

# Lecture 27

## An Overview of Spatial Interpolation

STAT 8020 Statistical Methods II  
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Gaussian Process Spatial Model

Spatial Interpolation

Parameter estimation

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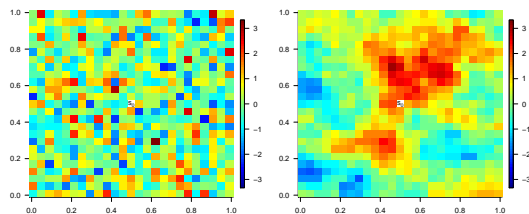
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### Toy Examples of Spatial Interpolation



**Question:** What is your best guess of the value of the missing pixel, denoted as  $Y(s_0)$ , for each case?

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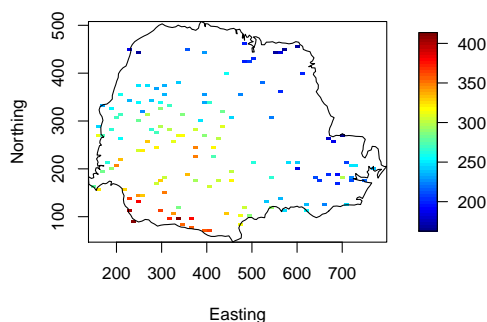
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### Interpolating Paraná State Precipitation Data



**Goal:** To interpolate the values in the spatial domain

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The Spatial Interpolation Problem

Given observations of a spatially varying quantity  $Y$  at  $n$  spatial locations

$y(s_1), y(s_2), \dots, y(s_n), \quad s_i \in \mathcal{S}, i = 1, \dots, n$

We want to estimate this quantity at any **unobserved location**

$Y(s_0), \quad s_0 \in \mathcal{S}$

Applications

- Mining: ore grade
- Climate: temperature, precipitation, ...
- Remote Sensing: CO<sub>2</sub> retrievals
- Environmental Science: air pollution levels, ...

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Some History

- Mining (Kriging 1951) Matheron (1960s), Forestry (Matérn 1960)
- More recent work: Cressie (1993) Stein (1999)



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## Linear Interpolation

The best guess (in a statistical sense) should be based on the conditional distribution  $[Y(s_0) | Y = y]$  where

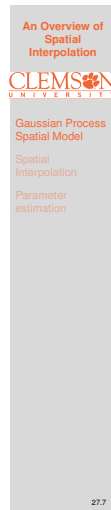
$$y = (y(s_1), \dots, y(s_n))^T$$

- Calculating this conditional distribution can be difficult

- Instead we use a **linear predictor**:

$$\hat{Y}(s_0) = \lambda_0 + \sum_{i=1}^n \lambda_i y(s_i)$$

- The best linear predictor is completely determined by the **mean** and **covariance** of  $\{Y(s), s \in S\}$ , and the observations  $y$



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## Gaussian Process (GP) Spatial Model

We assume that the observed data  $\{y(s_i)\}_{i=1}^n$  is one partial realization of a (continuously indexed) spatial GP  $\{Y(s)\}_{s \in S}$ .

**Model:**

$$Y(s) = m(s) + \epsilon(s), \quad s \in S \subset \mathbb{R}^d$$

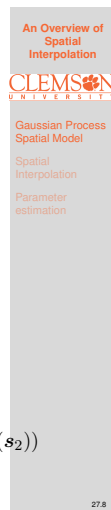
where

- Mean function:**

$$m(s) = E[Y(s)] = X^T(s)\beta$$

- Covariance function:**

$$\{\epsilon(s)\}_{s \in S} \sim \text{GP}(0, K(\cdot, \cdot)), \quad K(s_1, s_2) = \text{Cov}(\epsilon(s_1), \epsilon(s_2))$$



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## Assumptions on Covariance Function

In practice, the covariance must be estimated from the data  $(y(s_1), \dots, y(s_n))^T$ . We need to impose some structural assumptions

- Stationarity:**

$$\begin{aligned} K(s_1, s_2) &= \text{Cov}(\epsilon(s_1), \epsilon(s_2)) = C(s_1 - s_2) \\ &= \text{Cov}(\epsilon(s_1 + h), \epsilon(s_2 + h)) \end{aligned}$$

- Isotropy:**

$$K(s_1, s_2) = \text{Cov}(\epsilon(s_1), \epsilon(s_2)) = C(\|s_1 - s_2\|)$$



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## A Valid Covariance Function Must Be Positive Definite (p.d.)!

