

# Advanced Bayesian Computation Weeks 6 & 7

**Rajarshi Guhaniyogi**  
**Winter 2018**

February 23, 2018

# Linear Model Co-regionalization

- Let  $\mathbf{A} = ((a_{ij}))_{i,j=1}^m$ , such that the entries above lower triangle are all zero.
- Assign  $a_{ij} \sim N(0, 1)$  and  $\log(a_{ii}) \sim N(0, 1)$  for  $i > j$ .
- Assume  $v_k(\mathbf{s}) \sim GP(0, C_{1,\phi_k})$  independently.
- $\phi_k$ 's are assigned uniform priors as before.
- It is customarily assumed that  $\Psi = \text{diag}(\psi_1, \dots, \psi_m)$ ,  $\psi_1, \dots, \psi_m > 0$ .
- $\psi_k \sim IG(a, b)$  a-priori, for  $k = 1, \dots, m$ .
- Entries of  $\mathbf{B}$  are assigned normal priors.

- Need to define  $\text{Cov}(\mathbf{w}(\mathbf{s}), \mathbf{w}(\mathbf{s}'))$ , where  $h = \|\mathbf{s} - \mathbf{s}'\|$ .
- Amounts to defining  $\text{Cov}(w_k(\mathbf{s}), w_k(\mathbf{s}'))$  and  $\text{Cov}(w_k(\mathbf{s}), w_j(\mathbf{s}'))$ .
- $\text{Cov}(w_k(\mathbf{s}), w_k(\mathbf{s}')) = M(h|\nu_k, a_k)$ ,  
 $\text{Cov}(w_k(\mathbf{s}), w_j(\mathbf{s}')) = \alpha_{kj}M(h|\nu_{kj}, a_{kj})$ .
- Parsimonious Matern kernel defines  $a_{kj} = a_k = a$  and  $\nu_{kj} = \frac{\nu_k + \nu_j}{2}$ .
- $\alpha_{kj} = \zeta_{kj} \lambda_k \lambda_j$ ,  $\lambda_k, \lambda_j > 0$
- $\zeta_{kj} = \eta_{kj} \frac{\Gamma(\nu_k + d/2)^{1/2}}{\Gamma(\nu_k)^{1/2}} \frac{\Gamma(\nu_j + d/2)^{1/2}}{\Gamma(\nu_j)^{1/2}} \frac{\Gamma((\nu_k + \nu_j)/2)}{\Gamma((\nu_k + \nu_j)/2 + d/2)}$ .
- $\eta_{kk} = 1$  and  $((\eta_{kj}))_{k,j=1}^m$  is non-negative definite.
- This ensures a valid multivariate cross covariance matrix.

# Gaussian process High Dimensional Regression

- Consider modeling the situation  $y = f(\mathbf{x}) + \epsilon$ , where  $\mathbf{x} \in \mathbb{R}^p$  where  $p$  is large.
- We have already seen in the theoretical study of Gaussian process that the convergence rate of the fitted function to the truth is  $n^{-s/(2s+p)}(\log(n))^c$ , where  $c$  is a constant,  $s$  is the smoothness of the true surface,  $p$  is the number of predictors and  $n$  is the sample size.
- When  $p$  is large, convergence rate suffers a lot.
- We land in a hopeless situation (similar to the linear regression case) where we need to add some assumption in the true regression model to be able to recover it.
- Assumption: The regression function is affected only by a few covariates.
- Alternatively, one assumes that the covariates lie in a lower dimensional noisy manifold.

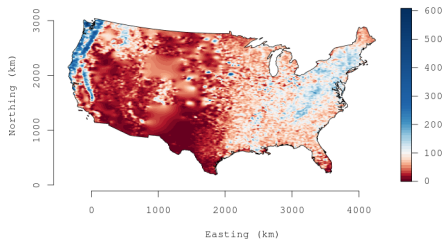
# Variable selection in Gaussian process

- Variable selection in Gaussian process is a very hard and unsolved problem.
- One idea was to employ a variant of the squared exponential covariance kernel.
- They define the covariance kernel
$$C_{\sigma^2, \phi, \lambda}(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp\left(-\sum_{j=1}^p \lambda_j (x_j - x'_j)^2\right).$$
- Use some penalty to select important  $\lambda_j$ 's.
- This is known as the automatic relevance determination (ARD).
- Full Bayesian updating of  $\lambda_j$ 's by adding a spike and slab prior and computing the posterior does not seem to work very well.

# Big data, large sample size $n$ and Gaussian Process

- In many machine learning or environmental applications number of predictors is small.
- Sample size is massive.
- Important data applications.
- It is a wide area with different strategies applied to different models.
- We will see a few strategies.

