

Day 1 – Spatial & Spatio-temporal Modelling

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Introduction

About me

- ▶ Completed a Bachelor's degree in Statistics at FUTA
- ▶ Master's in Mathematical Sciences at AIMS-Tanzania
- ▶ PhD in Statistics and Epidemiology at University of Lancaster
- ▶ Postdoc at University of Manchester
- ▶ Lecturer in Statistics at the University of Manchester

Overview of the 3 days

- ▶ Spatial and spatio-temporal analysis (different likelihoods)
- ▶ Joint modelling of multiple malaria processes
- ▶ Non-stationary spatial processes
- ▶ Hybrid machine learning + geostatistical models

Linear Regression

- ▶ Goal: Model a continuous response variable as a linear function of predictors.
- ▶ Model $Y = X\beta + \epsilon$, where $\epsilon \sim N(0, \sigma^2)$
- ▶ Key Assumption
 - ▶ Linearity
 - ▶ Independence
 - ▶ Homoscedasticity (constant variance)
 - ▶ Normality of errors

Generalized Linear Models (GLMs)

- ▶ Extension of linear models to handle non-normal response distributions.
- ▶ Three components:
 - ▶ Random component: Distribution from the exponential family (e.g., Binomial, Poisson).
 - ▶ Systematic component: Linear predictor $\eta = X\beta$.
 - ▶ Link function: Relates $E(Y)$ to η .
- ▶ Examples:
 - ▶ Logistic regression for binary outcomes – logit link function
 - ▶ Poisson regression for count data – log link function

Why Spatial Statistics?

► **Spatial Dependence:**

Observations collected at nearby locations are often more similar than those farther apart.

► **Ignoring Spatial Structure:**

- Leads to biased parameter estimates.
- Underestimates uncertainty.
- Misses important spatial patterns.

► **Applications:**

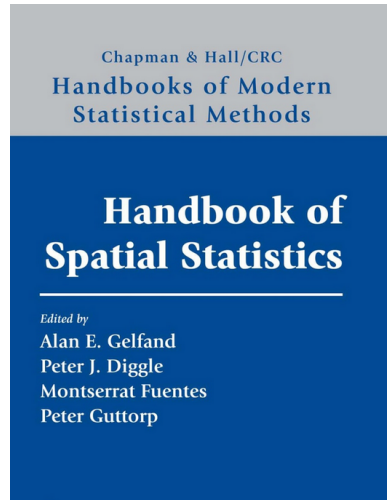
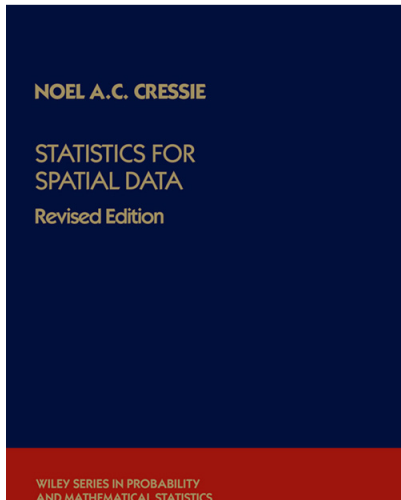
- Disease mapping
- Environmental monitoring
- Agricultural field trials

► **Goal:**

Account for spatial correlation to improve prediction and inference.

Spatial Analysis

Spatial Statistics



Classification of spatial statistics

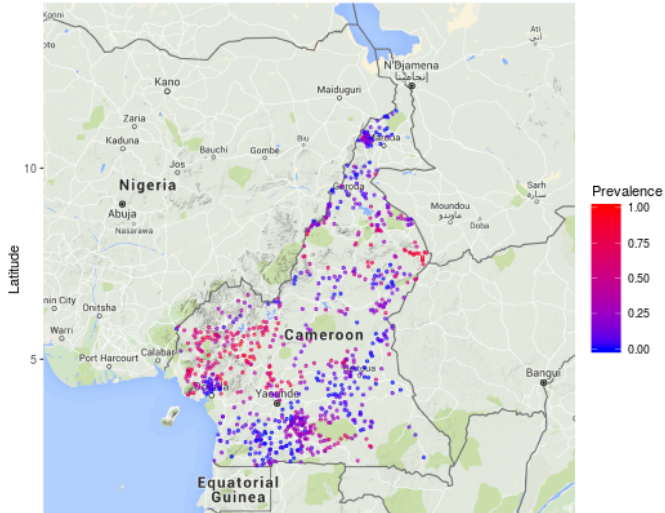
Cressie's book classifies spatial statistics according to **data format**:

1. Geostatistical data
2. Lattice data
3. Point patterns

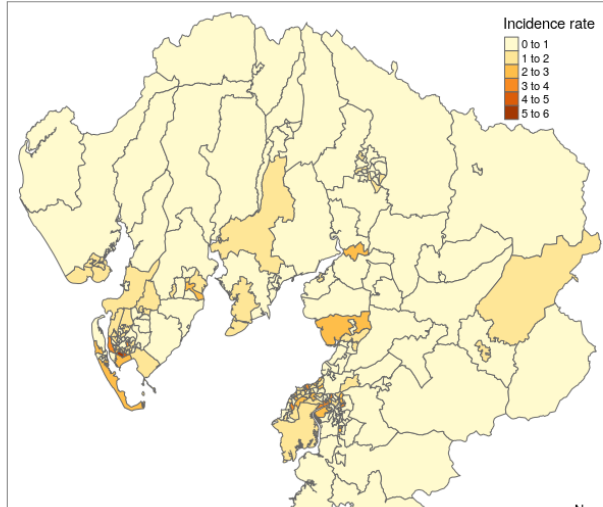
Gelfand's book classifies spatial statistics according to **spatial variation**:

1. Discrete spatial variation: Gaussian Markov Random Field (GMRF)
2. Continuous spatial variation: Gaussian Random Field (GMRF)

Geostatistical data: River blindness in Cameroon



Lattice Data: COPD emergency admission



Point pattern: Primary biliary cirrhosis data



Model-based Geostatistics

Modelling Geostatistical Data – Model-based Geostatistics

- ▶ The term **Model-based Geostatistics (MBG)** was coined by Peter Diggle in 1998 (Diggle, Tawn, and Moyeed 1998; Diggle and Giorgi 2019).
- ▶ MBG applies general principles of statistical modelling and inference to the analysis of geostatistical data.
- ▶ It emphasises the use of likelihood-based inference.
- ▶ **and the use of latent spatial process (Gaussian or stochastic process)**

Standard MBG model

$$Y_i = \beta_0 + \underbrace{\beta_1 d_1(x_i) + \beta_2 d_2(x_i)}_{\text{explained}} + \underbrace{S(x_i) + Z_j}_{\text{unexplained}},$$

where

- ▶ β_0 , β_1 , and β_2 are regression coefficients;
- ▶ $d_1(x)$ and $d_2(x)$ denote covariates/predictors at location x ;
- ▶ $S(x)$ is the stochastic spatial process;
- ▶ Z_j represents measurement error.

Modelling $S(x)$ and Z_j

- ▶ $Z_i \sim N(0, \tau^2)$
- ▶ We assume that $S(x)$ is a zero-mean **stationary and isotropic Gaussian process**. i.e $S \sim \text{MVN}(0, \Sigma)$
- ▶ The (i, j) th entry of Σ is

$$\Sigma_{ij} = \text{Cov}(S(x_i), S(x_j)) = \sigma^2 \rho(u)$$

- ▶ $u = \|x_i - x_j\|$ is the Euclidean distance between locations x_i and x_j
- ▶ **How do we choose parametric correlation function $\rho(\cdot)$?**

The Matérn correlation function

$$\rho(u; \phi, \kappa) = \frac{1}{2^{\kappa-1} \Gamma(\kappa)} \left(\frac{u}{\phi} \right)^{\kappa} K_{\kappa} \left(\frac{u}{\phi} \right),$$

► $K_{\kappa}(\cdot)$: modified Bessel function of order κ

► Interpretation

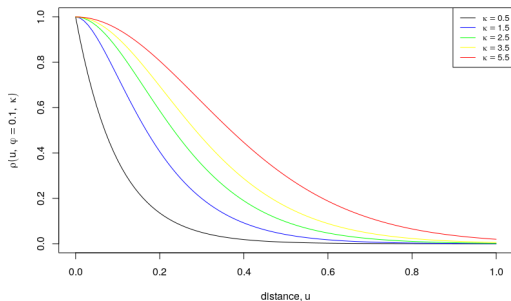
- κ determines the smoothness: $\kappa > r \Rightarrow S(x)$ is r times differentiable
- ϕ determines the scale of spatial correlation

► Special cases

- $\kappa = 0.5 \Rightarrow \rho(u) = \exp\{-u/\phi\}$
- $\kappa \rightarrow \infty \Rightarrow \rho(u) = \exp\{-(u/\phi)^2\}$
- Often sufficient to choose $\kappa \in \{0.5, 1.5, 2.5\}$