A covariance function is positive if

$$\sum_{i,j=1}^n a_i a_j C(\mathbf{s}_i - \mathbf{s}_j) \geq 0$$

for any finite locations  $\mathbf{s}_1, \dots, \mathbf{s}_n$ , and for any constants  $a_i, i = 1, \dots, n$

**Question:** what is the consequence if a covariance function is NOT p.d.?  $\Rightarrow$  weird things can happen

**Question:** How to guarantee a  $C(\cdot)$  is p.d.?

- Using a **parametric covariance function**
- Using **Bochner's Theorem** to construct a valid covariance function

## Notes

## Some Commonly Used Covariance Functions

- **Powered exponential:**

$$C(h) = \sigma^2 \exp\left(-\left(\frac{h}{\rho}\right)^\alpha\right), \quad \sigma^2 > 0, \rho > 0, 0 < \alpha \leq 2$$

- **Spherical:**

$$C(h) = \sigma^2 \left(1 - 1.5 \frac{h}{\rho} + 0.5 \left(\frac{h}{\rho}\right)^3\right) \mathbb{1}_{\{h \leq \rho\}}, \quad \sigma^2, \rho > 0$$

Note: it is only valid for 1,2, and 3 dimensional spatial domain.

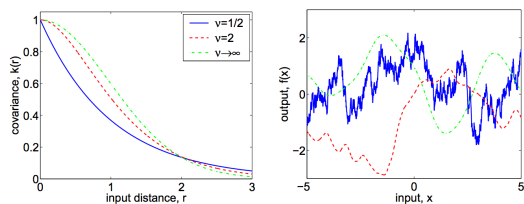
- **Matérn:**

$$C(h) = \sigma^2 \frac{(\sqrt{2\nu}h/\rho)^\nu K_\nu(\sqrt{2\nu}h/\rho)}{\Gamma(\nu)2^{\nu-1}}, \quad \sigma^2 > 0, \rho > 0, \nu > 0$$

*"Use the Matérn model" – Stein (1999, pp. 14)*

## Notes

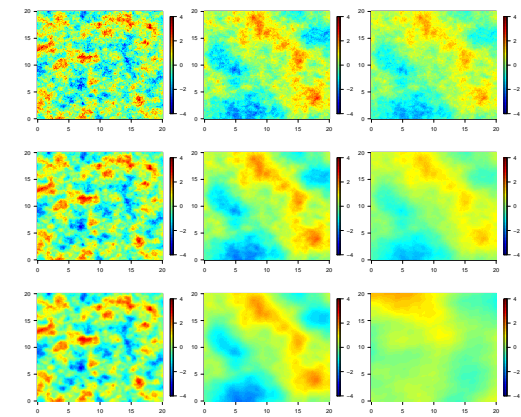
## 1-D Realizations from Matérn Model with Fixed $\sigma^2, \rho$



**Figure:** courtesy of Rasmussen & Williams 2006

## Notes

2-D Realizations from Matérn Model with Fixed  $\sigma^2$



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Conditional Distribution of Multivariate Normal

If 
$$\begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \sim N \left( \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} \right)$$

Then 
$$[Y_1|Y_2 = y_2] \sim N(\mu_{1|2}, \Sigma_{1|2})$$

where 
$$\begin{aligned} \mu_{1|2} &= \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(y_2 - \mu_2) \\ \Sigma_{1|2} &= \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} \end{aligned}$$

