Introduction to spatial statistics

Abhi Datta

January 26, 2018

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

Course Outline

- Introduction types of spatial data, exploratory data analysis
- Modeling univariate point referenced data Gaussian Processes (GP), spatial regression, estimation, spatial prediction (kriging)
- Bayesian modeling Metropolis Hastings, Gibbs sampler
- Large data computing challenges, efficient alternatives
- Areal data disease mapping

More about the course

- Materials available on https: //github.com/abhirupdatta/spatial-statistics-2018
- Texts for reference:
 - (Main) Banerjee, S., Carlin, B. P., and Gelfand, A. E. (2014), Hierarchical Modeling and Analysis for Spatial Data, Boca Raton, FL: Chapman and Hall/CRC, 2nd ed (BCG)
 - Cressie, N. A. C. and Wikle, C. K. (2011), Statistics for spatio-temporal data, Hoboken, NJ: Wiley, Wiley Series in Probability and Statistics

What is spatial data?

• Any data with some geographical information

What is spatial data?

- Any data with some geographical information
- Common sources of spatial data: climatology, forestry, ecology, environmental health, disease epidemiology, real estate marketing etc
 - have many important predictors and response variables
 - are often presented as maps

What is spatial data?

- Any data with some geographical information
- Common sources of spatial data: climatology, forestry, ecology, environmental health, disease epidemiology, real estate marketing etc
 - have many important predictors and response variables
 - are often presented as maps
- Other examples where spatial need not refer to space on earth:
 - Neuroimaging (data for each voxel in the brain)
 - Genetics (position along a chromosome)

• Three broad categories

- Point-referenced 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: Locations of scallops abundance data

- Areal data
 - Each observation is associated with a region like state, county etc.
 - Usually a result of aggregating point level data

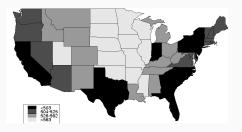


Figure: SAT scores across the 48 contiguous states in the US

- Point pattern data
 - The locations are viewed as "random"
 - Need not have variables at locations, just the pattern of points
 - Interest in the pattern of occurrences of an event like disease incidence, species distribution, crimes etc.



Figure: Locations of confirmed mountain lion sightings in the Bay area since 2004

Geostatistics – Analysis of 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

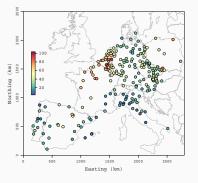


Figure: Pollutant levels in Europe in March, 2009

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).
 Euclidean space.
- Example: Data about pollution levels $Y(s_1), Y(s_2), \ldots, Y(s_n)$ at sites s_1, s_2, \ldots, s_n
- Conceptually: Pollutant level exists at all possible sites
- We can learn about Y(s) for any s in the region based on this data!
- Key to achieve this is exploiting structured dependence

Exploratory data analysis (EDA): Plotting the data

- At each s_i we observe the response $y(s_i)$ and a $p \times 1$ vector of covariates $x(s_i)'$
- Goals: Identify association between y and x, predict y(s) at any arbitrary s

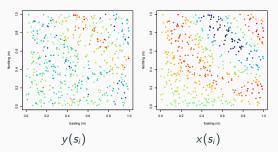


Figure: Response and covariate data for Dataset 1

Exploratory data analysis (EDA): Plotting the data

- At each s_i we observe the response $y(s_i)$ and a $p \times 1$ vector of covariates $x(s_i)'$
- Goals: Identify association between y and x, predict y(s) at any arbitrary s
- Surface plots of the data often helps to better understand spatial patterns

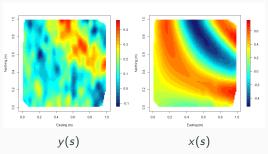


Figure: Response and covariate surface plots for Dataset 1

What's so special about spatial?

