Spatial Statistics

Introduction to Spatial Analysis

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Geostatistical Data

In this lecture we will cover:

- Mapping geostatistical data
- Exploratory tools for geostatistical data
- Definition of distance and projections
- The semivariogram
- Stationarity
- Empirical semivariograms
- Theoretical semivariograms
- Kriging for interpolation
- Non-parametric smoothing for interpolation

Geostatistical Data: Description

Data that varies continuously over space, but is measured only at discrete locations

Examples:

- field observations such as soil samples, air pollution measurements (environmental exposures)
- meteorological and climate data
- housing prices in a metropolitan area

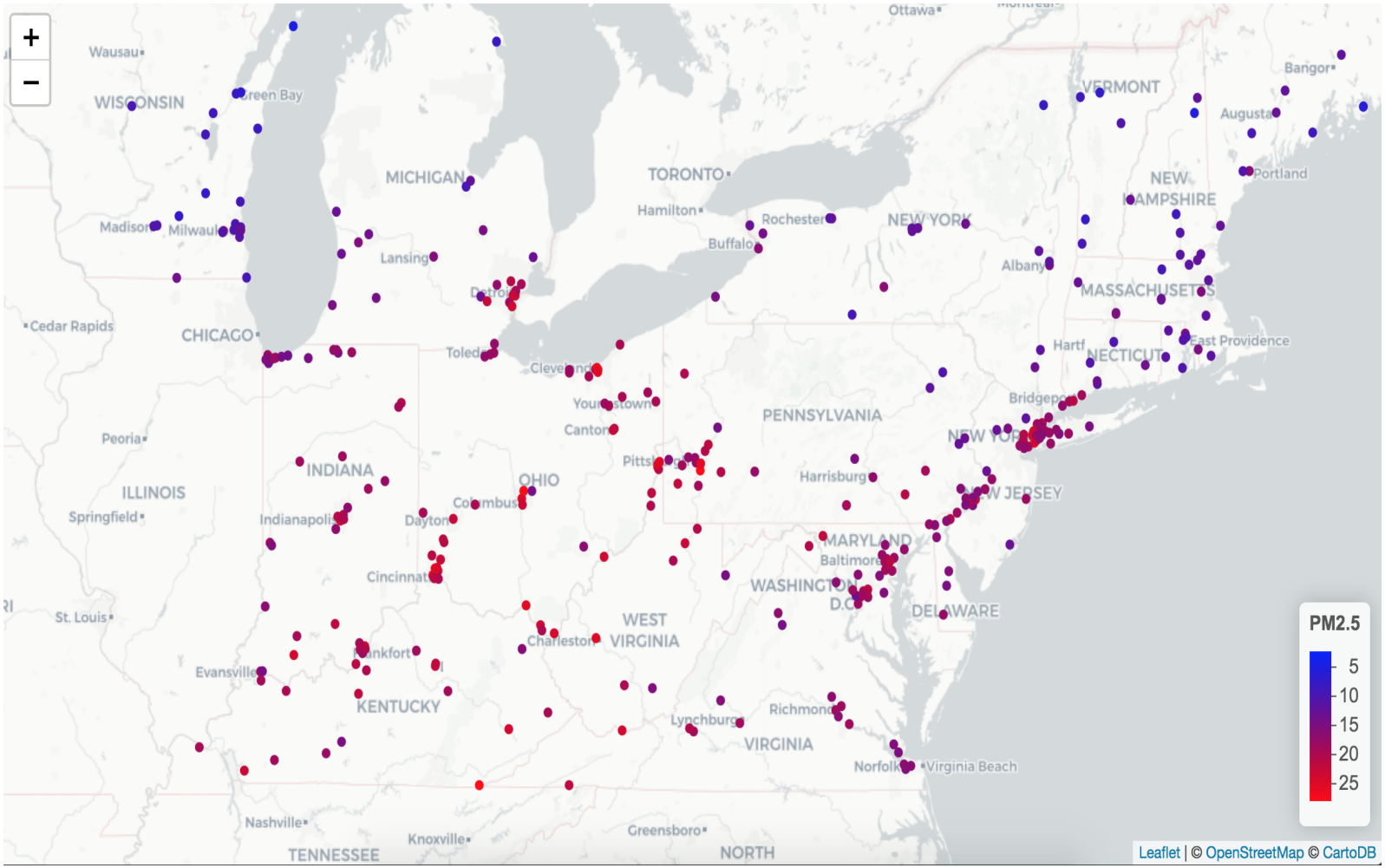
The common thread that links the data is a random process (also called stochastic process or random field)

$$Z(\mathbf{s}) : \mathbf{s} \in D$$

where D is a domain in $\mathbb{R}^d$ (d typically 2)

Geostatistical Data: Example

Recall our example of $PM_{2.5}$ in the northeast US. Here we have each point representing a location (latitude, longitude), and an associated Z(s) which is monthly $PM_{2.5}$ concentrations.



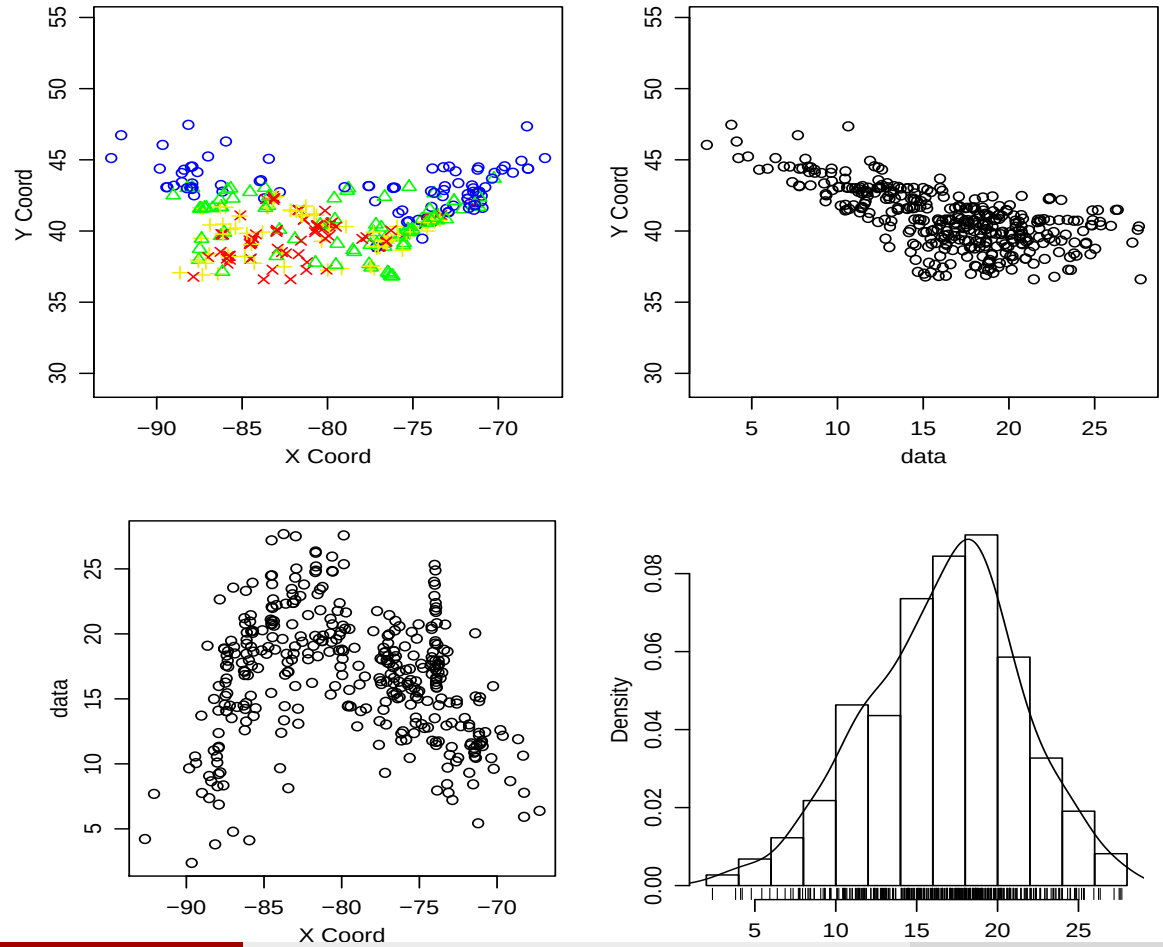
Geostatistical Data: Analytical Goals

Goals of spatial statistics applied to point referenced data

- Visualization of points on a map to look at distribution. Add colour scale to represent Z(s) values.
- Exploring the data to determine if there is a spatial pattern in the observations. (Often called spatial "structure")
- Testing null hypothesis of no spatial structure.
- Modeling the spatial correlation/covariance in the observations.
- Making predictions at unobserved locations: interpolation, smoothing.

