# Spatial Statistics 

## Geostatistical Data

Satyaki

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## Overview

## 1. Introduction

2. Formalization
3. Exploratory analysis
4. Semivariogram
5. Kriging

## A study on brain cancer

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## A study on brain cancer

- Navarre is a province in Spain.
- It is divided in 40 health districts.
- A study on the number of deaths due to brain cancer for years 1988-1994 was done in 2006 (Ugarte et al. (2006)).
- In each district, there is standardized morbidity ratio (SMR). This is calculated based on the observed data in a district.
- The data is given as Navarre.RData in the statistical software R.

Table: Glimps of the data

| NAME | SMR |
| :---: | :---: |
| ALLO | 1.8709074 |
| ALSASUA | 0.0000000 |
| ARTAJONA | 5.3980815 |
| $\vdots$ | $\vdots$ |

## Visualizing the data

histogram of smr


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## Spatial diagram



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- The data is available as LipCancer.RData in the statistical software R.


## Visualization

hist of population percentange


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hist of permuted population percentage


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- Majority of his time was engaged in developing of methodology for analysis of data arising from agricultural field trails.
- A data set was collected analyzed by Mercer (1911) that dealt with the wheat production at Rothamsted.
- Fisher encountered this type of data while working at Rothamsted.


## Mercer's wheat data



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- Fisher commented: "the widely verified fact that patches in close proximity are commonly more alike, ..., than those which are farther apart"
- He proposed blocking to tackle spatial variation: a form of covariate adjustment under the implicit assumption that systematic spatial variation, if it exists at all, is piecewise constant within blocks.


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- That essentially leads to Markov Random Field.
- In modern language, his proposal is similar to a conditional model for the distribution of the yield of the each plot, given the average yield, when the average is taken over "neighbouring" plots.
- Thus, the moral: "everything is related to everything else, but near things are more related than distant things". Tobler (1979)


## Different types of spatial data

- $(74.1,97]$
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- (54.7,61.2]
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Geostatistical Data or point referenced data

## Second type of spatial data



## Second type of spatial data



Areal data

## Third type of spatial data

longleaf

60
40 $\bigcirc$
$\bigcirc$

longleaf


Chicago Crimes


Point Pattern Data

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- Geostatistical Data or Point referenced data: $s_{1}, s_{2}, \ldots, s_{n}$ are fixed and $X_{s_{1}}, X_{s_{2}}, \ldots, X_{s_{n}}$ are random variables.
- Goal: modeling, identification and separation of small and large scale variations, prediction (or kriging) at unobserved sites.



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- Lattice data or areal data: $\mathbb{S}$ is fixed collection of countably many points.


## Formal definitions

- Lattice data or areal data: Here $s_{1}, s_{2}, \ldots, s_{n}$ denote the blocks and the observation $X_{s_{1}}, X_{s_{2}}, \ldots, X_{s_{n}}$ are random observations.
- Goal: Constructing models, quantifying spatial correlations.



## Formal definitions

- The spatial observations comes from a spatial process $\left\{X_{s}, s \in \mathbb{S}\right\} ;$ Generally, $\mathbb{S} \subset \mathbb{R}^{2}$.
- Geostatistical Data or Point referenced data: $s$ varies continuously in a fixed subset $\mathbb{S}$, which contains a two dimensional rectangle of positive volume. $Z_{s}$ is observed at fixed sites $\left\{s_{1}, \ldots, s_{n}\right\} \subset \mathbb{S}$.
- Lattice data or areal data: $\mathbb{S}$ is fixed and partitioned into a finite number of blocks with clearly defined boundaries.
- Point pattern data: Here the observation sites $\left\{s_{1}, \ldots, s_{n}\right\}$ is random and the number of observation site $n$ is also random. $X_{s}$ can simply be equal to 1 indicating the occurrence of an event. Additionally, we may have some covariate information at these locations.


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- Goal: Decide whether distribution of points are regular or completely random or aggregated?