- Linear regression model: $y(s_i) = x(s_i)'\beta + \epsilon(s_i)$
- $\epsilon(s_i)$ are iid $N(0, \tau^2)$ errors
- $y = (y(s_1), y(s_2), \dots, y(s_n))'; X = (x(s_1)', x(s_2)', \dots, x(s_n)')'$
- Inference: $\hat{\beta} = (X'X)^{-1}X'Y \sim N(\beta, \tau^2(X'X)^{-1})$
- Prediction at new location s_0 : $\widehat{y(s_0)} = x(s_0)'\hat{\beta}$
- Although the data is spatial, this is an ordinary linear regression model

Residual plots

• Surface plots of the residuals (y(s) - y(s)) help to identify any spatial patterns left unexplained by the covariates

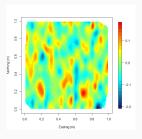


Figure: Residual plot for Dataset 1 after linear regression on x(s)

Residual plots

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

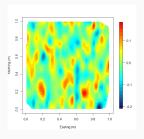
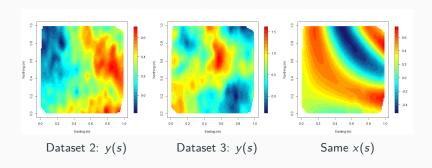


Figure: Residual plot for Dataset 1 after linear regression on x(s)

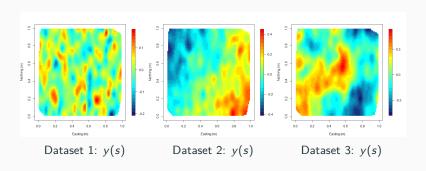
- No evident spatial pattern in plot of the residuals
- The covariate x(s) seem to explain all spatial variation in y(s)
- Does a non-spatial regression model always suffice?

Two more datasets



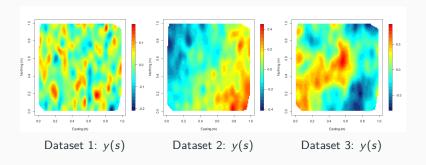
Residual plots

• Linear regression: $y(\mathbf{s}_i) = \beta_0 + x(\mathbf{s}_i)\beta_1 + \epsilon(\mathbf{s}_i)$



Residual plots

• Linear regression: $y(\mathbf{s}_i) = \beta_0 + x(\mathbf{s}_i)\beta_1 + \epsilon(\mathbf{s}_i)$



- Strong residual spatial pattern in datasets 2 and 3
- The covariate x(s) does not explain all spatial variation in y(s)

More EDA

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

More EDA

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

First law of geography

"Everything is related to everything else, but near things are more related than distant things." – Waldo Tobler

More EDA

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

First law of geography

"Everything is related to everything else, but near things are more related than distant things." – Waldo Tobler

- In general pairwise squared differences of the data should have higher values if the locations are far apart
- In other words: $(Y(s+h)-Y(s))^2$ should be roughly increasing with ||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:

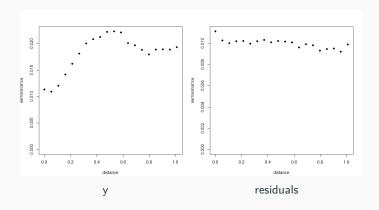
$$N(t_k) = \{(s_i, s_j) : ||s_i - s_j|| \in I_k\}, k = 1, \dots, K.$$

• Empirical semivariogram:

$$\gamma(t_k) = \frac{1}{2|N(t_k)|} \sum_{s_i, s_j \in N(t_k)} (Y(s_i) - Y(s_j))^2$$

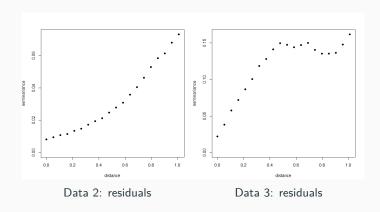
- ullet For spatial data, the $\gamma(t_k)$ is expected to roughly increase with t_k
- A flat semivariogram would suggest little spatial variation

Empirical semivariogram: Data 1



- variog command in the geoR package in R calculates empirical semivariograms
- Residuals display little spatial variation

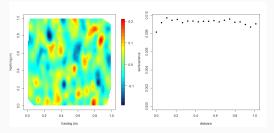
Empirical semivariograms: Data 2 and 3



• Semivariograms of the residuals point to spatial variation

 When covariates does not explain all variation, one needs to leverage the information from the locations

- When covariates does not explain all variation, one needs to leverage the information from the locations
- Linear regression with the co-ordinates added as regressors: $y(\mathbf{s}_i) = \beta_0 + x(\mathbf{s}_i)\beta_1 + s_{ix}\beta_2 + s_{iy}\beta_3 + \epsilon(\mathbf{s}_i)$