Geostatistical Data: Exploratory Analysis

Using the geoR library, we can do quick explorations of spatial data. Here we show the $PM_{2.5}$ concentrations, the $PM_{2.5}$ trend in each x (longitude) and y (latitude) directions, and a histogram of the $PM_{2.5}$ concentrations.
Create an `as.geodata()` object, and plot it.



Geostatistical Data: Statistical Definition

Statistical formulation

- Spatial pattern as a random process: $Z(\mathbf{s}) : \mathbf{s} \in D$ where the spatial domain D is fixed (e.g. Northeast US) and $\mathbf{s}$ are the spatial locations $s_1, s_2, ..., s_n$ in D (e.g. GPS locations of $PM_{2.5}$ monitor). The process is the collection of random variables $Z(\mathbf{s})$ (e.g. $Z(s_1) = PM_{2.5}$ concentration at location s_1)
- Since an infinite number of measurements could have been taken over the domain, D we think of the spatial locations we have measured $Z(\mathbf{s})$ as a realization of the random process

Geostatistical Data: Distance

- Understanding spatial structure based on covariance/correlation is key.
- How is distance defined?
- Irregular spacing leads to few (usually one) pair of points for a given distance.

Geostatistical Data: Covariance

- Covariance tells us whether knowing one observation gives us any information about another observation.
- Covariance allows borrowing of strength for local prediction and estimation, usually increasing efficiency (reduced uncertainty).

Definition of covariance and correlation between two variables

$$\text{Cov}(X_1, X_2) = E[(X_1 - E(X_1))(X_2 - E(X_2))]$$
$$\text{Corr}(X_1, X_2) = \frac{\text{Cov}(X_1, X_2)}{\sqrt{\text{Var}(X_1)\text{Var}(X_2)}}$$

- In the spatial setting, **covariance is a function of distance**.

Geostatistical Data: Covariance

Covariance and correlation for random processes are often called autocovariance and autocorrelation

$$C(h) = E[(Z(s) - E(Z(s))) \cdot (Z(s+h) - E(Z(s+h)))]$$
$$\text{Cov}(Z(s_i), Z(s_j)) = C(s_i - s_j) = C(h)$$

The covariance depends only on the distance, h, between locations s_i and s_j, not on the locations themselves. We will revisit this assumption later.

$$\rho(h) = \frac{C(h)}{C(0)} = \frac{C(h)}{Var(Z(s))}$$

Geostatistical Data: Distance

- How is distance, h, defined?
- Several ways to define spatial distances but they must satisfy several technical conditions
  1. symmetry ($d(s_i, s_j) = d(s_j, s_i)$)
  2. the distance between a point and itself is zero
  3. the triangle inequality ($d(s_i, s_j) \leq d(s_i) + d(s_i)$)
- Euclidean distance
  $d(s_i, s_j) = \sqrt{(s_{ix} - s_{jx})^2 + (s_{iy} - s_{jy})^2}$

Euclidean distance is by far the most common way to represent distance in spatial analysis.

Geostatistical Data: Semivariogram

- The most widely used quantification of spatial autocorrelation is the **semivariogram**.
- It measures the similarity of values as a function of the distance between their locations.
- Traditional geostatisticians tend to favor the semivariogram over the covariogram/correlogram for historical reasons and because the empirical semivariogram is an unbiased estimator of the true semivariogram, while the covariogram is biased.

Geostatistical Data: Semivariogram

- $\text{Var}[Z(s+h) - Z(s)] = E[(Z(s+h) - Z(s))^2]$
- This is the expected squared difference between values, which generally increases as a function of the distance between the locations.
- $\text{Var}[Z(s+h) - Z(s)] = 2\gamma((s+h) - s) = 2\gamma(h)$
- $2\gamma(h)$ is the variogram and $\gamma(h)$ is the semivariogram

Geostatistical Data: Stationarity

Some additional properties of the semivariogram

- An assumption that is made in spatial analysis is that the spatial process under study repeats itself over the domain D. Such a spatial process is said to be stationary. For a stationary process the absolute coordinates at which we observe the process are unimportant. All that matters are the orientated distances between the points. In a stationary process if we translate the entire set of coordinates by a specific amount in a specified direction, the entire process remains the same.

Geostatistical Data: Stationarity

- It is useful to view spatial data as multivariate, despite it being the same measurement (i.e. $PM_{2.5}$ concentration) at multiple locations
- We have a joint probability density:
  $F(Z(\mathbf{s})) = P(Z(s_1) \leq z_1, Z(s_2) \leq z_2, ..., Z(s_n) \leq z_n)$
- Strong stationarity means that the joint density is invariant under translation:
  $P(Z(s_1) \leq z_1, Z(s_2) \leq z_2, ..., Z(s_n) \leq z_n) = P(Z(s_1 + h) \leq z_1, Z(s_2 + h) \leq z_2, ..., Z(s_n + h) \leq z_n)$

Geostatistical Data: Stationarity

- A weaker form of stationarity assumes that the moments (mean, variance) of the joint density are invariant.
- Called second-order stationarity
- $E[Z(s)] = \mu$
- $Cov(Z(s+h), Z(s)) = C(h)$
- $C(h)$ only depends on distance, h where C is a covariogram

Geostatistical Data: Stationarity

A third form of stationarity is intrinsic stationarity. This is the version we often use because it applies a technique of differencing of the spatial process to obtain stationarity. It derives from weak stationarity, and is what gives us the semivariogram.

- Differencing in what we previously described: Z(s+h)-Z(s)
- It is intrinsic if it has a constant mean and the variance of the differences at pairs of locations only depends on the distance h between locations
- These properties allow us to define the semivariogram (variogram)

$$\frac{1}{2}(Z(s+h) - Z(s)) = \gamma(h)$$

This is the preferred method (and thus instrinsic stationarity is the primiary type of stationary) for characterizing geostatistical spatial processes.

Geostatistical Data: Stationarity

Some additional properties of the semivariogram

- Recall: when the random (spatial) process is stationary it is a function of the spatial lag, or distance only ($\gamma(h)$).
- $\gamma(-h) = \gamma(h)$
- $\gamma(0) = 0$ since $Var(Z(s) - Z(s)) = 0$.
- the spatial process is **isotropic** if $\gamma(h) = \gamma(||h||)$
- the semivariogram and the covariance function are related by:

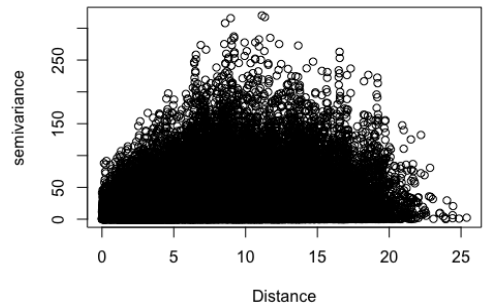
$$\begin{aligned}
\gamma(h) &= \frac{1}{2}E[(Z(s+h) - Z(s))^2] \\
&= \frac{1}{2}E[((Z(s+h) - \mu) - (Z(s) - \mu))^2] \\
&= -E[(Z(s+h) - \mu)(Z(s) - \mu)] + \frac{1}{2}E[(Z(s+h) - \mu)^2] \\
&\quad + \frac{1}{2}E[(Z(s) - \mu)^2] \\
&= -C(h) + C(0)
\end{aligned}$$

Geostatistical Data: Stationarity

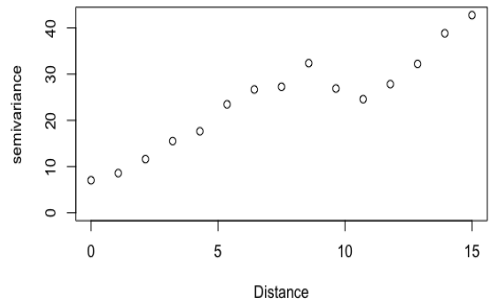
- Spatial processes have the assumption of stationarity, i.e. $E[Z(\mathbf{s})] = \mu$ for all $\mathbf{s} \in D$. This means the mean of the process does not depend on location.
- Stationarity also states that $Cov(Z(s_i), Z(s_j)) = C(s_i - s_j)$. This means that the covariance depends only on the difference between locations s_i and s_j and not on the locations themselves (stationarity). $C(\cdot)$ is the covariance function.

