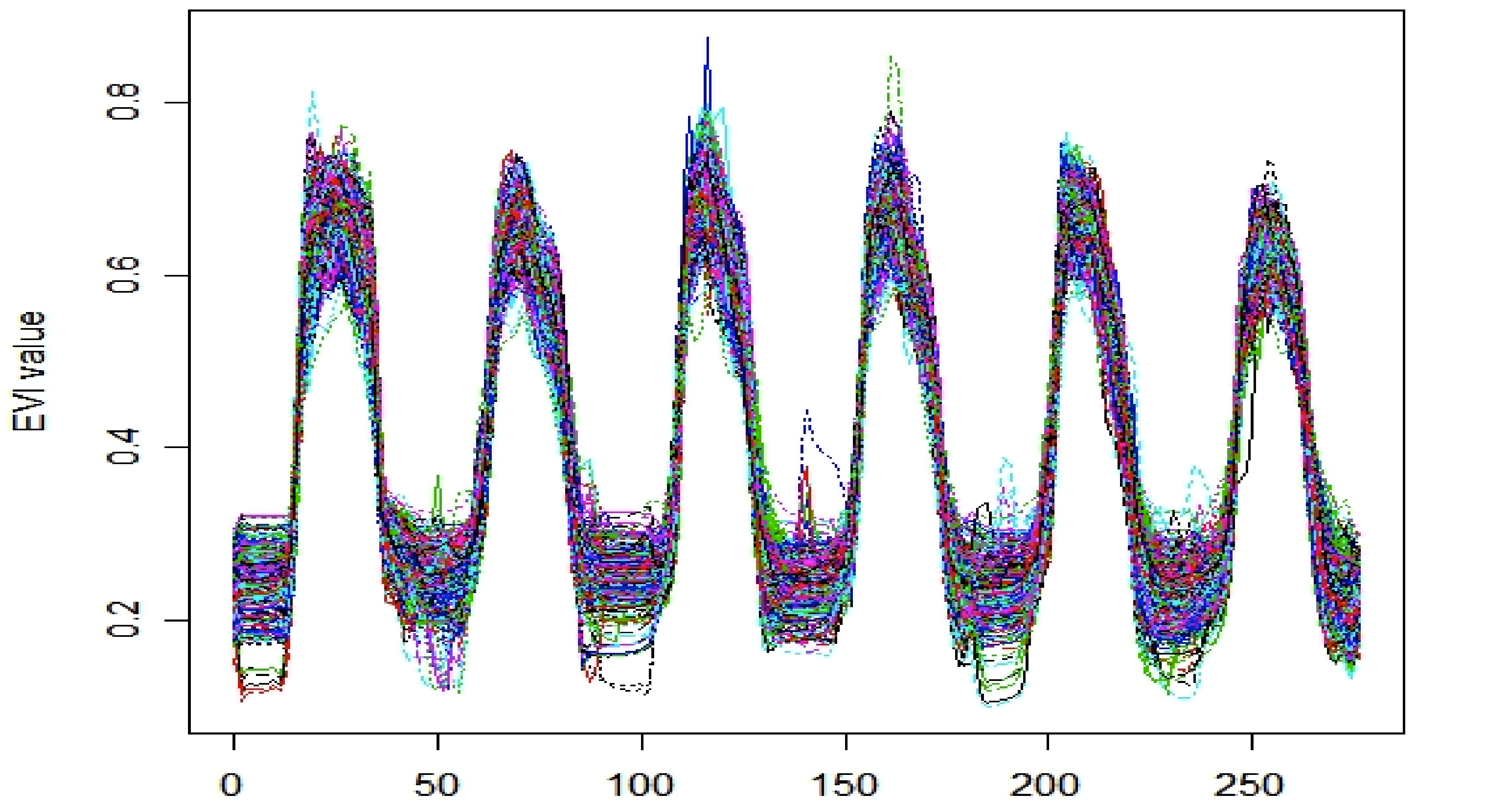
Strict geometric constraints for solving the EM steps.

- Hypothesize better convergence results from this approach.
- Following Peng and Paul's , 2009 paper on "A geometric approach to maximum likelihood estimation of the functional principal components from sparse longitudinal data"

Software:

- SPACE (Spatial Principal Analysis by Conditional Estimation)
- First version with limited spatial correlation choices.
- Follow up versions with more general spatial correlation.

Future Work



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- NSF Award No: #0947950: GLACIER-Global Change Initiative-Education & Research. 03/15/2010-03/14/2014

Related paper:

- Liu, C., Ray, S., Hooker, G., Friedl, M.F. (2012) Functional Factor Analysis For Periodic Remote Sensing Data. *Annals of Applied Statistics*, **6**:2, 601-624.