

# Statistics for spatio-temporal data

## *Reading group*

Part I

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# Course outline<sup>1</sup>

1. Introduction to spatial and spatio-temporal data
  - what are spatial data? why spatial modeling? types of spatial data
2. Point-level modeling
  - spatial regression, Gaussian processes, Kriging, large datasets and spatio-temporal models
3. Areal data models
  - spatial association, modeling areal data and spatio-temporal models
4. Introduction to point patterns
  - modeling point pattern and spatio-temporal analysis

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<sup>1</sup>Many of these slides were excerpted from Alan Gelfand's material.

## Reference books

- Banerjee, S., Carlin, B. P., and Gelfand, A. E. (2014), *Hierarchical Modeling and Analysis for Spatial Data*, Chapman and Hall/CRC, 2nd edition
- Cressie, N. and Wikle, C. (2011). *Statistics for Spatio-Temporal Data*. New York: Wiley.
- Finkenstädt B., Held L., Isham V. (2007) *Statistical methods for spatio-temporal systems*, Chapman and Hall/CRC.
- Gelfand, A.E., Diggle, P., Guttorp, P. and Fuentes, M. (2010) *Handbook of Spatial Statistics*, Boca Raton, FL: CRC Press.
- Wikle C. K., Zammit-Mangion A., Cressie N. (2019) *Spatio-Temporal Statistics with R*, Chapman and Hall/CRC.

# Outline

## 1 Introduction to spatial and spatio-temporal data

- What are spatial data?
- Why spatial modeling?
- Types of spatial data

## 2 Point-referenced modeling

- EDA
- Gaussian Processes
- Spatial linear regression
- Parameter estimation
- Kriging
- Model comparison
- Large spatial data

## 3 Spatio-temporal models

- Continuous space-time models
- Discrete-time spatial models

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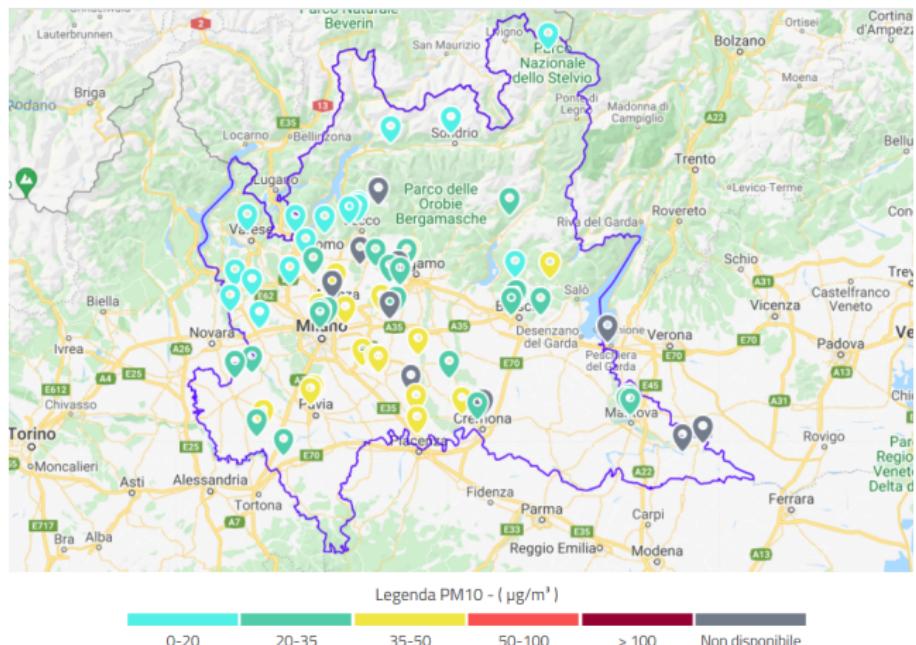
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# Spatial data examples



**Figure:** PM<sub>10</sub> collected at the monitoring network over Lombardia on September 26, 2021. Source: ARPA Lombardia.

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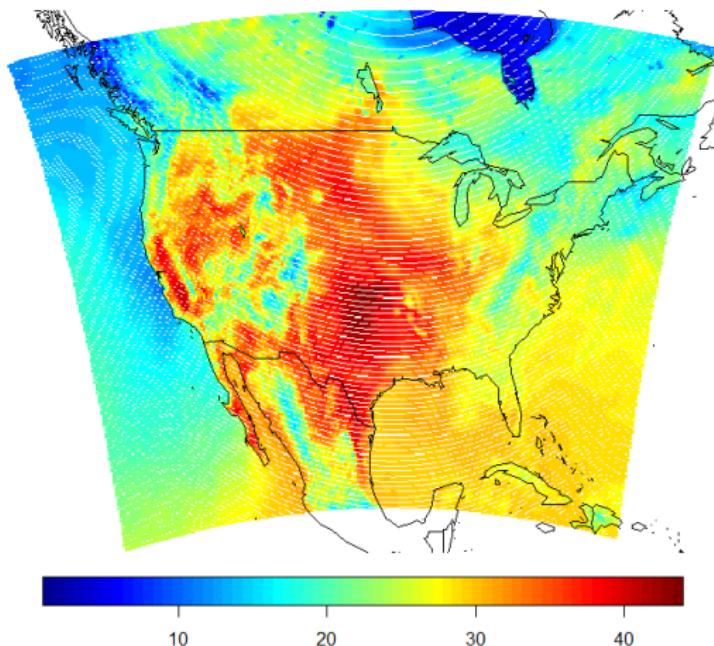
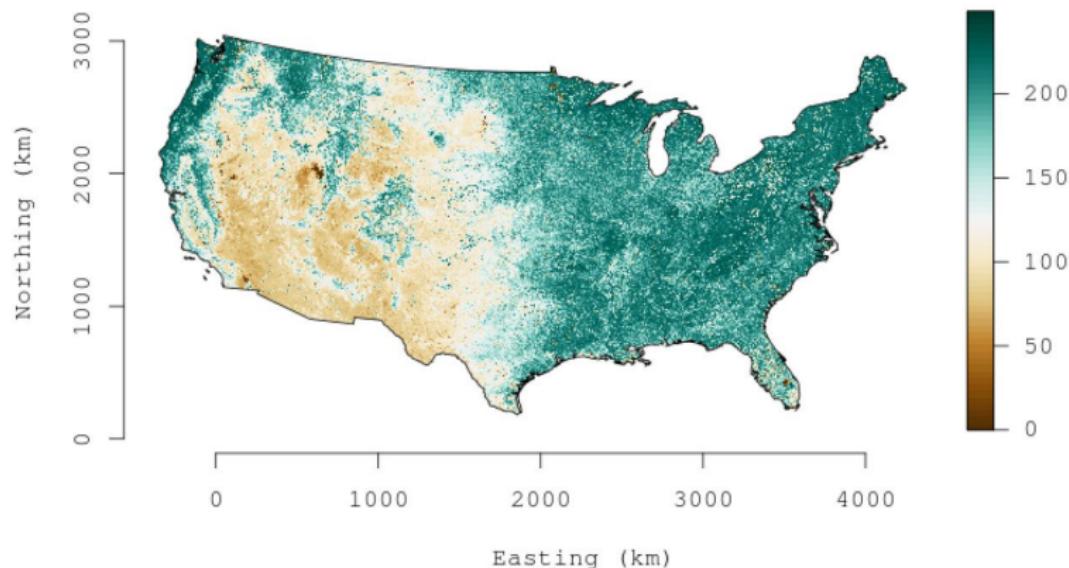


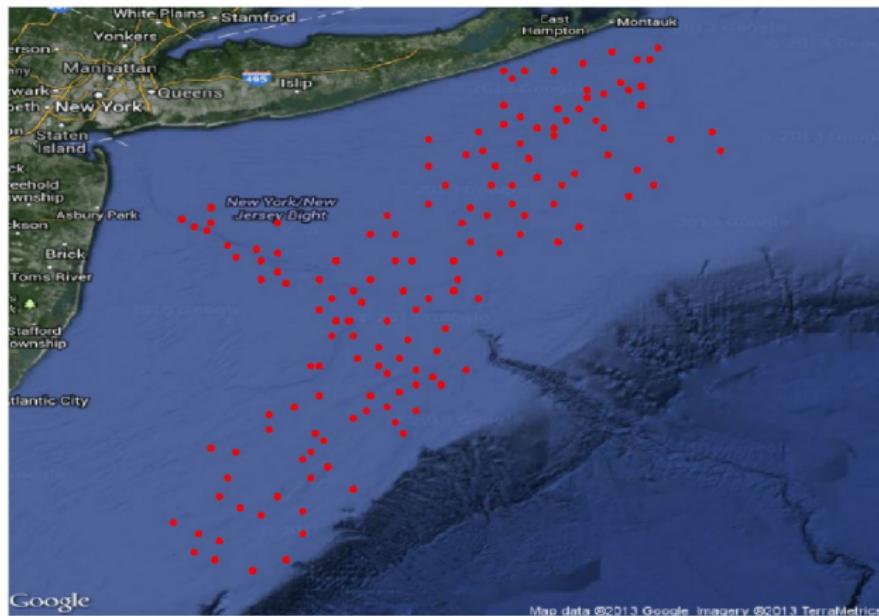
Figure: Temperature surface predicted by a computer model over US (Paci et al., 2015).

## Spatial data examples



**Figure:** Normalized Difference Vegetation Index (NDVI) image from the MODerate-resolution Imaging Spectroradiometer (MODIS) sensor (Datta et al., 2016).

# Spatial data examples



**Figure:** Locations of scallop counts off the New Jersey and Long Island coastline (Banerjee et al., 2014).

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Figure: Covid-19 deaths from March 1, 2020 to September 26, 2021 in Italy. Source: StatGroup-19.

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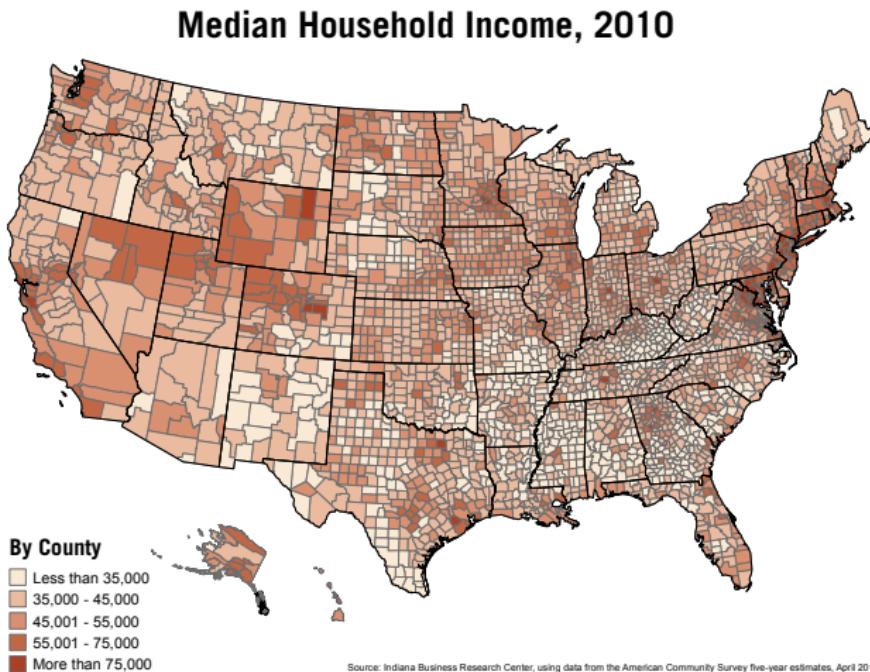


Figure: Median household income by US county in 2010. Source: Indiana's Public Data Utility.