## Exploratory analysis on point referenced data



- Part of river Meuse in Netherlands
- Zinc concentration measurements
- Collected in a flood plain
- The concentration seems to be decreasing as distance increases from the river


## Scatter plot and simple linear regression



## Scatter plot and simple linear regression



- Clearly correlated.
- A simple linear regression can be tested.
- $y=a_{0}+a_{1} x+\epsilon$


## Fitted and the residuals



- $[-1.283,-0.7073]$
[0.1312,0.4448]
$\left[\begin{array}{l}-0.1312,0.4448] \\ 0.4448,1.021]\end{array}\right.$
(1.021,1.597]


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- However, the residuals do not seems to be spatially uncorrelated.
- More analysis, taking the spatial structure into the account, required.


## Covariogram

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- Weak stationary essentially mean that the covariance relationship between the
- $E(X(s))=\mu, \forall s \in \mathbb{S}$
- $\operatorname{Cov}\left(X\left(s_{1}\right), X\left(s_{2}\right)\right)=C\left(s_{2}-s_{1}\right)=C(\mathbf{h})$ values of the process at any two locations can be summarized by a function $C(\mathbf{h})$, depending on the separation vector $\mathbf{h}=s_{2}-s_{1}$.


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- Weak stationary essentially mean that the covariance relationship between the values of the process at any two locations can be summarized by a function $C(\mathbf{h})$, depending on the separation vector $\mathbf{h}=s_{2}-s_{1}$.
- $E(X(s))=\mu, \forall s \in \mathbb{S}$
- $\operatorname{Cov}\left(X\left(s_{1}\right), X\left(s_{2}\right)\right)=C\left(s_{2}-s_{1}\right)=C(\mathbf{h})$
- If $C(\mathbf{h})=\psi(\|\mathbf{h}\|)$, then the covariance function is called isotropic.

Covariance function is also known as covariogram.

## Important Properties

- $|C(\mathbf{h})| \leq C(0)$.
- $C(\mathbf{h})$ is positive semidefinite.
- If $C(\mathbf{h})$ is continuous at the origin then it is continuous everywhere.


## Intrinsic stationarity (Mathéron (1962))

- $E\left(X\left(s_{i}\right)-X\left(s_{j}\right)\right)=0$ and
- $E\left(X\left(s_{i}\right)-X\left(s_{j}\right)\right)^{2}=2 \gamma\left(s_{j}-s_{i}\right)=2 \gamma(\mathbf{h})$


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- Then the process is said to be intrinsic stationary.
- $\gamma(\mathbf{h})$ is called semivariogram.
- If the process is stationary, then $\gamma(\mathbf{h})=C(0)-C(\mathbf{h})$.
- If $\gamma(\mathbf{h})=\phi(\|\mathbf{h}\|)$, then the semivariogram is called isotropic.


## Important Properties

- $\gamma(\mathbf{h}) \geq 0$
- $\gamma(\mathbf{h})=\gamma(-\mathbf{h})$
- $\gamma(\mathbf{h})$ is conditionally negative definite.


## Reminder: $\gamma(\mathbf{h})$ is property of difference

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- even the $X(s) \mid X\left(s^{\prime}\right)$ and $X\left(s^{\prime}\right) \mid X(s)$ have proper density
- but $\left(X(s), X\left(s^{\prime}\right)\right)$ does not have one.


## Examples of $\gamma(h)$

- Linear:

$$
\gamma(\|\mathbf{h}\|)= \begin{cases}\tau^{2}+\sigma^{2}\|\mathbf{h}\| & \text { if }\|\mathbf{h}\|>0 \\ 0 & \text { otherwise }\end{cases}
$$

linear semivariogram


## Examples of $\gamma(h)$

- Spherical: $\gamma(\|\mathbf{h}\|)= \begin{cases}\tau^{2}+\sigma^{2} & \text { if }\|\mathbf{h}\|>1 / \phi \\ \tau^{2}+\sigma^{2}\left(\frac{3 \phi\|h\|}{2}-\frac{1}{2}(\phi\|h\|)^{3}\right) & \text { if } 0<\|\mathbf{h}\| \leq 1 / \phi \\ 0 & \text { otherwise }\end{cases}$


