Lecture 14

Interpolation of Spatial Data I

DSA 8020 Statistical Methods II

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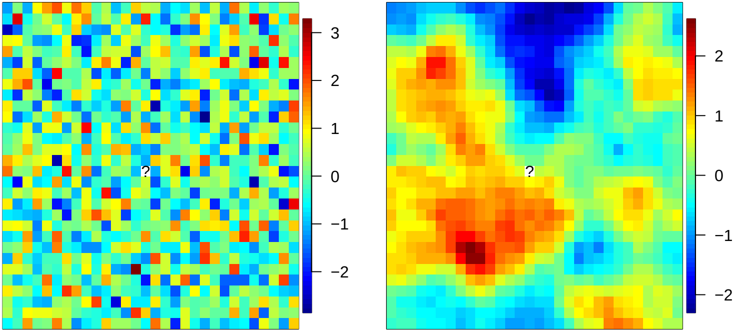
Agenda

1. Background
2. Gaussian Process Spatial Model
3. Spatial Interpolation

Toy Examples of Spatial Interpolation

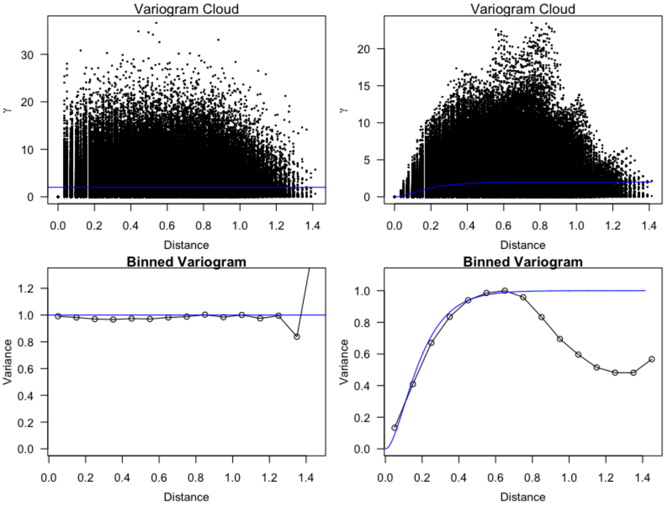
Let's consider two spatial images, each with a missing pixel



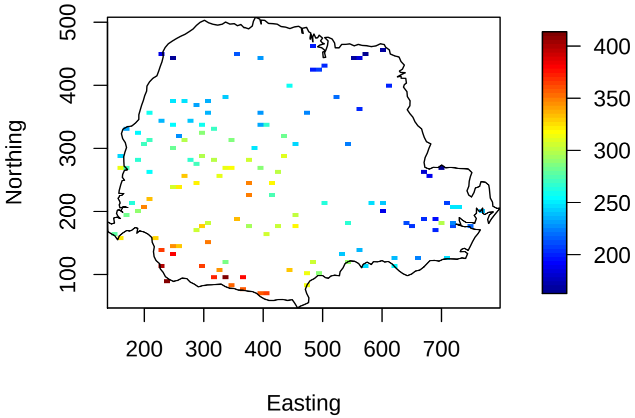
Question: What is your best guess of the value of the missing pixel, denoted as $Y(s_0)$, for each case?

Visualizing Spatial Dependence Structure

Similar to time series analysis, we can compute the covariance between data points in space to examine the degree of spatial dependence.



Interpolating Paraná State Precipitation Data



Goal: To interpolate the values in the spatial domain

The Spatial Interpolation Problem

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

$$y(\boldsymbol{s}_1), y(\boldsymbol{s}_2), \cdots, y(\boldsymbol{s}_n), \qquad \boldsymbol{s}_i \in \mathcal{S}, \, i = 1, \cdots, n$$

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

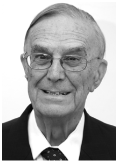
$$Y(\boldsymbol{s}_0), \qquad \boldsymbol{s}_0 \in \mathcal{S}$$

Applications

- Mining: ore grade
- Climate: temperature, precipitation, $\cdots$
- Remote Sensing: CO_2 retrievals
- Environmental Science: air pollution levels, $\cdots$

Some History of Spatial Statistics

- Mining (Krige 1951) Matheron (1960s), Forestry (Matérn 1960)



- More recent work: Cressie (1993) Stein (1999)


