Analysis of univariate point referenced spatial data

Abhi Datta

January 26, 2018

Department of Biostatistics, Bloomberg School of Public Health, Johns Hopkins University, Baltimore, Maryland

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:
  $y(s) = x(s)'\beta + w(s) + \epsilon(s)$ for all $s \in D$
- How to choose the function $w(\cdot)$?
- Since we want to predict at any location over the entire domain D, this choice will amount to choosing a surface $w(s)$
- How to do this ?

Gaussian Processes (GPs)

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

Valid covariance functions and isotropy

- $C(\cdot,\cdot)$ needs to be valid. For all n and all $\{s_1, s_2, ..., s_n\}$, the resulting covariance matrix $C(s_i, s_j)$ for $(w(s_1), w(s_2), ..., w(s_n))$ must be positive definite
- So, $C(\cdot,\cdot)$ needs to be a positive definite function
- Simplifying assumptions:
  - Stationarity: $C(s_1, s_2)$ only depends on $h = s_1 - s_2$ (and is denoted by $C(h)$)
  - Isotropic: $C(h) = C(||h||)$
  - 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	$C(t) = \begin{cases} \sigma^2 \exp(-\|\phi t\|^p) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$
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

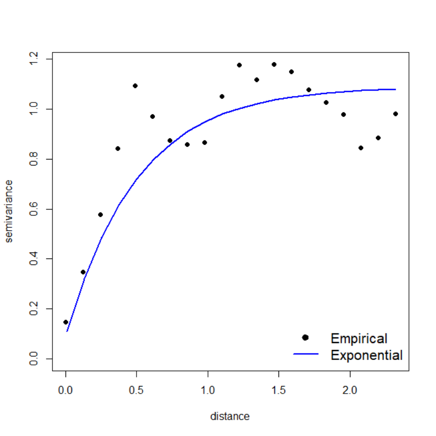
$$C(t) = \begin{cases} \tau^2 + \sigma^2 & \text{if } t = 0 \\ \sigma^2 \exp(-\phi t) & \text{if } t > 0 \end{cases}.$$

- 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.

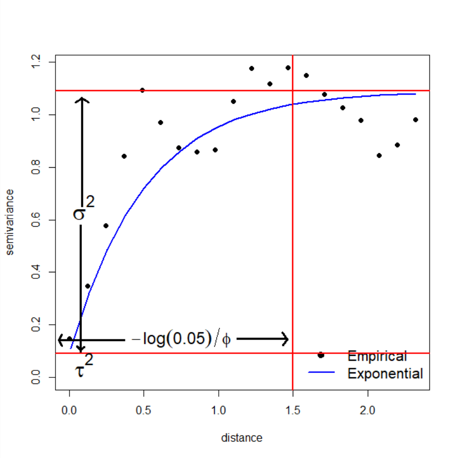
Covariance functions and semivariograms

- Recall: Empirical semivariogram: $\gamma(t_k) = \frac{1}{2|N(t_k)|} \sum_{s_i, s_j \in N(t_k)} (Y(s_i) - Y(s_j))^2$
- For any stationary GP, $E(Y(s+h) - Y(s))^2/2 = C(0) - C(h) = \gamma(h)$
- $\gamma(h)$ is the semivariogram corresponding to the covariance function $C(h)$
- 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 $t = ||h||$

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 $w = (w(s_1), w(s_2), \ldots, w(s_n))'$, predict $w(s_0)$ for a new location s_0
- If $w(s)$ is modeled as a GP, then $(w(s_0), w(s_1), \ldots, w(s_n))'$ jointly follow multivariate normal distribution
- $w(s_0) \,|\, w$ follows a normal distribution with
    - Mean (kriging estimator): $m(s_0) + c'C^{-1}(w - m)$
    - where $m = E(w)$, $C = Cov(w)$, $c = Cov(w, w(s_0))$
    - Variance: $C(s_0, s_0) - c'C^{-1}c$
- The GP formulation gives the full predictive distribution of $w(s_0)|w$

Modeling with GPs

Spatial linear model

$$y(s) = x(s)'\beta + w(s) + \epsilon(s)$$

- $w(s)$ modeled as $GP(0, C(\cdot \mid \theta))$ (usually without a nugget)
- $\epsilon(s) \stackrel{\text{iid}}{\sim} N(0, \tau^2)$ contributes to the nugget
- Under isotropy: $C(s+h, s) = \sigma^2 R(||h|| \,; \phi)$
- $w = (w(s_1), \ldots, w(s_n))' \sim N(0, \sigma^2 R(\phi))$ where $R(\phi) = \sigma^2(R(||s_i - s_j|| \,; \phi))$
- $y = (y(s_1), \ldots, y(s_n))' \sim N(X\beta, \sigma^2 R(\phi) + \tau^2 I)$