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exponential semivariogram



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Gaussian semivariogram


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- Matérn: $\gamma(\|\mathbf{h}\|)= \begin{cases}\tau^{2}+\sigma^{2}\left(1-\frac{(2 \sqrt{\nu} \phi\|h\|)^{\nu}}{2^{\nu-1} \Gamma(\nu)} K_{\nu}(2 \sqrt{\nu} \phi\|\mathbf{h}\|)\right) & \text { if }\|\mathbf{h}\|>0 \\ 0 & \text { otherwise }\end{cases}$
- $\gamma(\|\mathbf{h}\|)=\left\{\begin{array}{lc}\tau^{2}+\sigma^{2}(1-(1+\phi\|h\|) \exp (-\phi\|h\|)) & \text { if }\|\mathbf{h}\|>0 \\ 0 & \text { otherwise }\end{array}\right.$


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- $\widehat{\gamma}(d)=$
$\frac{1}{2|(N(d))|} \sum_{\left(s_{i}, s_{j}\right) \in N(d)}\left[x\left(s_{i}\right)-x\left(s_{j}\right)\right]^{2}$
- $N(d)$ : set of pairs of points such that
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- $|N(d)|:$ Cardinality of $N(d)$.
- Problem: The distances between the pairs can be all different. So it is of no use.
- Replace the $N(d)$ by $N\left(d_{k}\right)=$ $\left\{\left(s_{i}, s_{j}\right): d_{k-1}<\left\|s_{i}-s_{j}\right\|<d_{k}\right\}$, for $k=1, \ldots, K$.
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estimated semivariogram



## Semivariogram fitting

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## Spatial prediction: kriging

- Task: Given observations of $\mathbf{X}=\left(X\left(s_{1}\right), \ldots, X\left(s_{n}\right)\right)^{T}$, predict $X\left(s_{0}\right)$ at a location $s_{0}$, where it is not observed.


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- How to choose $\ell$ 's?
- Two requirements: $E\left(X\left(s_{0}\right)-\sum_{i} \ell_{i} X\left(s_{i}\right)\right)=0$ and $E\left(X\left(s_{0}\right)-\sum_{i} \ell_{i} X\left(s_{i}\right)\right)^{2}$ gets minimized w.r.t. $\ell$ 's.
- Defining $a_{0}=1, a_{i}=-\ell_{i}, \forall i=1, \ldots, n$, the above criteria become $E\left(\sum_{i=0}^{n} a_{i} X\left(s_{i}\right)\right)^{2}$ with $\sum_{i=0}^{n} a_{i}=0$.


## Ordinary kriging contd.

- Expansion of $E\left(\sum_{i=0}^{n} a_{i} X\left(s_{i}\right)\right)^{2}$ with the assumption of intrinsic stationarity, and with $\sum_{i} a_{i}=0$, leads to $-\sum_{i} \sum_{j} a_{i} a_{j} \gamma\left(s_{i}-s_{j}\right)$.
- Now defining $\gamma_{i j}=\gamma\left(s_{i}-s_{j}\right)$, for $i, j \in\{1, \ldots, n\}$ and $\gamma_{0 j}=\gamma\left(s_{0}-s_{j}\right)$, differentiating $E\left(X\left(s_{0}\right)-\sum_{i} \ell_{i} X\left(s_{i}\right)\right)^{2}$ w.r.t. $\ell$, equating to zero will lead to the solution for $\ell$ 's.
- However, the so obtained $\ell$ s are dependent on the unknown $\gamma$ and hence to be estimated from the data.


## Universal kriging

- Task: Given observations of $\mathbf{X}=\left(X\left(s_{1}\right), \ldots, X\left(s_{n}\right)\right)^{T}$, predict $X\left(s_{0}\right)$ at a location $s_{0}$, where it is not observed.


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- Assume that $X(s)$ is related to $p$-dimensional covariates $z\left(s_{1}\right), z\left(s_{2}\right), \ldots, z\left(s_{n}\right)$ by the model: $X=Z \boldsymbol{\beta}+\boldsymbol{\epsilon}, \boldsymbol{\epsilon} \sim N(0, \Sigma)$.