Outline

Linear Interpolation

The best guess (in a statistical sense) should be based on the conditional distribution $[Y(\boldsymbol{s}_0)|\boldsymbol{Y} = \boldsymbol{y}]$ where

$$\boldsymbol{y} = (y(\boldsymbol{s}_1), \cdots, y(\boldsymbol{s}_n))^{\mathrm{T}}$$

- Calculating this conditional distribution can be difficult
- Instead we use a linear predictor:

$$\hat{Y}(\boldsymbol{s}_0) = \lambda_0 + \sum_{i=1}^{n} \lambda_i y(\boldsymbol{s}_i)$$

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

Next, we will introduce a class of spatial model where the distribution is fully determined by its mean and covariance

Gaussian Process (GP) Spatial Model

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

Model:

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

where

- Mean function:

$$m(\boldsymbol{s}) = \mathrm{E}\left[Y(\boldsymbol{s})\right] = \boldsymbol{X}^T(\boldsymbol{s})\boldsymbol{\beta}$$

- Covariance function:

$$\{\epsilon(\boldsymbol{s})\}_{\boldsymbol{s}\in\mathcal{S}} \sim \mathrm{GP}\left(0, K\left(\cdot,\cdot\right)\right), \quad K(\boldsymbol{s}_1, \boldsymbol{s}_2) = \mathrm{Cov}\left(\epsilon(\boldsymbol{s}_1), \epsilon(\boldsymbol{s}_2)\right)$$

Assumptions on Covariance Function

In practice, the covariance must be estimated from the data $(y(\boldsymbol{s}_1), \cdots, y(\boldsymbol{s}_n))^{\mathrm{T}}$. We need to impose some structural assumptions

- Stationarity:

$$\begin{aligned} K(\boldsymbol{s}_1, \boldsymbol{s}_2) &= \mathrm{Cov}\left(\epsilon(\boldsymbol{s}_1), \epsilon(\boldsymbol{s}_2)\right) = C(\boldsymbol{s}_1 - \boldsymbol{s}_2) \\ &= \mathrm{Cov}\left(\epsilon(\boldsymbol{s}_1 + \boldsymbol{h}), \epsilon(\boldsymbol{s}_2 + \boldsymbol{h})\right) \end{aligned}$$

- Isotropy:

$$K(\boldsymbol{s}_1, \boldsymbol{s}_2) = \mathrm{Cov}\left(\epsilon(\boldsymbol{s}_1), \epsilon(\boldsymbol{s}_2)\right) = C(\|\boldsymbol{s}_1 - \boldsymbol{s}_2\|)$$

A Valid Covariance Function Must Be Positive Definite!

A covariance function is positive definite (p.d.) if

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

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

Question: what is the consequence if a covariance function is NOT p.d.? ⇒ We can get a negative variance

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

- Using a parametric covariance function (see some examples in next slide)
- Using Bochner's Theorem to construct a valid covariance function

Some Commonly Used Covariance Functions

- Powered exponential:

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

- Spherical:

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

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

- Matérn:

$$C(h) = \sigma^2 \frac{\left(\sqrt{2\nu}h/\rho\right)^\nu \mathcal{K}_\nu\left(\sqrt{2\nu}h/\rho\right)}{\Gamma(\nu)2^{\nu-1}}, \qquad \sigma^2 > 0,\ \rho > 0,\ \nu > 0$$

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

1-D Realizations from Matérn Model with Fixed σ^2, ρ

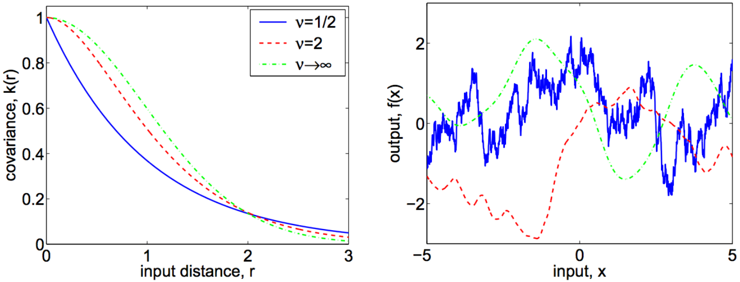
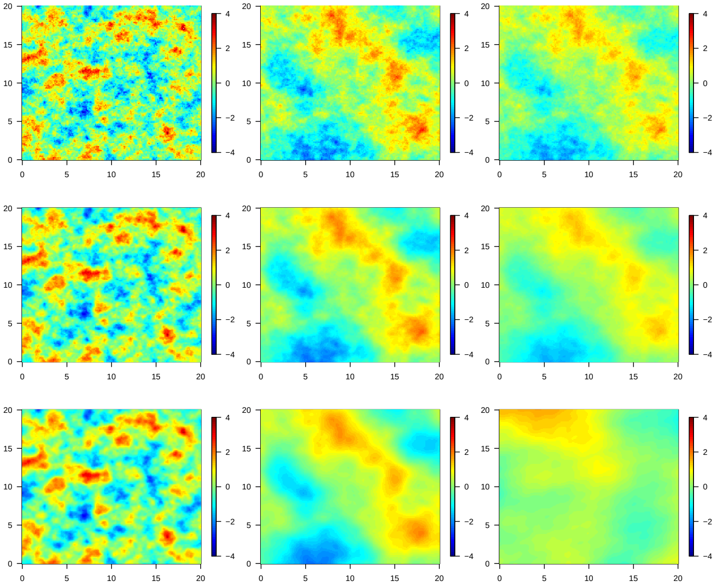