Matérn correlation function – κ

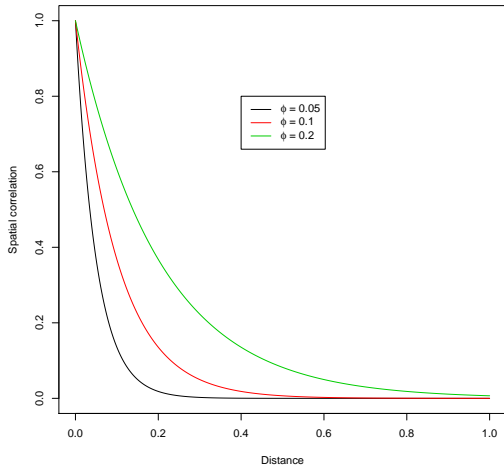
$$\rho(u; \phi, \kappa) = \frac{1}{2^{\kappa-1} \Gamma(\kappa)} \left(\frac{u}{\phi} \right)^{\kappa} K_{\kappa} \left(\frac{u}{\phi} \right),$$



Exponential correlation functions: $\rho(u; \psi = 0.5)$

$\rho(u; \psi = 1.0)$

The scale of the spatial correlation – ϕ



Do we need the process $S(x)$?

- Regression residuals

$$\hat{r}_i = Y_i - \hat{Y}_i$$

from a GLM

- Each \hat{r}_i estimates

$$S(x_i) + Z_i$$

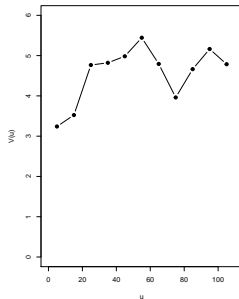
The variogram

► Empirical variogram

$$\hat{V}(u) = \frac{1}{2|N(u)|} \sum_{(i,j) \in N(u)} (\hat{r}_i - \hat{r}_j)^2$$

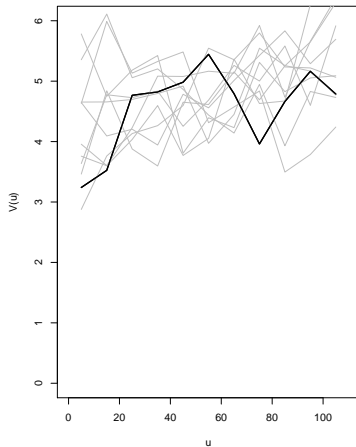
► where

$$N(u) = \{(i, j) : \|x_i - x_j\| = u\}$$



Confirming existence of spatial correlation

1. Randomly permute the \hat{r}_i while holding the locations x fixed
2. Compute the empirical variogram using the permuted \hat{r}_i
3. Repeat steps 1–2 B times
4. Use the resulting B variograms to compute **pointwise 95% tolerance bands** at each distance bin
5. If the observed variogram lies outside the 95% band, this indicates **residual spatial correlation**



Inference: Maximum likelihood estimation

► Multivariate Gaussian distribution

$$Y \sim \text{MVN}(D\beta, \sigma^2 R + \tau^2 I)$$

- D : matrix of covariates, $[D]_{ik} = d_k(x_i)$
- R : spatial correlation matrix,
 $[R]_{ij} = \rho(u_{ij})$, with $u_{ij} = \|x_i - x_j\|$

► Fitting process

1. Initialise β (e.g. using ordinary least squares)
2. Initialise θ (e.g. using the empirical variogram)
3. Maximise

$$\ell(\theta) = \log\{f(y; \beta, \theta)\},$$

where $f(\cdot; \beta, \theta)$ is the multivariate Gaussian density

Beyond Gaussian responses

So far, we assumed:

$$Y \sim \text{MVN}(D\beta, \sigma^2 R + \tau^2 I)$$

However, many geostatistical datasets are:

- ▶ Binary (presence / absence)
- ▶ Counts (number of cases)
- ▶ Rates or proportions

A Gaussian likelihood is no longer appropriate

Separating data and process models

Model-based geostatistics distinguishes between:

► **Observation model (likelihood):**

$$Y_i \mid \eta_i \sim \pi(y_i \mid \eta_i)$$

► **Latent process model:**

$$\eta_i = X_i\beta + S(x_i) + Z_i$$

Key idea:

- Non-Gaussian data
- Gaussian latent structure

Common likelihoods in practice

► Gaussian

$$Y_i \mid \eta_i \sim N(\eta_i, \sigma^2)$$

Continuous measurements (e.g. pollution levels)