## Spatial data examples

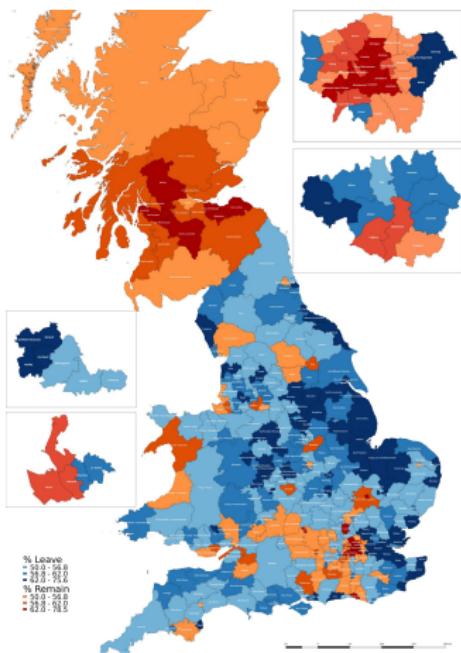


Figure: Brexit results by UK county. Source: Wikipedia.

# Spatial data examples

Earthquake map from 2021-08-28 10:24:35 to 2021-09-27 10:17:50

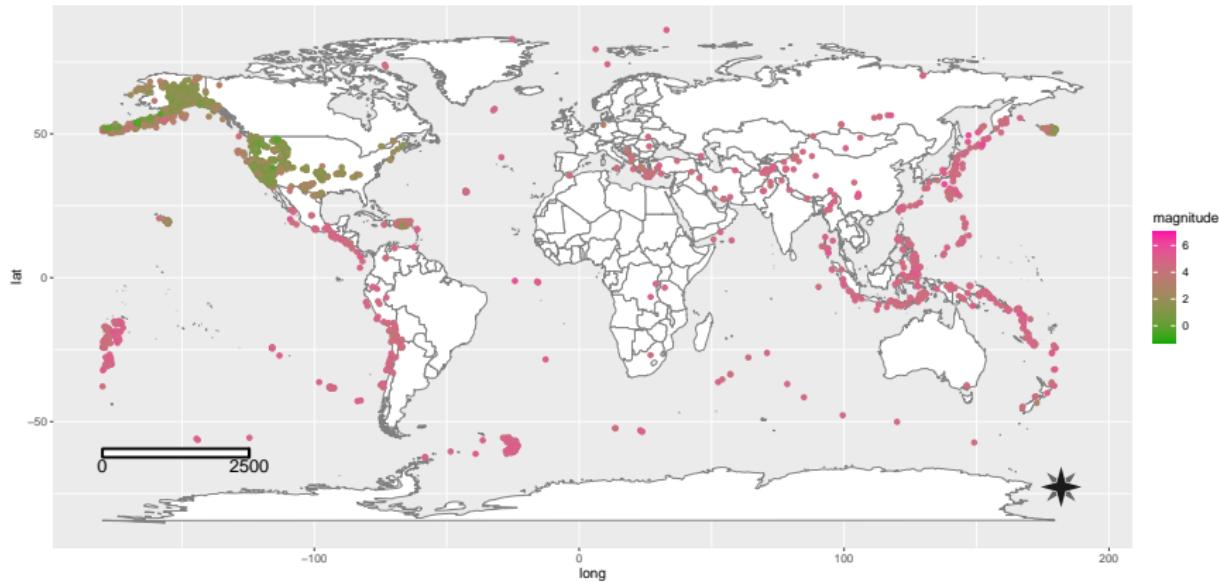


Figure: Earthquakes occurred from August 28 to September 27, 2021.

## Spatial data examples

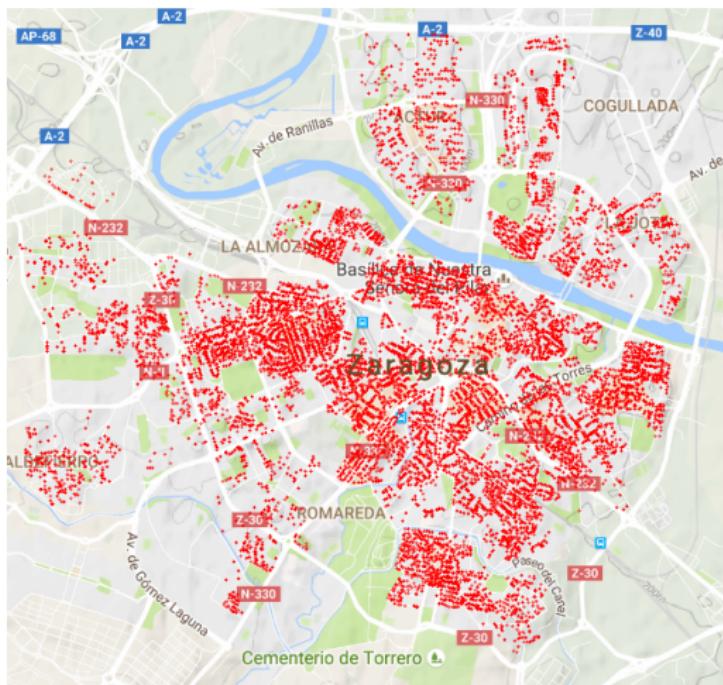


Figure: Property sales in Zaragoza during the period 2006-2014, consisting of  $\sim 30,000$  transactions (Paci et al., 2017).

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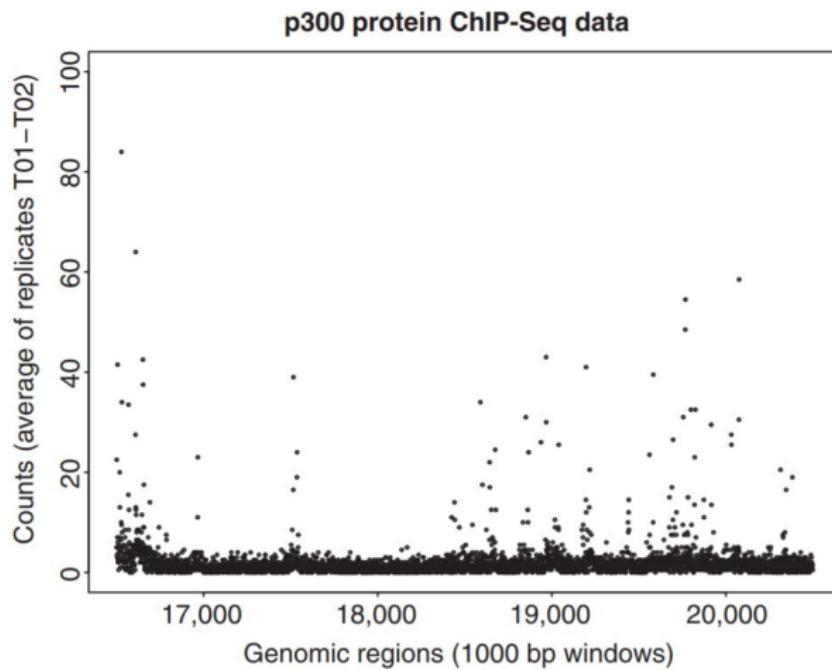


Figure: Chromatin Immunoprecipitation Sequencing (ChIP-Seq) data (Ranciati et al., 2017).

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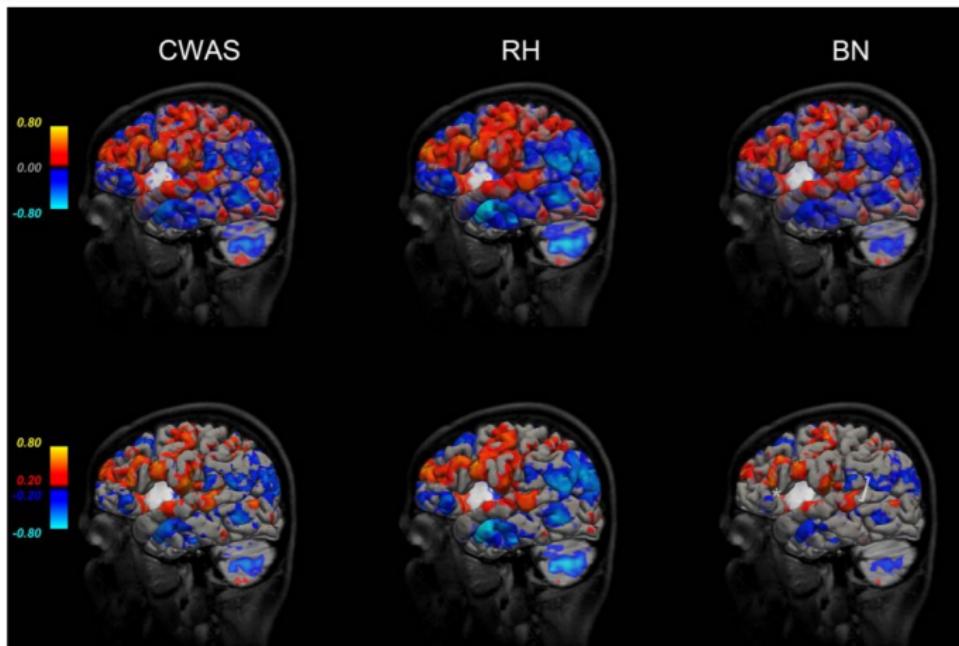


Figure: Pre-surgical functional magnetic resonance imaging (fMRI) data (Liu et al., 2016).

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- ⇒ Motivate data analysis and statistical modeling for complex spatial and spatio-temporal data sets.