Parameter estimation

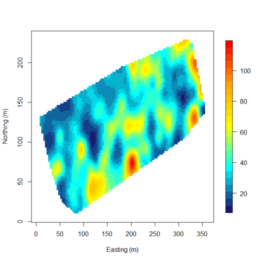
- $y = (y(s_1), \ldots, y(s_n))' \sim N(X\beta, \sigma^2 R(\phi) + \tau^2 I)$
- We can obtain MLEs of parameters $\beta, \tau^2, \sigma^2, \phi$ based on the above model and use the estimates to krige at new locations
- In practice, the likelihood is often very flat with respect to the spatial covariance 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

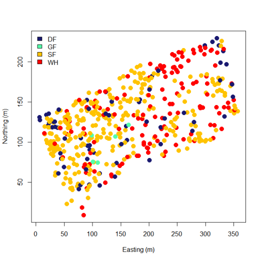
- For k total parameters and sample size n:
    - AIC: $2k - 2\log(l(y \mid \hat{\beta}, \hat{\theta}, \hat{\tau^2}))$
    - BIC: $\log(n)k - 2\log(l(y \mid \hat{\beta}, \hat{\theta}, \hat{\tau^2}))$
- Prediction based approaches using holdout data:
    - Root Mean Square Predictive Error (RMSPE): $\sqrt{\frac{1}{n_{out}} \sum_{i=1}^{n_{out}} (y_i - \hat{y}_i)^2}$
    - 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

Western Experimental Forestry (WEF) data

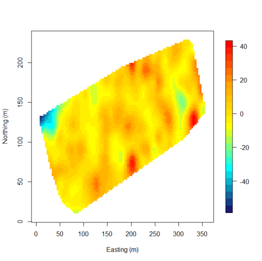
- Data consist of a census of all trees in a 10 ha. stand in Oregon
- Response of interest: Diameter at breast height (DBH)
- Covariate: Tree species (Categorical variable)



DBH



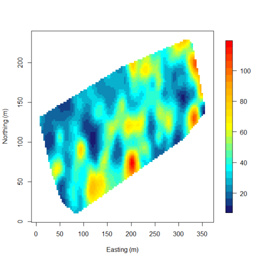
Species



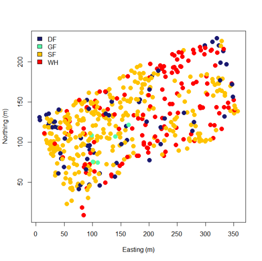
Residuals

Western Experimental Forestry (WEF) data

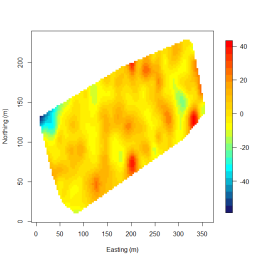
- Data consist of a census of all trees in a 10 ha. stand in Oregon
- Response of interest: Diameter at breast height (DBH)
- Covariate: Tree species (Categorical variable)



DBH



Species

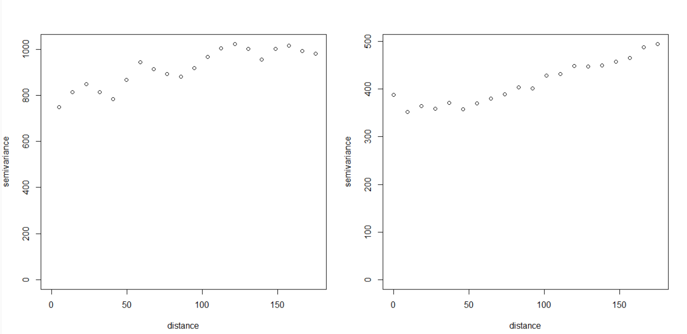


Residuals

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

Empirical semivariograms

- Regression model: DBH $\sim$ Species



DBH | Residuals

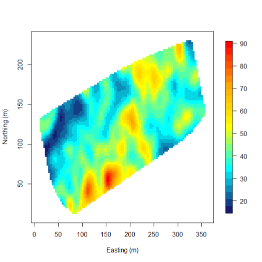
- Semivariogram of the residuals confirm unexplained spatial variation

Model comparisons

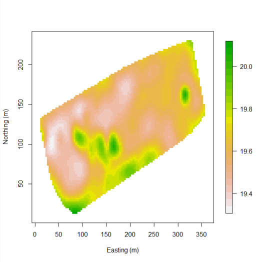
Table: Model comparison

	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