# Forest Biomass Data

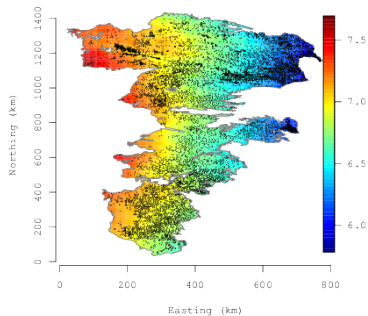


- Biomass is the biological material in a living or recently dead organism.
- Prediction of forest biomass is important to understand current carbon stock and flux, bio-feedstock for emerging bio-economies, and impact of deforestation.
- **Forest Inventory and Analysis (FIA)** under USDA collects data on Biomass regularly.

Depth of water table data between 1935 to 2013.



(a) High Plain Aquifer



(b) Depth of water table

Modeling of spatio-temporal trend of water table



# Problem with Gaussian processes with big data

- $\mathbf{y} = (y_1, \dots, y_n)'$  are observed data and  $\mathbf{x}_1, \dots, \mathbf{x}_n$  are the corresponding predictors.
- Let  $\mathbf{X} = [\mathbf{x}_1 : \dots : \mathbf{x}_n]'$  be the predictor matrix.
- Model:  $\mathbf{y} \sim N(\mu \mathbf{1}_n, \mathbf{C}_\theta + \tau^2 \mathbf{I})$ .
- Estimating parameters  $\theta$  from the likelihood

$$-\frac{1}{2} \log(\det(\mathbf{C}_\theta + \tau^2 \mathbf{I})) - \frac{1}{2} (\mathbf{y} - \mu \mathbf{1}_n)' (\mathbf{C}_\theta + \tau^2 \mathbf{I})^{-1} (\mathbf{y} - \mu \mathbf{1}_n)$$

## Challenges

- Store  $\mathbf{C}_\theta + \tau^2 \mathbf{I}$
- Compute  $\text{Chol}(\mathbf{C}_\theta + \tau^2 \mathbf{I}) = \mathbf{L}\mathbf{L}'$ .

# Low Rank Model

- Approximate  $\mathbf{C}_\theta \approx \mathbf{B}_\theta \mathbf{C}_\theta^{*-1} \mathbf{B}_\theta' + \mathbf{D}_\theta$
- $\mathbf{B}_\theta$  is the  $n \times r$  spatial basis matrix  $r \ll n$ .
- $\mathbf{C}_\theta^*$  is an  $r \times r$  spatial covariance matrix.
- $\mathbf{D}_\theta$  is either sparse or diagonal.
- Different choices of basis functions leads to different low rank models.
- The computational complexity  $O(r^3 + nr^2) \leq O(n^3)$ .

# Kernel Convolution

- Use a finite basis representation to approximate a Gaussian process.
- $f(\mathbf{x}) = \int K(\mathbf{x} - \mathbf{z}, \boldsymbol{\theta}) du(\mathbf{z})$ , where  $u(\mathbf{z})$  is a white noise process.
- This is called Kernel convolution of white noise processes and is widely used in environmental applications.
- An approximation of the  $f(\mathbf{x})$  by a finite sum is given by

$$f(\mathbf{x}) \approx \sum_{j=1}^J K(\mathbf{x} - \mathbf{z}_j^*, \boldsymbol{\theta}) u_j,$$

$\mathbf{z}_1^*, \dots, \mathbf{z}_J^*$  are “knot” points in  $\mathbb{R}^p$  and  $u_1, \dots, u_J \sim N(0, \sigma^2)$ .

- $J \ll n$ , i.e. number knots is much lesser than the sample size.
- Choice of  $K(\cdot, \boldsymbol{\theta})$  is important for the method to work.
- In the spatial context this idea was proposed in 2001 by David Higdon.

# Kernel Convolution

- Model

$$y = \mu + \sum_{j=1}^J K(\mathbf{x} - \mathbf{z}_j^*, \boldsymbol{\theta}) u_j + \epsilon, \quad \epsilon \sim N(0, \tau^2).$$

- With data  $(y_1, \mathbf{x}_1), \dots, (y_n, \mathbf{x}_n)$ , the data equation is given by

$$\mathbf{y} = \mu \mathbf{1}_n + \mathbf{K} \mathbf{u} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim N(0, \tau^2 \mathbf{I})$$

where the  $i$ th row of  $\mathbf{K}$  is given by  $(K(\mathbf{x}_i - \mathbf{z}_1^*, \boldsymbol{\theta}), \dots, K(\mathbf{x}_i - \mathbf{z}_J^*, \boldsymbol{\theta}))'$ .

