Introduction to Geostatistics

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May 15, 2023

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- Course materials available at https://doserjef.github.io/CASANR23-Spatial-Modeling/

What is spatial data?

- Any data with some geographical information (i.e., spatially indexed)
- Common sources of spatial data: agricultural, climatology, forestry, ecology, environmental health, disease epidemiology, product marketing, etc.
    - have many important predictors and response variables
    - are often presented as maps

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  - are often presented as maps
- Other examples where spatial need not refer to space on earth:
  - Genetics (position along a chromosome)
  - Neuroimaging (data for each voxel in the brain)

Point-referenced spatial data

- Each observation is associated with a location (point)
- Data represents a sample from a continuous spatial domain
- Also referred to as geocoded or geostatistical data

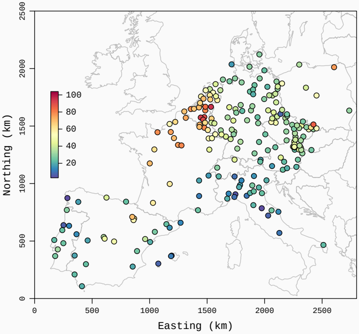


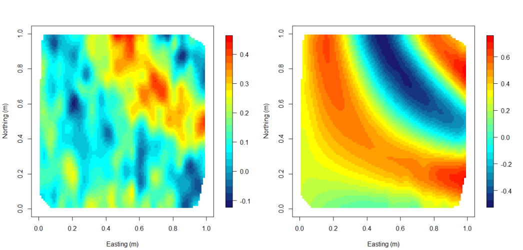
Figure: Pollutant levels in Europe in March, 2009

Point level modeling

- Point-level modeling refers to modeling of point-referenced data collected at locations referenced by coordinates (e.g., lat-long, Easting-Northing).
- Data from a spatial process $\{Y(\mathbf{s}) : \mathbf{s} \in \mathscr{D}\}$, $\mathscr{D}$ is a subset in Euclidean space.
- Example: $Y(\mathbf{s})$ is a pollutant level at site $\mathbf{s}$
- Conceptually: Pollutant level exists at all possible sites
- Practically: Data will be a partial realization of a spatial process – observed at $\{\mathbf{s}_1, \ldots, \mathbf{s}_n\}$
- Statistical objectives: Inference about the process $Y(\mathbf{s})$; predict at new locations.
- Remarkable: Can learn about entire $Y(\mathbf{s})$ surface. The key: Structured dependence

Exploratory data analysis (EDA): Plotting the data

- A typical setup: Data observed at n locations $\{\mathbf{s}_1, \ldots, \mathbf{s}_n\}$
- At each $\mathbf{s}_i$ we observe the response $y(\mathbf{s}_i)$ and a $p \times 1$ vector of covariates $\mathbf{x}(s_i)$
- Surface plots of the data often helps to understand spatial patterns



$y(\mathbf{s})$ $\quad$ $x(\mathbf{s})$

Figure: Response and covariate surface plots for Dataset 1

What's so special about spatial?

- Linear regression model: $y(\mathbf{s}_i) = \mathbf{x}(s_i)^\top \beta + \epsilon(\mathbf{s}_i)$
- $\epsilon(\mathbf{s}_i)$ are iid $N(0, \tau^2)$ errors
- $\mathbf{y} = (y(\mathbf{s}_1), \dots, y(\mathbf{s}_n))^\top$; $\mathbf{X} = (\mathbf{x}(\mathbf{s}_1)^\top, \dots, \mathbf{x}(\mathbf{s}_n)^\top)^\top$
- Inference: $\hat{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \sim N(\beta, \tau^2 (\mathbf{X}^\top \mathbf{X})^{-1})$
- Prediction at new location $\mathbf{s}_0$: $\widehat{y(s_0)} = \mathbf{x}(s_0)^\top \hat{\beta}$
- Although the data is spatial, this is an ordinary linear regression model

Residual plots

- Surface plots of the residuals $(y(\mathbf{s}) - \widehat{y(\mathbf{s})})$ help to identify any spatial patterns left unexplained by the covariates