Geostatistical Data: Empirical Semivariograms

Plot the separation distance $||h||$ vs $\gamma(h)$ for all pairs of points, but this is difficult to interpret.

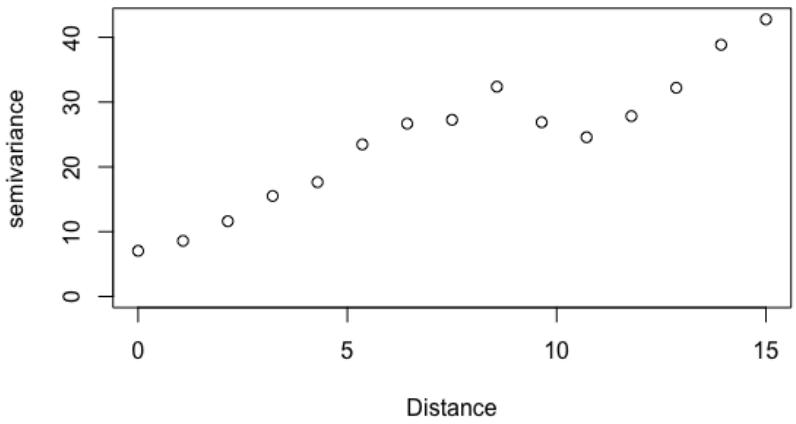


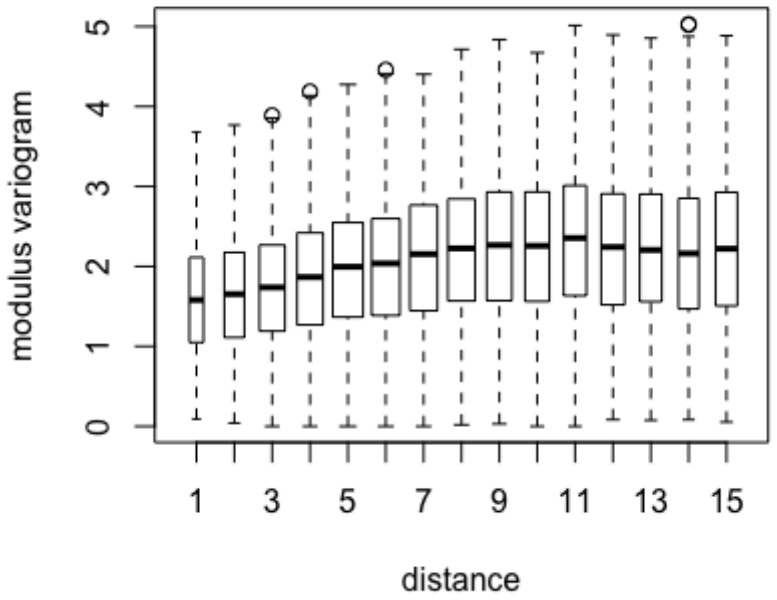
Instead an empirical estimate can be calculated by binning the distances:
$\hat{\gamma} = \frac{1}{2N(h)} \sum_{N(h)} [Z(s_i) - Z(s_j)]^2$



Geostatistical Data: Empirical Semivariograms

- Divide distance into K intervals $I_1 = (0, h_1), ..., I_K = (h_{K-1}, h_K)$
- $\hat{\gamma}(h_k) = \frac{1}{2N(h_k)} \sum_{N(h)} [Z(s_i) - Z(s_j)]^2$
- $N(h_k)$ is the set of pairs in the interval I_k