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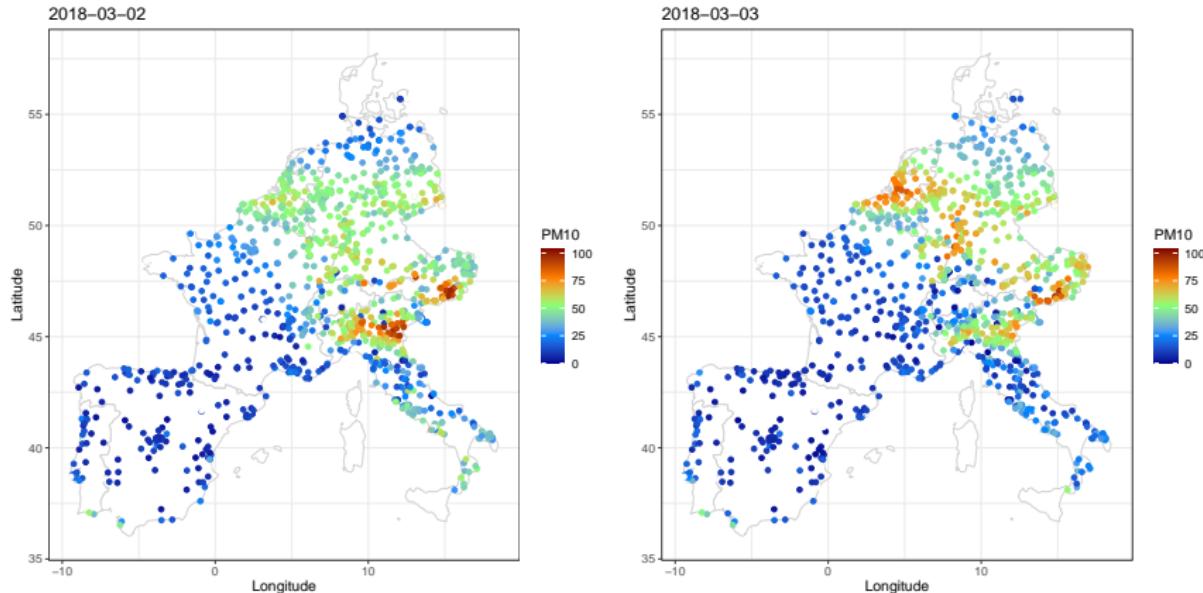
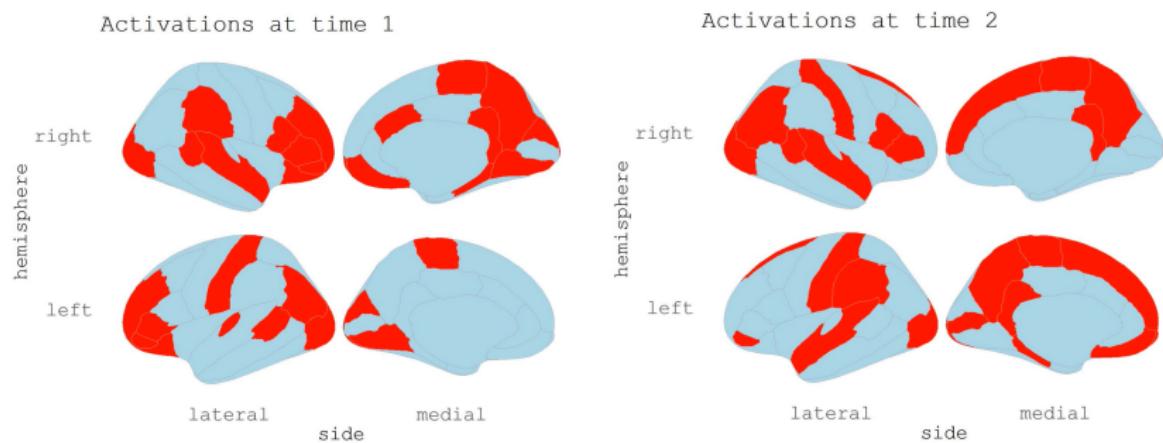


Figure: PM<sub>10</sub> observed across Europe in two consecutive days.

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**Figure:** Spontaneous activations of brain regions over time, detected from resting state fMRI data (Gasperoni et al., 2021).

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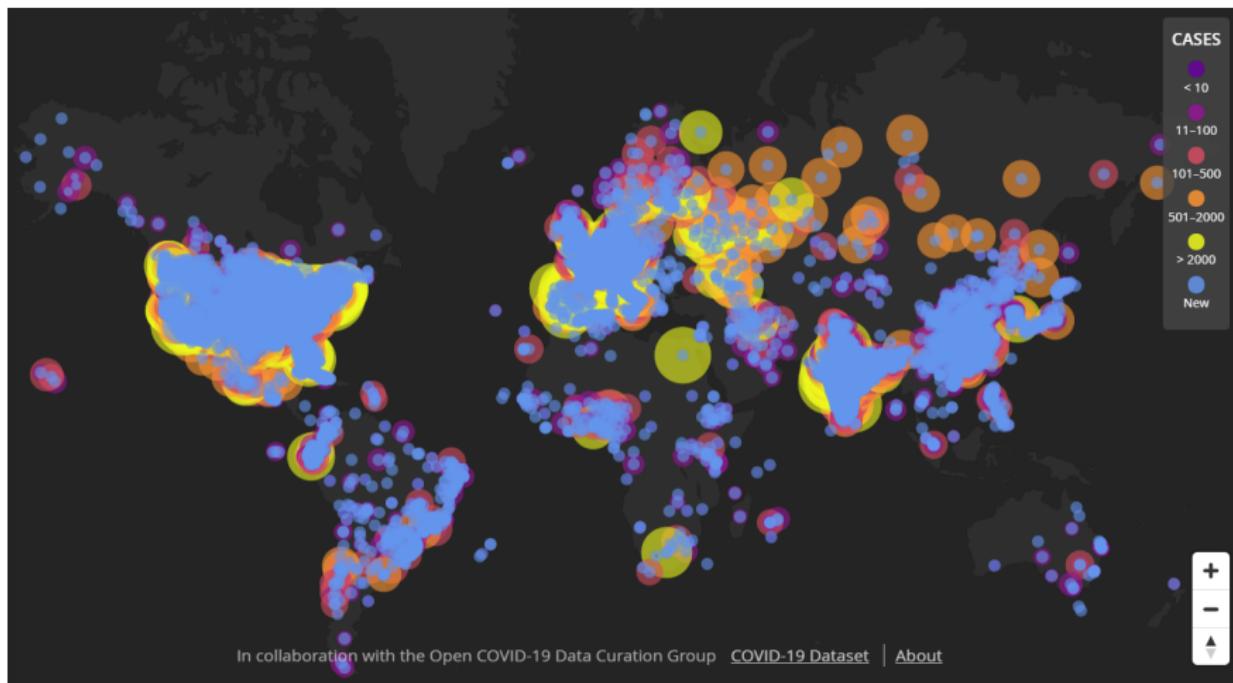


Figure: COVID-19 confirmed cases worldwide. Source: [www.healthmap.org](http://www.healthmap.org).

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- Answers to the problems come as **inference**, i.e., estimates or predictions along with a quantification of their uncertainties.

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2. **Predict** at unobserved locations (smoothing, interpolation) and/or times (forecasting)
3. More specific goals might include data assimilation, computer-model emulation, and design of spatio-temporal monitoring networks

# Spatial data analysis

Statistical inference for spatial processes is often challenging, but is necessary when we try to draw conclusions about questions of interest, such as:

- Does the spatial patterning of disease incidences give rise to the conclusion that they are clustered, and if so, are the clusters found related to factors such as age, relative poverty, or pollution sources?
- Given a number of observed soil samples, which part of a study area is polluted?
- Given scattered air quality measurements, how many people are exposed to high levels of black smoke or particulate matter (e.g. PM<sub>10</sub>) and where do they live?
- Do governments tend to compare their policies with those of their neighbors, or do they behave independently?

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- Early on, much of the statistical methodology was developed quite independently and grew primarily from the different areas of application, including:
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- For many years spatial statistics labored on the fringe of mainstream statistics. However, the past 30 years has seen an explosion of interest in space and space-time problems.
- This has been largely fueled by the increased availability of inexpensive, high-speed computing that has:
  - enabled the collection of large spatial and spatio-temporal datasets across many fields,
  - facilitated the widespread usage of sophisticated geographic information systems (GIS) software to create attractive displays,
  - has endowed the ability to investigate (fit and infer under) challenging, evermore appropriate and realistic models.

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- Locations:
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- Location generation process
  - known or unknown
  - fixed or random

# Notation

- $\mathcal{S}$ : the space of all possible locations (we will consider  $\mathbb{R}^2$ )
- $D \subseteq \mathcal{S}$ : fixed subset of  $\mathcal{S}$  (study region)
- $\mathbf{s} \in D$ : given point in  $D$
- $\mathbf{s}_1, \dots, \mathbf{s}_n$ : locations of  $n$  observations
- $y(\mathbf{s}_1), \dots, y(\mathbf{s}_n)$ : observations of the variable of interest

# Types of spatial data

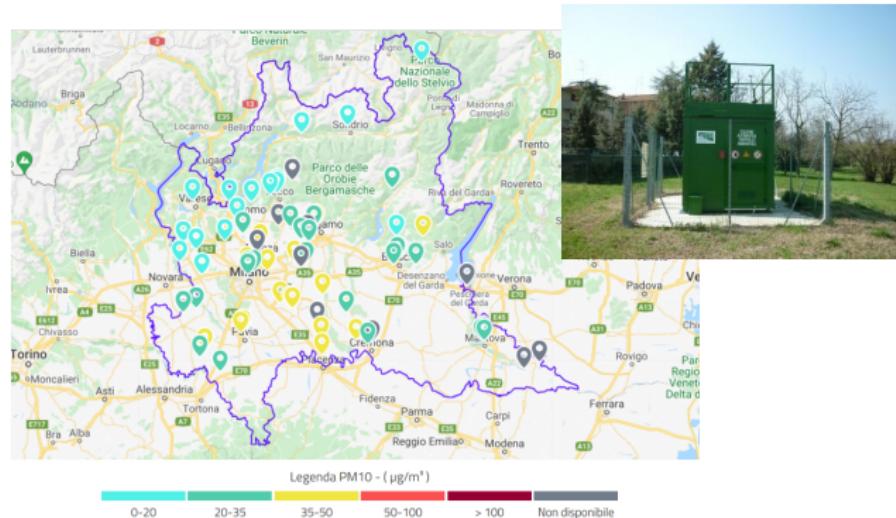
There are three broad categories:

1. Point-referenced data (or geostatistical data)
2. Areal data
3. Point pattern data

# Types of spatial data

## Point-referenced data

- Each observation is associated with a fixed known location (point)
- Data represents a sample from a *continuous spatial domain*
- The variable of interest does exist in all points of the domain but it is observed only at a finite set of points
- Also referred to as geocoded or **geostatistical** data

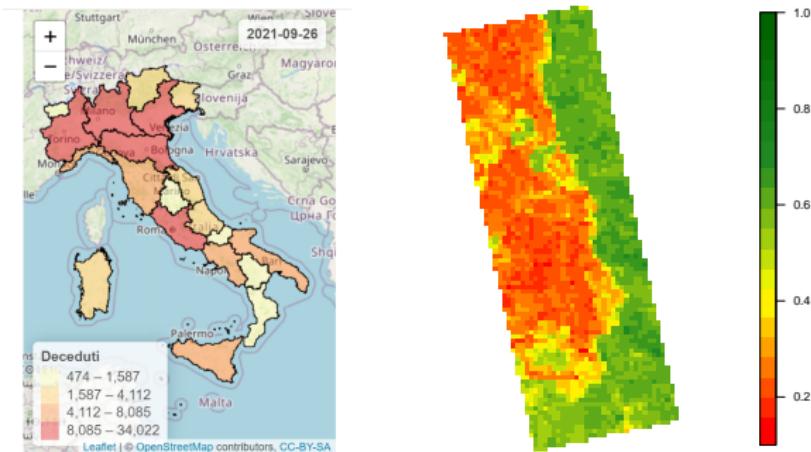


**Figure:** PM<sub>10</sub> collected at the monitoring network over Lombardia on September 26, 2021. Source: ARPA Lombardia.