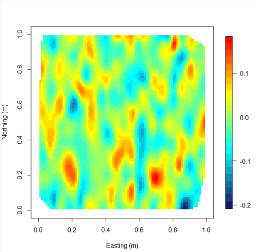


Figure: Residual plot for Dataset 1 after linear regression on $x(\mathbf{s})$

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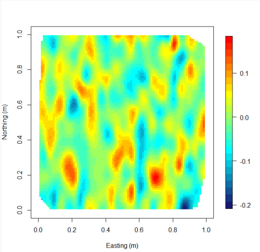
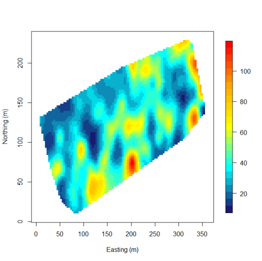


Figure: Residual plot for Dataset 1 after linear regression on $x(\mathbf{s})$

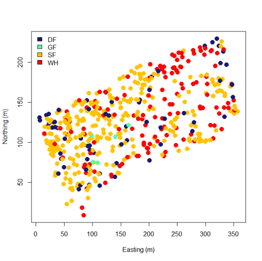
- No evident spatial pattern in plot of the residuals
- The covariate $x(\mathbf{s})$ seem to explain all spatial variation in $y(\mathbf{s})$
- Does a non-spatial regression model always suffice?

Western Experimental Forestry (WEF) data

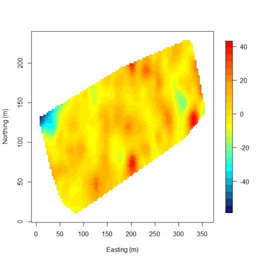
- Data consist of a census of all trees in a 10 ha. stand in Oregon
- Response of interest: Diameter at breast height (DBH)
- Covariate: Tree species (Categorical variable)



DBH



Species



Residuals

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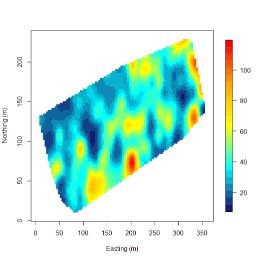
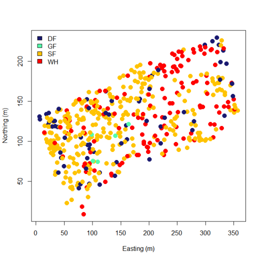


DBH



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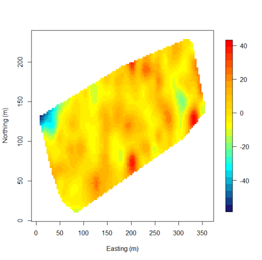

Residuals

- Local spatial patterns in the residual plot
- Simple regression on species seems to be not sufficient

More EDA

- Besides eyeballing residual surfaces, how to do more formal EDA to identify spatial pattern?

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First law of geography

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- In general $(Y(\mathbf{s}+\mathbf{h}) - Y(\mathbf{s}))^2$ roughly increasing with $||\mathbf{h}||$ will imply a spatial correlation
- Can this be formalized to identify spatial pattern?

Empirical semivariogram

- Binning: Make intervals $I_1 = (0, m_1)$, $I_2 = (m_1, m_2)$, and so forth, up to $I_K = (m_{K-1}, m_K)$. Representing each interval by its midpoint t_k, we define:

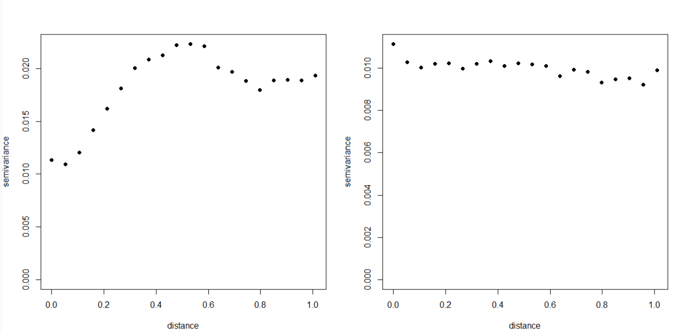
$$N(t_k) = \{(\mathbf{s}_i, \mathbf{s}_j) : \|\mathbf{s}_i - \mathbf{s}_j\| \in I_k\}, k = 1, \ldots, K.$$

- Empirical semivariogram:

$$\gamma(t_k) = \frac{1}{2|N(t_k)|} \sum_{\mathbf{s}_i, \mathbf{s}_j \in N(t_k)} (Y(\mathbf{s}_i) - Y(\mathbf{s}_j))^2$$

- For spatial data, the $\gamma(t_k)$ is expected to roughly increase with t_k
- A flat semivariogram would suggest little spatial variation