Figure: courtesy of Rasmussen & Williams 2006

The larger ν is, the smoother the process is

2-D Realizations from Matérn Model with Fixed σ^2



Outline

Conditional Distribution of Multivariate Normal

If

$$\begin{pmatrix} \boldsymbol{Y}_1 \\ \boldsymbol{Y}_2 \end{pmatrix} \sim \mathrm{N}\left(\begin{pmatrix} \boldsymbol{\mu_1} \\ \boldsymbol{\mu_2} \end{pmatrix}, \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} \right)$$

Then

$$[\boldsymbol{Y}_1 | \boldsymbol{Y}_2 = \boldsymbol{y}_2] \sim \mathrm{N}\left(\boldsymbol{\mu_{1|2}}, \Sigma_{1|2}\right)$$

where

$$\boldsymbol{\mu_{1|2}} = \boldsymbol{\mu_1} + \Sigma_{12}\Sigma_{22}^{-1}\left(\boldsymbol{y}_2 - \boldsymbol{\mu_2}\right)$$
$$\Sigma_{1|2} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}$$

GP-Based Spatial Interpolation: Kriging

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

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

We have

$$[Y_0 | \boldsymbol{Y} = \boldsymbol{y}] \sim \mathrm{N}\left(m_{Y_0|\boldsymbol{Y}=\boldsymbol{y}}, \sigma^2_{Y_0|\boldsymbol{Y}=\boldsymbol{y}}\right)$$

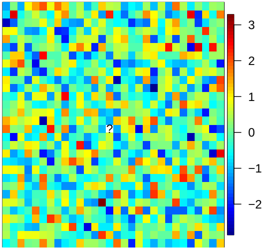
where

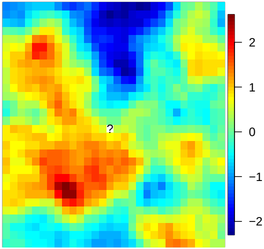
$$\begin{aligned} m_{Y_0|\boldsymbol{Y}=\boldsymbol{y}} &= m_0 + k^{\mathrm{T}}\Sigma^{-1}(\boldsymbol{y} - \boldsymbol{m}) \\ \sigma^2_{Y_0|\boldsymbol{Y}=\boldsymbol{y}} &= \sigma_0^2 - k^{\mathrm{T}}\Sigma^{-1}k \end{aligned}$$

Next, we are going to revisit our toy examples

Toy Examples Revisited

For simplicity, we assume $m(s) = 0$ for $s \in \mathcal{S}$, the spatial covariance only depends on distance





$$m_{Y_0|\boldsymbol{Y}=\boldsymbol{y}} = 0 + k^{\mathrm{T}}\Sigma^{-1}(\boldsymbol{y} - \boldsymbol{0}), \quad \sigma^2_{Y_0|\boldsymbol{Y}=\boldsymbol{y}} = \sigma_0^2 - k^{\mathrm{T}}\Sigma^{-1}k$$

Spatial uncorrelated field:

- $m_{Y_0|\boldsymbol{Y}} = 0$
- $\sigma^2_{Y_0|\boldsymbol{Y}=\boldsymbol{y}} = \sigma_0^2$

Spatial correlated field:

- $m_{Y_0|\boldsymbol{Y}} = k^{\mathrm{T}}\Sigma^{-1}\boldsymbol{y}$
- $\sigma^2_{Y_0|\boldsymbol{Y}=\boldsymbol{y}} = \sigma_0^2 - k^{\mathrm{T}}\Sigma^{-1}k$