# Types of spatial data

## Areal data

- Each observation is associated with a areal unit with well-defined boundaries of *regular* or *irregular* shape, like pixels, regions, county etc...
- The variable of interest is observed only at a finite set of regions
- Usually a result of aggregating point level data
- Also referred to as [lattice](#) data

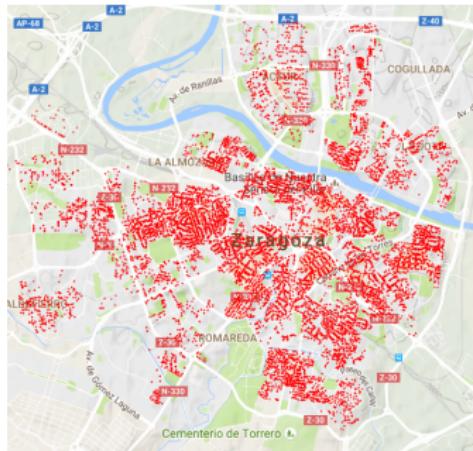
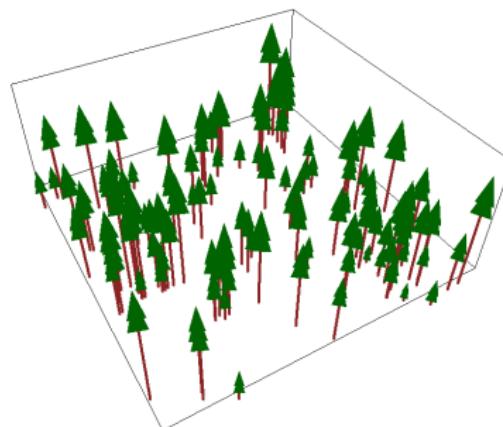


**Figure:** Left panel: Covid-19 deaths from March 1, 2020 to September 26, 2021 in Italy; source: StatGroup-19. Right panel: NDVI values over the Zuera region, Spain in 1986; source Landsat.

# 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.
- Sometimes, also a response variable (*mark*) is associated with the random locations



**Figure:** Left panel: Pines in a Finnish forest. Right panel: property sales in Zaragoza during the period 2006-2014 (Paci et al., 2017).

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- To achieve this: exploiting the **structured dependence**

# Plotting the data

$$Y(\mathbf{s}_i), i = 1, \dots, n = 213$$

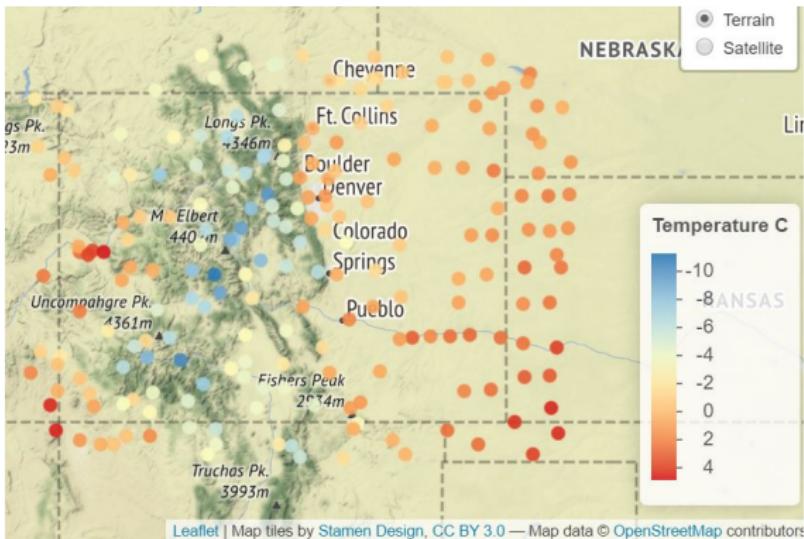


Figure: Temperature data collected at 213 monitoring sites in Colorado (US).

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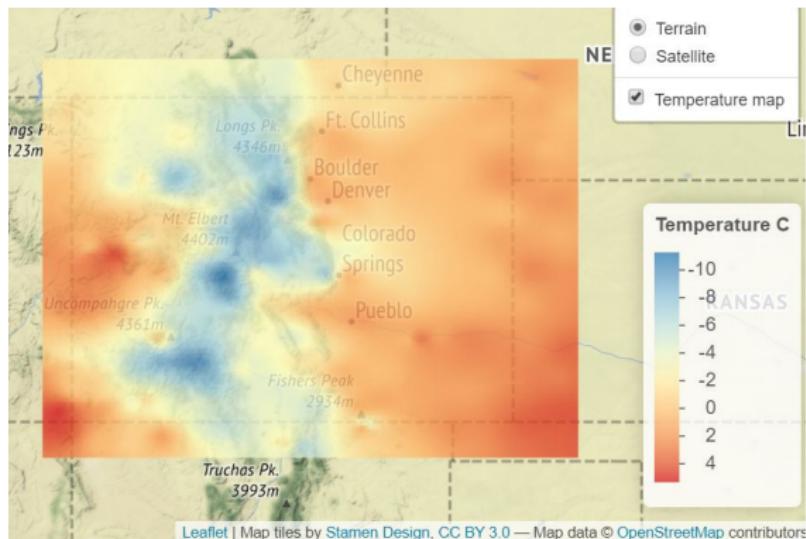


Figure: Interpolated map; **surface plots** of the data often helps to understand spatial patterns.

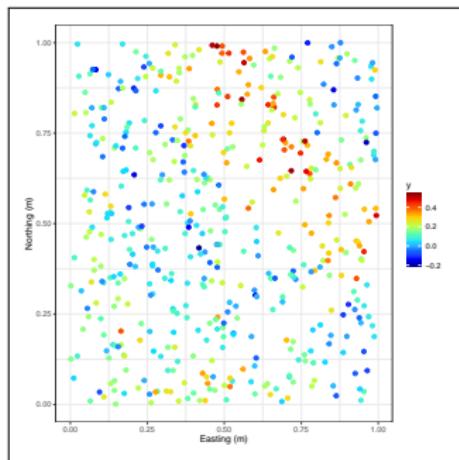
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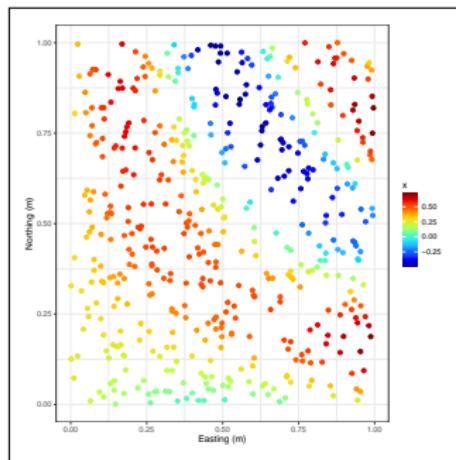
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- Data observed at  $n$  fixed spatial locations  $\{\mathbf{s}_1, \dots, \mathbf{s}_n\}$
- At each location  $\mathbf{s}_i$  we observe the response  $y(\mathbf{s}_i)$  and a  $p \times 1$  vector of covariates  $\mathbf{x}(\mathbf{s}_i)$

Dataset 1


 $y(\mathbf{s}_1), \dots, y(\mathbf{s}_n)$ 

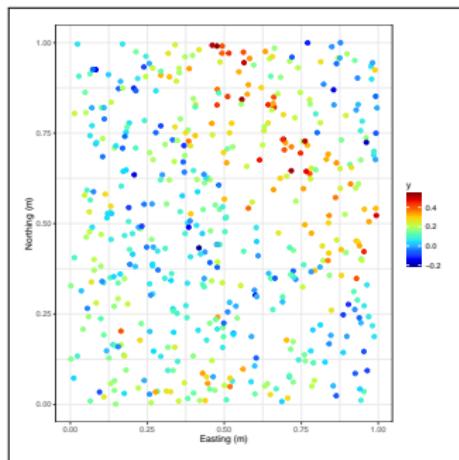
Covariate


 $x(\mathbf{s}_1), \dots, x(\mathbf{s}_n)$

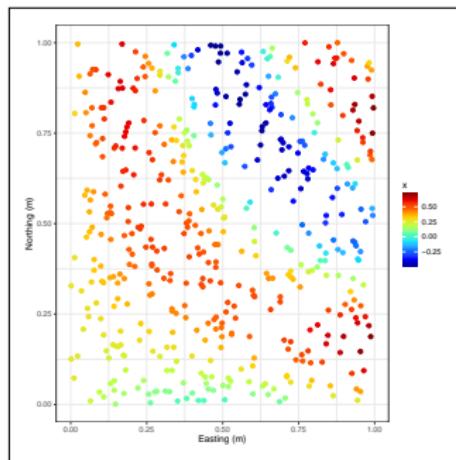
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Dataset 1


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Covariate

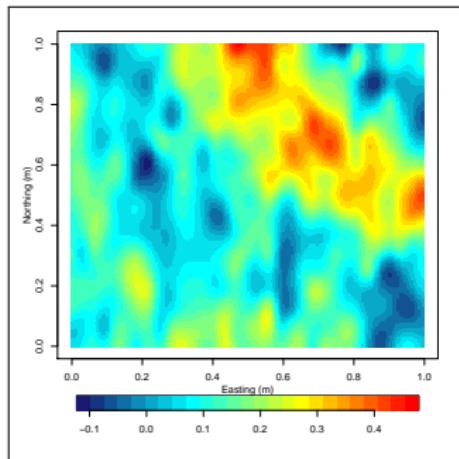

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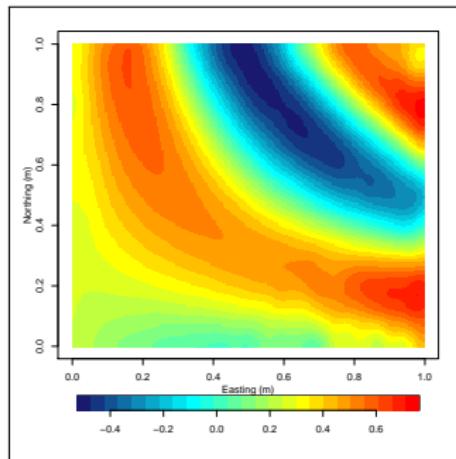
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- Although the data is spatial, this is an ordinary linear regression model
- $\mathbf{y} = (y(\mathbf{s}_1), y(\mathbf{s}_2), \dots, y(\mathbf{s}_n))'$ ;  $\mathbf{X} = (\mathbf{x}(s_1)', \mathbf{x}(s_2)', \dots, \mathbf{x}(s_n)')$
- **Inference - OLS:**  $\hat{\boldsymbol{\beta}} = (\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}' \mathbf{y}$
- **Prediction** at new location  $\mathbf{s}_0$ :  $\hat{y}(\mathbf{s}_0) = \mathbf{x}(\mathbf{s}_0)' \hat{\boldsymbol{\beta}}$