Empirical variogram: Data 1

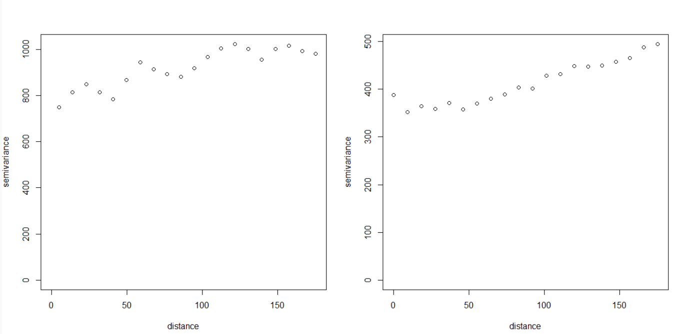


y residuals

- Residuals display little spatial variation

Empirical variograms: WEF data

- Regression model: DBH $\sim$ Species



DBH　　　Residuals

- Variogram of the residuals confirm unexplained spatial variation

Modeling with the locations

- When purely covariate based models does not suffice, one needs to leverage the information from locations
- General model using the locations:
  $y(\mathbf{s}) = \mathbf{x}(\mathbf{s})^\top \beta + w(\mathbf{s}) + \epsilon(\mathbf{s})$ for all $\mathbf{s} \in \mathscr{D}$
- How to choose the function $w(\cdot)$?
- Since we want to predict at any location over the entire domain $\mathscr{D}$, this choice will amount to choosing a surface $w(\mathbf{s})$
- How should such a surface be chosen?

Gaussian Processes (GPs)

- One popular approach to model $w(\mathbf{s})$ is via Gaussian Processes (GP)
- The collection of random variables $\{w(\mathbf{s}) \,|\, \mathbf{s} \in \mathscr{D}\}$ is a GP if
  - it is a valid stochastic process
  - all finite dimensional densities $\{w(\mathbf{s}_1), \ldots, w(\mathbf{s}_n)\}$ follow multivariate Gaussian distribution
- A GP is completely characterized by a mean function $m(\mathbf{s})$ and a covariance function $C(\cdot, \cdot)$
- Advantage: Likelihood based inference.
  $w = (\mathbf{w}(s_1), \ldots, w(\mathbf{s}_n))^\top \sim N(\mathbf{m}, \mathbf{C})$ where
  $\mathbf{m} = (m(\mathbf{s}_1), \ldots, m(\mathbf{s}_n))^\top$ and $\mathbf{C} = C(\mathbf{s}_i, \mathbf{s}_j)$

Valid covariance functions and isotropy

- $C(\cdot,\cdot)$ needs to be valid. For all n and all $\{\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_n\}$, the resulting covariance matrix $C(\mathbf{s}_i, \mathbf{s}_j)$ for $(w(\mathbf{s}_1), w(\mathbf{s}_2), \dots, w(\mathbf{s}_n))$ must be positive definite
- So, $C(\cdot,\cdot)$ needs to be a positive definite function
- Simplifying assumptions:
  - Stationarity: $C(\mathbf{s}_1, \mathbf{s}_2)$ only depends on $\mathbf{h} = \mathbf{s}_1 - \mathbf{s}_2$ (and is denoted by $C(\mathbf{h})$)
  - Isotropic: $C(\mathbf{h}) = C(||\mathbf{h}||)$
  - Anisotropic: Stationary but not isotropic
- Isotropic models are popular because of their simplicity, interpretability, and because a number of relatively simple parametric forms are available as candidates for C.

Some common isotropic covariance functions

Model	Covariance function, $C(t) = C(\|\|h\|\|)$
Spherical	$C(t) = \begin{cases} 0 & \text{if } t \geq 1/\phi \\ \sigma^2 \left[1 - \frac{3}{2}\phi t + \frac{1}{2}(\phi t)^3\right] & \text{if } 0 < t \leq 1/\phi \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$
Exponential	$C(t) = \begin{cases} \sigma^2 \exp(-\phi t) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$
Powered exponential	$C(t) = \begin{cases} \sigma^2 \exp(-\lvert\phi t\rvert^p) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$
Matérn at $\nu = 3/2$	$C(t) = \begin{cases} \sigma^2 (1 + \phi t) \exp(-\phi t) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$

