

Spatial Reading Group

Optional Subtitle

February 15, 2017

Outline

Motivation

Classical Frequentist Spatial Stats

Spatial Relationships

Variograms

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?

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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

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

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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.

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 μ 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 μ 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.

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 β , covariance of a parametric model for $S(x)$, and nugget variance τ^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 ν and ϕ ; 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 σ^2/ϕ is more stable than σ^2 and ϕ
- ▶ Computational tool: **profile log-likelihood**:
Assume a model with parameters (α, ψ) ,

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

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 |

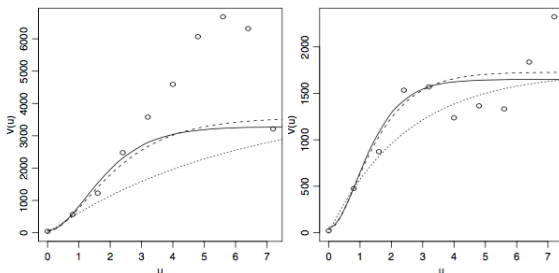


Figure: left: constant mean model; right: linear trend surface
 circle: sample variogram; solid line $\kappa = 2.5$; dashed line $\kappa = 1.5$; dotted line $\kappa = 0.5$

Preferential Sampling

The Problem

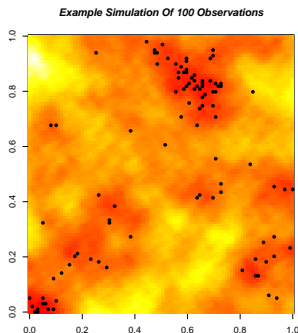
- ▶ So far we have assumed the sampling locations X are fixed, or assumed known.
- ▶ What if the sampling locations depend on the underlying field S ?

Example

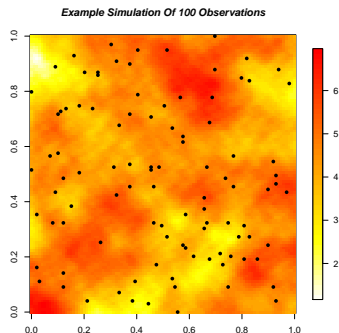
- ▶ Pollution data from measuring stations
- ▶ Ocean temperature data from marine mammals
- ▶ Lead concentration in Galicia (to be shown)

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 ϕ 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 θ .
- ▶ 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

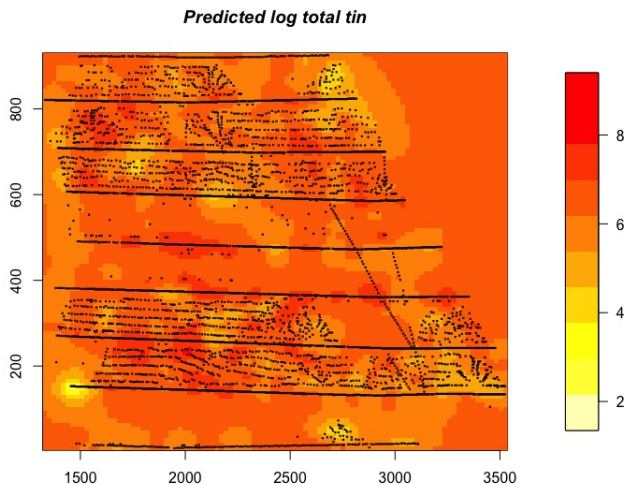
- ▶ Due to the flexibility of the Matern correlation function, many different combinations of the correlation parameters ϕ fit the data equally well.
- ▶ A consequence of this is that the posterior distribution of $[\theta|Y]$ has non-negligible probability mass across a wide range of the parameter space.
- ▶ 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.)

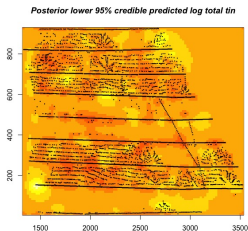
Real example: Predicting total Tin in Cornwall, UK

Figure: Predicted mean field .

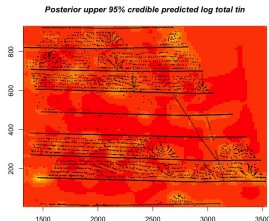


Real example: Predicting total Tin in Cornwall, UK

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.