

# Spatial Reading Group

## Optional Subtitle

February 15, 2017

# Outline

Motivation

Classical Frequentist Spatial Stats

Spatial Relationships

Variograms

Kriging

Maximum Likelihood Estimation

Extension - Preferential Sampling

Bayesian Estimation and Prediction

# Motivation

## Why Spatial Data needs Spatial Stats

- ▶ Spatial Data are continuous but measured discretely.
- ▶ The data tend to be correlated.
- ▶ The measurements are rarely taken at random

# Assumptions

- ▶ Smooth data
- ▶ Stationary data
  - ▶ Does a trend extend beyond the bounds of the study?
  - ▶ Is the covariance consistent in the bounds of the study?

# Outline

Motivation

Classical Frequentist Spatial Stats

Spatial Relationships

Variograms

Kriging

Maximum Likelihood Estimation

Extension - Preferential Sampling

Bayesian Estimation and Prediction

# Covariance

- ▶ Smooth data
- ▶ Stationary data
  - ▶ Does a trend extend beyond the bounds of the study?
  - ▶ Is the covariance consistent in the bounds of the study?

# Mattern Function

- ▶  $\rho(x) = \{2^{\kappa-1}\Gamma(\kappa)\}^{-1} \frac{u}{\phi}^{\kappa} K_{\kappa}(\frac{u}{\phi})$
- ▶  $\kappa$  is order of differentiation, smoothness
- ▶  $\phi$  is scale, degree of decay over time
- ▶  $\kappa$  and  $\phi$  are not orthogonal.

# Outline

Motivation

Classical Frequentist Spatial Stats

Spatial Relationships

Variograms

Kriging

Maximum Likelihood Estimation

Extension - Preferential Sampling

Bayesian Estimation and Prediction



## Second Slide Title

- ▶ First item.

## Second Slide Title

- ▶ First item.
- ▶ Second item.

## Second Slide Title

- ▶ First item.
- ▶ Second item.
- ▶ Third item.

## Second Slide Title

- ▶ First item.
- ▶ Second item.
- ▶ Third item.
- ▶ Fourth item.

## Second Slide Title

- ▶ First item.
- ▶ Second item.
- ▶ Third item.
- ▶ Fourth item.
- ▶ Fifth item.

## Second Slide Title

- ▶ First item.
- ▶ Second item.
- ▶ Third item.
- ▶ Fourth item.
- ▶ Fifth item. Extra text in the fifth item.

# Maximum Likelihood Estimation

- ▶ Gaussian model

$$Y \sim N(D\beta, \sigma^2 R(\phi) + \tau^2 I)$$

with covariates matrix  $D_{n \times p}$ , regression coefficients  $\beta$ , covariance of a parametric model for  $S(x)$ , and nugget variance  $\tau^2$ .

- ▶ The log-likelihood function is

$$\begin{aligned} L(\beta, \tau^2, \sigma^2, \phi) = & -0.5 \{ n \log(2\pi) + \log\{ |(\sigma^2 R(\phi) + \tau^2 I)| \} \\ & + (y - D\beta)^T (\sigma^2 R(\phi) + \tau^2 I)^{-1} (y - D\beta) \} \end{aligned}$$

- ▶ Let  $\nu^2 = (\tau^2/\sigma^2)$ ,  $V = R(\phi) + \nu I$ , then  $L(\beta, \tau^2, \sigma^2, \phi)$  is maximized at

$$\hat{\beta}(V) = (D^T V^{-1} D)^{-1} D^T V^{-1} y \quad (1)$$

$$\hat{\sigma}^2(V) = n^{-1} \{ y - D\hat{\beta}(V) \}^T V^{-1} \{ y - D\hat{\beta}(V) \} \quad (2)$$