- $\mathbf{u} = (u_1, \dots, u_J)' \sim N(0, \sigma^2 \mathbf{I})$ .
- Marginalizing over  $\mathbf{u}$ , the likelihood is  $N(\mathbf{y} | \mu \mathbf{1}_n, \sigma^2 \mathbf{K} \mathbf{K}' + \tau^2 \mathbf{I})$ .
- More generally, if one assumes  $u_1, \dots, u_J$  are correlated and  $\mathbf{u} \sim N(0, \sigma^2 \mathbf{D})$  then the likelihood is  $N(\mathbf{y} | \mu \mathbf{1}_n, \sigma^2 \mathbf{K} \mathbf{D} \mathbf{K}' + \tau^2 \mathbf{I})$ .

$$p(\mu, \sigma^2, \tau^2) \propto N(\mathbf{y} | \mu \mathbf{1}_n, \sigma^2 \mathbf{K} \mathbf{D} \mathbf{K}' + \tau^2 \mathbf{I}) \times p(\mu) \\ \times p(\tau^2) \times p(\sigma^2).$$

- $\mathbf{K}$  is a  $n \times J$  matrix.
- Inverting the  $n \times n$  matrix  $\mathbf{H} = \sigma^2 \mathbf{K} \mathbf{D} \mathbf{K}' + \tau^2 \mathbf{I}$  can be made easy with simple trick.
- This technique is called Sherman-Woodbury-Morrison matrix identity.
- The main computational cost comes from inverting a  $J \times J$  matrix.

# Posterior predictive distribution and estimation of regression function

- Posterior distribution of  $\mathbf{u}$  can be obtained easily.
- Note that  $p(\mathbf{u}|-) \propto N(\mathbf{y}|\mu\mathbf{1}_n + \mathbf{K}\mathbf{u}, \tau^2\mathbf{I}) \times N(\mathbf{u}|\mathbf{0}, \sigma^2\mathbf{D})$ .
- $\mathbf{u}|-$  follows a multivariate normal distribution.
- Prediction at new predictor  $\mathbf{x}$  can be obtained as before.
- $y \sim N(\mu + \sum_{j=1}^J K(\mathbf{x} - \mathbf{z}_j^*, \boldsymbol{\theta})u_j, \tau^2)$ . Draw posterior predictive samples from this distribution corresponding to every posterior sample of the parameters.

# Choice of the kernel function

- Choice of the kernel function plays important role in the kernel convolution method.
- Popular choices are radial basis functions, wavelet basis functions etc.
- There can be drastic differences with different choices of the basis function.
- Can the kernel choice be automated?

# Predictive Process Model (Banerjee et al., 2008)/Sparse Gaussian Process

- Consider a set of  $n^*$  knots  $\mathcal{S}^* = \{\mathbf{s}_1^*, \dots, \mathbf{s}_{n^*}^*\}$  with  $n^* \ll n$ .



# Predictive Process Model (Banerjee et al., 2008)/Sparse Gaussian Process

- Consider a set of  $n^*$  knots  $\mathcal{S}^* = \{\mathbf{s}_1^*, \dots, \mathbf{s}_{n^*}^*\}$  with  $n^* \ll n$ .
- Process realization over knots:  
 $\mathbf{w}^* = (w(\mathbf{s}_1), \dots, w(\mathbf{s}_{n^*}))' \sim N(\mathbf{0}, \sigma^2 \mathbf{R}^*)$ .

# Predictive Process Model (Banerjee et al., 2008)/Sparse Gaussian Process

- Consider a set of  $n^*$  knots  $\mathcal{S}^* = \{\mathbf{s}_1^*, \dots, \mathbf{s}_{n^*}^*\}$  with  $n^* \ll n$ .
- Process realization over knots:  
 $\mathbf{w}^* = (w(\mathbf{s}_1), \dots, w(\mathbf{s}_{n^*}))' \sim N(\mathbf{0}, \sigma^2 \mathbf{R}^*)$ .
- $\mathbf{R}^* = [\rho(\mathbf{s}_i^*, \mathbf{s}_j^*; \phi)]$  is an  $n^* \times n^*$ .

# Predictive Process Model (Banerjee et al., 2008)/Sparse Gaussian Process

- Consider a set of  $n^*$  knots  $\mathcal{S}^* = \{\mathbf{s}_1^*, \dots, \mathbf{s}_{n^*}^*\}$  with  $n^* \ll n$ .
- Process realization over knots:  
 $\mathbf{w}^* = (w(\mathbf{s}_1), \dots, w(\mathbf{s}_{n^*}^*))' \sim N(\mathbf{0}, \sigma^2 \mathbf{R}^*)$ .
- $\mathbf{R}^* = [\rho(\mathbf{s}_i^*, \mathbf{s}_j^*; \phi)]$  is an  $n^* \times n^*$ .
- Correlation between  $w(\mathbf{s})$  and  $\mathbf{w}^*$ :  $\mathbf{r}(\mathbf{s}) = [\rho(\mathbf{s}, \mathbf{s}_i^*; \phi)]$ .