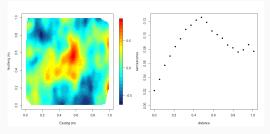


New residuals for data 2 Empirical semivariogram

 The linear model for the co-ordinates explains most of the spatial variation in dataset 2

• Linear regression with the co-ordinates added as regressors:

$$y(\mathbf{s}_i) = \beta_0 + x(\mathbf{s}_i)\beta_1 + s_{ix}\beta_2 + s_{iy}\beta_3 + \epsilon(\mathbf{s}_i)$$



Residuals for data 3 Empirical semivariogram

Dataset 3 still exhibits strong spatial correlation

- Linear model for the co-ordinates often does not suffice
- More general model: $y(\mathbf{s}_i) = \beta_0 + x(\mathbf{s}_i)\beta_1 + w(\mathbf{s}_i) + \epsilon(\mathbf{s}_i)$
- How to choose the function $w(\cdot)$?
- Since we want to predict at any location over the entire domain, this choice will amount to choosing a surface w(s)
- How to do this?

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. $w = (w(s_1), \dots, w(s_n))' \sim N(m, C)$ where $m = (m(s_1), \dots, m(s_n))'$ 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, $C(t) = C(h)$
	$ \qquad \qquad \qquad \text{if } t \geq 1/\phi $
Spherical	$C(t) = \left\{egin{array}{ll} 0 & ext{if } t \geq 1/\phi \ \sigma^2 \left[1 - rac{3}{2}\phi t + rac{1}{2}(\phi t)^3 ight] & ext{if } 0 < t \leq 1/\phi \ au^2 + \sigma^2 & ext{otherwise} \end{array} ight.$
	$ au^2 + \sigma^2$ otherwise
Exponential	$C(t) = \left\{ egin{array}{ll} \sigma^2 \exp(-\phi t) & ext{if } t > 0 \ au^2 + \sigma^2 & ext{otherwise} \end{array} ight.$
LAponential	$\tau^2 + \sigma^2 \qquad \text{otherwise}$
Powered	$C(t) = \int \sigma^2 \exp(- \phi t ^p)$ if $t > 0$
exponential	$C(t) = \left\{ egin{array}{ll} \sigma^2 \exp(- \phi t ^p) & ext{if } t>0 \ au^2 + \sigma^2 & ext{otherwise} \end{array} ight.$
Matérn	$C(t) = \left\{ egin{array}{ll} \sigma^2 \left(1 + \phi t ight) \exp(-\phi t) & ext{if } t > 0 \ au^2 + \sigma^2 & ext{otherwise} \end{array} ight.$
at $\nu=3/2$	$\tau^2 + \sigma^2 \qquad \text{otherwise}$

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 au^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

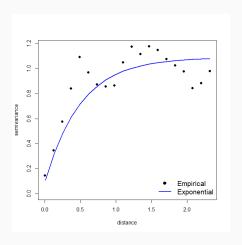
• Recall: Empirical semivariogram:

$$\gamma(t_k) = \frac{1}{2|N(t_k)|} \sum_{s_i, s_j \in N(t_k)} (Y(s_i) - Y(s_j))^2$$

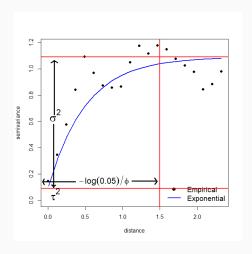
• For any stationary GP, $E(Y(s+h) - Y(s))^2/2 = C(0) - C(h) = \gamma(h)$

- $\gamma(h)$ is the semivariogram corresponding to the covariance function C(h)
- $\begin{aligned} \bullet & \text{ Example: For exponential GP,} \\ \gamma(t) = \left\{ \begin{array}{cc} \tau^2 + \sigma^2(1 \exp(-\phi t)) & \text{if } t > 0 \\ 0 & \text{if } t = 0 \end{array} \right., \text{ where } t = ||h|| \end{aligned}$

Covariance functions and semivariograms



Covariance functions and semivariograms



Summary

- Geostatistics Analysis of point-referenced spatial data
- Surface plots of data and residuals
- EDA with empirical semivariograms
- Modeling unknown surfaces with Gaussian Processes
- Relationship between covariance functions anf variograms