# Maximum Likelihood Estimation

- ▶ Plug (1) and (2) into  $L(\beta, \tau^2, \sigma^2, \phi)$  and obtain the **concentrated log-likelihood**:  
$$L_0(\nu^2, \phi) = -0.5\{n \log(2\pi) + n \log \hat{\sigma}^2(V) + \log|V| + n\}$$
- ▶ Optimize  $L_0(\nu^2, \phi)$  numerically with respect to  $\nu$  and  $\phi$ ; back substitution to obtain  $\hat{\sigma}^2$  and  $\hat{\beta}$
- ▶ Re-parameterisation of  $V$  can be used to obtain more stable estimation, e.g the ratio  $\sigma^2/\phi$  is more stable than  $\sigma^2$  and  $\phi$
- ▶ Computational tool: **profile log-likelihood**:  
Assume a model with parameters  $(\alpha, \psi)$ ,

$$L_p(\alpha) = L(\alpha, \hat{\psi}(\alpha)) = \max_{\psi} (L(\alpha, \psi))$$



# Maximum Likelihood Estimation

- ▶ Non-Gaussian data:  
(1): transformation to Gaussian (2) generalized linear model
- ▶ (1) E.g. Box-Cox transformation; denote the transformed responses  $Y^* = (Y_1^*, \dots, Y_n^*)$ , and fit a Gaussian model

$$Y^* \sim N(D\beta, \sigma^2\{R(\phi) + \tau^2 I\})$$

Computationally demanding, transformation may impede scientific interpretation

- ▶ (2) Generalized linear model

$$L(\theta|S) = \prod_{i=1}^n f_i(y_i|S, \theta)$$

$$L(\theta, \phi) = \int_S \prod_{i=1}^n f_i(y_i|s, \theta) g(s|\phi) ds$$

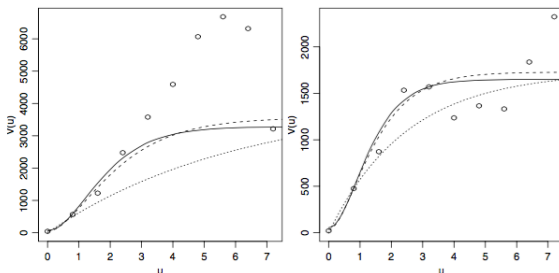
Involve high dimensional integration; need MCMC/Hierarchical likelihood/Generalized estimating equations

# Maximum Likelihood Estimation (An Example)

Model with constant mean							
Model	$\hat{\mu}$		$\hat{\sigma}^2$	$\hat{\phi}$	$\hat{\tau}^2$		logL
$\kappa = 0.5$	863.71		4087.6	6.12	0		-244.6
$\kappa = 1.5$	848.32		3510.1	1.2	48.16		-242.1
$\kappa = 2.5$	844.63		3206.9	0.74	70.82		-242.33

Model with linear trend							
Model	$\hat{\beta}_0$	$\hat{\beta}_1$	$\hat{\beta}_2$	$\hat{\sigma}^2$	$\hat{\phi}$	$\hat{\tau}^2$	logL
$\kappa = 0.5$	919.1	-5.58	-15.52	1731.8	2.49	0	-242.71
$\kappa = 1.5$	912.49	-4.99	-16.46	1693.1	0.81	34.9	-240.08
$\kappa = 2.5$	912.14	-4.81	-17.11	1595.1	0.54	54.72	-239.75



**Figure:** left: constant mean model; right: linear trend surface  
 circle: sample variogram; solid line  $\kappa = 2.5$ ; dashed line  $\kappa = 1.5$ ; dotted line  $\kappa = 0.5$

# Kriging

- ▶ Suppose our objective is to predict the value of the signal at an arbitrary location  $S(x)$ .
- ▶ Note that  $(S(x), Y)$  is multivariate Gaussian with mean vector  $\mu \mathbf{1}$  and covariance matrix

$$\begin{pmatrix} \sigma^2 & \sigma^2 r^T \\ \sigma^2 r & \sigma^2 V \end{pmatrix},$$

where  $r$  is a vector with elements  $r_i = \rho(\|x - x_i\|)$  and  $V = \sigma^2 R + \tau^2 I$ .