# Predictive Process Model (Banerjee et al., 2008)/Sparse Gaussian Process

- Consider a set of  $n^*$  knots  $\mathcal{S}^* = \{\mathbf{s}_1^*, \dots, \mathbf{s}_{n^*}^*\}$  with  $n^* \ll n$ .
- Process realization over knots:  
 $\mathbf{w}^* = (w(\mathbf{s}_1), \dots, w(\mathbf{s}_{n^*}))' \sim N(\mathbf{0}, \sigma^2 \mathbf{R}^*)$ .
- $\mathbf{R}^* = [\rho(\mathbf{s}_i^*, \mathbf{s}_j^*; \phi)]$  is an  $n^* \times n^*$ .
- Correlation between  $w(\mathbf{s})$  and  $\mathbf{w}^*$ :  $\mathbf{r}(\mathbf{s}) = [\rho(\mathbf{s}, \mathbf{s}_i^*; \phi)]$ .
- predictive process:  $\tilde{w}(\mathbf{s}) = E[w(\mathbf{s}) | \mathbf{w}^*] = \mathbf{r}(\mathbf{s})' \mathbf{R}^{*-1} \mathbf{w}^*$

# Predictive Process Model (Banerjee et al., 2008)/Sparse Gaussian Process

- Consider a set of  $n^*$  knots  $\mathcal{S}^* = \{\mathbf{s}_1^*, \dots, \mathbf{s}_{n^*}^*\}$  with  $n^* \ll n$ .
- Process realization over knots:  
 $\mathbf{w}^* = (w(\mathbf{s}_1), \dots, w(\mathbf{s}_{n^*}^*))' \sim N(\mathbf{0}, \sigma^2 \mathbf{R}^*)$ .
- $\mathbf{R}^* = [\rho(\mathbf{s}_i^*, \mathbf{s}_j^*; \phi)]$  is an  $n^* \times n^*$ .
- Correlation between  $w(\mathbf{s})$  and  $\mathbf{w}^*$ :  $\mathbf{r}(\mathbf{s}) = [\rho(\mathbf{s}, \mathbf{s}_i^*; \phi)]$ .
- predictive process:  $\tilde{w}(\mathbf{s}) = E[w(\mathbf{s}) | \mathbf{w}^*] = \mathbf{r}(\mathbf{s})' \mathbf{R}^{*-1} \mathbf{w}^*$

predictive process model

$$y(\mathbf{s}) = \mathbf{x}(\mathbf{s})' \boldsymbol{\beta} + \tilde{w}(\mathbf{s}) + \epsilon(\mathbf{s}), \quad \epsilon(\mathbf{s}) \sim N(0, \tau^2)$$

# Predictive Process Model (Banerjee et al., 2008)/Sparse Gaussian Process

- Consider a set of  $n^*$  knots  $\mathcal{S}^* = \{\mathbf{s}_1^*, \dots, \mathbf{s}_{n^*}^*\}$  with  $n^* \ll n$ .
- Process realization over knots:  
 $\mathbf{w}^* = (w(\mathbf{s}_1), \dots, w(\mathbf{s}_{n^*}))' \sim N(\mathbf{0}, \sigma^2 \mathbf{R}^*).$

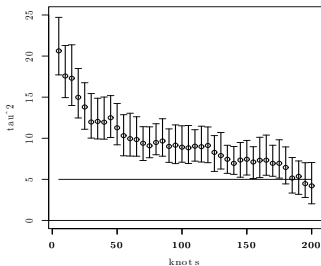
Dimension reduction comes from applying Sherman-Woodbury-Morrison matrix identity

Only inverting an  $n^* \times n^*$  matrix inversion is required at each stage of MCMC.

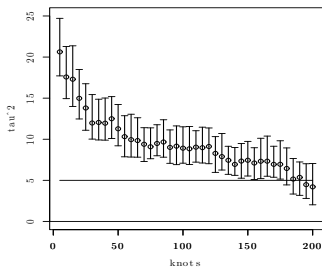
predictive process model

$$y(\mathbf{s}) = \mathbf{x}(\mathbf{s})'\beta + \tilde{w}(\mathbf{s}) + \epsilon(\mathbf{s}), \epsilon(\mathbf{s}) \sim N(0, \tau^2)$$

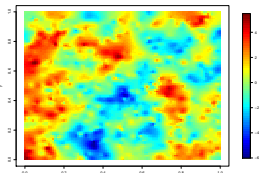
# Issues with PP: Overestimated Nugget & Smoothed Spatial Surface



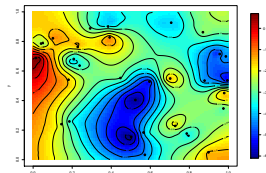
# Issues with PP: Overestimated Nugget & Smoothed Spatial Surface



