Introduction to Spatial Data and Models

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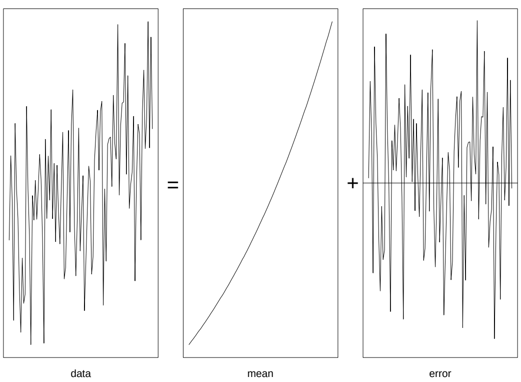
- Researchers in diverse areas such as climatology, ecology, environmental health, and real estate marketing are increasingly faced with the task of analyzing data that are:
  - highly multivariate, with many important predictors and response variables,
  - geographically referenced, and often presented as maps, and
  - temporally correlated, as in longitudinal or other time series structures.

⇒ motivates hierarchical modeling and data analysis for complex spatial (and spatiotemporal) data sets.

- point-referenced data, where $Y(\mathbf{s})$ is a random vector at a location $\mathbf{s} \in \Re^r$, where $\mathbf{s}$ varies continuously over D, a fixed subset of $\Re^r$ that contains an r-dimensional rectangle of positive volume;
- areal data, where D is again a fixed subset (of regular or irregular shape), but now partitioned into a finite number of areal units with well-defined boundaries;
- point pattern data, where now D is itself random; its index set gives the locations of random events that are the spatial point pattern. $Y(\mathbf{s})$ itself can simply equal 1 for all $\mathbf{s} \in D$ (indicating occurrence of the event), or possibly give some additional covariate information (producing a marked point pattern process).

- First step in analyzing data
- First Law of Geography: Mean + Error
- Mean: first-order behavior
- Error: second-order behavior (covariance function)
- EDA tools examine both first and second order behavior
- Preliminary displays: Simple locations to surface displays

First Law of Geography

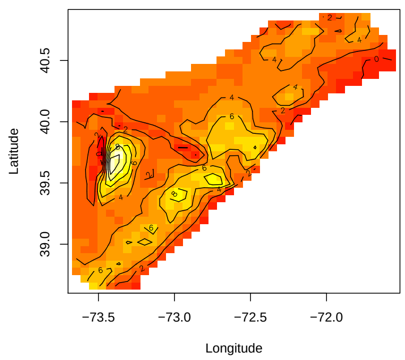


Scallops Sites

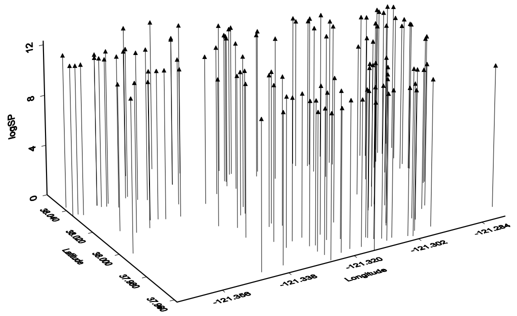
- Spatial surface observed at finite set of locations $\mathscr{S} = \{\mathbf{s}_1, \mathbf{s}_2, ..., \mathbf{s}_n\}$
- Tessellate the spatial domain (usually with data locations as vertices)
- Fit an interpolating polynomial:

$$f(\mathbf{s}) = \sum_i w_i(\mathscr{S}; \mathbf{s}) f(\mathbf{s}_i)$$

- "Interpolate" by reading off $f(\mathbf{s}_0)$.
- Issues:
  - Sensitivity to tessellations
  - Choices of multivariate interpolators
  - Numerical error analysis



