Introduction to spatial statistics

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Course Outline

- Introduction – types of spatial data, exploratory data analysis
- Modeling univariate point referenced data – Gaussian Processes (GP), spatial regression, frequentist and Bayesian estimation and spatial prediction (kriging)
- Large data – computing challenges, efficient alternatives, spatial machine learning
- Areal data – disease mapping
- *Point-pattern data – cluster/hotspot detection
- *Spatially varying relationships, change-of-support problems

More about the course

- Materials available on https://github.com/abhirupdatta/advanced-spatial-statistics-2021
- 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
    - Cressie, N. A. C. and Wikle, C. K. (2011), Statistics for spatio-temporal data, Hoboken, NJ: Wiley, Wiley Series in Probability and Statistics

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    - have many important predictors and response variables
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- 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)

Types of spatial data

- Three broad categories

Types of spatial data

- 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

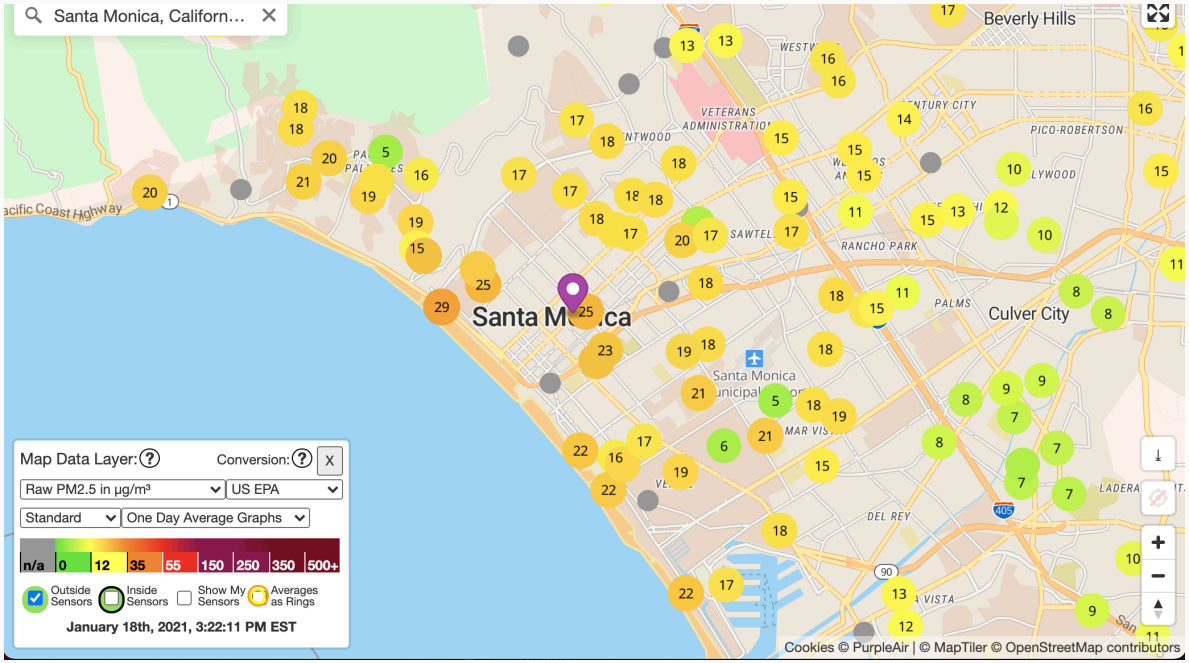


Figure: $PM_{2.5}$ readings in μgm^{-3} from PurpleAir low-cost sensors in Santa Monica, CA on Jan 18, 2021.[1]