True Spatial Surface

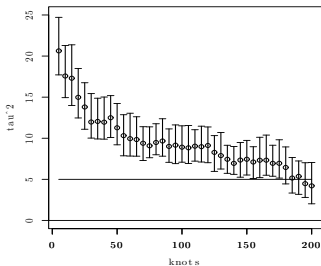


Predictive Process Surface





# Issues with PP: Overestimated Nugget & Smoothed Spatial Surface



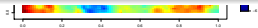
True Spatial Surface

Predictive Process Surface

## Quantified underestimation

$$\text{var}(w(\mathbf{s})) = \text{var}(\tilde{w}(\mathbf{s})) + \text{var}(w(\mathbf{s}) - \tilde{w}(\mathbf{s})) \geq \text{var}(\tilde{w}(\mathbf{s}))$$

$$\tilde{\epsilon}(\mathbf{s}) = w(\mathbf{s}) - \tilde{w}(\mathbf{s}) \sim GP(0, C_{\tilde{\epsilon}}(\mathbf{s}_1, \mathbf{s}_2; \theta))$$



# Model Based Bias Adjustments

▶ TPP slide

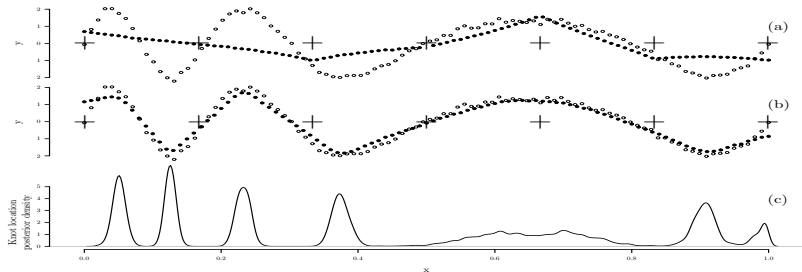
$$y(\mathbf{s}) = \mathbf{x}(\mathbf{s})'\boldsymbol{\beta} + \tilde{w}(\mathbf{s}) + \tilde{\epsilon}(\mathbf{s}) + \epsilon(\mathbf{s})$$

Modified predictive process (Finley et al., 2009)

$$\tilde{\epsilon}(\mathbf{s}_i) \stackrel{ind}{\sim} N(0, \delta^2(\mathbf{s}_i; \boldsymbol{\theta})); \quad \delta^2(\mathbf{s}; \boldsymbol{\theta}) = C_{\tilde{\epsilon}}(\mathbf{s}, \mathbf{s}; \boldsymbol{\theta}).$$

|            | True | Non-spatial        | PP                   | Modified PP         |
|------------|------|--------------------|----------------------|---------------------|
| $\beta_0$  | 8.25 | 8.26 (8.15 , 8.27) | 10.83 (9.29 , 12.60) | 9.21 (7.83 , 10.97) |
| $\sigma^2$ | 6    | –                  | 8.95 (2.68 , 15.81)  | 5.07 (3.44 , 7.32)  |
| $\tau^2$   | 0.5  | 3.59 (3.30 , 3.88) | 2.20 (2.02 , 2.40)   | .73 (.39 , 1.17)    |
| $\phi$     | 4    | –                  | 2.78 (2.32 , 3.62)   | 2.73 (2.23 , 5.38)  |
| G          | –    | 3959.95            | 2397.21              | 347.16              |
| P          | –    | 3943.83            | 2502.70              | 1471.05             |
| D          | –    | 7903.79            | 4899.91              | 1818.22             |
| $PD$       | –    | 1.95               | 31.79                | 731.42              |
| DIC        | –    | 2509.32            | 2000.50              | 1628.88             |

# Knots are Learning from The Data



- Observed data  $\circ$  drawn from normal distribution with varying frequency sine function mean and .01 variance
- knots are assigned  $U(0,1)$  prior.

+ naive knot starting locations

• posterior predictive means of 100 new locations

## Hierarchical adaptive predictive process model with random knots

$$[\boldsymbol{\beta}, \boldsymbol{\theta}_1, \mathcal{S}^*, \boldsymbol{\theta}_2 \mid \mathbf{y}, \mathcal{S}, n^*] \propto \times [\boldsymbol{\theta}_1] \times N(\boldsymbol{\beta} \mid \boldsymbol{\mu}_\beta, \boldsymbol{\Sigma}_\beta) \\ \times N(\mathbf{y} \mid \mathbf{X}\boldsymbol{\beta}, \boldsymbol{\Sigma}_y(\mathcal{S}^*, \mathcal{S}; \boldsymbol{\theta}_1)).$$