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- $\Sigma=\sigma^{2} H(\phi)+\tau^{2} I_{n}, H(\phi)_{i, j}=\rho\left(\phi ; d_{i, j}\right)$.
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- $d_{i, j}=\left\|s_{i}-s_{j}\right\|, \tau^{2}$ can be 0 if we assume there is not nugget effect.
- Then the predicted value of $X(\cdot)$ at $s_{0}$, will be

$$
E\left(X\left(s_{0}\right) \mid \mathbf{X}=\mathbf{x}\right)=\boldsymbol{z}_{0}^{T} \boldsymbol{\beta}+\gamma^{T} \Sigma^{-1}(\mathbf{x}-Z \boldsymbol{\beta}), \text { with }
$$

- $\operatorname{Var}\left(X\left(s_{0}\right) \mid \mathbf{X}=\mathbf{x}\right)=\sigma^{2}+\tau^{2}-\gamma^{T} \Sigma^{-1} \gamma$.
- $\gamma$ : a vector containing the covariance between $X\left(s_{0}\right)$ and the other $X$ 's.


## Kriging contd

- $\beta, \gamma$ and $\Sigma$ have to be estimated.


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- $\widehat{X\left(s_{0}\right)}=z_{0}^{T} \widehat{\boldsymbol{\beta}}+\widehat{\gamma}^{T} \widehat{\Sigma}^{-1}(\mathbf{x}-Z \widehat{\boldsymbol{\beta}})$
- Prediction error variance $\sigma^{2}\left(s_{0}\right)=\sigma^{2}+\tau^{2}-\gamma^{T} \Sigma^{-1} \gamma+\delta^{T}\left(X^{T} \Sigma^{-1} X\right)^{-1} \boldsymbol{\delta}$,


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Question: What if $z(\cdot)$ is not known at $s_{0}$ ?

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Question: What if $z(\cdot)$ is not known at $s_{0}$ ? $\odot$

## Kriging contd.

$$
\begin{aligned}
& \widehat{X\left(s_{0}\right)}=\boldsymbol{z}_{0}^{T} \widehat{\boldsymbol{\beta}}+\widehat{\gamma}^{T} \widehat{\Sigma}^{-1}(\mathbf{x}-Z \widehat{\boldsymbol{\beta}}) \text { can also be written as } \boldsymbol{\lambda}^{T} \boldsymbol{x} \text {, where } \\
& \bullet \boldsymbol{\lambda}=\widehat{\Sigma}^{-1} \widehat{\gamma}+\widehat{\Sigma}^{-1} Z\left(Z^{T} \widehat{\Sigma}^{-1} Z\right)^{-1}\left(z\left(s_{0}\right)-Z^{T} \widehat{\Sigma}^{-1} \widehat{\gamma}\right)
\end{aligned}
$$

## Kriging contd.

$\widehat{X\left(s_{0}\right)}=\boldsymbol{z}_{0}^{T} \widehat{\boldsymbol{\beta}}+\widehat{\gamma}^{T} \widehat{\Sigma}^{-1}(\mathbf{x}-Z \widehat{\boldsymbol{\beta}})$ can also be written as $\boldsymbol{\lambda}^{T} \boldsymbol{x}$, where

- $\boldsymbol{\lambda}=\widehat{\Sigma}^{-1} \widehat{\gamma}+\widehat{\Sigma}^{-1} Z\left(Z^{T} \widehat{\Sigma}^{-1} Z\right)^{-1}\left(z\left(s_{0}\right)-Z^{T} \widehat{\Sigma}^{-1} \widehat{\gamma}\right)$
- Multiplying $\lambda$ with $Z^{T}$ from the left, we get

$$
z\left(s_{0}\right)=Z^{T} \boldsymbol{\lambda}
$$

- Iterative procedure will lead us estimates of $z\left(s_{0}\right)$ and $X\left(s_{0}\right)$.


## Meuse data kriging



Meuse data kriging


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