[1] Source: https://www.purpleair.com/

Types of spatial data

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

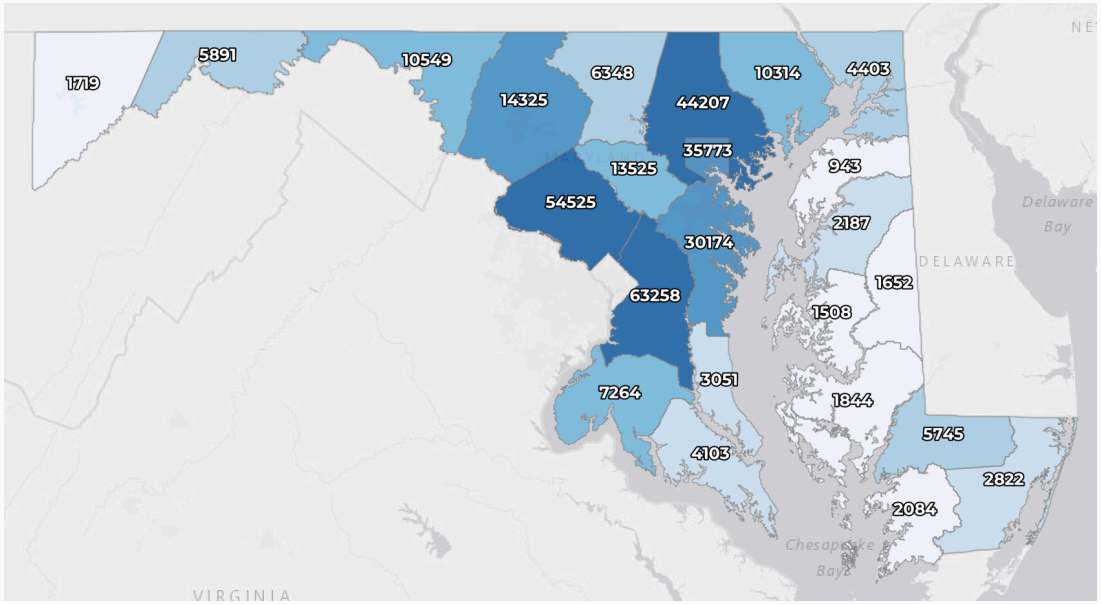


Figure: COVID cases for Maryland counties on Jan 18, 2021[1]

[1] Source: https://coronavirus.maryland.gov/datasets/

Types of spatial data

- 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.

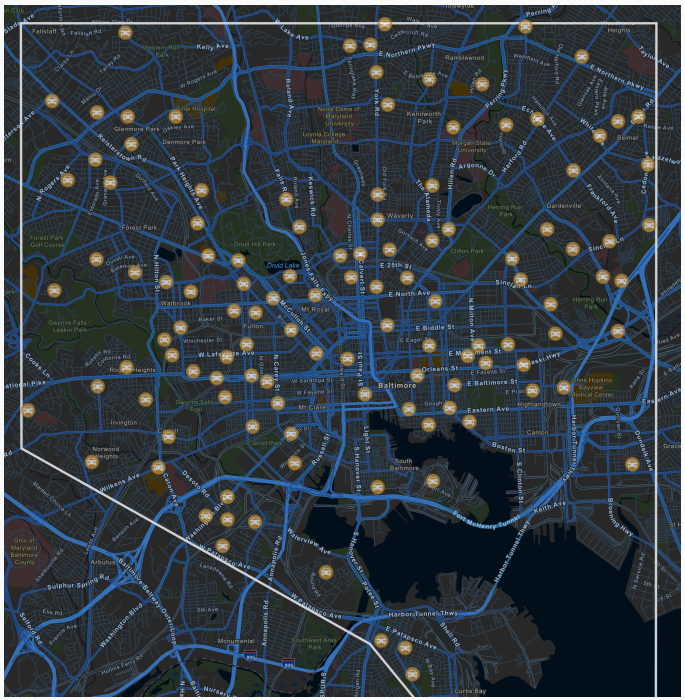
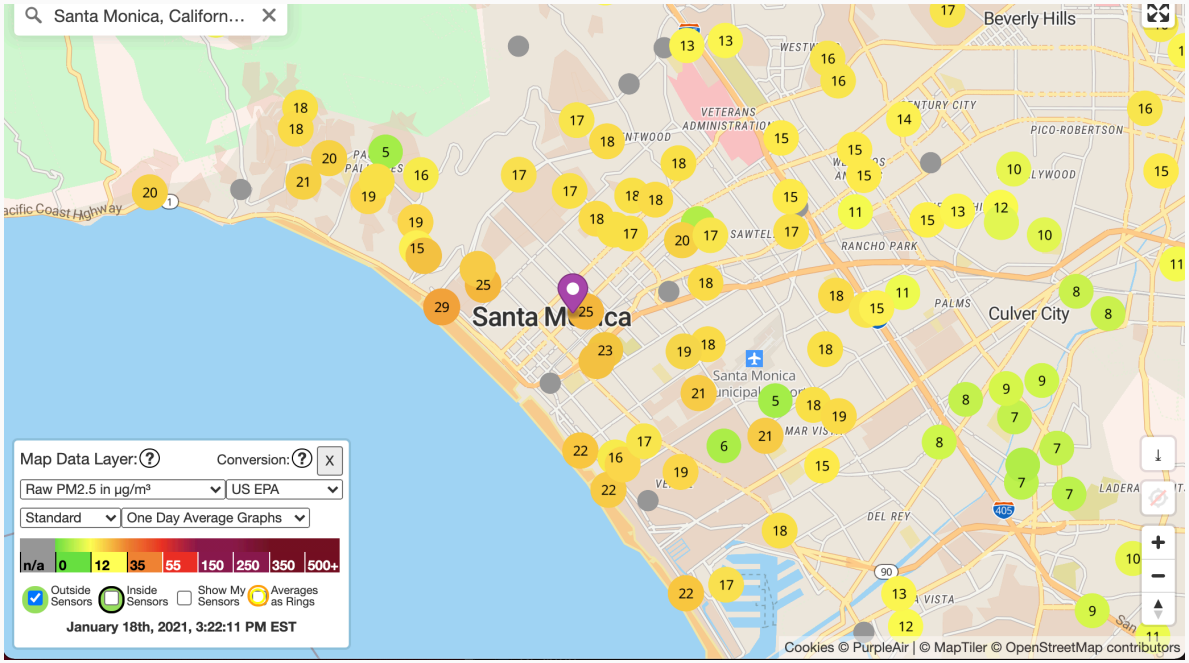