# Kriging

- ▶ Conditional mean and variance:

$$E(S(x)|Y) = \mu + r^T V^{-1}(Y - \mu \mathbf{1}),$$

$$\text{Var}(S(x)|Y) = \sigma^2(1 - r^T V^{-1}r).$$

- ▶ Two types:

- ▶ Ordinary kriging: replace  $\mu$  by its weighted least squares estimator

$$\hat{\mu} = (\mathbf{1}^T V^{-1} \mathbf{1})^{-1} \mathbf{1}^T V^{-1} Y.$$

- ▶ Simple kriging: replace  $\mu$  by  $\hat{\mu} = \bar{y}$ .
- ▶ Both kriging predictors can be expressed as a linear combination:  $\hat{S}(x) = \sum_{i=1}^n a_i(x) Y_i$ , but  $\sum_{i=1}^n a_i(x) = 1$  only for ordinary kriging.

# Preferential Sampling

## The Problem

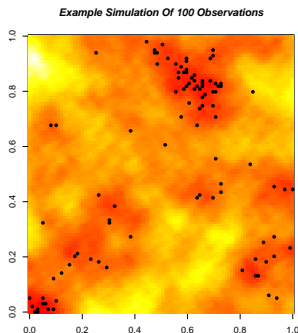
- ▶ So far we have assumed the sampling locations  $X$  are fixed, or assumed known.
- ▶ What if the sampling locations depend on the underlying field  $S$ ?

## Example

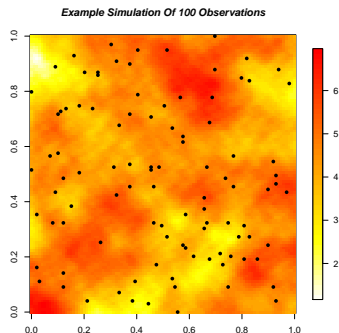
- ▶ Pollution data from measuring stations
- ▶ Ocean temperature data from marine mammals
- ▶ Lead concentration in Galicia (to be shown)

# Preferential Sampling

**Figure:** Example of a single realisation of  $S$  and corresponding 100 sampling locations selected using a spatial Poisson Process with intensity  $\lambda(x) = \exp(\beta S(x))$ .



(a) Example of 100 preferentially sampled locations ( $\beta = 2$ )



(b) Example of 100 non-preferentially sampled locations ( $\beta = 0$ )

# Preferential Sampling

## Solution

- ▶ We must account for the dependence between  $X$  and  $S$ .

$$L(\theta) = \int [X, Y, S] dS. \quad (3)$$

- ▶ Diggle et al. 2010 - Monte Carlo
- ▶ Integrated Nested Laplace Approximation (INLA) - Joe
- ▶ Template Model Builder - Danny

# Preferential Sampling

## Results

Model	Parameter	Standard MLE	<i>TMB</i>
Preferential	Bias	(0.77, 1.36)	(0.41, 0.94)
Preferential	Root-mean-square error	(0.86, 1.40)	(0.60, 1.05)

**Table:** Comparison of approximate 95% confidence intervals for the root-mean-square errors and bias between standard MLE and *TMB* over 50 independent simulations for preferential ( $\beta = 2$ ) at location  $x_0 = (0.49, 0.49)$ .



# Problems with the MLE approach

- ▶ MLE method separates parameter estimation and spatial prediction as two distinct problems.
- ▶ First the model is formulated, and it's parameters estimated.
- ▶ These estimated parameters are assumed true and spatial prediction equations are computed with these estimates plugged-in.
- ▶ Parameter uncertainty is ignored when making spatial prediction.
- ▶ Parameter uncertainty is often VERY HIGH. Even with seemingly large datasets ( $n > 10,000$ ), the positive correlation dilutes the information present. Largely different values of correlation parameters  $\phi$  often fit the data equally well.