- Process parameter in data likelihood

## Hierarchical adaptive predictive process model with random knots

$$[\beta, \theta_1, \mathcal{S}^*, \theta_2 | \mathbf{y}, \mathcal{S}, n^*] \propto [\theta_2] \times [\theta_1] \times N(\beta | \mu_\beta, \Sigma_\beta) \\ \times [\mathcal{S}^* | \theta_2] \times N(\mathbf{y} | \mathbf{X}\beta, \Sigma_{\mathbf{y}}(\mathcal{S}^*, \mathcal{S}; \theta_1)).$$

- Process parameter in data likelihood

## Hierarchical adaptive predictive process model with random knots

$$[\beta, \theta_1, \mathcal{S}^*, \theta_2 | \mathbf{y}, \mathcal{S}, n^*] \propto [\theta_2] \times [\theta_1] \times N(\beta | \mu_\beta, \Sigma_\beta) \\ \times [\mathcal{S}^* | \theta_2] \times N(\mathbf{y} | \mathbf{X}\beta, \Sigma_{\mathbf{y}}(\mathcal{S}^*, \mathcal{S}; \theta_1)).$$

- Process parameter in data likelihood
- Parameters in the intensity surface for the knots.

## Hierarchical adaptive predictive process model with random knots

$$[\beta, \theta_1, \mathcal{S}^*, \theta_2 | \mathbf{y}, \mathcal{S}, n^*] \propto [\theta_2] \times [\theta_1] \times N(\beta | \mu_\beta, \Sigma_\beta) \\ \times [\mathcal{S}^* | \theta_2] \times N(\mathbf{y} | \mathbf{X}\beta, \Sigma_{\mathbf{y}}(\mathcal{S}^*, \mathcal{S}; \theta_1)).$$

- Process parameter in data likelihood
- Parameters in the intensity surface for the knots.
- Idea of modeling knots is applicable to any knot based low rank model.



## Modelling the intensity surface for knots

$$[\mathcal{S}^* | \eta_D, n^*] = \prod_{i=1}^{n^*} \frac{\eta(\mathbf{s}_i^*)}{\int_D \eta(\mathbf{s}) d\mathbf{s}}$$

## Modelling the intensity surface for knots

$$[\mathcal{S}^* | \eta_D, n^*] = \prod_{i=1}^{n^*} \frac{\eta(\mathbf{s}_i^*)}{\int_D \eta(\mathbf{s}) d\mathbf{s}}$$

- Parametric option:

$$\log \eta(\mathbf{s}; \boldsymbol{\theta}_2) = \frac{1}{m} \sum_{j=1}^m N_{2D}(\mathbf{s} | \mathbf{u}_j, \Sigma_\eta),$$

## Modelling the intensity surface for knots

$$[\mathcal{S}^* | \eta_D, n^*] = \prod_{i=1}^{n^*} \frac{\eta(\mathbf{s}_i^*)}{\int_D \eta(\mathbf{s}) d\mathbf{s}}$$

- Parametric option:

$$\log \eta(\mathbf{s}; \boldsymbol{\theta}_2) = \frac{1}{m} \sum_{j=1}^m N_{2D}(\mathbf{s} | \mathbf{u}_j, \Sigma_\eta),$$

- A log-Gaussian approach:

$$\eta(\mathbf{s}) = \exp\{\alpha w_2(\mathbf{s})\}; \quad w_2(\mathbf{s}) \sim GP(0, \rho_2(\cdot; \phi_2)),$$

## Modelling the intensity surface for knots

$$[\mathcal{S}^* | \eta_D, n^*] = \prod_{i=1}^{n^*} \frac{\eta(\mathbf{s}_i^*)}{\int_D \eta(\mathbf{s}) d\mathbf{s}}$$

- Parametric option:

$$\log \eta(\mathbf{s}; \boldsymbol{\theta}_2) = \frac{1}{m} \sum_{j=1}^m N_{2D}(\mathbf{s} | \mathbf{u}_j, \Sigma_\eta),$$

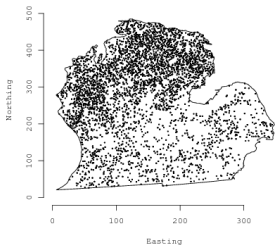
- A log-Gaussian approach:

$$\eta(\mathbf{s}) = \exp\{\alpha w_2(\mathbf{s})\}; w_2(\mathbf{s}) \sim GP(0, \rho_2(\cdot; \phi_2)),$$

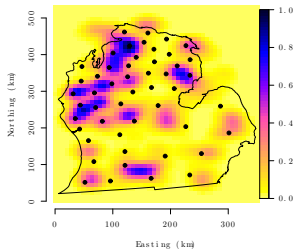
- Any other random measure on  $[\mathcal{S}^* | n^*]$ .