# Residual plot

## Dataset 1

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

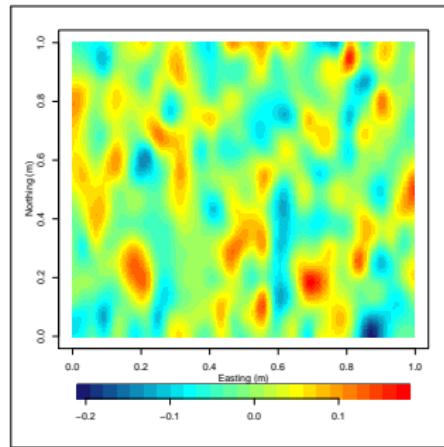


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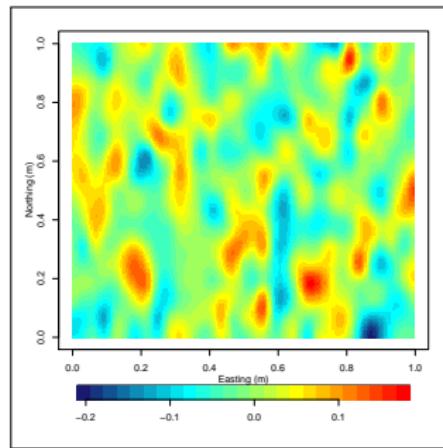
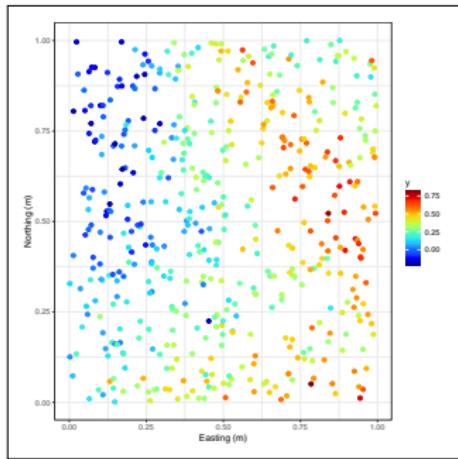


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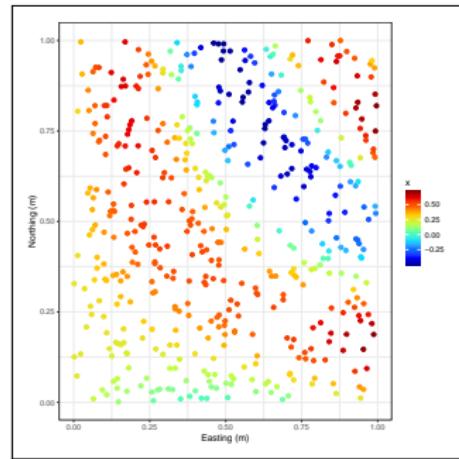
- No evident spatial pattern in plot of the residuals
- The covariate  $X(\mathbf{s})$  seems to explain all the spatial variation in  $Y(\mathbf{s})$

# One more dataset

Dataset 2

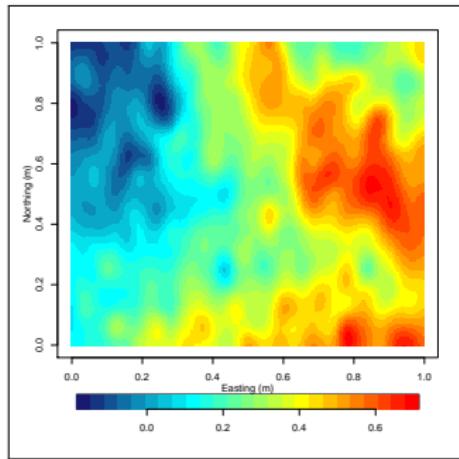
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Same covariate

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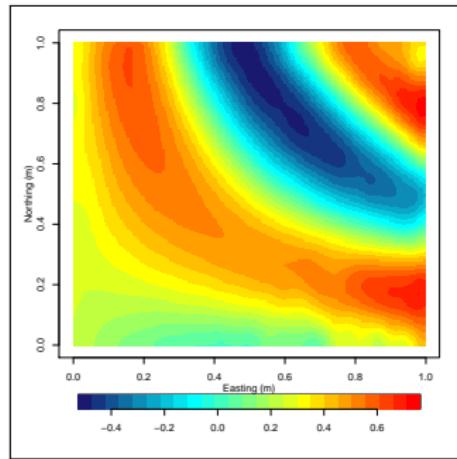
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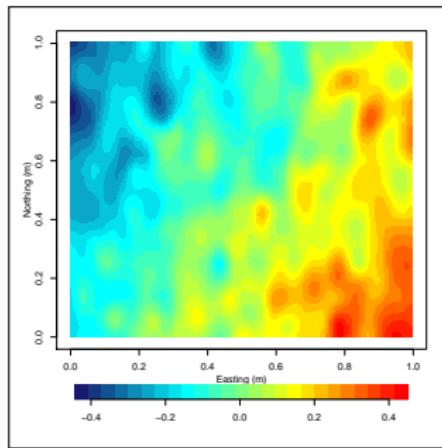


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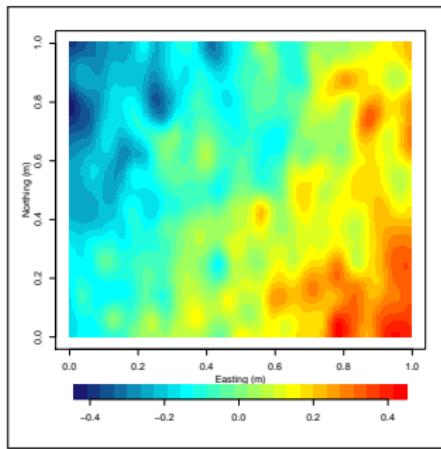


Figure: Residual plot of Dataset 2 after linear regression on  $X(\mathbf{s})$ .

- Strong residual spatial pattern in Dataset 2
- The covariate  $X(\mathbf{s})$  does not explain all the spatial variation in  $Y(\mathbf{s})$
- Simple regression seems to be not enough

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- Can this be formalized to identify spatial pattern?

## Empirical variogram

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

# Empirical variogram

## Dataset 1

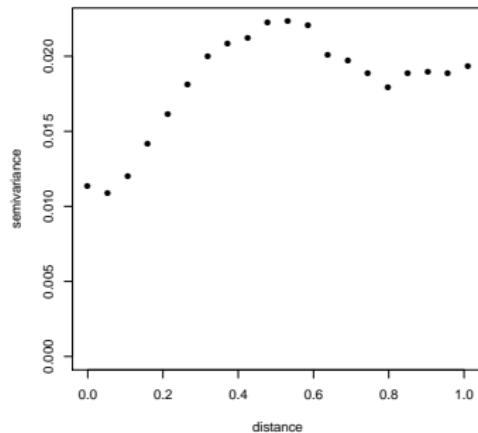


Figure: Empirical variogram on  $y_1(s)$ .

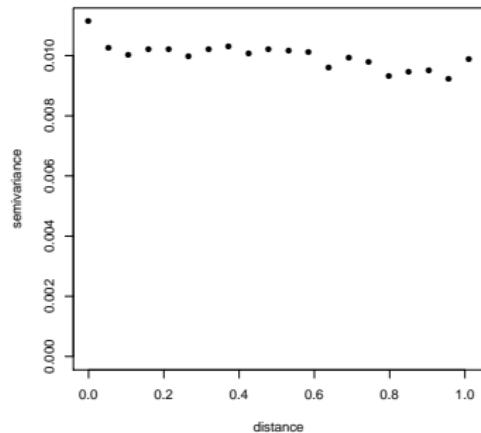


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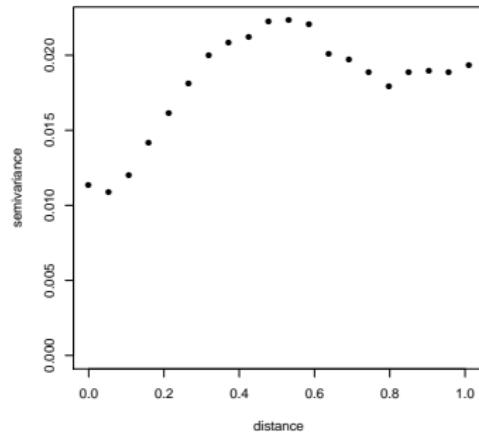


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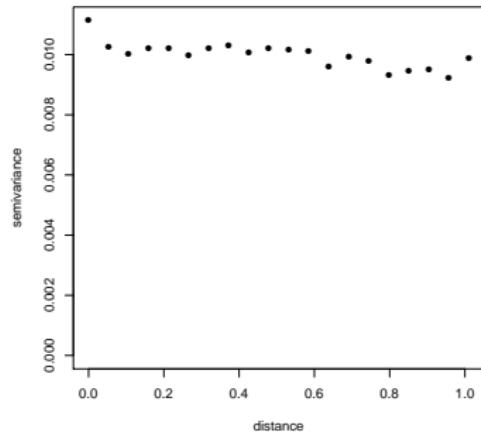


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- Residuals display little spatial variation

# Empirical variogram

## Dataset 2

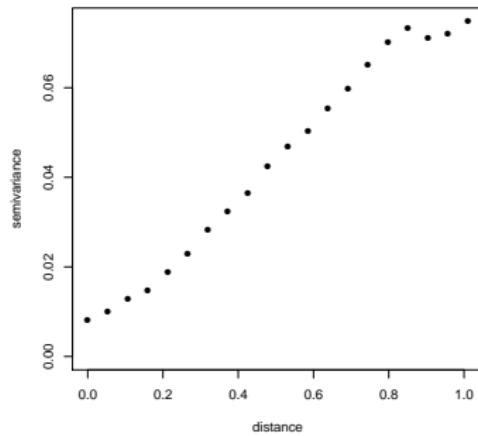


Figure: Empirical variogram of  $y_2(\mathbf{s})$ .