Drop-line scatter plot



Surface plot

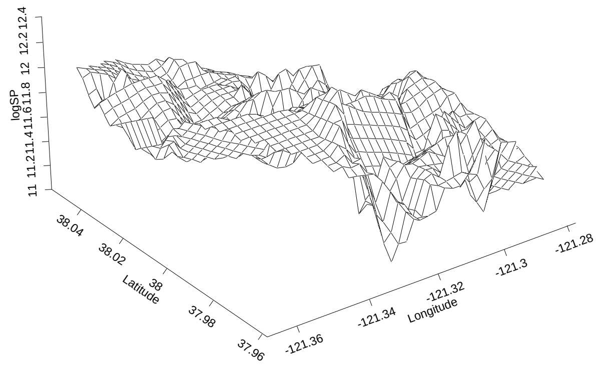
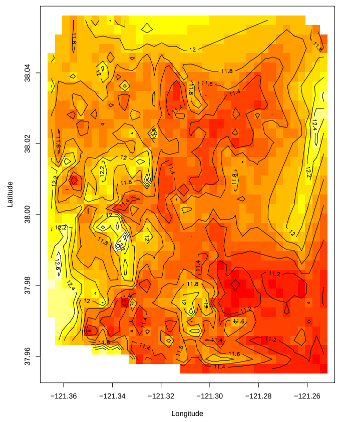
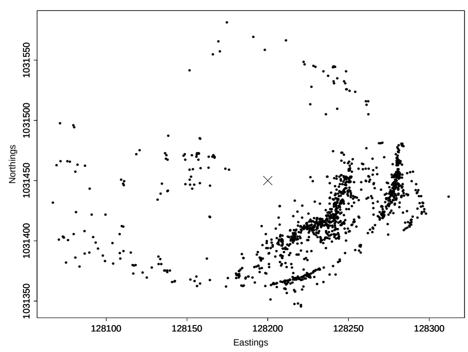


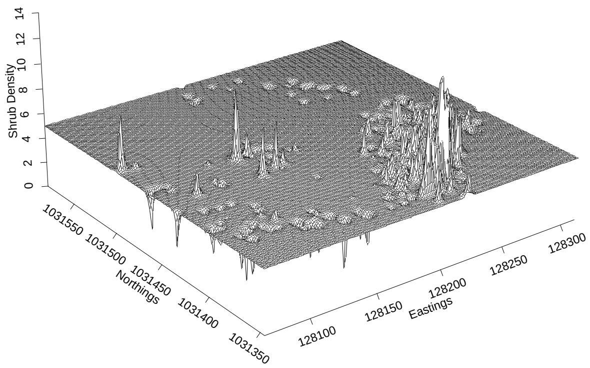
Image contour plot



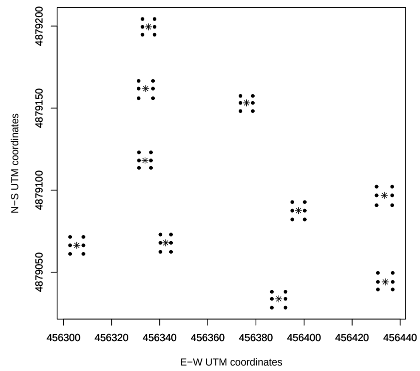
Locations form patterns



Surface features



Interesting plot arrangements



- Point-level modelling refers to modelling of spatial datacollected at locations referenced by coordinates (e.g., lat-long, Easting-Northing).
- Fundamental concept: Data from a spatial process $\{Y(\mathrm{s}) : \mathrm{s} \in D\}$, where D is a fixed subset in Euclidean space.
- Example: $Y(\mathrm{s})$ is a pollutant level at site s
- Conceptually: Pollutant level exists at all possible sites
- Practically: Data will be a partial realization of a spatial process – observed at $\{\mathrm{s}_1, \ldots, \mathrm{s}_n\}$
- Statistical objectives: Inference about the process $Y(\mathrm{s})$; predict at new locations.

Suppose our spatial process has a mean, $\mu(\mathbf{s}) = E(Y(\mathbf{s}))$, and that the variance of $Y(\mathbf{s})$ exists for all $\mathbf{s} \in D$.