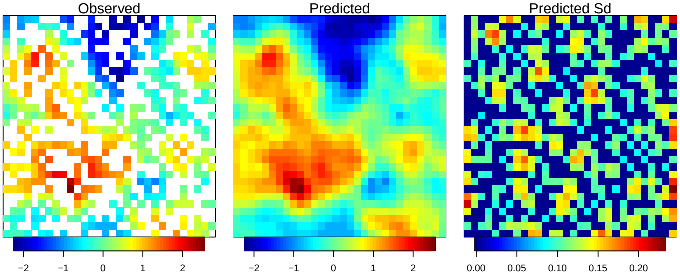
Interpolating Multiple Points in Space

In practice, we would like to predict the values at many locations. The Gaussian conditional distribution formula can still be used:

$$[\boldsymbol{Y}_0 | \boldsymbol{Y} = \boldsymbol{y}] \sim \mathrm{N}\left(\boldsymbol{m}_{\boldsymbol{Y}_0|\boldsymbol{Y}=\boldsymbol{y}}, \Sigma_{\boldsymbol{Y}_0|\boldsymbol{Y}=\boldsymbol{y}}\right)$$

where

$$\boldsymbol{m}_{\boldsymbol{Y}_0|\boldsymbol{Y}=\boldsymbol{y}} = \boldsymbol{m}_0 + \boldsymbol{k}^{\mathrm{T}} \Sigma^{-1} (\boldsymbol{y} - \boldsymbol{m})$$
$$\Sigma_{\boldsymbol{Y}_0|\boldsymbol{Y}=\boldsymbol{y}} = \Sigma_0 - \boldsymbol{k}^{\mathrm{T}} \Sigma^{-1} \boldsymbol{k}$$



GP-Based Spatial Interpolation: Kriging

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

$$\begin{pmatrix} \boldsymbol{Y}_0 \\ \boldsymbol{Y} \end{pmatrix} \sim \mathrm{N}\left(\begin{pmatrix} \boldsymbol{m}_0 \\ \boldsymbol{m} \end{pmatrix}, \begin{pmatrix} \Sigma_0 & \boldsymbol{k}^{\mathrm{T}} \\ \boldsymbol{k} & \Sigma \end{pmatrix} \right)$$

We have

$$[\boldsymbol{Y}_0 | \boldsymbol{Y} = \boldsymbol{y}] \sim \mathrm{N}\left(\boldsymbol{m}_{\boldsymbol{Y}_0|\boldsymbol{Y}=\boldsymbol{y}}, \Sigma_{\boldsymbol{Y}_0|\boldsymbol{Y}=\boldsymbol{y}} \right)$$

where

$$\begin{aligned} \boldsymbol{m}_{\boldsymbol{Y}_0|\boldsymbol{Y}=\boldsymbol{y}} &= \boldsymbol{m}_0 + \boldsymbol{k}^{\mathrm{T}} \Sigma^{-1} (\boldsymbol{y} - \boldsymbol{m}) \\ \Sigma_{\boldsymbol{Y}_0|\boldsymbol{Y}=\boldsymbol{y}} &= \Sigma_0 - \boldsymbol{k}^{\mathrm{T}} \Sigma^{-1} \boldsymbol{k} \end{aligned}$$

Question: what if we don't know $m(s; \boldsymbol{\beta}), c(h; \boldsymbol{\theta})$?

$\Rightarrow$ We need to estimate the mean and covariance from the data $\boldsymbol{y}$.

Summary

These slides cover:

- The problem of spatial interpolation
- Stationarity and Isotropy of a spatial process
- Gaussian Process Spatial Models

R functions/tricks to know:

- `vgram` (under the package `fields`) for visualizing spatial dependence
- `image.plot` (under the package `fields`) for visualizing spatial images
- Some matrix calculation tricks for speeding up computation

Bochner's Theorem

A complex-valued function C on $\mathbb{R}^{\mathrm{d}}$ is the covariance function for a weakly stationary mean square contituous complex-valued random process on $\mathbb{R}^d$ if and only if it can be represented as

$$C(\boldsymbol{h}) = \int_{\mathbb{R}^d} \exp(i\omega^{\mathrm{T}}\boldsymbol{h})F(d\boldsymbol{\omega}),$$

with F a positive finite measure. When F has a density with respect to Lebesgue measure, we have the spectral density f and

$$f(\omega) = \frac{1}{2\pi}\int_{\mathbb{R}^d} \exp(-i\omega^{\mathrm{T}}\boldsymbol{h})C(\boldsymbol{h})\,d\boldsymbol{h}$$