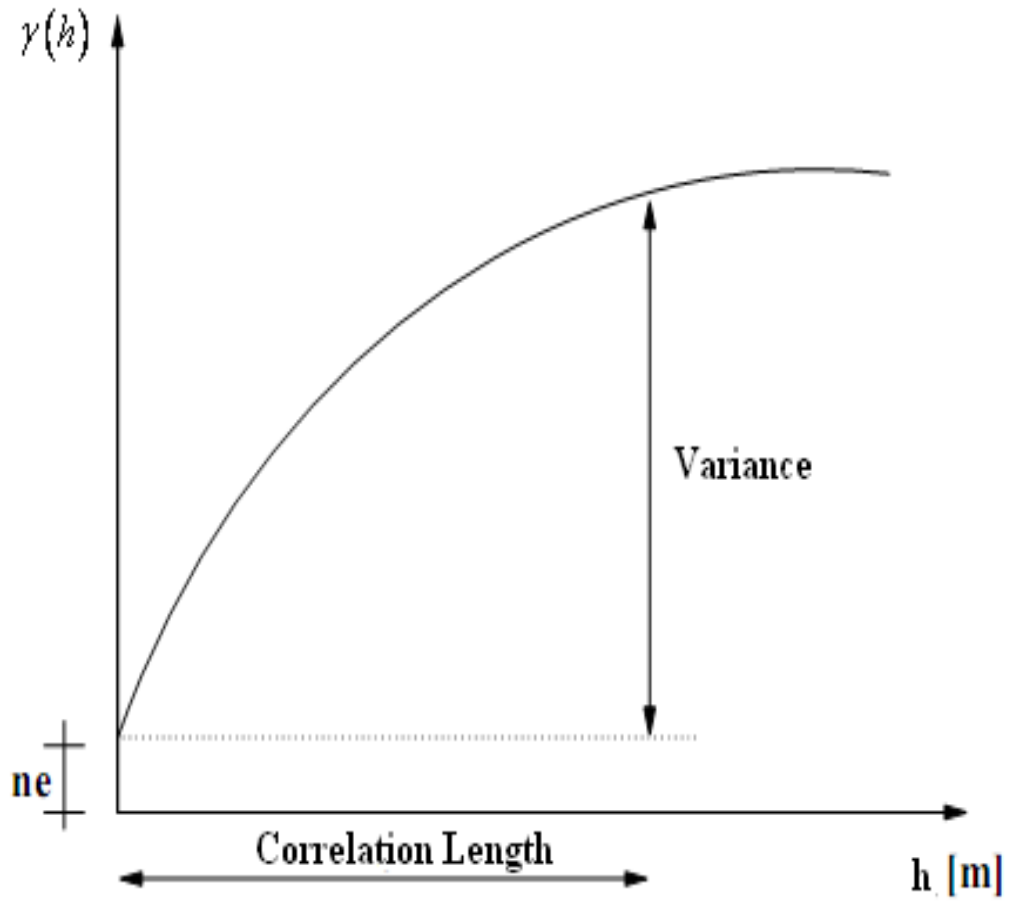




Geostatistical Data: Empirical Semivariograms

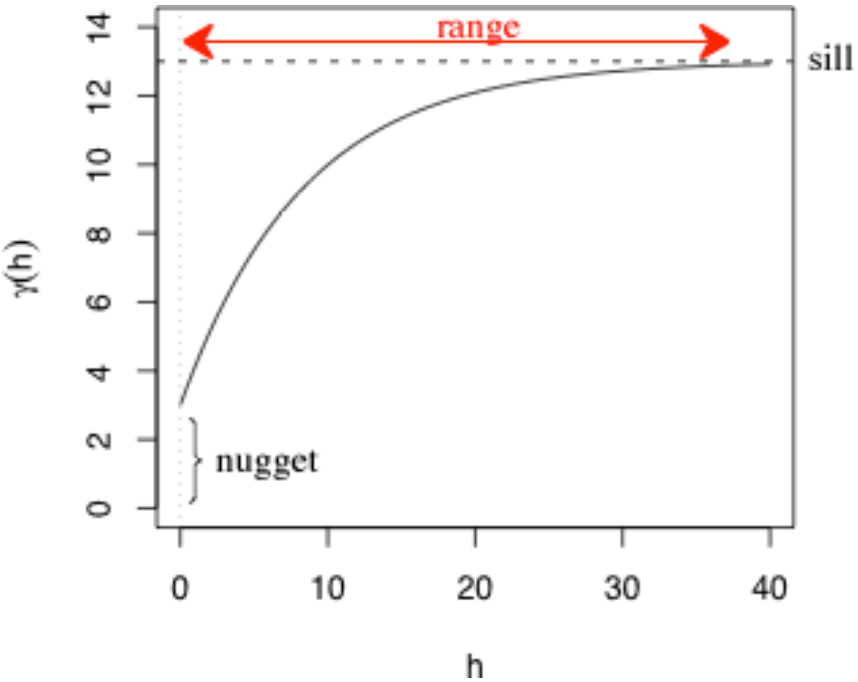
- There is a more robust estimate of the variogram by Cressie and Hawkins
- Less sensitive to outliers
- $\hat{\gamma}(h_k) = \frac{1}{N(h_k)} \sum_{N(h)} |Z(s_i) - Z(s_j)|^{1/2}$
- Again, $N(h_k)$ is the set of pairs in the interval I_k

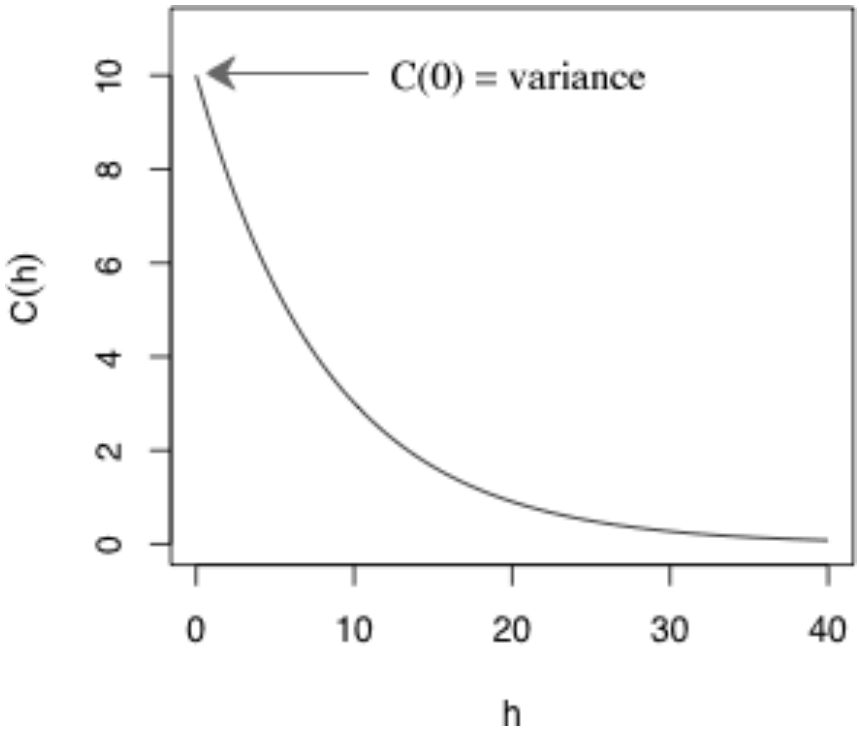
Geostatistical Data: Semivariogram Interpretation



- Observations that are close together are more alike than those far apart: increasing variance in pairwise difference with increasing h means decreasing autocorrelation.

Geostatistical Data: Semivariogram Interpretation





Geostatistical Data: Semivariogram Interpretation

- Strength of spatial structure is based on where the semivariogram reaches an asymptote. This distance is called the **range**, ρ. Beyond this distance, it is assumed that there is no autocorrelation.
- The semivariance where the asymptote is reached is the **sill**, σ^2.
- The discontinuity at the origin is called the **nugget**, τ^2.
- If there is a nugget, be careful to interpret the sill as the value after subtracting the nugget (the 'effective' sill).
- Recall that if the process is not stationary $C(h)$ doesn't exist.

Geostatistical Data: Theoretical Semivariograms

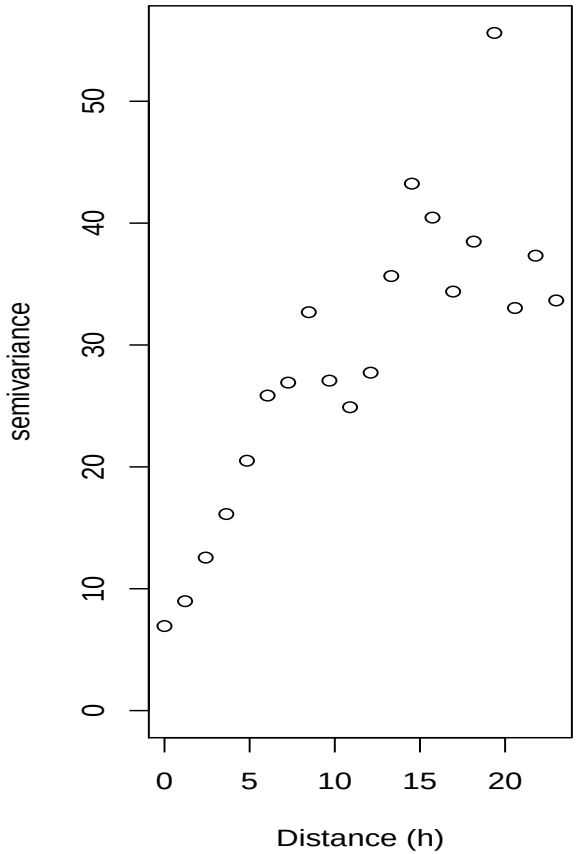
We want to fit a theoretical model to our "empirical" semivariogram to describe the shape of the spatial process.
Common parametric semivariogram functions:

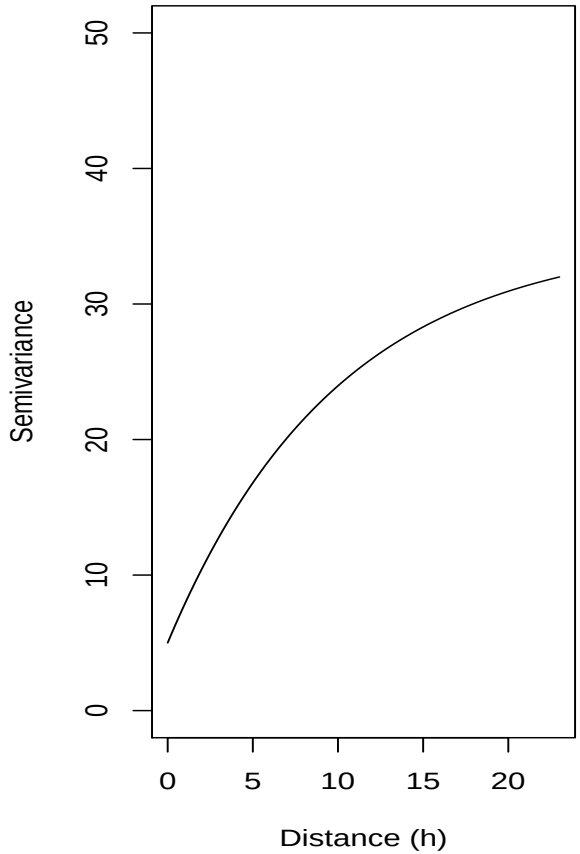
- Exponential
- Spherical
- Gaussian
- Matern