Figure: Locations of auto-theft in Baltimore city in Dec 2020 - Jan 2021[1]

[1] Source: https://arcgisportal.baltimorepolice.org/publiccrimemap/

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



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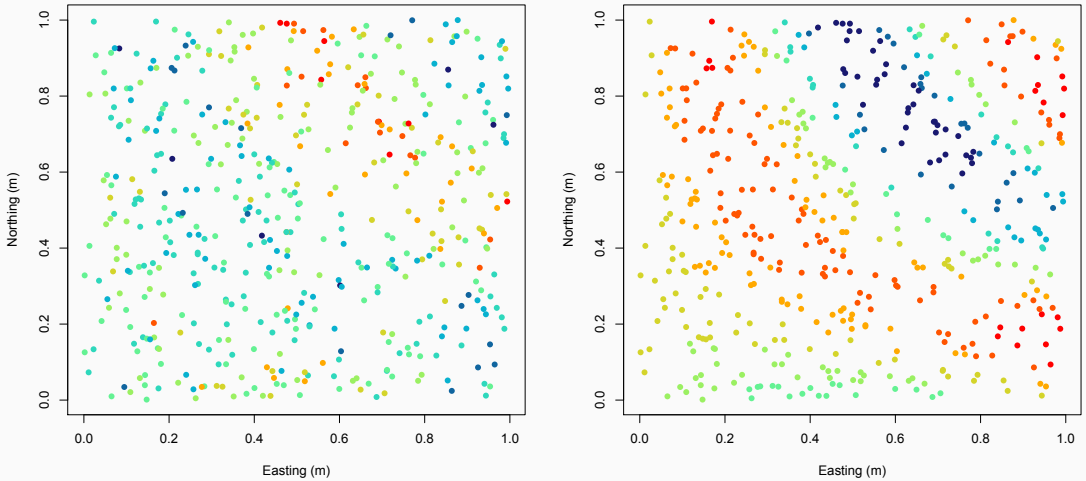
Point level modeling

- Point-level modeling refers to modeling of point-referenced data collected at locations referenced by coordinates (e.g., lat-long).
- 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
- Data are realizations from a spatial process $\{Y(s) : s \in D\}$, D is a subset in Euclidean space.
- 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



$y(s_i)$ $x(s_i)$

Figure: Response and covariate data for Dataset 1

Exploratory data analysis (EDA): Plotting the data

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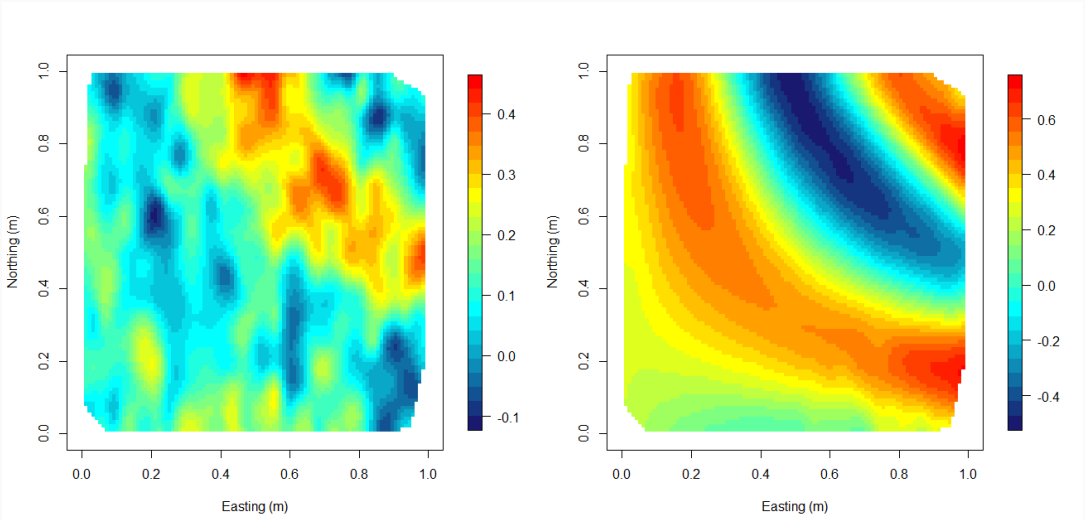
- Surface plots of the data often helps to better understand spatial patterns



$y(s)$ $x(s)$

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
- $y = (y(s_1), y(s_2), \ldots, y(s_n))'$; $X = (x(s_1)', x(s_2)', \ldots, x(s_n)')'$
- 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 $(y(s) - \widehat{y(s)})$ help to identify any spatial patterns left unexplained by the covariates