# Estimated Spatial Surface: PP vs. APP

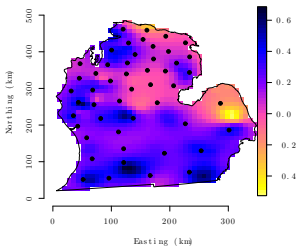
data locations



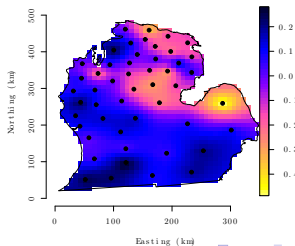
Knot density



APP: residual surface



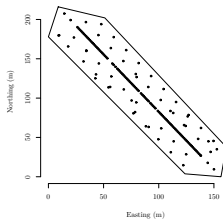
PP: residual surface



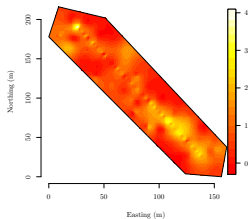
# Motivating Dataset on Soil Nutrients

▶ LMC

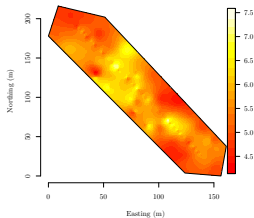
Soil sample locations



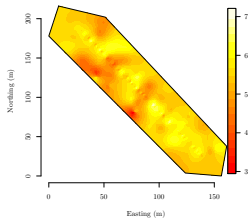
Phosphorus (P)



Sum of base cations (SBC)



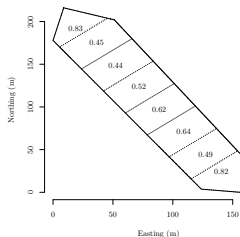
Sum of nitrogen (SN)



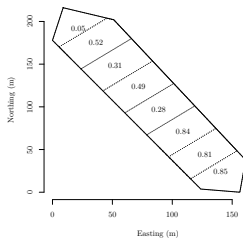
# Correlations Between Soil Nutrients are Space Varying

sub-domain correlation among the soil nutrient outcomes

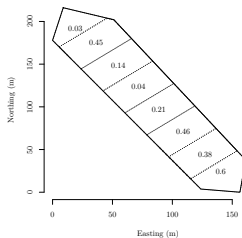
*PP,SBC*



*PP,SN*



*PSN,SBC*



# Multivariate Spatial Modeling

► Figure: Soil Nutrients

$$\mathbf{Y}(\mathbf{s}) = \boldsymbol{\mu}(\mathbf{s}) + \mathbf{W}(\mathbf{s}) + \boldsymbol{\epsilon}(\mathbf{s})$$

- Multivariate response
- Fixed effects
- Multivariate spatial function
- Multivariate error

$$\mathbf{Y}(\mathbf{s}) = (y_1(\mathbf{s}), \dots, y_m(\mathbf{s}))' \quad \mathbf{W}(\mathbf{s}) = (w_1(\mathbf{s}), \dots, w_m(\mathbf{s}))'$$

$$\boldsymbol{\epsilon}(\mathbf{s}) = (\epsilon_1(\mathbf{s}), \dots, \epsilon_m(\mathbf{s}))' \stackrel{iid}{\sim} N(\mathbf{0}, \boldsymbol{\Psi})$$

In our case  $m = 3$



# Linear Model Coregionalization

Constructive approach following factor analysis ideas:

$$\begin{pmatrix} w_1(\mathbf{s}) \\ \vdots \\ \vdots \\ w_m(\mathbf{s}) \end{pmatrix} = \begin{pmatrix} a_{11} & 0 & \dots & \dots & 0 \\ a_{21} & a_{22} & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{m1} & \dots & \dots & \dots & a_{mm} \end{pmatrix} \begin{pmatrix} v_1(\mathbf{s}) \\ \vdots \\ \vdots \\ v_m(\mathbf{s}) \end{pmatrix}$$

$W(\mathbf{s})$

controls correlation in  $w_i$ 's

$v_i(\cdot) \stackrel{ind}{\sim} GP(\cdot, \cdot; \theta_1)$

# Space Varying Linear Model Coregionalization

$$\begin{pmatrix} w_1(\mathbf{s}) \\ \vdots \\ w_m(\mathbf{s}) \end{pmatrix} = \begin{pmatrix} a_{11}(\mathbf{s}) & 0 & \dots & \dots & 0 \\ a_{21}(\mathbf{s}) & a_{22}(\mathbf{s}) & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{m1}(\mathbf{s}) & \dots & \dots & \dots & a_{mm}(\mathbf{s}) \end{pmatrix} \begin{pmatrix} v_1(\mathbf{s}) \\ \vdots \\ v_m(\mathbf{s}) \end{pmatrix}$$