Geostatistical Data: Empirical vs Theoretical

Exponential:

$$\gamma(h) = \tau^2 + \sigma^2(1 - exp(-h/\rho))$$

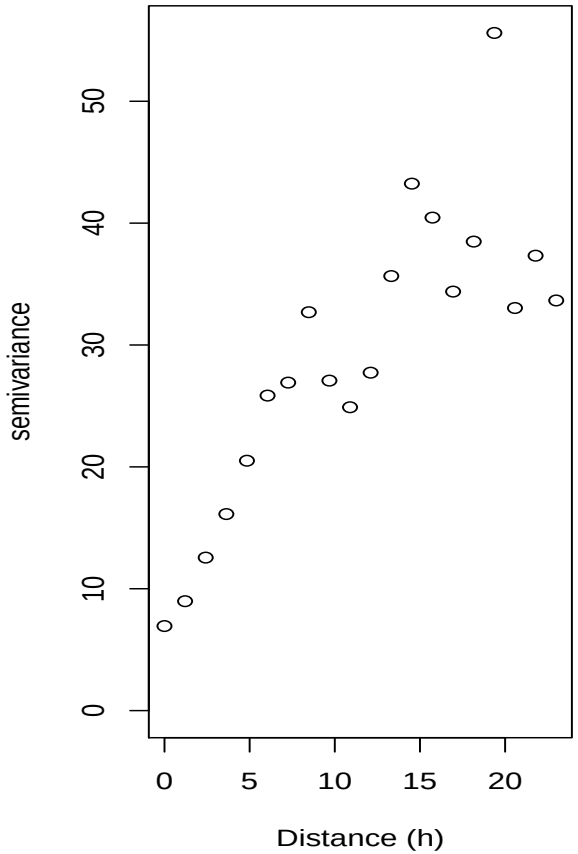


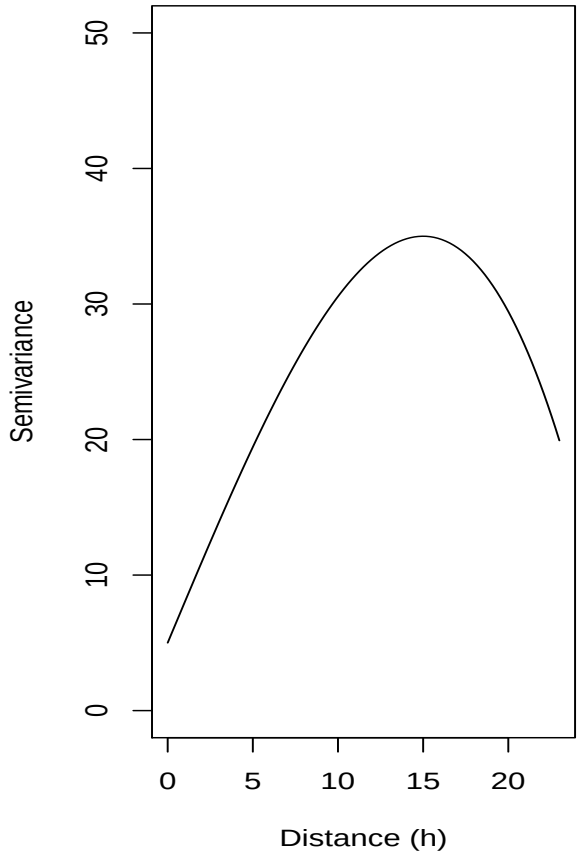


Geostatistical Data: Empirical vs Theoretical

Spherical:

$$\gamma(h) = \tau^2 + \sigma^2(3/2(h/\rho) - 1/2(h/\rho)^3)$$

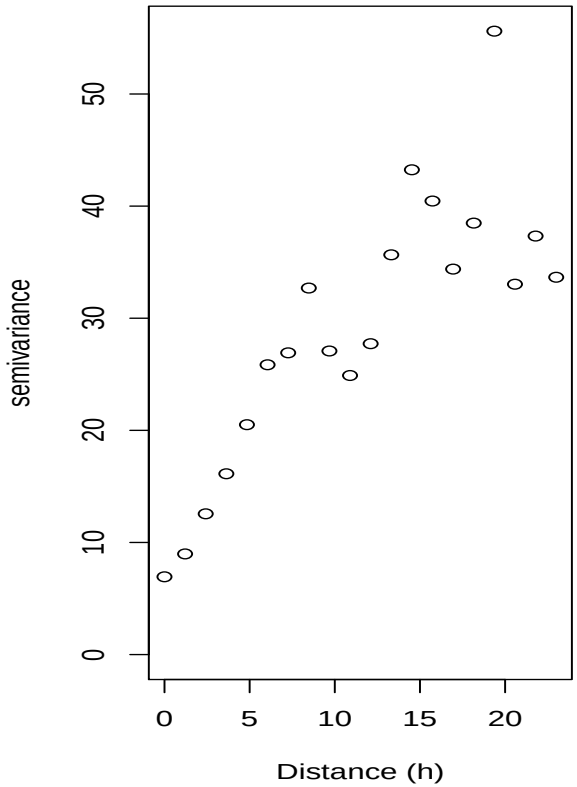


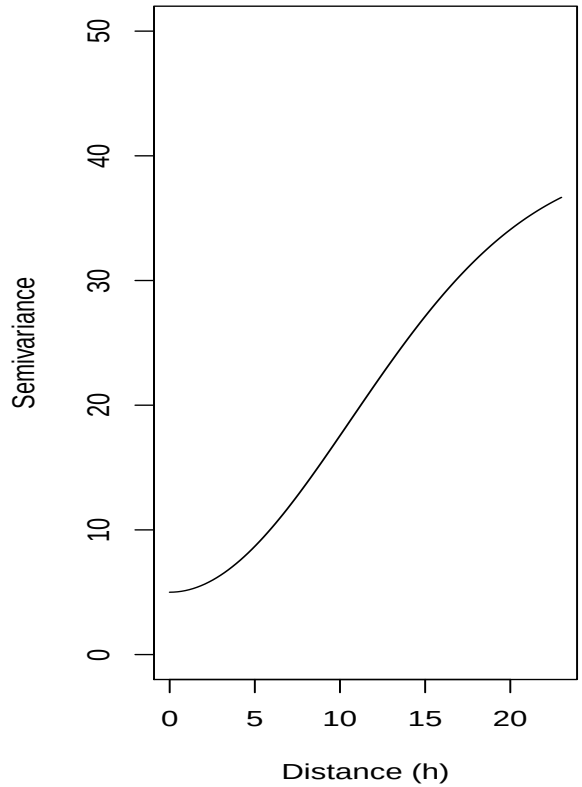


Geostatistical Data: Empirical vs Theoretical

Gaussian:

$$\gamma(h) = \tau^2 + \sigma^2(1 - exp(-\frac{h^2}{\rho^2}))$$





Geostatistical Data: Fitting a Semivariogram

Eyeballing the semivariogram is useful for exploratory purposes and to find the approximate shape of the spatial process, but we would rather find a valid theoretical semivariogram function that reflects the empirical semivariogram. Ordinary Least Squares: find the parameters $\theta = (\tau^2, \sigma^2, \rho)$ that minimize the squared vertical distance between the empirical and theoretical semivariograms.

$$(\hat{\gamma}(h) - \gamma(h;\theta))^T (\hat{\gamma}(h) - \gamma(h;\theta))$$

where $\hat{\gamma}(h)$ is the empirical semivariogram and $\gamma(h;\theta)$ is the theoretical semivariogram with parameters θ

Geostatistical Data: Fitting a Semivariogram Model

We use the binned semivariogram,

$$\hat{\gamma}(h) = \frac{1}{2N(h)} \sum_{N(h)} [Z(s_i) - Z(s_j)]^2$$

- The relationship between $\hat{\gamma}(h)$ and h is nonlinear (semivariogram model is not a linear function)
- Use generalized least squares, solved numerically
- Minimize SSE $\sum_j^K [\hat{\gamma}(h_j) - \gamma(h_j)]^2$
- K bins from our empirical semivariogram