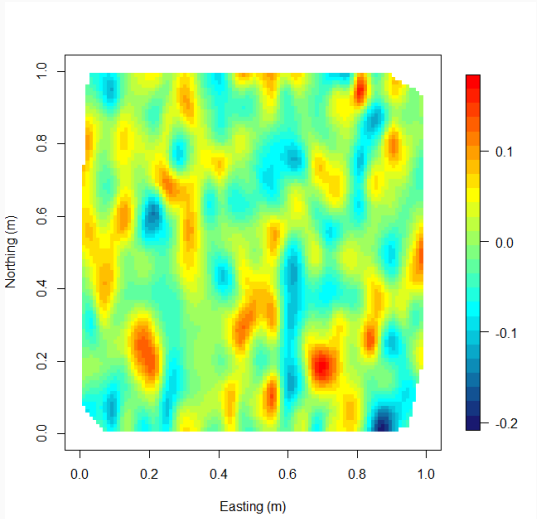


Figure: Residual plot for Dataset 1 after linear regression on $x(s)$

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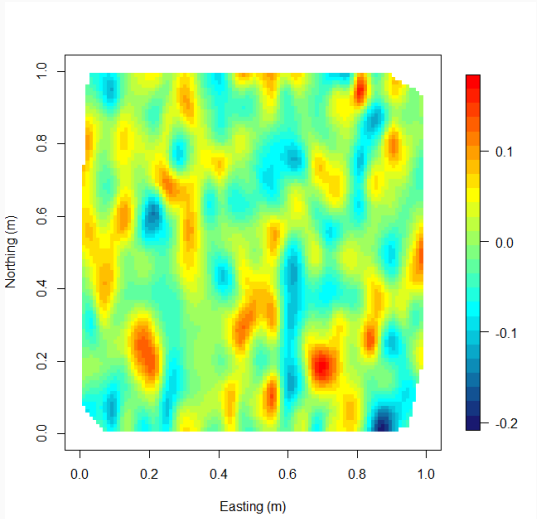
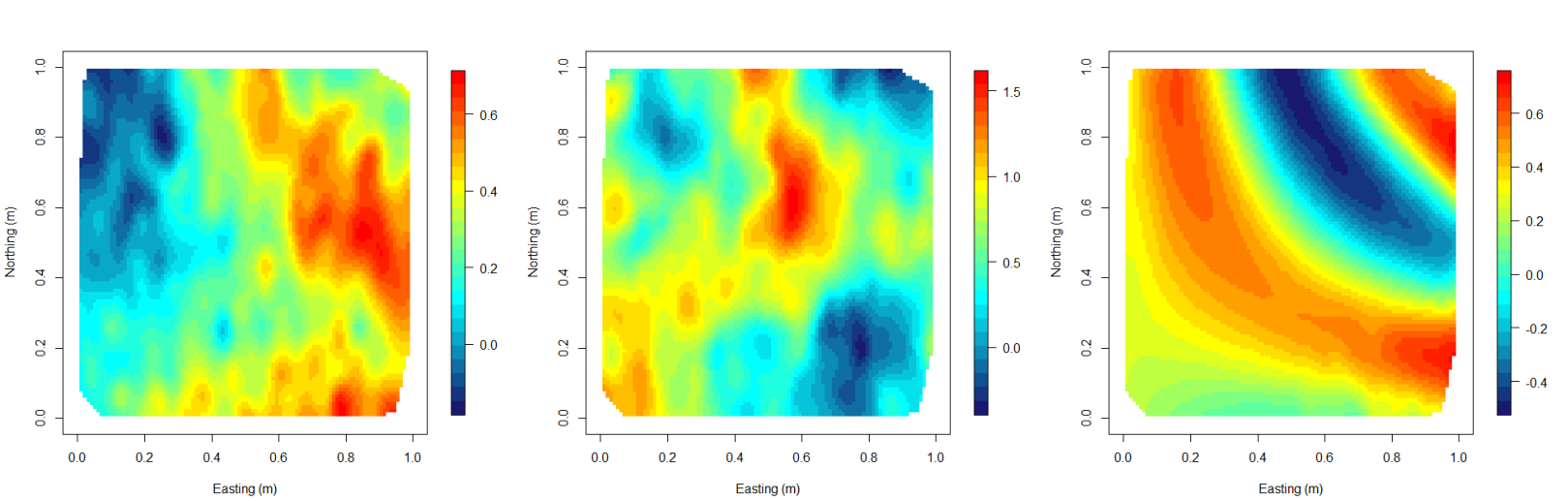


Figure: Residual plot for Dataset 1 after linear regression on $x(s)$

- 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?