► Binomial

$$Y_i \mid \eta_i \sim \text{Binomial}(n_i, p_i), \quad \text{logit}(p_i) = \eta_i$$

Prevalence survey data

► Poisson

$$Y_i \mid \eta_i \sim \text{Poisson}(\lambda_i), \quad \log(\lambda_i) = \eta_i$$

Disease counts, event data

Link functions

The linear predictor enters the likelihood via a link:

$$g(\mu_i) = \eta_i = X_i\beta + S(x_i) + Z_i$$

Examples:

- ▶ Identity link \rightarrow Gaussian data
- ▶ Logit link \rightarrow Binomial data
- ▶ Log link \rightarrow Poisson data

This gives a **generalized linear mixed model (GLMM)** structure

Computational challenges

For non-Gaussian likelihoods:

- ▶ The marginal likelihood requires:

$$L(\theta) = \int \pi(y \mid S, \theta) \pi(S \mid \theta) dS$$

- ▶ High-dimensional integral over latent field x
- ▶ No closed-form solution

Consequences:

- ▶ Maximum likelihood is expensive
- ▶ Bayesian inference via MCMC is slow

Classical solutions and limitations

- ▶ Laplace approximation
- ▶ Penalised quasi-likelihood (PQL)
- ▶ MCMC-based Bayesian inference

Limitations:

- ▶ Poor scalability for large spatial fields
- ▶ Long runtimes
- ▶ Difficult model exploration

Key takeaway

We want:

- ▶ Flexible likelihoods (Binomial, Poisson, etc.)
- ▶ Spatial and spatio-temporal random effects
- ▶ Bayesian inference
- ▶ Computational efficiency

This motivates **Integrated Nested Laplace Approximation (INLA)**

From likelihoods to INLA

Hierarchical models setup:

- ▶ Data likelihood: possibly non-Gaussian
- ▶ Latent field: Gaussian with spatial dependence
- ▶ Hyperparameters: low-dimensional

This class of models is known as **Latent Gaussian Models**

INLA is designed specifically for this class

Why INLA?

- ▶ Fully Bayesian inference for latent Gaussian models is often computationally expensive
- ▶ Markov chain Monte Carlo (MCMC):
 - ▶ Accurate but slow for large spatial datasets
 - ▶ Poor scaling with dimension of latent field
- ▶ **INLA** provides:
 - ▶ Deterministic (non-sampling) approximation
 - ▶ Orders-of-magnitude speed-ups
 - ▶ Accurate marginal posterior distributions

Latent Gaussian models

INLA is designed for **latent Gaussian models (LGMs)**:

$$y_i \mid \eta_i, \theta \sim \pi(y_i \mid \eta_i, \theta), \quad \eta = AS$$

where

- ▶ $S \sim \mathcal{N}(0, Q(\theta)^{-1})$ is a latent Gaussian field
- ▶ A is a known design / projection matrix
- ▶ θ are low-dimensional hyperparameters

Examples of S :

- ▶ Spatial Gaussian random fields
- ▶ Temporal effects
- ▶ Random effects and smoothers

Key idea: sparsity

- ▶ Latent field \mathcal{S} is modelled as a **Gaussian Markov Random Field (GMRF)**
- ▶ GMRFs have **sparse precision matrices** $Q(\theta)$

Why this matters:

- ▶ Sparse matrix algebra is fast
- ▶ Enables scalable inference for large spatial problems
- ▶ Crucial for INLA's computational efficiency

Stage 1: Hyperparameter inference

Goal:

$$\pi(\theta \mid y) \propto \frac{\pi(y \mid S, \theta) \pi(S \mid \theta) \pi(\theta)}{\pi(S \mid y, \theta)}$$

- ▶ INLA uses a **Laplace approximation** to integrate out S
- ▶ Produces an accurate approximation to:

$$\pi(\theta \mid y)$$

Key point:

- ▶ θ is low-dimensional \rightarrow numerical optimisation is feasible

Stage 2: Latent field given θ

- Conditional on θ , INLA approximates:

$$\pi(S \mid \theta, y)$$

- Approximation:
 - Gaussian
 - Centered at the mode of the conditional posterior
 - Uses local curvature (Hessian)

This step exploits:

- Gaussian structure of S
- Sparse precision matrix

Stage 3: Marginal posteriors

Final goal:

$$\pi(S_i | y), \quad \pi(\theta_j | y)$$

INLA computes:

$$\pi(S_i | y) = \int \pi(S_i | \theta, y) \pi(\theta | y) d\theta$$

- ▶ Integration performed numerically
- ▶ Output:
 - ▶ Marginal posterior means
 - ▶ Credible intervals
 - ▶ Full marginal densities

GRF vs GMRF: concept vs computation

Lindgren, Rue, and Lindström (2011) provides the link between the two.