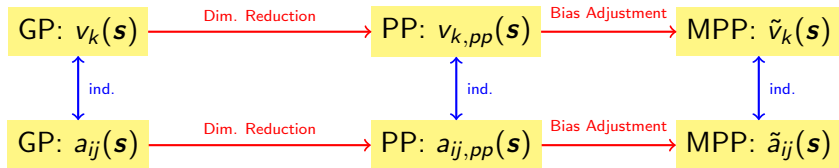
$W(\mathbf{s})$

$a_{ij}(\cdot) \stackrel{ind}{\sim} GP(\cdot, \cdot; \theta_{1,a})$

$v_i(\cdot) \stackrel{ind}{\sim} GP(\cdot, \cdot; \theta_1)$

- **Big-N** problem is encountered in updating  $\mathbf{v}_i = (v_i(\mathbf{s}_1), \dots, v_i(\mathbf{s}_n))'$ ,  $\mathbf{a}_{ij} = (a_{ij}(\mathbf{s}_1), \dots, a_{ij}(\mathbf{s}_n))'$ .

# Dimension Reduction



$$\tilde{W}(\mathbf{s}) = \tilde{A}(\mathbf{s}) \tilde{v}(\mathbf{s})$$

$$\begin{pmatrix} \tilde{w}_1(\mathbf{s}) \\ \vdots \\ \tilde{w}_m(\mathbf{s}) \end{pmatrix} = \begin{pmatrix} \tilde{a}_{11}(\mathbf{s}) & 0 & \cdots & \cdots & 0 \\ \tilde{a}_{21}(\mathbf{s}) & \tilde{a}_{22}(\mathbf{s}) & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \tilde{a}_{m1}(\mathbf{s}) & \cdots & \cdots & \cdots & \tilde{a}_{mm}(\mathbf{s}) \end{pmatrix} \begin{pmatrix} \tilde{v}_1(\mathbf{s}) \\ \vdots \\ \tilde{v}_m(\mathbf{s}) \end{pmatrix}$$



$\tilde{W}(\mathbf{s})$



$\tilde{a}_{ij}(\cdot) \stackrel{ind}{\sim} MPP(\cdot, \cdot; \theta_{1,a})$



$\tilde{v}_i(\cdot) \stackrel{ind}{\sim} MPP(\cdot, \cdot; \theta_1)$

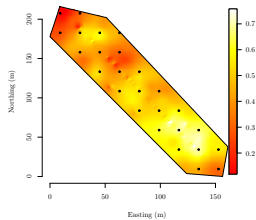
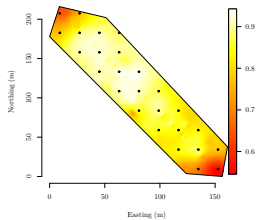
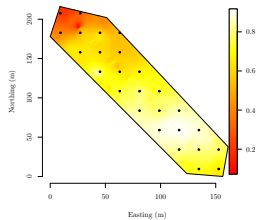
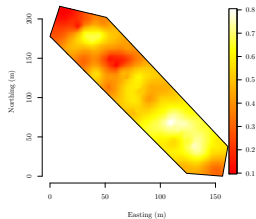
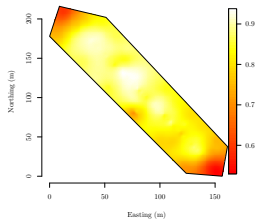
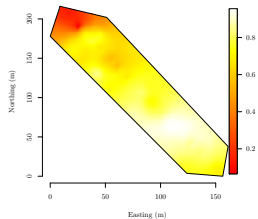
# Soil Nutrient Data Analysis

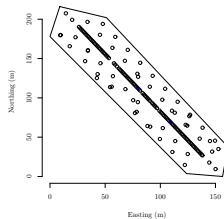
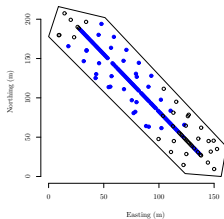
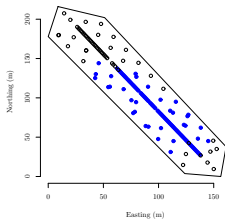
- 1 Modified predictive process models with varying number of knots are fitted.

|   | <b>Stationary</b> | <b>Non-stationary full</b> | <b>Non-stationary MPP<br/>26 knots</b> |
|---|-------------------|----------------------------|--|
| G | 39.45             | 28.02                      | 24.4                                   |
| P | 92.62             | 79.9                       | 77.28                                  |
| D | 132.07            | 107.92                     | 101.68                                 |

## Advantages over space varying full model

- 1 5 hours of running time for modified predictive process, 21 hours of running time for full model.
- 2 Better model fit.





- Observed points with statistically significant correlations given in blue.
- Left to right  $\rho(\mathbf{s})_{P,SBC}$ ,  $\rho(\mathbf{s})_{P,SN}$  and  $\rho(\mathbf{s})_{SN,SBC}$ .
- P, SN are highly correlated; so are P and SBC.