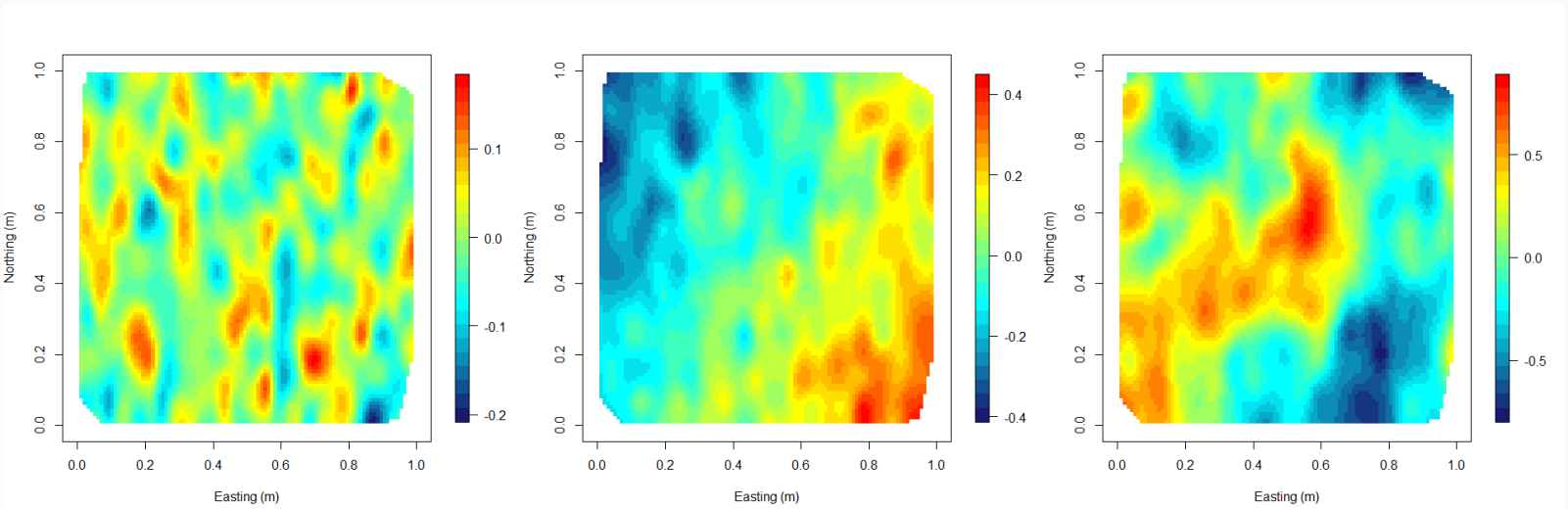
Two more datasets



Dataset 2: $y(s)$ Dataset 3: $y(s)$ Same $x(s)$

Residual plots

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



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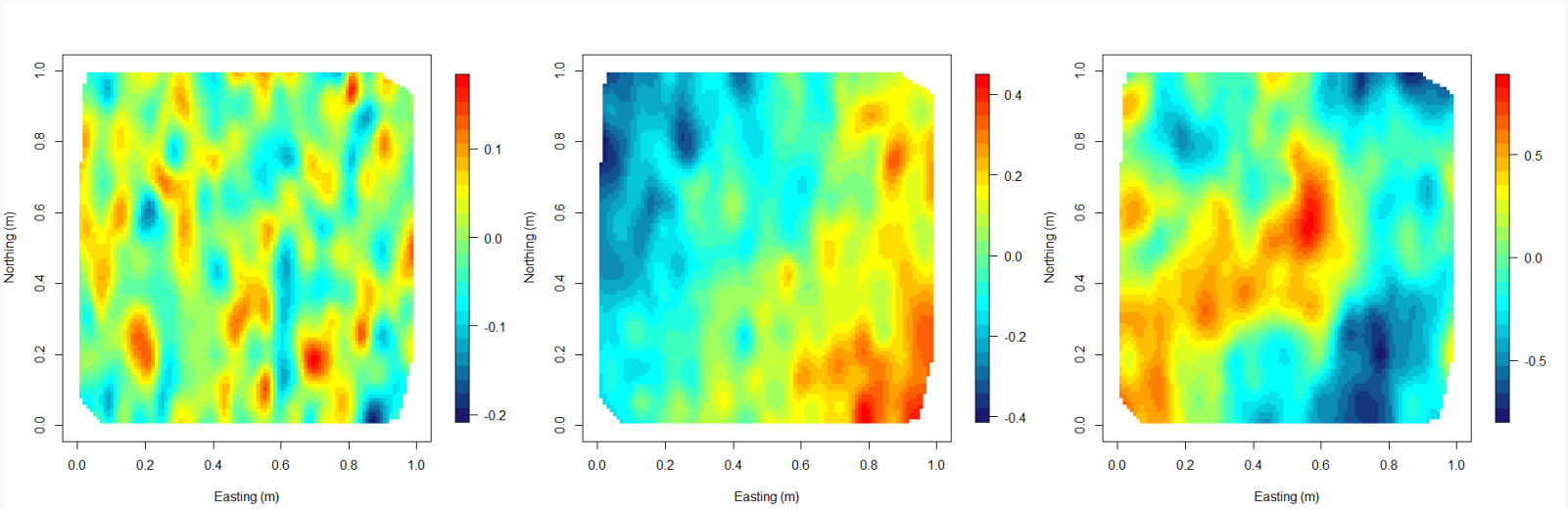