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GP-Based Spatial Interpolation: Kriging

If  $\{Y(s)\}_{s \in \mathcal{S}}$  follows a GP, then

$$\begin{pmatrix} Y_0 \\ \mathbf{Y} \end{pmatrix} \sim N \left( \begin{pmatrix} m_0 \\ \mathbf{m} \end{pmatrix}, \begin{pmatrix} \sigma_0^2 & k^T \\ k & \Sigma \end{pmatrix} \right)$$

We have

$$[Y_0 | \mathbf{Y} = \mathbf{y}] \sim N \left( m_{Y_0 | \mathbf{Y} = \mathbf{y}}, \sigma_{Y_0 | \mathbf{Y} = \mathbf{y}}^2 \right)$$

where

$$\begin{aligned} m_{Y_0 | \mathbf{Y} = \mathbf{y}} &= m_0 + k^T \Sigma^{-1} (\mathbf{y} - \boldsymbol{\mu}) \\ \sigma_{Y_0 | \mathbf{Y} = \mathbf{y}}^2 &= \sigma_0^2 - k^T \Sigma^{-1} k \end{aligned}$$

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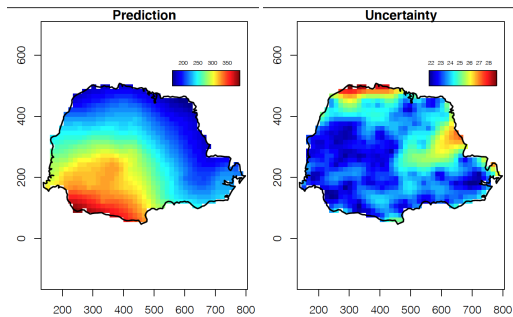
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Spatial Prediction of Paraná State Rainfall



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GP-Based Spatial Interpolation: Kriging

If  $\{Y(s)\}_{s \in \mathcal{S}}$  follows a GP, then

$$\begin{pmatrix} Y_0 \\ \mathbf{Y} \end{pmatrix} \sim N \left( \begin{pmatrix} m_0 \\ \mathbf{m} \end{pmatrix}, \begin{pmatrix} \sigma_0^2 & k^T \\ k & \Sigma \end{pmatrix} \right)$$

We have

$$[Y_0 | \mathbf{Y} = \mathbf{y}] \sim N \left( m_{Y_0 | \mathbf{Y} = \mathbf{y}}, \sigma_{Y_0 | \mathbf{Y} = \mathbf{y}}^2 \right)$$

where

$$\begin{aligned} m_{Y_0 | \mathbf{Y} = \mathbf{y}} &= m_0 + k^T \Sigma^{-1} (\mathbf{y} - \boldsymbol{\mu}) \\ \sigma_{Y_0 | \mathbf{Y} = \mathbf{y}}^2 &= \sigma_0^2 - k^T \Sigma^{-1} k \end{aligned}$$

Question: what if we don't know  $m_0, \mathbf{m}, \sigma_0^2, \Sigma$ ?  
⇒ We need to estimate the mean and covariance from the data  $\mathbf{y}$ .

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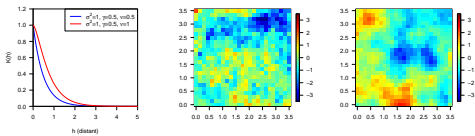
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Gaussian Process

We assume that the observed data  $\{y(s_i)\}_{i=1}^n$  is one partial realization of a (continuously indexed) spatial stochastic process  $\{Y(s)\}_{s \in \mathcal{S}}$ .