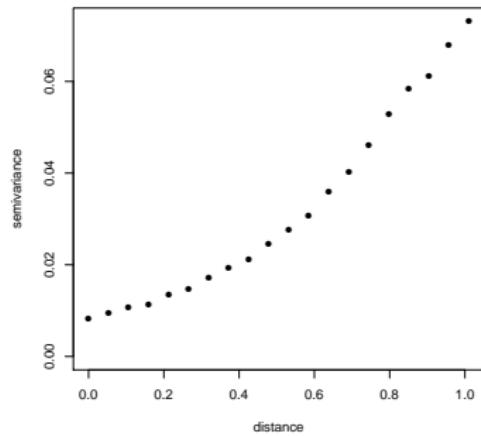


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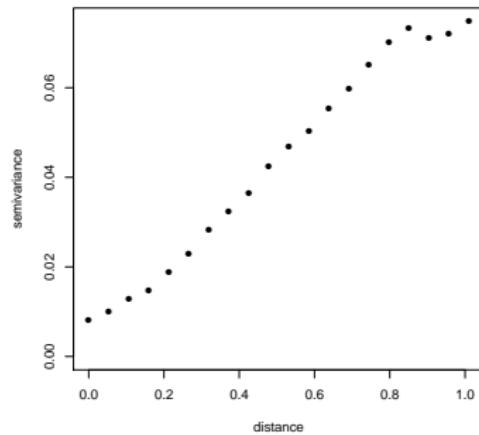


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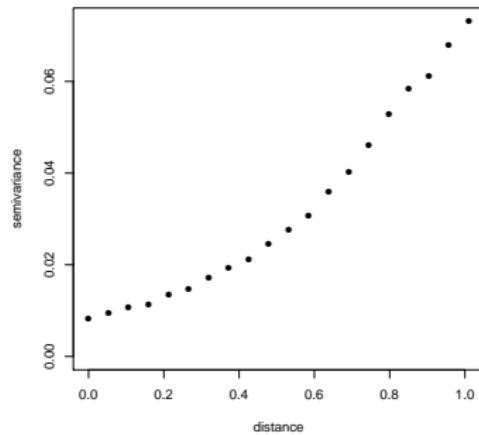


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- Variogram of the residuals suggests **unexplained spatial variation**

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- Model  $w(\mathbf{s})$  as a stochastic process

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- A GP is completely characterized by a mean function  $m(\mathbf{s})$  and a covariance function  $C(\cdot, \cdot)$
- **Advantage:** Likelihood based inference

$$\mathbf{w} = (w(\mathbf{s}_1), \dots, w(\mathbf{s}_n))' \sim \mathcal{N}(m, C)$$

where  $m = (m(\mathbf{s}_1), \dots, m(\mathbf{s}_n))'$  and  $C = C(\mathbf{s}_i, \mathbf{s}_j)$ .

# Covariance function

- $C(\cdot, \cdot)$  needs to be **valid**, i.e., for all  $n$  and all  $\{\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_n\}$ , the resulting covariance matrix  $C = C(\mathbf{s}_i, \mathbf{s}_j)$  for  $(w(\mathbf{s}_1), \dots, w(\mathbf{s}_n))$  must be positive definite
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- So,  $C(\cdot, \cdot)$  needs to be a **positive definite** function
- Construct valid covariance functions by using properties of characteristic functions:
  - Multiply valid covariance functions (corresponds to summing independent random variables)
  - Mixing covariance functions (corresponds to mixing distributions)
  - Convolving covariance functions, i.e., if  $c_1$  and  $c_2$  are valid then  $c_{12}(\mathbf{s}) = \int c_1(\mathbf{s} - \mathbf{u})c_2(\mathbf{u})d\mathbf{u}$  is valid.

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In words, the covariance between the values of the process at any two locations  $\mathbf{s}$  and  $\mathbf{s} + \mathbf{h}$  can be summarized by a covariance function  $C(\mathbf{h})$  (sometimes called a [covariogram](#)), and this function depends only on the separation vector  $\mathbf{h}$ .

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**Isotropic models** are popular because of their [simplicity](#), [interpretability](#), and because a number of relatively simple [parametric forms](#) are available as candidates for  $C$ .

# Common isotropic covariance functions

Model	Covariance function, $C(t)$
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	$C(t) = \begin{cases} \sigma^2 \exp(- \phi t ^p) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$
Gaussian	$C(t) = \begin{cases} \sigma^2 \exp(-\phi^2 t^2) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$
Rational quadratic	$C(t) = \begin{cases} \sigma^2 \left( 1 - \frac{t^2}{(1+\phi t^2)} \right) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$
Wave	$C(t) = \begin{cases} \sigma^2 \frac{\sin(\phi t)}{\phi t} & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$
Matérn	$C(t) = \begin{cases} \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)} (2\sqrt{\nu}t\phi)^{\nu} K_{\nu}(2\sqrt{\nu}t\phi) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$

## Exponential covariance function

$$C(t) = \begin{cases} \tau^2 + \sigma^2 & \text{if } t = 0 \\ \sigma^2 \exp(-\phi t) & \text{if } t > 0 \end{cases}$$

- The **effective range**,  $t_0$ , as the distance at which the 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**  $\tau^2$  is often viewed as a “**nonspatial effect variance**”.
- The **partial sill**  $\sigma^2$  is viewed as a “**spatial effect variance**”.
- The **sill**  $\tau^2 + \sigma^2$  gives the maximum total variance
- Note discontinuity at 0 due to the nugget. This is intentional! To account for measurement error or micro-scale variability.

# Covariance functions and variograms

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$$\gamma(\mathbf{h}) = \frac{1}{2} E [(Y(\mathbf{s} + \mathbf{h}) - Y(\mathbf{s}))^2]$$

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- So given  $C(\mathbf{h})$ , we are able to determine  $\gamma(\mathbf{h})$ .

# Covariance functions and variograms

- Recall the empirical semivariogram:

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

- The theoretical semivariogram is defined as

$$\gamma(\mathbf{h}) = \frac{1}{2} E [(Y(\mathbf{s} + \mathbf{h}) - Y(\mathbf{s}))^2]$$

If the variogram depends only on  $\mathbf{h}$  and not the particular choice of  $\mathbf{s}$ , we say the process is **intrinsically stationary**.

- For any stationary GP:

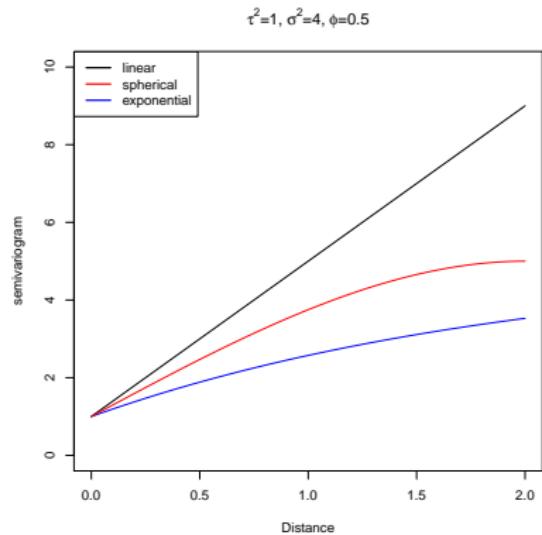
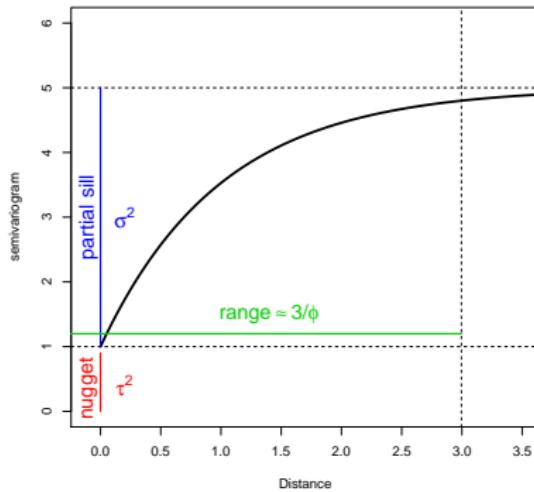
$$\gamma(\mathbf{h}) = C(\mathbf{0}) - C(\mathbf{h})$$

- So given  $C(\mathbf{h})$ , we are able to determine  $\gamma(\mathbf{h})$ .
- Example: For exponential (isotropic) GP

$$\gamma(t) = \begin{cases} 0 & \text{if } t = 0 \\ \tau^2 + \sigma^2(1 - \exp(-\phi t)) & \text{if } t > 0 \end{cases}$$

# Variograms

## Examples



# The Matérn Correlation Function

- The Matérn is a very versatile family:

$$C(t) = \begin{cases} \tau^2 + \sigma^2 & \text{if } t = 0 \\ \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)}(\phi t)^\nu K_\nu(\phi t) & \text{if } t > 0 \end{cases}$$

where  $K_\nu$  is the modified Bessel function of order  $\nu$  (computationally tractable)

- $\nu$  is a smoothness parameter controlling process smoothness:
  - $\nu = 1/2$  gives the exponential covariance function
  - $\nu = 3/2$  gives a convenient closed form
  - $\nu = \infty$  gives the Gaussian covariance function

# Modeling point-referenced data

## Spatial linear model

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- $w(\mathbf{s})$  is the spatial error (spatial random effects) and it is modeled as a stationary GP  $(0, C(\cdot, \cdot | \theta))$
- Under isotropy:  $C(\mathbf{s} + \mathbf{h}, \mathbf{s} | \theta) = \sigma^2 \mathbf{R}(|h|; \phi)$
- $\mathbf{w} = (w(\mathbf{s}_1), \dots, w(\mathbf{s}_n))' \sim N(\mathbf{0}, \sigma^2 \mathbf{R}(\phi))$  where  $\mathbf{R}(\phi)_{ij} = \rho(|\mathbf{s}_i - \mathbf{s}_j|; \phi)$ , introducing the partial sill ( $\sigma^2$ ) and range ( $\phi$ ) parameters.

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- $\varepsilon(\mathbf{s}) \sim \text{iid } N(0, \tau^2)$  is the **non-spatial error** and contributes to the nugget  $\tau^2$
- Interpretations attached to  $\varepsilon(\mathbf{s})$ :
  - pure error term; model is not perfectly spatial;
  - measurement error or replication variability causing discontinuity in spatial surface  $Y(\mathbf{s})$ ;
  - microscale uncertainty; distances smaller than the smallest inter-location distance.

## Parameter estimation

- Gaussian spatial models are special cases of the general linear model, with a particular specification of the covariance matrix:  $\Sigma_\theta = \sigma^2 \mathbf{R}(\phi) + \tau^2 I_n$
- The sampling model is given by

$$\mathbf{y} | \boldsymbol{\theta}, \boldsymbol{\beta} \sim N_n (\mathbf{X}\boldsymbol{\beta}, \Sigma_\theta)$$

where  $\boldsymbol{\theta} = (\sigma^2, \tau^2, \phi)$ .