Dataset 1: $y(s)$ Dataset 2: $y(s)$ Dataset 3: $y(s)$

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

More EDA

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First law of geography

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- 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:

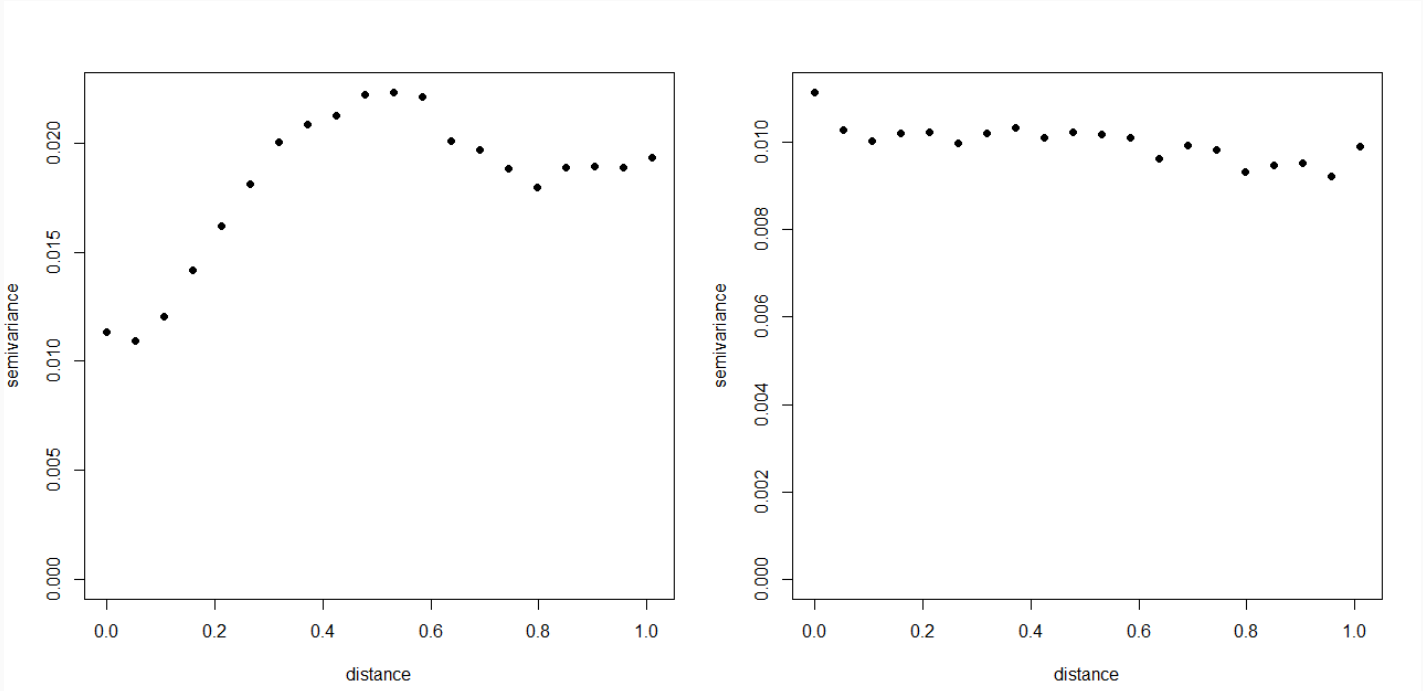
$$N(t_k) = \{(s_i, s_j) : \|s_i - s_j\| \in I_k\}, k = 1, \ldots, K.$$

- Empirical semivariogram:

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

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

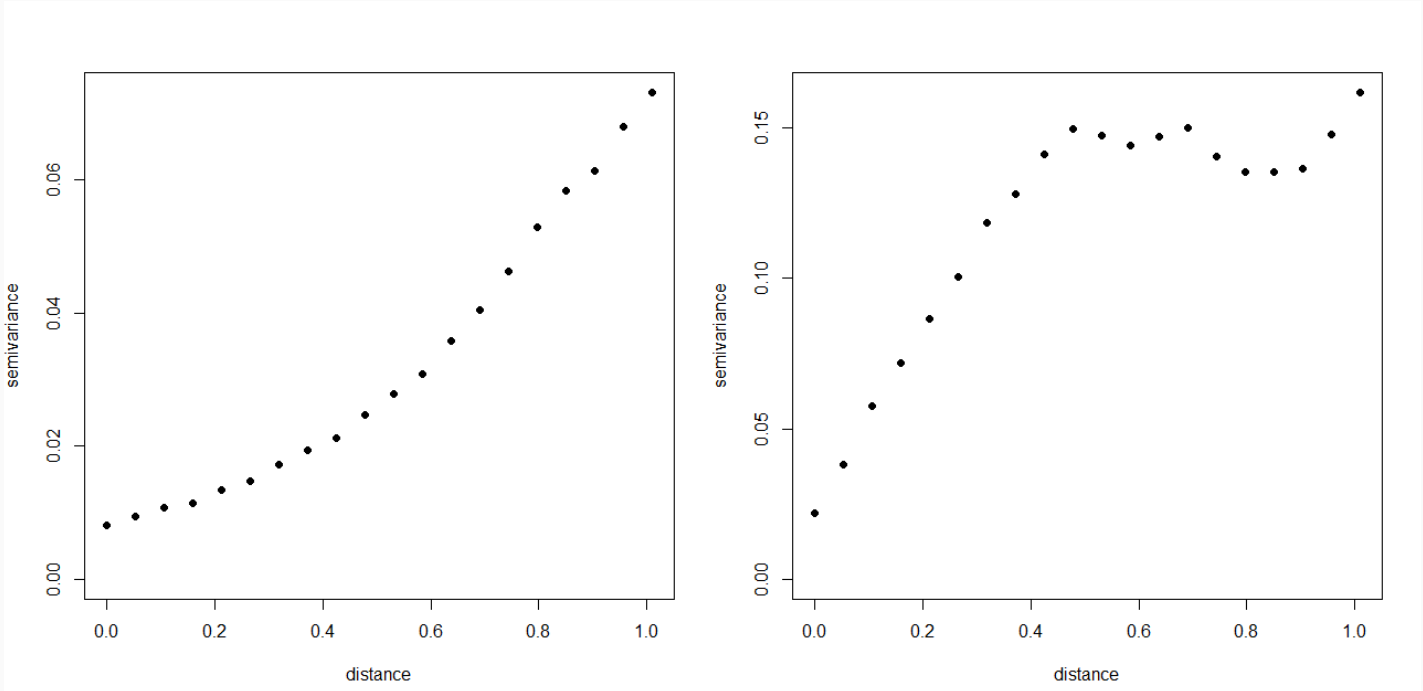
Empirical semivariogram: Data 1



y residuals

- *variog* command in the *geoR* package in R calculates empirical semivariograms
- Variogram of residuals suggests very little spatial variation

Empirical semivariograms: Data 2 and 3



Data 2: residuals

Data 3: residuals

- Semivariograms of the residuals point to spatial variation

Using the locations

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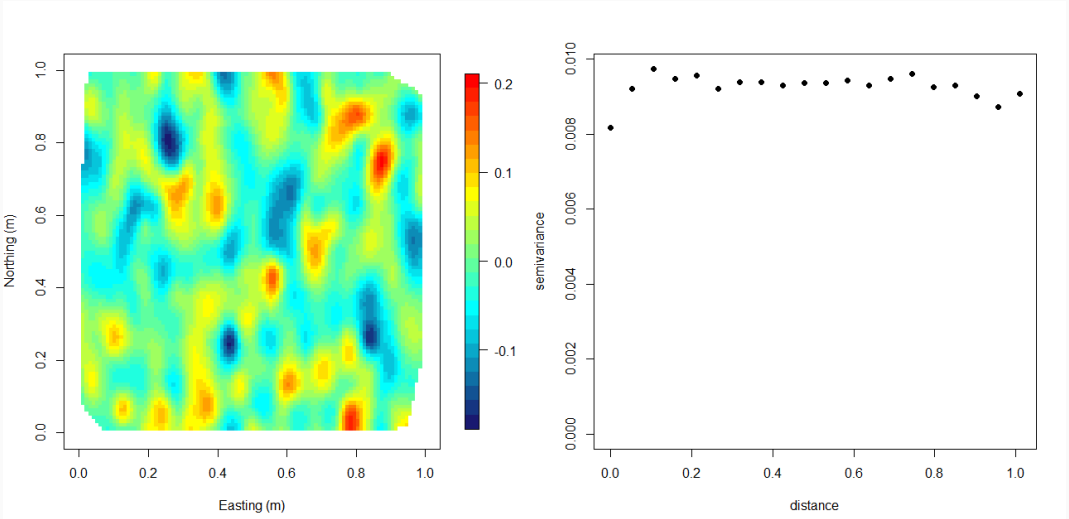
- Linear regression with the co-ordinates added as regressors:
  $y(\mathbf{s}_i) = \beta_0 + x(\mathbf{s}_i)\beta_1 + s_{ix}\beta_2 + s_{iy}\beta_3 + \epsilon(\mathbf{s}_i)$