# Bayesian approach

- ▶ Account for parameter uncertainty when making spatial prediction and hence make more conservative estimates of prediction accuracy.

$$[S|Y] = \int [S|Y, \theta][\theta|Y]d\theta$$

- ▶ The Bayesian predictive distribution is a weighted average of plug-in predictive distributions  $[S|Y, \hat{\theta}]$ , weighted by the posterior uncertainty of the model values  $\theta$ .
- ▶ Arbitrary nonlinear functional  $T(S)$  of  $S$  can be estimated (along with credible intervals, standard errors etc) by simple deterministic transformations of the posterior samples of  $S$ .

# Problems with Bayesian implementation

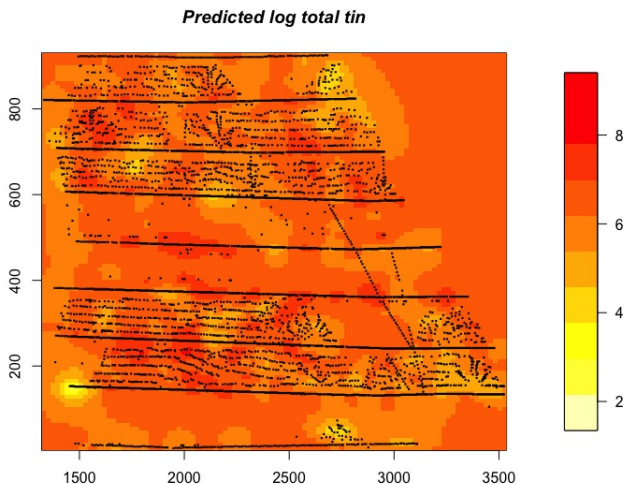
- ▶ Due to the flexibility of the Matern correlation function, many different combinations of the correlation parameters  $\phi$  fit the data equally well.
- ▶ A consequence of this is that the posterior distribution of  $[\theta|Y]$  has non-negligible probability mass across a wide range of the parameter space.
- ▶ The first consequence of this is that posterior distributions are extremely sensitive to prior distributions. Apparently 'diffuse' priors can still heavily affect the location and scale of the posterior distribution.
- ▶ Secondly, MCMC samplers must be formulated with large transition jumps to ensure the whole parameter space is explored. This leads to VERY LONG MCMC chains needing to be run (100,000 +).

# The joy of INLA

- ▶ INLA enables **very** accurate deterministic approximations to both  $[\theta|Y]$  and  $\int[S|Y, \theta][\theta|Y]d\theta$  to be obtained.
- ▶ INLA handles most well-known response functions (Binomial, Poisson, Gamma etc), enabling Generalized Geostatistical Models to be fit.
- ▶ Through a combination of high-accuracy Laplace approximations and cubic spline interpolation, values from INLA are often indistinguishable from the 'true' values from an MCMC chain.
- ▶ INLA is FAST. Taking only seconds - minutes to run compared with the hours - days that MCMC can take.
- ▶ Multiple responses can be fit to the same spatial process! (E.g poisson process and intensity process enabling preferential sampling to be investigated.)

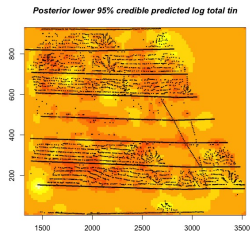
# Real example: Predicting total Tin in Cornwall, UK

Figure: Predicted mean field .

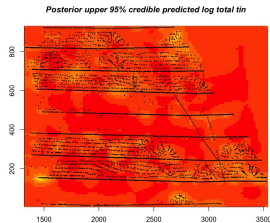


# Real example: Predicting total Tin in Cornwall, UK

Figure: Upper and lower 95% credible fields.



(a)



(b)

# Summary

- ▶ The **first main message** of your talk in one or two lines.
- ▶ The **second main message** of your talk in one or two lines.
- ▶ Perhaps a **third message**, but not more than that.
- ▶ Outlook
  - ▶ Something you haven't solved.
  - ▶ Something else you haven't solved.

# For Further Reading I



A. Author.

*Handbook of Everything.*

Some Press, 1990.



S. Someone.

On this and that.

*Journal of This and That*, 2(1):50–100, 2000.