- So the likelihood is

$$\mathcal{L}(\boldsymbol{\beta}, \boldsymbol{\theta}; \mathbf{y}) \propto |\Sigma_\theta|^{-1/2} \exp \left\{ -\frac{1}{2} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top \Sigma_\theta^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \right\}$$

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- The Maximum Likelihood Estimates (MLE) of  $\boldsymbol{\beta}$  and  $\boldsymbol{\theta}$  are  $\hat{\boldsymbol{\beta}}$  and  $\hat{\boldsymbol{\theta}}$  that maximizes the likelihood above
- $\hat{\boldsymbol{\beta}}_{MLE} = \hat{\boldsymbol{\beta}}_{GLS} = (\mathbf{X}' \Sigma_\theta^{-1} \mathbf{X})^{-1} \mathbf{X}' \Sigma_\theta^{-1} \mathbf{y}$

# Parameter estimation

- In practice, the likelihood is often very flat with respect to the spatial covariance parameters and choice of initial values is important
- Initial values can be eyeballed from empirical semivariogram of the residuals from ordinary linear regression
- Estimated parameter values can be used for prediction (*kriging*)

# Parameter estimation

## Example: Ozone data

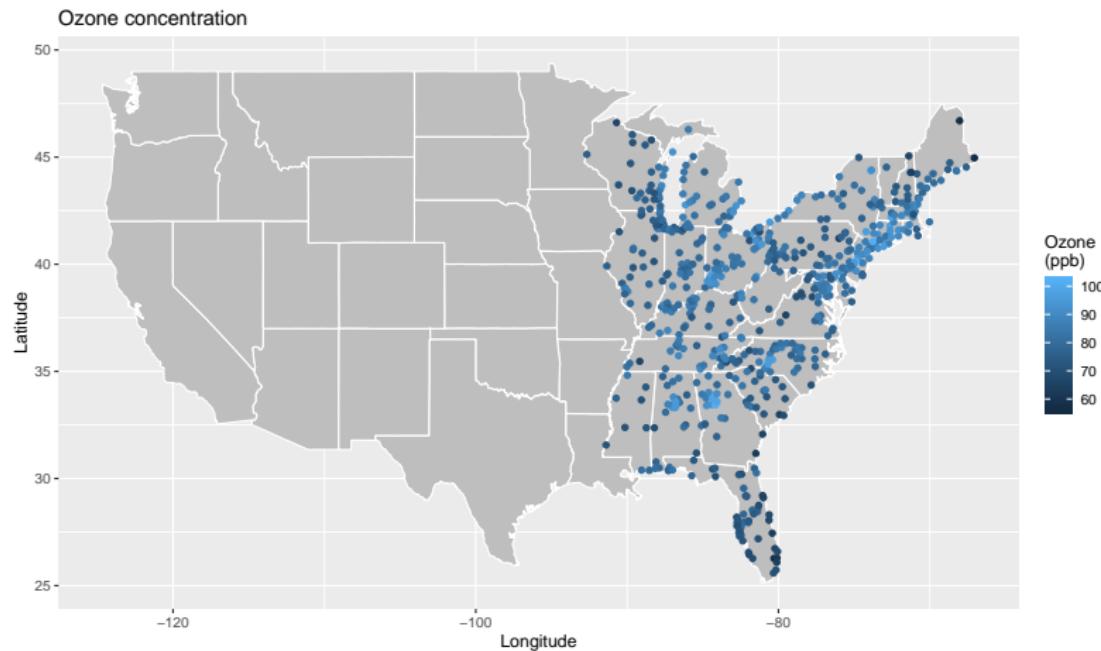


Figure: Ozone concentrations at  $n = 631$  monitoring stations in the Eastern US.

# Parameter estimation

## Example: Ozone data

- Model:  $y(\mathbf{s}) = \beta_0 + w(\mathbf{s}) + \varepsilon(\mathbf{s})$
- $w(\mathbf{s}) \sim \text{GP}(0, C)$ ,  $C(\mathbf{s}_i, \mathbf{s}_j) = \sigma^2 \exp(-\phi ||\mathbf{s}_i - \mathbf{s}_j||)$ ,  $\varepsilon(\mathbf{s}) \sim N(0, \tau^2)$

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- MLE obtained using `likfit` function of `geoR` R package

```
fit_mle <- likfit(Y, coords, fix.nugget = FALSE,
                     cov.model="exponential", ini = c(var(Y), 1))
summary(fit_mle)

Parameters of the mean component (trend): beta0  76.1311

Parameters of the spatial component:
correlation function: exponential
  (estimated) variance parameter sigmasq (partial sill) = 47.82
  (estimated) cor. fct. parameter phi (range parameter) = 197
```

```
anisotropy parameters:
  (fixed) anisotropy angle = 0  ( 0 degrees )
  (fixed) anisotropy ratio = 1
```

```
Parameter of the error component:
  (estimated) nugget = 15.7
```

Practical Range with cor=0.05 for asymptotic range: 590.0498

## Hierarchical modeling

- Alternatively, the **Bayesian** posterior distribution of  $(\beta, \theta)$  can be derived (and sampled from). A prior distribution of  $(\beta, \theta)$  is required.
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First stage (Data Model): [data | process, parameters]

$$\mathbf{y} | \beta, \mathbf{w}, \tau^2 \sim N_n (\mathbf{X}\beta + \mathbf{w}, \tau^2 I_n)$$

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**Third stage** (Parameter Model): [(hyper)parameters]

priors on  $(\beta, \theta)$

## Bayesian posterior inference

- Markov chain Monte Carlo methods can be used to sample from the posterior distribution  $p(\beta, \theta | \mathbf{y})$
  - The model can be fitted either as:
    - \*  $f(\mathbf{y} | \beta, \theta)p(\beta, \theta)$
    - \*  $f(\mathbf{y} | \beta, \theta, \mathbf{w})p(\mathbf{w} | \theta)p(\beta, \theta)$
- ⇒ **Exercise:** derive the forms of the full conditional distributions for  $\beta$ ,  $\sigma^2$ ,  $\tau^2$ ,  $\phi$  and  $\mathbf{w}$  in the exponential covariance model

# Parameter estimation

## Example: Ozone data

Posterior inference obtained from `spBayes` R package (Finley et al., 2015)

```
starting <- list(phi = 3/(0.5 * d.max), sigma.sq = 5, tau.sq = 5)
tuning   <- list(phi = 0.5, sigma.sq = 0.05, tau.sq = 0.05)
priors   <- list("beta.Flat", phi.Unif = c(3/d.max, 3/(0.01 * d.max)),
                 sigma.sq.IG = c(2, 5), tau.sq.IG = c(2, 5))

fit_bayes <- spLM(Y ~ 1, coords = coords.utm, cov.model = "exponential",
                     starting = starting, tuning = tuning, priors = priors,
                     n.samples = 5000, n.report = 2000)

round(apply(fit_bayes$p.theta.samples, 2, quantile))

      sigma.sq    tau.sq     phi
0%     4.776    6.356   0.001
25%    40.310   14.439   0.004
50%    45.558   15.588   0.005
75%    53.145   16.857   0.006
100%   191.853   36.265   0.010
```

# Kriging: spatial prediction at new locations

- Kriging: Named in honor of **D.G. Krige**, a South African mining engineer whose seminal work on empirical methods for geostatistical data inspired the general approach.
- **Goal:** given the observations  $\mathbf{y}$ , predict  $Y$  at new site  $\mathbf{s}_0$  where  $\mathbf{s}_0$  has not been observed

# Conditional normal distribution

- $$\begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{pmatrix} \sim N \left( \begin{pmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{pmatrix}, \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} \right)$$

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- Then,  $\mathbf{X}_1 | \mathbf{X}_2 \sim N(\boldsymbol{\mu}_{1|2}, \Sigma_{1|2})$ , where
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- The conditional mean is the “best” predictor of  $\mathbf{X}_1$  based on  $\mathbf{X}_2$ , i.e.,  $\boldsymbol{\mu}_{1|2}$  minimize the mean-squared prediction error

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- Recalling the linear spatial model with GP, we have

$$\begin{pmatrix} y(\mathbf{s}_0) \\ \mathbf{y} \end{pmatrix} \sim N \left( \begin{pmatrix} \mathbf{x}'_0 \boldsymbol{\beta} \\ \mathbf{X} \boldsymbol{\beta} \end{pmatrix}, \begin{pmatrix} \tau^2 + \sigma^2 & \boldsymbol{\gamma}'_\phi \\ \boldsymbol{\gamma}_\phi & \Sigma_\theta \end{pmatrix} \right)$$

where  $\boldsymbol{\gamma}'_\phi = (\sigma^2 \rho(||\mathbf{s}_1 - \mathbf{s}_0||; \phi), \dots, \sigma^2 \rho(||\mathbf{s}_n - \mathbf{s}_0||; \phi))$  and  $\Sigma_\theta = \sigma^2 \mathbf{R}(\phi) + \tau^2 I_n$ .

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- Substituting these values into the conditional mean and variance, we obtain

$$E[Y(\mathbf{s}_0) | \mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}] = \mathbf{x}'_0 \boldsymbol{\beta} + \boldsymbol{\gamma}'_\phi \Sigma_\theta^{-1} (\mathbf{y} - \mathbf{X} \boldsymbol{\beta}) \quad \text{kriging estimator}$$

$$\text{Var}[Y(\mathbf{s}_0) | \mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}] = \tau^2 + \sigma^2 - \boldsymbol{\gamma}'_\phi \Sigma_\theta^{-1} \boldsymbol{\gamma}_\phi$$

# Kriging: spatial prediction at new locations

- Plugging-in ML estimates:

$$\hat{Y}(\mathbf{s}_0) = \mathbf{x}'_0 \hat{\boldsymbol{\beta}}_{MLE} + \hat{\boldsymbol{\gamma}}'_\phi \hat{\Sigma}_\theta^{-1} (\mathbf{y} - \mathbf{X} \hat{\boldsymbol{\beta}}_{MLE})$$
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- Bayesian Kriging computes (simulates) posterior predictive density:

$$p(y(\mathbf{s}_0) | \mathbf{y}) = \int p(\mathbf{s}_0 | \mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}) p(\boldsymbol{\beta}, \boldsymbol{\theta} | \mathbf{y}) d\boldsymbol{\beta} d\boldsymbol{\theta}$$

# Kriging: spatial prediction at new locations

Example: Ozone data

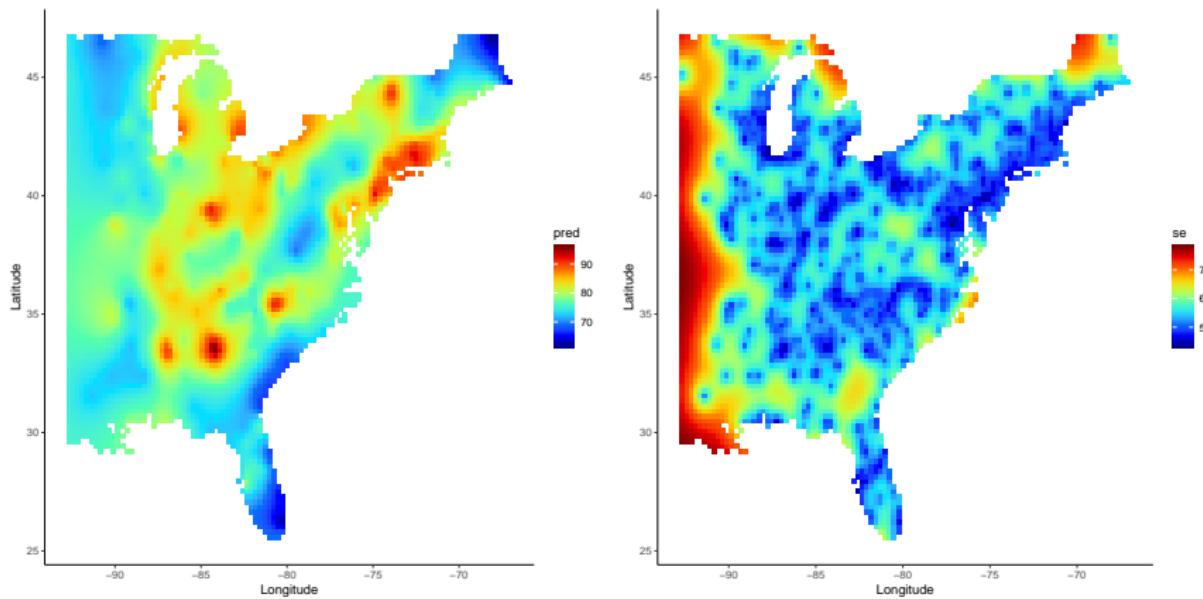


Figure: Kriged surface (left panel) and predicted standard error (right panel).