Geostatistical Data: Fitting a Semivariogram Model

In Generalized Least Squares (GLS) we introduce the covariance matrix, V

$$(\hat{\gamma}(h) - \gamma(h, \theta))^T V(h, \theta)^{-1} (\hat{\gamma}(h) - \gamma(h, \theta))$$

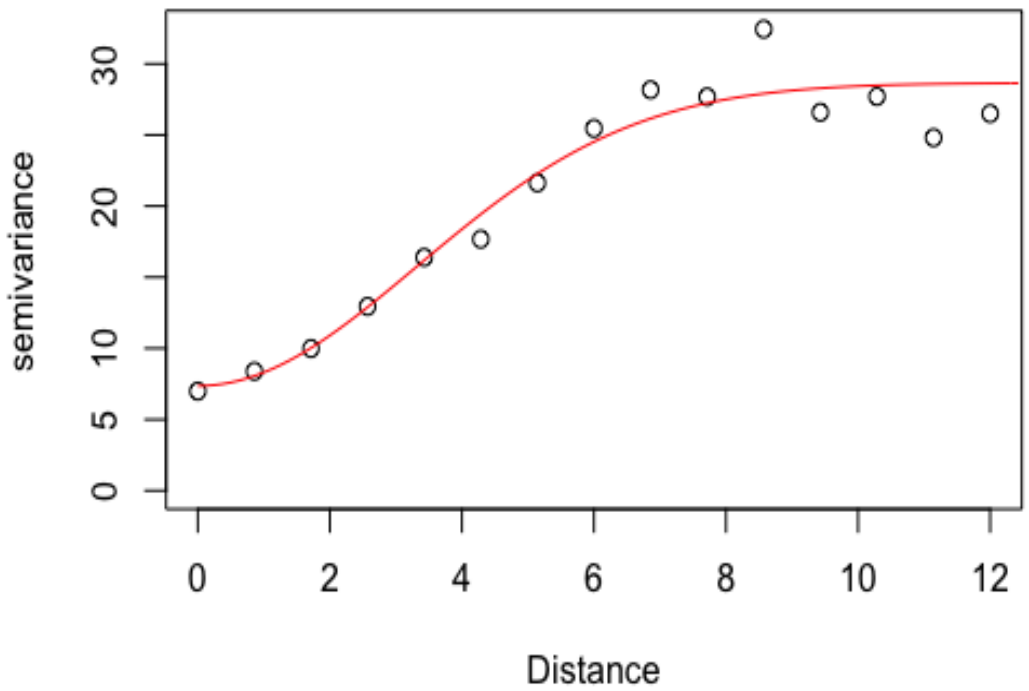
- Correlation among bins is accounted for with $V(h, \theta)^{-1}$
- Difficult to calculate this since θ are unknown, computationally intensive
- Use approximation and weighted least squares which accounts for unequal variance of bins (Cressie 1985)
- WLS still does not account for correlation, but is better than OLS as it gives more weight to bins having more data

Geostatistical Data: Fitting a Semivariogram Model

- $V(h;\theta)^{-1}$ =I gives the OLS equation
- Taking $V(h;\theta)^{-1}$ = diag $Var[\hat{\gamma}(h_1)], ..., Var[\hat{\gamma}(h_K)]$ gives a weighted least squares estimator
- $Var[\hat{\gamma}(h_j)] \approx 2[\hat{\gamma}(h_j)]^2/N(h_j)$
- now we minimize WSSE $\frac{1}{2}\sum_{j}^{K} \frac{N(h_j)}{\hat{\gamma}(h_j)}[\hat{\gamma}(h_j) - \gamma(h_j)]^2$

Geostatistical Data: Fitting a Semivariogram Model

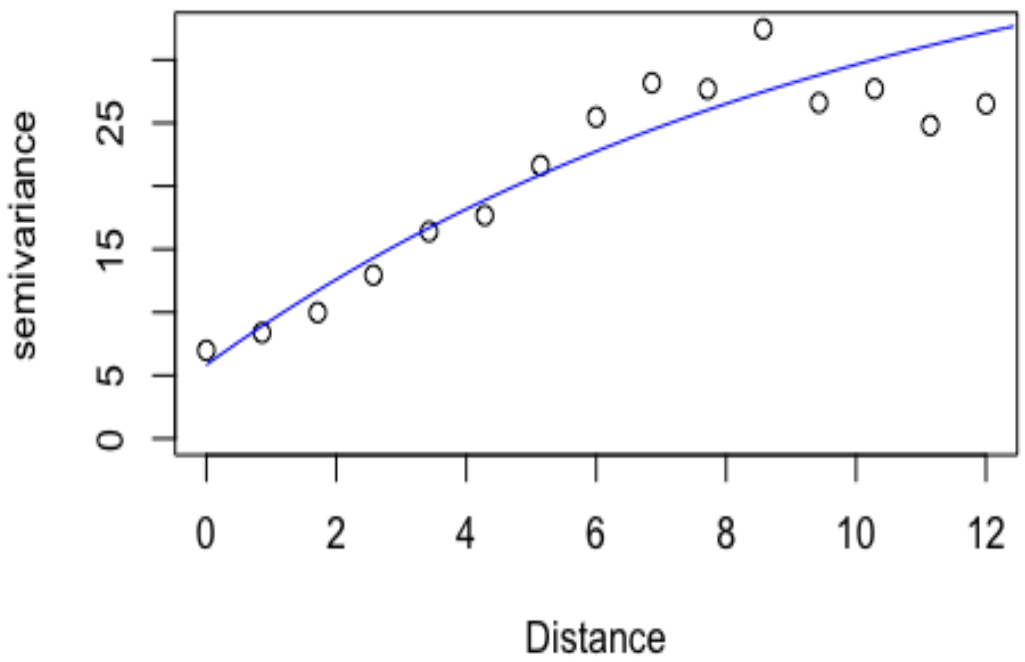
Result of fitting a Gaussian semivariogram by WLS to binned empirical semivariogram. In R use variofit() with weights="cressie"



Estimated parameters: $\hat{\sigma}^2 = 21.2972$, $\hat{\phi} = 4.6864$, $\hat{\tau}^2 = 7.3589$; SSE: 253.5

Geostatistical Data: Fitting a Semivariogram Model

Result of fitting an exponential semivariogram by WLS to binned empirical semivariogram. In R use variofit() with weights="cressie"



Estimated parameters: $\hat{\sigma}^2 = 38.2043$, $\hat{\phi} = 10.2684$, $\hat{\tau}^2 = 5.8442$; SSE: 479.8

Geostatistical Data: Fitting a Semivariogram Model

- There is extensive literature on fitting semivariograms, but approach is somewhat arbitrary and unsatisfying statistically.
- The objective that is minimized (deviation of empirical semivariogram values from semivariogram model) is based on pseudo-data.
- Fitting is basically just curve fitting and is sensitive to the binning and maximum distance chosen.
- Calculations based on semivariograms are fast, even with many observations.
- Semivariogram modeling is not based on a particular probability model for the data, so it may be more resistant to violations of assumptions.
- Compare SSE different models fit by one method (i.e. exponential vs spherical WLS). Don't compare SSE from WLS and OLS.