- Gaussian Processes GP  $(m(\cdot), K(\cdot, \cdot))$  are widely used in modeling spatial stochastic processes
- Spatial statisticians often focus on the covariance function. e.g.  $K(h) = \sigma^2 \frac{(\sqrt{2\nu}h/\gamma)^\nu K_\nu(\sqrt{2\nu}h/\gamma)}{\Gamma(\nu)2^{\nu-1}}$



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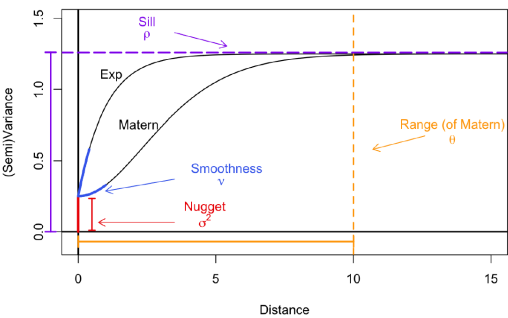
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Semivariogram  $\{\frac{1}{2} \text{Var}(Y(s_i, s_j))\}_{i,j}$



Source: fields vignette by Wiens and Krock, 2019

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Variogram, Semivariogram, and Covariance Function

Under the stationary and isotropic assumptions

Variogram:

$$\begin{aligned} 2\gamma(s_i, s_j) &= \text{Var}(Y(s_i) - Y(s_j)) \\ &= E\left\{((Y(s_i) - \mu(s_i)) - (Y(s_j) - \mu(s_j)))^2\right\} \\ &= E\left\{(Y(s_i) - Y(s_j))^2\right\} \\ &= 2\gamma(\|s_i - s_j\|) = 2\gamma(h) \end{aligned}$$

Semivariogram and covariance function:

$$\gamma(h) = C(0) - C(h)$$

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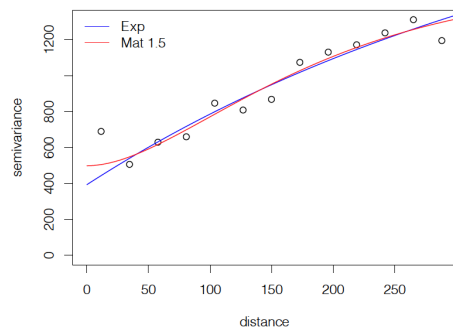
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Estimation: Least Squares Method

$$\underset{\theta}{\operatorname{argmin}} \sum_u \frac{n_u}{\gamma(h_u; \theta)^2} [\hat{\gamma}(h_u) - \gamma(h_u; \theta)]^2$$



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Maximum Likelihood Estimation (MLE)

Log-likelihood:

Given data  $\mathbf{y} = (y(s_1), \dots, y(s_n))^T$

$$\ell_n(\beta, \theta; \mathbf{y}) \propto -\frac{1}{2} \log |\Sigma_\theta| - \frac{1}{2} (\mathbf{y} - \mathbf{X}^T \beta)^T [\Sigma_\theta]_{n \times n}^{-1} (\mathbf{y} - \mathbf{X}^T \beta)$$

where  $\Sigma_\theta(i, j) = \sigma^2 \rho_{\rho, \nu}(\|s_i - s_j\|) + \tau^2 \mathbb{1}_{\{s_i = s_j\}}, i, j = 1, \dots, n$

for any fixed  $\theta_0 \in \Theta$  the unique value of  $\beta$  that maximizes  $\ell_n$  is given by

$$\hat{\beta} = \left( \mathbf{X}^T \Sigma_{\theta_0}^{-1} \mathbf{X} \right)^{-1} \mathbf{X}^T \Sigma_{\theta_0} \mathbf{y}$$

Then we obtain the profile log likelihood

$$\ell_n(\theta; \mathbf{y}) \propto -\frac{1}{2} \log |\Sigma_\theta| - \frac{1}{2} \mathbf{y}^T P(\theta) \mathbf{y}$$

where

$$P(\theta) = \Sigma_\theta^{-1} - \Sigma_\theta^{-1} \mathbf{X} \left( \mathbf{X}^T \Sigma_\theta^{-1} \mathbf{X} \right)^{-1} \mathbf{X}^T \Sigma_\theta$$

Solve the maximization problem above to get the MLE

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