- Strong stationarity: If for any given set of sites, and any displacement $\mathbf{h}$, the distribution of $(Y(\mathbf{s}_1), ..., Y(\mathbf{s}_n))$ is the same as, $(Y(\mathbf{s}_1 + \mathbf{h}), ..., Y(\mathbf{s}_n + \mathbf{h}))$.
- Weak stationarity: Constant mean $\mu(\mathbf{s}) = \mu$, and $Cov(Y(\mathbf{s}), Y(\mathbf{s} + \mathbf{h})) = C(\mathbf{h})$: the covariance depends only upon the displacement (or separation) vector.
- Strong stationarity implies weak stationarity
- The process isGaussian if $\mathbf{Y} = (Y(\mathbf{s}_1), \ldots, Y(\mathbf{s}_n))$ has a multivariate normal distribution.
- For Gaussian processes, strong and weak stationarity are equivalent.

Variograms

- Suppose we assume $E[Y(\mathbf{s} + \mathbf{h}) - Y(\mathbf{s})] = 0$ and define
  $$E[Y(\mathbf{s} + \mathbf{h}) - Y(\mathbf{s})]^2 = Var\left(Y(\mathbf{s} + \mathbf{h}) - Y(\mathbf{s})\right) = 2\gamma(\mathbf{h}) \ .$$
  This is sensible if the left hand side depends only upon $\mathbf{h}$. Then we say the process is intrinsically stationary.
- $\gamma(\mathbf{h})$ is called the *semivariogram* and $2\gamma(\mathbf{h})$ is called the *variogram*.

Note that intrinsic stationarity defines only the first and second moments of the differences $Y(\mathbf{s} + \mathbf{h}) - Y(\mathbf{s})$. It says nothing about the joint distribution of a collection of variables $Y(\mathbf{s}_1), \ldots, Y(\mathbf{s}_n)$, and thus provides no likelihood.

Intrinsic Stationarity and Ergodicity

- Relationship between $\gamma(\mathbf{h})$ and C($\mathbf{h}$):
  $$\begin{aligned} 2\gamma(\mathbf{h}) &= Var(Y(\mathbf{s} + \mathbf{h})) + Var(Y(\mathbf{s})) - 2Cov(Y(\mathbf{s} + \mathbf{h}), Y(\mathbf{s})) \\ &= C(\mathbf{0}) + C(\mathbf{0}) - 2C(\mathbf{h}) \\ &= 2[C(\mathbf{0}) - C(\mathbf{h})]. \end{aligned}$$
- Easy to recover γ from C. The converse needs the additional assumption of *ergodicity*: $\lim_{\|\mathbf{u}\| \to \infty} C(\mathbf{u}) = 0$.
- So $\lim_{\|\mathbf{u}\| \to \infty} \gamma(\mathbf{u}) = C(\mathbf{0})$, and we can recover C from γ as long as this limit exists.
  $$C(\mathbf{h}) = \lim_{\|\mathbf{u}\| \to \infty} \gamma(\mathbf{u}) - \gamma(\mathbf{h}).$$

- When $\gamma(\mathbf{h})$ or $C(\mathbf{h})$ depends upon the separation vector only through the distance $||\mathbf{h}||$, we say that the process is *isotropic*. In that case, we write $\gamma(||\mathbf{h}||)$ or $C(||\mathbf{h}||)$. Otherwise we say that the process is *anisotropic*.
- If the process is intrinsically stationary and isotropic, it is also called homogeneous.

Isotropic processes are popular because of their simplicity, interpretability, and because a number of relatively simple parametric forms are available as candidates for C (and γ). Denoting $||\mathbf{h}||$ by t for notational simplicity, the next two tables provide a few examples...