New residuals for data 2 Empirical semivariogram

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

Using the locations

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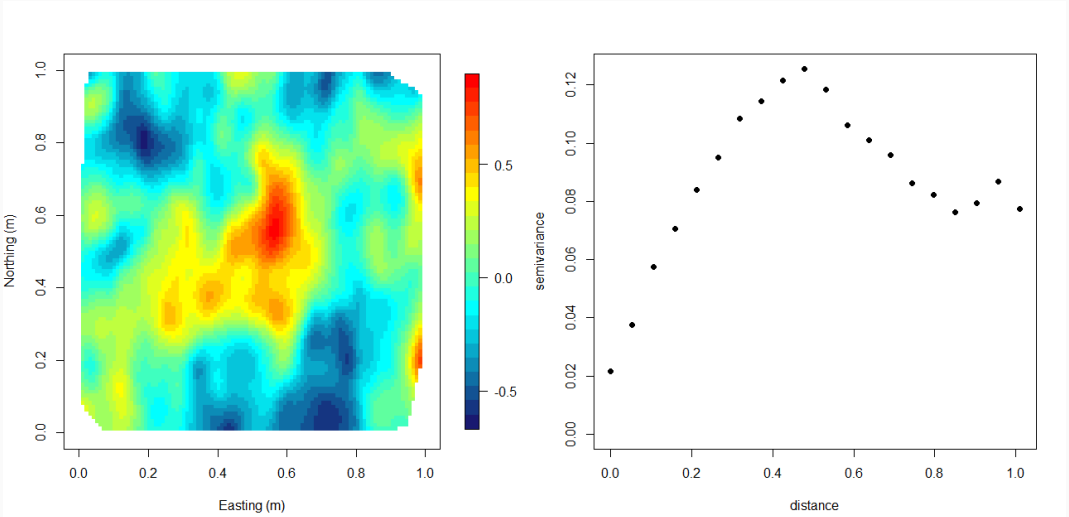

Residuals for data 3 Empirical semivariogram

- Dataset 3 still exhibits strong spatial correlation

Modeling with the locations

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

General idea

- Model: $y(s) = x(s)'\beta + w(s) + \epsilon(s)$
- Optimize $\|y - X\beta - w\|_2^2 + P(w)$ where $y = (y(s_1), \ldots, y(s_n))'$, X and w are similarly defined, $P(w)$ is some 'roughness' penalty (regularization term) shrinking towards smooth estimates of the function $w(\cdot)$
- Many approaches are related to this general approach: basis function expansions, penalized regression splines, Gaussian Processes

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- In this course, we will focus on Gaussian Processes

Gaussian Processes (GPs)

- One popular approach to model w(s) is via Gaussian Processes (GP)
- GP is a distribution over the class of functions, whose support is the space of 'suitably smooth' functions
- The collection of random variables $\{w(s) \,|\, s \in D\}$ is a GP if
  - it is a valid stochastic process (Kolmogorov consistency)
  - 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 $C = (C(s_i, s_j))$ 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
  - Non-stationary: Does not use any of these assumptions (most general)
- Isotropic models are popular because of their interpretability, and because a number of relatively simple parametric forms are available as candidates for C.

The Matérn covariance family

The stationary (isotropic) Matérn covariance function is specified by

$$C(\|h\|_2) = \sigma^2 \frac{2^{1-\nu}\left(\sqrt{2}\phi\|h\|_2\right)^{\nu}}{\Gamma(\nu)} \mathscr{K}_{\nu}\left(\sqrt{2}\phi\|h\|_2\right),$$

where $\mathscr{K}_{\nu}$ is the modified Bessel function of second kind.

- $\sigma^2 = Cov(w(s)) =$ Marginal variance for all s
- $\nu =$ Smoothness parameter; a GP $w(\cdot)$ with Matérn covariance with smoothness ν is $(\lceil \nu \rceil - 1)$-times (mean square) differentiable functions (Stein, 1999[3])
- $\phi =$ Spatial decay (inverse scale) parameter

[3] Stein, M. L. (2012). Interpolation of spatial data: some theory for kriging. Springer Science & Business Media

The Matérn covariance family (special cases)

- $\nu = 1/2 \implies$ exponential covariance function;

$$C(\|h\|_2) = \sigma^2 \exp(-\phi\|h\|_2)$$

- $\nu = 3/2 \implies$ smoother than exponential;

$$C(\|h\|_2) = \sigma^2(1 + \phi\|h\|_2)\exp(-\phi\|h\|_2)$$

- $\nu = \infty \implies$ squared exponential (or Gaussian) covariance function (very smooth);

$$C(\|h\|_2) = \sigma^2 \exp(-\phi\|h\|_2^2)$$

Some traditional terminology

$w(\cdot) \sim GP(0, C)$ with marginal variance σ^2 and $\epsilon(s) \overset{\text{iid}}{\sim} N(0, \tau^2)$,
$\implies w(\cdot) + \epsilon(\cdot) \sim GP(0, C^*)$ where $C^* = C + \delta$ with
$\delta(s, s') = \tau^2 I(s = s')$.

- E.g. If C is the exponential covariance function, then $C^*(\|h\|) = \tau^2 I(h = 0) + \sigma^2 \exp(-\phi\|h\|)$
- τ^2 (called the nugget) is the noise (measurement error) or "micro-scale variance".
- Note discontinuity at 0 due to the nugget.
- The partial sill (σ^2) is the "spatial effect variance."
- $\sigma^2 + \tau^2$ is the sill $=$ partial sill $+$ nugget, i.e., the total variance.
- 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 $\log(0.05) \approx -3$.

Summary

- Geostatistics – Analysis of point-referenced spatial data
- Surface plots of data and residuals
- EDA with empirical semivariograms
- Basics of Gaussian Processes and covariance functions
- Modeling unknown surfaces with GP (to be contd.)