Notes on exponential model

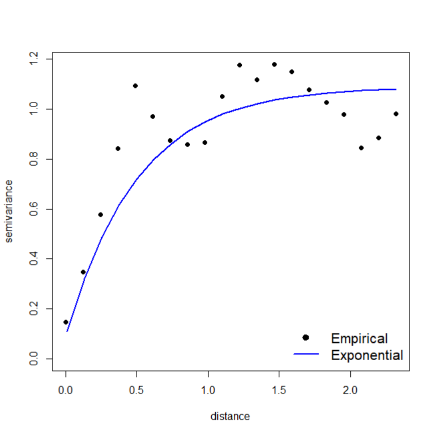
$$C(t) = \begin{cases} \tau^2 + \sigma^2 & \text{if } t = 0 \\ \sigma^2 \exp(-\phi t) & \text{if } t > 0 \end{cases} .$$

- We define the effective range, t_0, as the distance at which this correlation has dropped to only 0.05. Setting $\exp(-\phi t_0)$ equal to this value we obtain $t_0 \approx 3/\phi$, since $\log(0.05) \approx -3$.
- The nugget τ^2 is often viewed as a "nonspatial effect variance,"
- The partial sill (σ^2) is viewed as a "spatial effect variance."
- $\sigma^2 + \tau^2$ gives the maximum total variance often referred to as the sill
- Note discontinuity at 0 due to the nugget. Intentional! To account for measurement error or micro-scale variability.

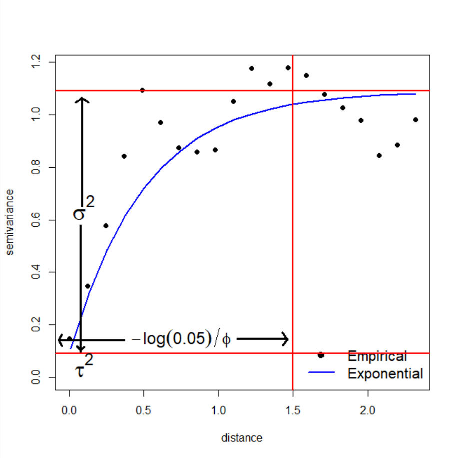
Covariance functions and semivariograms

- Recall: Empirical semivariogram:
  $\gamma(t_k) = \frac{1}{2|N(t_k)|} \sum_{\mathbf{s}_i, \mathbf{s}_j \in N(t_k)} (Y(\mathbf{s}_i) - Y(\mathbf{s}_j))^2$
- For any stationary GP,
  $E(Y(\mathbf{s}+\mathbf{h}) - Y(\mathbf{s}))^2/2 = C(\mathbf{0}) - C(\mathbf{h}) = \gamma(\mathbf{h})$
- $\gamma(\mathbf{h})$ is the semivariogram corresponding to the covariance function $C(\mathbf{h})$
- Example: For exponential GP,
  $\gamma(t) = \begin{cases} \tau^2 + \sigma^2(1 - \exp(-\phi t)) & \text{if } t > 0 \\ 0 & \text{if } t = 0 \end{cases}$, where $t = ||\mathbf{h}||$

Covariance functions and semivariograms



Covariance functions and semivariograms



The Matèrn covariance function

- The Matèrn is a very versatile family:

$$C(t) = \begin{cases} \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)}(2\sqrt{\nu}t\phi)^\nu K_\nu(2\sqrt(\nu)t\phi) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{if } t = 0 \end{cases}$$

  K_ν is the modified Bessel function of order ν (computationally tractable)

- ν is a smoothness parameter controlling process smoothness. Remarkable!
- $\nu = 1/2$ gives the exponential covariance function

Kriging: Spatial prediction at new locations

- Goal: Given observations $\mathbf{w} = (w(\mathbf{s}_1), w(\mathbf{s}_2), \ldots, w(\mathbf{s}_n))^\top$, predict $w(\mathbf{s}_0)$ for a new location $\mathbf{s}_0$
- If $w(\mathbf{s})$ is modeled as a GP, then $(w(\mathbf{s}_0), w(\mathbf{s}_1), \ldots, w(\mathbf{s}_n))^\top$ jointly follow multivariate normal distribution
- $w(\mathbf{s}_0) \,|\, \mathbf{w}$ follows a normal distribution with
  - Mean (kriging estimator): $m(\mathbf{s}_0) + \mathbf{c}^\top \mathbf{C}^{-1}(\mathbf{w} - \mathbf{m})$
  - where $m = E(\mathbf{w})$, $\mathbf{C} = Cov(\mathbf{w})$, $\mathbf{c} = Cov(\mathbf{w}, w(\mathbf{s}_0))$
  - Variance: $\mathbf{C}(\mathbf{s}_0, \mathbf{s}_0) - \mathbf{c}^\top \mathbf{C}^{-1}\mathbf{c}$
- The GP formulation gives the full predictive distribution of $w(\mathbf{s}_0)|\mathbf{w}$