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- What happens when  $\mathbf{s}_0$  is far away from all the  $\mathbf{s}_i$ 's ?
- $(\rho(\mathbf{s}_1, \mathbf{s}_0; \phi), \dots, \rho(\mathbf{s}_n, \mathbf{s}_0; \phi))' \approx (0, \dots, 0)'$
- Kriging mean:  $\approx \mu(\mathbf{s}_0)$  = unconditional mean
- Kriging variance:  $\approx C(\mathbf{s}_0, \mathbf{s}_0)$  = unconditional variance
- $w(\mathbf{s}_0)$  is almost independent of the  $w(\mathbf{s}_i)$ 's i.e., we are not exploiting much information on the process at far away locations

# Model comparison

- Likelihood-based criteria. For  $k$  total parameters and sample size  $n$ :
  - AIC:  $2k - 2\log(L(\mathbf{y} \mid \hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\theta}}))$
  - BIC:  $\log(n)k - 2\log(L(\mathbf{y} \mid \hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\theta}}))$

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  - BIC:  $\log(n)k - 2\log(L(\mathbf{y} | \hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\theta}}))$
- Prediction-based approaches using holdout data:
  - Root Mean Square Predictive Error (RMSPE):
$$\sqrt{\frac{1}{n_{out}} \sum_{i=1}^{n_{out}} (y(\mathbf{s}_i) - \hat{y}(\mathbf{s}_i))^2}$$
  - Coverage probability (CP):
$$\frac{1}{n_{out}} \sum_{i=1}^{n_{out}} I(y(\mathbf{s}_i) \in (\hat{y}(\mathbf{s}_i)_{0.025}, \hat{y}(\mathbf{s}_i)_{0.975}))$$
  - Width of 95% confidence interval (CIW):
$$\frac{1}{n_{out}} \sum_{i=1}^{n_{out}} (\hat{y}(\mathbf{s}_i)_{0.025} - \hat{y}(\mathbf{s}_i)_{0.975})$$
  - The last two approaches compares the distribution of  $y(\mathbf{s}_i)$  instead of comparing just their point predictions

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  - Land use classification at a location (not ordinal)
- Replace Gaussian likelihood by an appropriate non-Gaussian likelihood  $f(y(\mathbf{s}_i)|\boldsymbol{\beta}, w(\mathbf{s}_i), \delta)$  such that

$$g(E(Y(\mathbf{s}_i))) = \eta(\mathbf{s}_i) = \mathbf{x}'(\mathbf{s}_i)\boldsymbol{\beta} + w(\mathbf{s}_i),$$

where  $\eta$  is a canonical link function (such as a logit) and  $\delta$  is a dispersion parameter.

## The “big $n$ problem”

- $\mathcal{S} = \{\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_n\}$  are locations where data are observed
- $y(\mathbf{s}_i)$  is outcome at the  $i$ -th location and  $\mathbf{y} = (y(\mathbf{s}_1), y(\mathbf{s}_2), \dots, y(\mathbf{s}_n))'$
- Model:  $\mathbf{y} \sim N(\mathbf{X}\boldsymbol{\beta}, \Sigma_\theta)$ , where  $\Sigma_\theta = \Sigma(\sigma^2, \phi)$
- Estimating process parameters from the likelihood:

$$-\frac{1}{2} \log \det(\Sigma_\theta) - \frac{1}{2} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \Sigma_\theta^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

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- Model:  $\mathbf{y} \sim N(\mathbf{X}\boldsymbol{\beta}, \Sigma_\theta)$ , where  $\Sigma_\theta = \Sigma(\sigma^2, \phi)$
- **Estimating process** parameters from the likelihood:

$$-\frac{1}{2} \log \det(\Sigma_\theta) - \frac{1}{2} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \Sigma_\theta^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

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- Need to calculate  $\det(\Sigma_\theta)$  and quadratic forms of  $\Sigma_\theta^{-1}$ .

# The “big $n$ problem”

- Conditional predictive density

$$p(y(\mathbf{s}_0) | \mathbf{y}, \boldsymbol{\theta}, \boldsymbol{\beta}) = N(y(\mathbf{s}_0) | \mu(\mathbf{s}_0), \sigma^2(\mathbf{s}_0))$$

- Classig Kriging, spatial prediction/interpolation

$$E[Y(\mathbf{s}_0) | \mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}] = \mathbf{x}'_0 \boldsymbol{\beta} + \boldsymbol{\gamma}' \boldsymbol{\Sigma}_{\theta}^{-1} (\mathbf{y} - \mathbf{X} \boldsymbol{\beta})$$

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- Again need to evaluate quadratic forms of  $\boldsymbol{\Sigma}_{\boldsymbol{\theta}}^{-1}$ .
- Challenge:** evaluating the density requires  $O(n^3)$  operations and  $O(n^2)$  memory which can quickly overwhelm computing systems when  $n$  is only moderately large.

## Literature on spatial big data

1. Low rank methods: typically involve reducing the  $n \times n$  matrix  $\Sigma_\theta$  ([Fixed Rank Kriging](#), [Predictive process](#));

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4. Algorithmic approaches: differ from the previous approaches in that they focus more on fitting schemes than model building ([Metakriging](#), [Gapfill](#), [Local Approximate Gaussian Processes](#)).

## A case study competition

- Heaton, M.J., Datta, A., Finley, A.O., Furrer, R., Guinness, J., Guhaniyogi, R., Gerber, F., Gramacy, R.B., Hammerling, D., Katzfuss, M. and Lindgren, F. (2018), A case study competition among methods for analyzing large spatial data. *Journal of Agricultural, Biological and Environmental Statistics*, pp.1-28.
- A case study competition between various research groups across the globe who each implemented their own method to analyze the same spatial datasets.
- Data and code available at:  
<https://github.com/finnlindgren/heatoncomparison>

# Outline

- 1 Introduction to spatial and spatio-temporal data
  - What are spatial data?
  - Why spatial modeling?
  - Types of spatial data
- 2 Point-referenced modeling
  - EDA
  - Gaussian Processes
  - Spatial linear regression
  - Parameter estimation
  - Kriging
  - Model comparison
  - Large spatial data
- 3 Spatio-temporal models
  - Continuous space-time models
  - Discrete-time spatial models

# Spatio-temporal analysis

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## Continuous time vs discretized time

$$\{Y(\mathbf{s}, t), \mathbf{s} \in D_s, t \in D_t\}$$

- Spatio-temporal domain:  
 $D = D_s \times D_t$ , where  $D_s \subset \mathbb{R}^r$  and  $D_t \subset \mathbb{R}^+$
- Each observation has a space-time coordinate

$$\{Y_t(\mathbf{s}), \mathbf{s} \in D_s, t = 1, \dots, T\}$$

- Geo-referenced time series
- Restricted to data observed at *regular* time intervals (hourly, daily, etc)
- Interpolation at finer temporal resolution not possible

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## Spatio-temporal covariance function

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- Separability:

$$\text{Cov}(w(\mathbf{s}, t), w(\mathbf{s}', t')) = \sigma^2 \rho_1(\mathbf{s} - \mathbf{s}'; \phi_1) \rho_2(t - t'; \phi_2)$$

where  $\rho_1$  is a valid two-dimensional correlation function and  $\rho_2$  is a valid one-dimensional correlation function.

- Separable models do **not** allow for space-time interaction

# Spatio-temporal covariance function

## Non-separable models

- Non-separable covariance function (e.g., De Iaco et al. 2002; Gneiting 2002; Stein 2005) allows space-time interaction

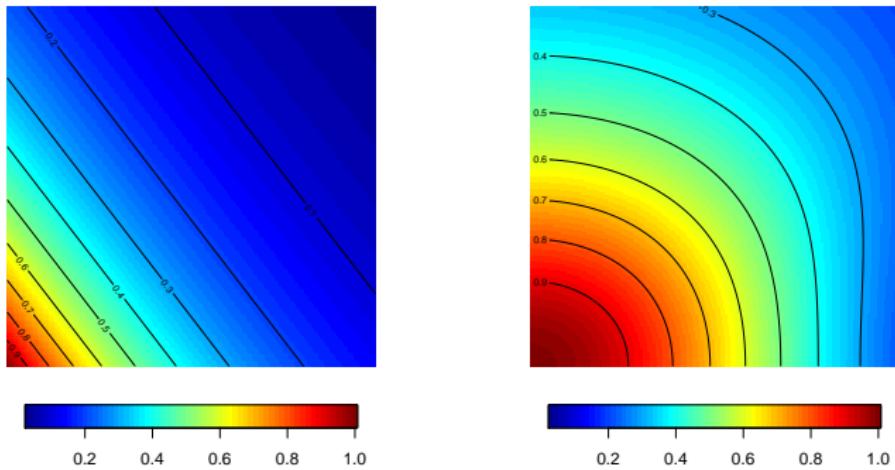


Figure: Separable vs non-separable correlation function.

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where  $\otimes$  is the Kronecker product (separable model).

- Fast likelihood evaluation by properties of Kronecker.

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- Fast likelihood evaluation by properties of Kronecker.
- Spatio-temporal predictions (kriging) through  $w(\mathbf{s}_0, t_0) \mid \mathbf{w}$

## Discrete-time spatial models

$$y_t(\mathbf{s}) = \mu_t(\mathbf{s}) + w_t(\mathbf{s}) + \varepsilon_t(\mathbf{s})$$

- $\mu_t(\mathbf{s})$  is the mean structure, usually set to as  $\mu_t(\mathbf{s}) = \mathbf{x}'_t(\mathbf{s})\boldsymbol{\beta}_t(\mathbf{s})$ ;
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- $w_t(\mathbf{s})$  is the **spatio-temporal random effect**;
  - *additive form* (or multiplicative)  $w_t(\mathbf{s}) = \alpha_t + v(\mathbf{s})$
  - *independent-in-time* spatial processes  $w_t(\mathbf{s}), \forall t$
  - **dynamic spatio-temporal models**

$$w_t(\mathbf{s}) = w_{t-1}(\mathbf{s}) + \eta_t(\mathbf{s}),$$

where  $\eta_t(\mathbf{s})$  are independent-in-time spatial processes

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# Discrete-time spatial models

## Dynamic spatio-temporal models

- State-space formulation (West and Harrison, 1997)
- $\mathbf{y}_t = (y_t(\mathbf{s}_1), \dots, y_t(\mathbf{s}_n))'$

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### 1. Stage: Measurement equation

$$\mathbf{y}_t = f(\mathbf{z}_t \mid \boldsymbol{\theta}) + \boldsymbol{\varepsilon}_t,$$

where  $\mathbf{z}_t$  is the state vector, not observable but generated by a first-order Markovian process and  $\boldsymbol{\varepsilon}_t$  is a white noise process

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### 2. Stage: Transition equation

$$\mathbf{z}_t = g(\mathbf{z}_{t-1} \mid \boldsymbol{\gamma}) + \boldsymbol{\eta}_t,$$

where  $\boldsymbol{\eta}_t$  is a discrete-time spatial process.

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