Some common isotropic variograms

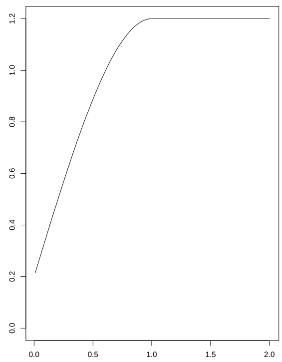
model	Variogram, $\gamma(t)$
Linear	$\gamma(t) = \begin{cases} \tau^2 + \sigma^2 t & \text{if } t > 0 \\ 0 & \text{otherwise} \end{cases}$
Spherical	$\gamma(t) = \begin{cases} \tau^2 + \sigma^2 & \text{if } t \geq 1/\phi \\ \tau^2 + \sigma^2 \left[\frac{3}{2}\phi t - \frac{1}{2}(\phi t)^3\right] & \text{if } 0 < t \leq 1/\phi \\ 0 & \text{otherwise} \end{cases}$
Exponential	$\gamma(t) = \begin{cases} \tau^2 + \sigma^2(1 - \exp(-\phi t)) & \text{if } t > 0 \\ 0 & \text{otherwise} \end{cases}$
Powered exponential	$\gamma(t) = \begin{cases} \tau^2 + \sigma^2(1 - \exp(-\lvert\phi t\rvert^p)) & \text{if } t > 0 \\ 0 & \text{otherwise} \end{cases}$
Matérn at $\nu = 3/2$	$\gamma(t) = \begin{cases} \tau^2 + \sigma^2 \left[1 - (1 + \phi t)\, e^{-\phi t}\right] & \text{if } t > 0 \\ 0 & \text{o/w} \end{cases}$

Examples: Spherical Variogram

$$\gamma(t) = \begin{cases} \tau^2 + \sigma^2 & \text{if } t \geq 1/\phi \\ \tau^2 + \sigma^2 \left[\frac{3}{2}\phi t - \frac{1}{2}(\phi t)^3\right] & \text{if } 0 < t \leq 1/\phi \\ 0 & \text{if } t = 0. \end{cases}$$

- While $\gamma(0) = 0$ by definition, $\gamma(0^+) \equiv lim_{t \to 0^+} \gamma(t) = \tau^2$; this quantity is the *nugget*.
- $\lim_{t \to \infty} \gamma(t) = \tau^2 + \sigma^2$; this asymptotic value of the semivariogram is called the *sill*. (The sill minus the nugget, σ^2 in this case, is called the *partial sill*.)
- Finally, the value $t = 1/\phi$ at which $\gamma(t)$ first reaches its ultimate level (the sill) is called the *range*, $R \equiv 1/\phi$.

Examples: Spherical Variogram



b) spherical; a0 = 0.2 , a1 = 1 , R = 1

Some common isotropic covariograms

Model	Covariance function, $C(t)$
Linear	$C(t)$ does not exist
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 $\log(0.05) \approx -3$.
- Finally, the form of $C(t)$ shows why the nugget τ^2 is often viewed as a "nonspatial effect variance," and the partial sill (σ^2) is viewed as a "spatial effect variance."

The Matèrn Correlation Function

- Much of statistical modelling is carried out through correlation functions rather than variograms
- 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 (a *fractal*) controlling process smoothness

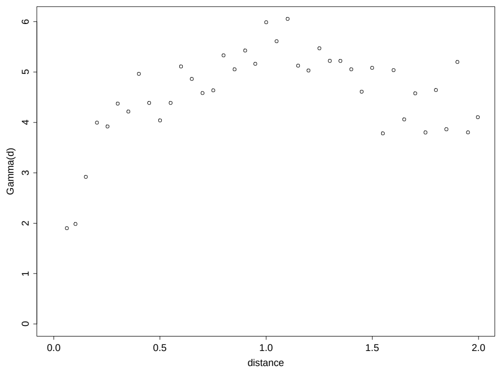
- How do we select a variogram? Can the data really distinguish between variograms?
- Empirical Variogram:

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

  where $N(t)$ is the number of points such that $\|\mathbf{s}_i - \mathbf{s}_j\| = t$ and $|N(t)|$ is the number of points in $N(t)$.
- Grid up the t space into intervals $I_1 = (0, t_1)$, $I_2 = (t_1, t_2)$, and so forth, up to $I_K = (t_{K-1}, t_K)$. Representing t values in each interval by its midpoint, 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 variogram: scallops data



Empirical variogram: scallops data