Modeling with GPs

Spatial linear model

$$y(\mathbf{s}) = x(\mathbf{s})^\top \beta + w(\mathbf{s}) + \epsilon(\mathbf{s})$$

- $w(\mathbf{s})$ modeled as $GP(0, C(\cdot \mid \boldsymbol{\theta}))$ (usually without a nugget)
- $\epsilon(\mathbf{s}) \overset{\text{iid}}{\sim} N(0, \tau^2)$ contributes to the nugget
- Under isotropy: $C(\mathbf{s} + \mathbf{h}, \mathbf{s}) = \sigma^2 R(||\mathbf{h}||\,; \phi)$
- $\mathbf{w} = (w(\mathbf{s}_1), \ldots, w(\mathbf{s}_n))^\top \sim N(\mathbf{0}, \sigma^2 \mathbf{R}(\phi))$ where $\mathbf{R}(\phi) = \sigma^2(R(||s_i - s_j||\,; \phi))$
- $\mathbf{y} = (y(\mathbf{s}_1), \ldots, y(\mathbf{s}_n))^\top \sim N(\mathbf{X}\beta, \sigma^2 \mathbf{R}(\phi) + \tau^2 \mathbf{I})$

Parameter estimation

- $\mathbf{y} = (y(\mathbf{s}_1), \ldots, y(\mathbf{s}_n))^\top \sim N(\mathbf{X}\beta, \sigma^2\mathbf{R}(\phi) + \tau^2\mathbf{I})$
- We can obtain MLEs of parameters $\beta, \tau^2, \sigma^2, \phi$ based on the above model and use the estimates to krige at new locations
- In practice, the likelihood is often very flat with respect to the spatial covariance parameters and choice of initial values is important
- Initial values can be eyeballed from empirical semivariogram of the residuals from ordinary linear regression
- Estimated parameter values can be used for kriging

Model comparison

- For k total parameters and sample size n:
  - AIC: $2k - 2\log(l(\mathbf{y} \mid \hat{\beta}, \hat{\theta}, \hat{\tau^2}))$
  - BIC: $\log(n)k - 2\log(l(\mathbf{y} \mid \hat{\beta}, \hat{\theta}, \hat{\tau^2}))$

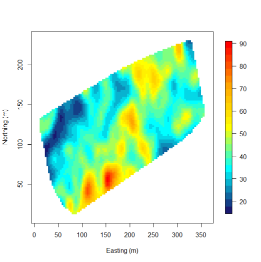
- Prediction based approaches using holdout data:
  - Root Mean Square Predictive Error (RMSPE): $\sqrt{\frac{1}{n_{out}} \sum_{i=1}^{n_{out}} (y_i - \hat{y}_i)^2}$
  - Coverage probability (CP): $\frac{1}{n_{out}} \sum_{i=1}^{n_{out}} I(y_i \in (\hat{y}_{i,0.025}, \hat{y}_{i,0.975}))$
  - Width of 95% confidence interval (CIW): $\frac{1}{n_{out}} \sum_{i=1}^{n_{out}} (\hat{y}_{i,0.975} - \hat{y}_{i,0.025})$
  - The last two approaches compares the distribution of y_i instead of comparing just their point predictions

Back to WEF data

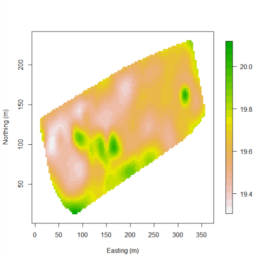
Table: Model comparison

	Spatial	Non-spatial
AIC	4419	4465
BIC	4448	4486
RMSPE	18	21
CP	93	93
CIW	77	82

WEF data: Kriged surfaces



DBH Estimates



Standard errors

Summary

- Geostatistics – Analysis of point-referenced spatial data
- Surface plots of data and residuals
- EDA with empirical semivariograms
- Modeling unknown surfaces with Gaussian Processes
- Kriging: Predictions at new locations
- Spatial linear regression using Gaussian Processes