Geostatistical Data: Fitting a Covariance Model

Fitting covariance models by maximum likelihood

- The more standard statistical approach is to fit a covariance model by maximum likelihood (ML)
- ML is the most common approach in statistics to fit models by estimating parameter values
- Recall, in linear regression with normal (uncorrelated) errors, least squares is the same as maximum likelihood estimation.
- ML requires specification of a probability model (the likelihood) for the data
- Likelihoods involve unknown parameters that must be estimated from data
- Our spatial data must follow a multivariate Gaussian distribution and have second-order stationarity (Covariance exists)

Geostatistical Data: Fitting a Covariance Model

Fitting covariance models by maximum likelihood

- Gaussian process: MVN, mean $= \mu$, Cov$=\sum(\theta)$
- Can think of this as spatial regression: $E(Z(s)) = \mu + \epsilon(s) = X\beta + \epsilon(s)$
- Where $\epsilon(s) \sim N(0, \sum(\theta))$
- The log-likelihood function has the form:
  $L(\beta, \theta; Z) = -\frac{1}{2} log|\sum(\theta)| - \frac{1}{2}(Z - X\beta)^T \sum(\theta)^{-1}(Z - X\beta)$
- Restricted maximum likelihood (REML) is an alternative and is based on maximizing the likelihood when the data are differences

Geostatistical Data: Fitting a Covariance Model

Fitting covariance models by maximum likelihood

- The goal is to maximize the probability of the data relative to different parameter values
- The parameter values are treated as unknown and the data as fixed, and the parameter values that give the highest likelihood are chosen
- ML/REML is done in this case by numerical methods (there is no closed form solution) and can be intensive for large datasets (more than a few hundred observations)

Geostatistical Data: Choosing a Model

Choosing among models fit by ML

- The traditional way is to use Akaike's Information Criterion, which in its general form minimizes:
- AIC $= 2\log($maximized likelihood$) + 2($number of parameters$)$
- AIC can be used for non-nested models. It compares the likelihoods of different models and penalizes models with more parameters:
- Models with smaller AIC are favoured

Geostatistical Data: Kriging

- Kriging is the spatial prediction of our process at unobserved locations
- Based on the fitted covariance function and the spatial regression model $E(Z(s)) = \mu + \epsilon(s) = X\beta + \epsilon(s)$
- Objective: To estimate the value of $Z(s)$ at one or more unsampled locations in our region D based on our observed samples $z(s_1), z(s_2), ..., z(s_n)$

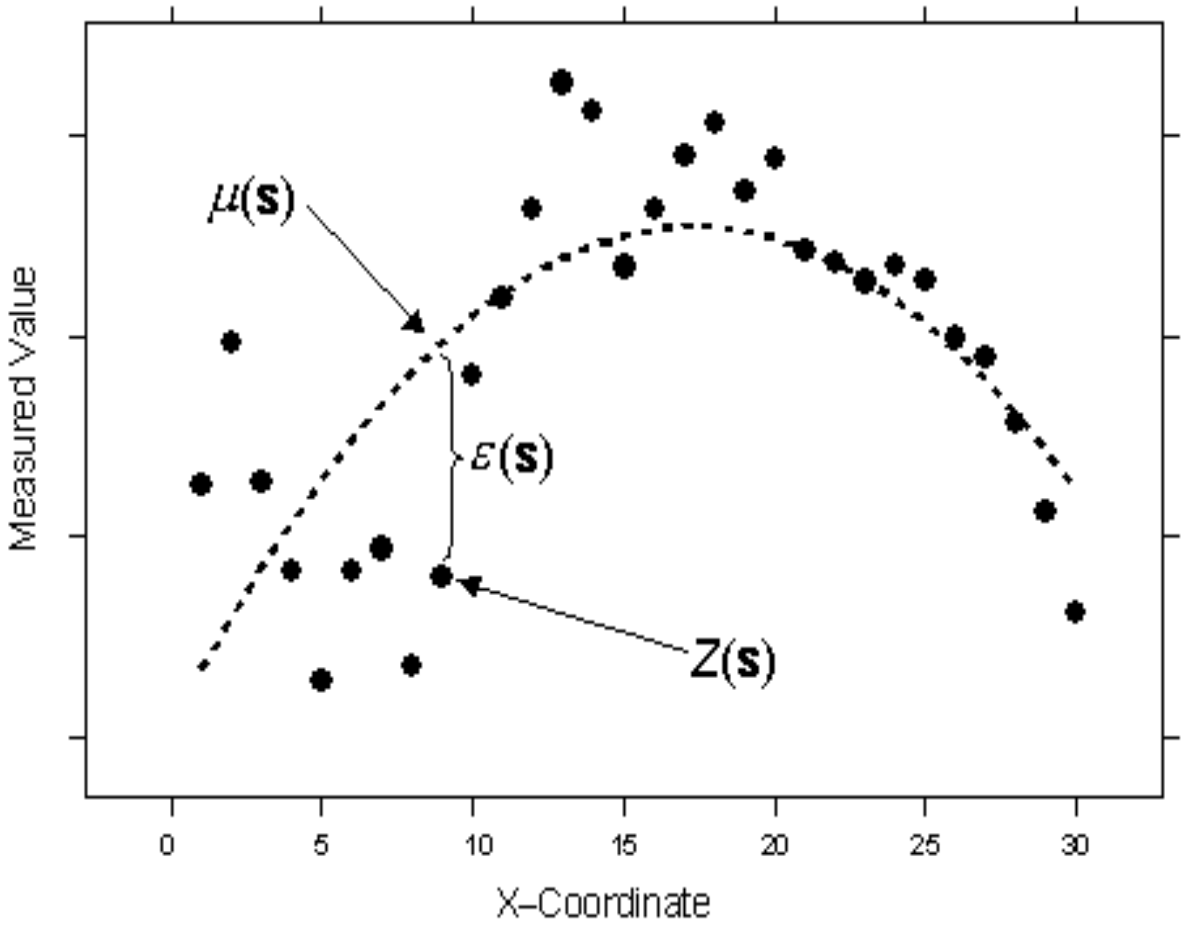
Geostatistical Data: Kriging

- The basic kriging recipe:
  1. Choose a parametric model for the semivariogram or covariance function
  2. Estimate the semivariogram/covariance parameters.
  3. Make predictions and uncertainty estimates given the parameter estimates.
- The kriging predictions are weighted averages of the observations. The covariance/semivariogram indicates the strength of spatial association and determines the weighting.
- The issue is how heavily to weight the observations based on distance from the location.

Geostatistical Data: Kriging

- The kriging predictor at new location s_0 is $\hat{Z}(s_0) = \sum \lambda_i Z(s_i)$
- Goal: to minimize squared error loss $E[(\hat{Z}(s_0) - Z(s_0))^2]$
- The best prediction of this is the conditional mean: $E(Z(s_0)|Z)$ which is the expected value of what you don't know given what you do know.
- This calculation assumes you know the covariance function (or have estimated it).
- In R we use the `krig.conv()` function in the geoR library.