- ▶ **Gaussian Random Field (GRF):**
 - ▶ Defined on a continuous spatial domain
 - ▶ Used for geostatistical modelling
 - ▶ Dense covariance structure
- ▶ **Gaussian Markov Random Field (GMRF):**
 - ▶ Defined on a finite set of locations
 - ▶ Sparse precision matrix
 - ▶ Computationally efficient

Key point:

In INLA, a **GMRF** is used as a computational approximation to a continuous **GRF**

Spatial modelling in INLA: SPDE approach

- ▶ Continuous Gaussian random fields are represented via: **Stochastic Partial Differential Equations (SPDEs)**

Key ideas:

- ▶ Start with a Matérn GRF (continuous)
- ▶ Approximate it on a triangulated mesh
- ▶ Obtain a **computational GMRF**
- ▶ Retain Matérn covariance structure

Benefits:

- ▶ Sparse precision matrix
- ▶ Fast Bayesian inference with INLA

Why the SPDE approach?

- ▶ In geostatistics, we often model spatial dependence using **Gaussian random fields (GRFs)** with Matérn covariance
- ▶ For observations at locations x_1, \dots, x_n :
 - ▶ Covariance matrix is **dense**
 - ▶ Computational cost is $\mathcal{O}(n^3)$

This becomes infeasible for large spatial datasets

Gaussian random fields

A spatial Gaussian random field is defined as:

$$S(x) \sim \text{GRF}(0, C(\cdot))$$

with covariance function:

$$\text{Cov}\{S(x), S(x')\} = C(\|x - x'\|)$$

- ▶ The Matérn family is widely used
- ▶ Defined on a **continuous spatial domain**

From covariance to SPDE

A key result (Whittle, 1954):

A Matérn GRF is the solution to the SPDE:

$$(\kappa^2 - \Delta)^{\alpha/2} S(x) = \mathcal{W}(x),$$

where: - Δ is the Laplacian operator - $\mathcal{W}(x)$ is Gaussian white noise - Parameters (κ, α) control range and smoothness

Discretising the SPDE

- ▶ The spatial domain is discretised using a **triangular mesh**
- ▶ The continuous field is approximated as:

$$S(x) \approx \sum_{k=1}^K w_k \psi_k(x)$$

where:

- ▶ $\psi_k(x)$ are basis functions
- ▶ w_k are random weights

Local support of basis functions sparsity

From GRF to GMRF

- ▶ The SPDE discretisation yields

$$\mathbf{w} \sim \mathcal{N}(0, Q^{-1})$$

- ▶ Precision matrix Q is **sparse**
- ▶ This defines a **Gaussian Markov Random Field (GMRF)**

Key consequence: - Fast computation - Scales to large spatial problems

SPDE approach: summary

- ▶ Specify a Matérn Gaussian random field
- ▶ Use its equivalent SPDE representation
- ▶ Approximate the SPDE on a triangulated mesh
- ▶ Obtain a sparse GMRF representation
- ▶ Perform fast Bayesian inference using INLA

When should you use INLA?

INLA is well suited for:

- ▶ Spatial and spatio-temporal models
- ▶ Latent Gaussian models
- ▶ Large datasets with structured dependence

INLA is less suitable for:

- ▶ Highly non-Gaussian latent structures
- ▶ Very high-dimensional hyperparameter spaces
- ▶ Models requiring full joint posterior samples

INLA and inlabru R packages

What is inlabru?

- ▶ An R package built on top of INLA
- ▶ Designed for spatial and spatio-temporal modelling using **Integrated Nested Laplace Approximation (INLA)**
- ▶ Provides an intuitive interface for:
 - ▶ Spatial point process models
 - ▶ Geostatistical models
- ▶ Install INLA: <https://www.r-inla.org/download-install>
- ▶ Examples and documentation: <https://inlabru-org.github.io/inlabru/>

Key features

- ▶ Formula-based model specification
- ▶ Flexible integration with `sf`, `sp`, and `raster`

References

- Diggle, Peter, and Emanuele Giorgi. 2019. *Model-Based Geostatistics*. CRC Press.
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- Lindgren, Finn, Håvard Rue, and Johan Lindström. 2011. "An Explicit Link Between Gaussian Fields and Gaussian Markov Random Fields: The Stochastic Partial Differential Equation Approach." *Journal of the Royal Statistical Society Series B: Statistical Methodology* 73 (4): 423–98.