Geostatistical Data: Kriging

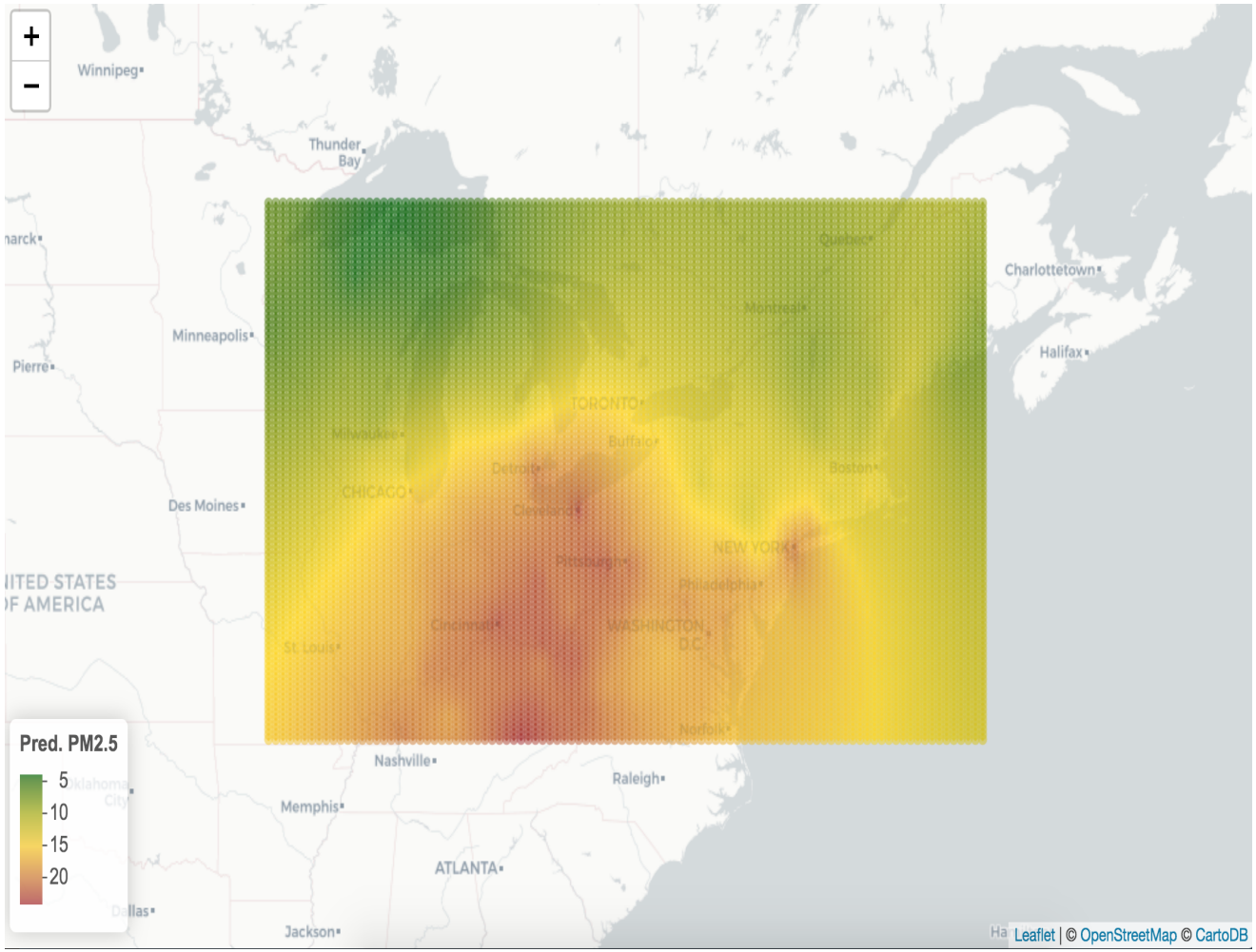


Geostatistical Data: Kriging Types

There are different kriging types for different assumptions and analytical goals. The types are:

- Simple Kriging: assumes a constant known mean $\mu = c$. This type is not often used because for unbiasedness constraint to be applicable in kriging equations, we must estimate the expected value.
- Ordinary Kriging: assumes a constant unknown mean (mean needs to be estimated) $Z(s) = \mu + \epsilon(s)$.
- Universal Kriging: assumes a trend in x and y, and may include other spatially varying covariates $Z(s) = \mu(s) + \epsilon(s)$ where $\mu(s) = \sum_{k=1}^{p} \beta_k x_k(s_i)$.

Geostatistical Data: Ordinary Kriging Result



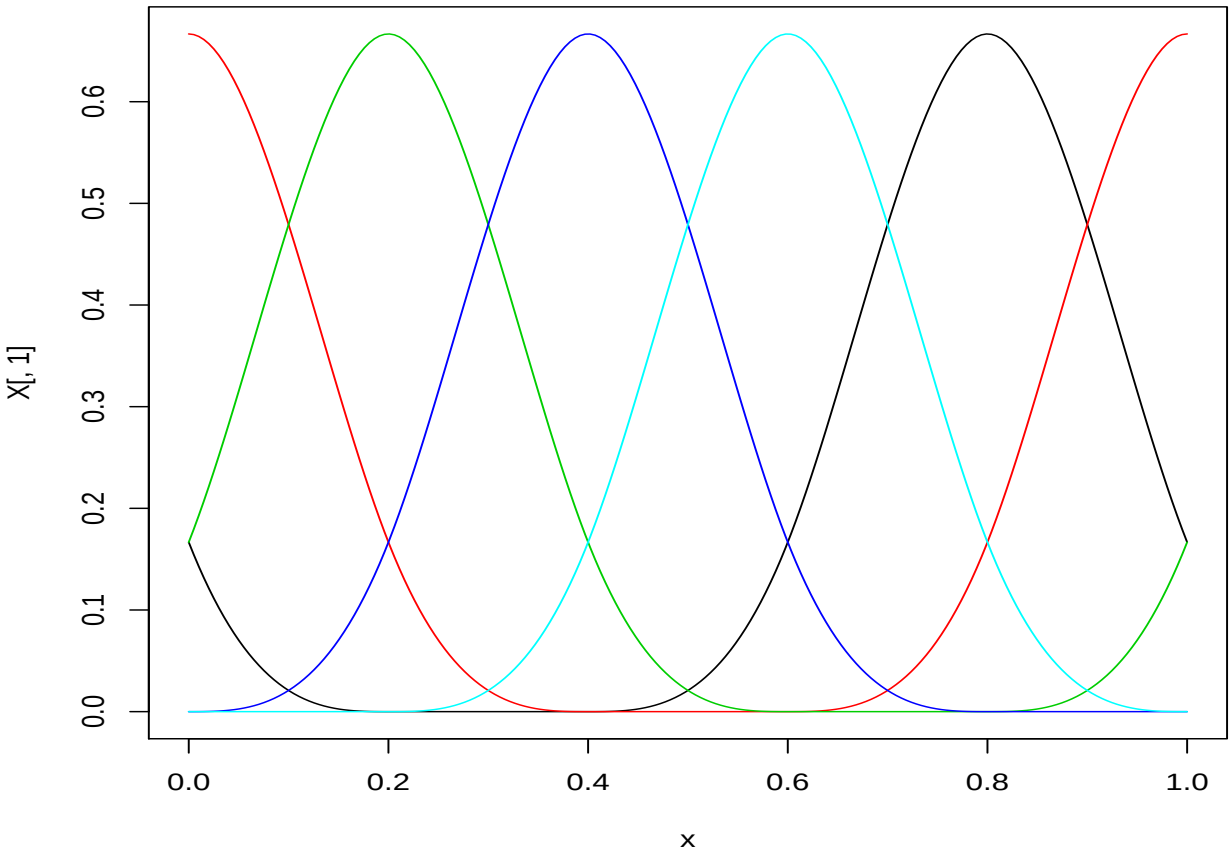
Geostatistical Data: Smoothing

- Here we focus on modeling the spatial component in the mean part of a regression model rather than in the covariance
- In general, $Z(s) = f(s) + \epsilon$ where errors are not correlated
- $f(s)$ is a "smooth" function described by a basis function, and consists of non-linear terms
- This is considered statistical smoothing because we can get an estimate of the prediction errors

Geostatistical Data: Splines

- In general, splines are curves that are formed by combining pieces of a polynomial.
- There are several types of splines including natural, cubic, and b-splines (the b stands for basis).
- $f(t_i) = \sum_{j=1}^{4} t^j \beta_j$
- B-spline curves are made up of polynomial pieces and are defined by a set of knots
- Choosing the number of knots defines how smooth (few) or wiggly (many) your functions

Geostatistical Data: Splines



Geostatistical Data: Splines

- Smoothing splines with penalty allows us to estimate where to put the knots by penalizing the wiggliness of the function
- Minimize the function $\sum_i (y_i - f(t_i))^2 + \lambda \int f''(t)^2 \mathrm{d}t$
- Here, λ is a penalty parameter that controls how much to penalize wiggly functions
- Tradeoff between the goodness of fit (the sum of squares) and the wiggliness of the function (the integral)
- Start by putting a knot at every data point, then penalize
- It is an optimization problem m where we minimize:

$$\sum_i (y_i - B_i^T \beta)^2 + \lambda \beta^T S \beta$$

- the matrix S is constructed by using the spline basis we chose, B is the basis matrix

Geostatistical Data: 2-D Splines

- Thin plate splines are smoothing splines in 2-d
- Extend the 1-d case to:

$$\sum_i (z_i - g(s_1, s_2))^2 + \iint g''(s_1, s_2)^2 \mathrm{d}s_1 \mathrm{d}s_2$$

- The thin plate spline can be implemented as an extension to the linear model in what's called a generalized additive model (GAM).

Geostatistical Data: 2-D Splines

- Can use the spline model to predict as we did with kriging.
- Also useful as we can generate standard errors for our predictions.
- Implemented in R using the `gam()` and `predict.gam()` functions in the mgcv library.

Geostatistical Data: 2-D Splines