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 Mathamatical 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)

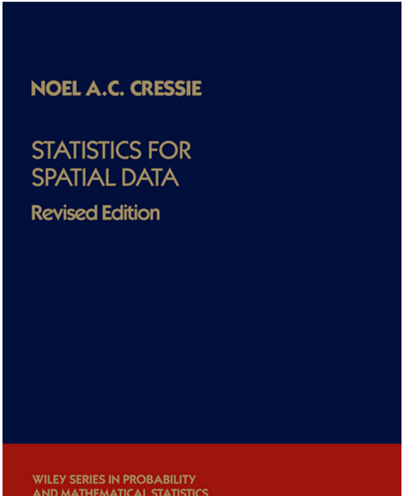
- Extension of linear models to handle non-normal response distributions.
- Three components:
  - Random component: Distribution from the exponential family (e.g., Binomial, Poisson).
  - Systematic component: Linear predictor $\eta = X\beta$.
  - Link function: Relates $E(Y)$ to η.
- Examples:
  - Logistic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

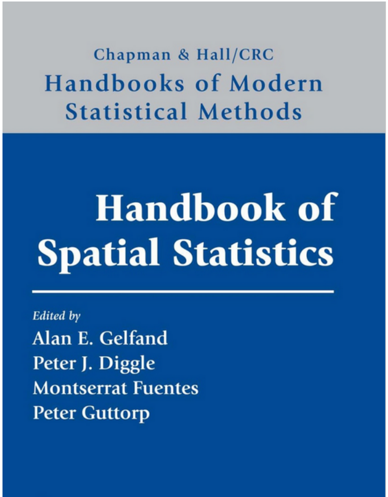
Why Spatial Statistics?

- **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

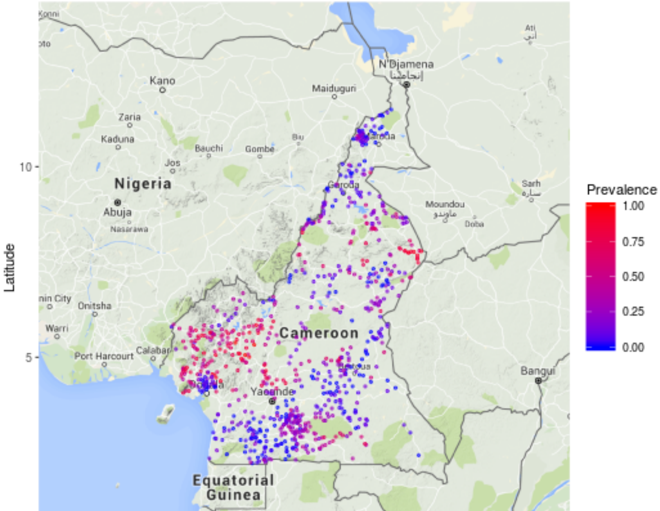
Cressie's book classifies spatial statistics according to **data format**:

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

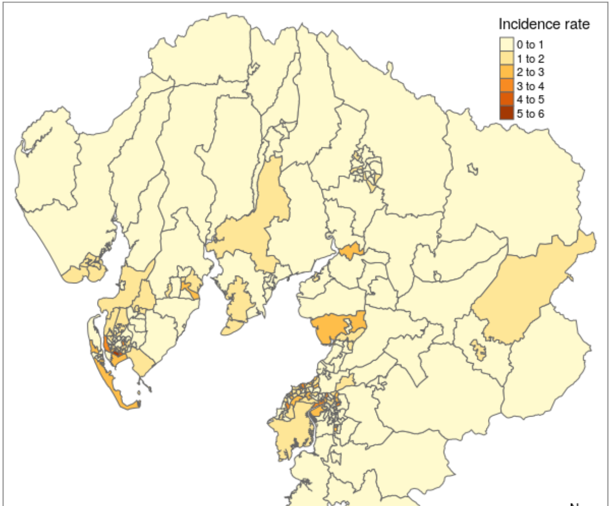
Gelfand's book classifies spatial statistics according to **spatial variation**:

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

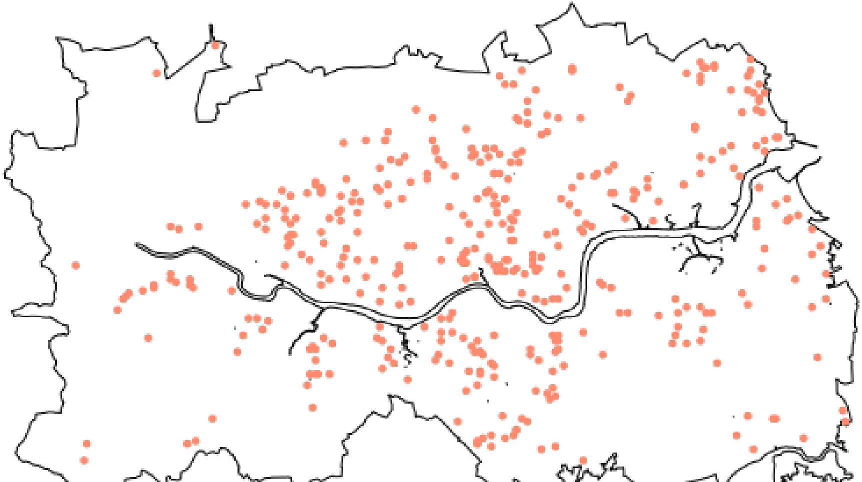
Geostatistical data: River blindness in Cameroon



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

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

where

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

Modelling $S(s)$ and Z_j

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

$$\Sigma_{ij} = \text{Cov}\left(S(s_i), S(s_j)\right) = \sigma^2 r(u)$$

- $u = \|s_i - s_j\|$ is the Euclidean distance between locations s_i and s_j
- **How do we choose parametric correlation function $r(\cdot)$?**

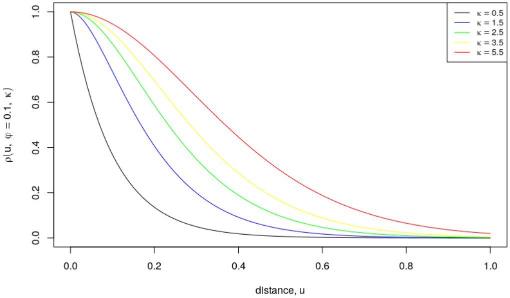
The Matérn correlation function

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

- $K_\nu(\cdot)$: modified Bessel function of order ν
- **Interpretation**
  - ν determines the smoothness: $\nu > r \Rightarrow S(s)$ is r times differentiable
  - ρ determines the scale/range of spatial correlation
- **Special cases**
  - $\nu = 0.5 \Rightarrow r(u) = \exp\{-u/\rho\}$
  - $\nu \to \infty \Rightarrow r(u) = \exp\{-(u/\rho)^2\}$
- Often sufficient to choose $\nu \in \{0.5, 1.5, 2.5\}$

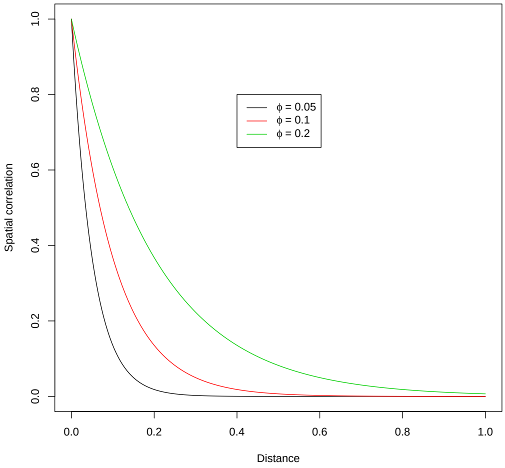
Matérn correlation function – ν

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



Exponential correlation function: $r(u; \nu = 0.5) = \exp\{-u/\rho\}$

The scale of the spatial correlation – ρ



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

- Regression residuals

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

  from a GLM
- Each $\hat{r}_i$ estimates

$$S(s_i) + Z_i$$

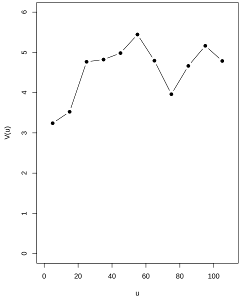
The variogram

- **Empirical variogram**

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

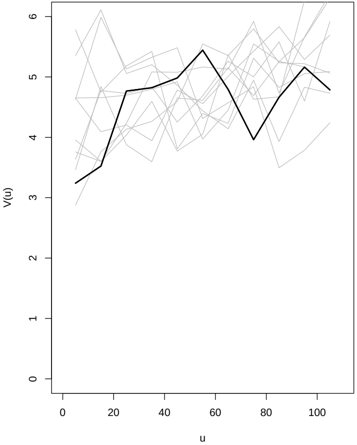
- where

$$N(u) = \{(i,j) : \|s_i - s_j\| = u\}$$



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**

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

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

- **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:

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

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:**

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

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**

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

  Prevalence survey data

- **Poisson**

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

  Disease counts, event data

Link functions

The linear predictor enters the likelihood via a link:

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

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)**:

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

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 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

Gaussian Markov Random Fields (GMRFs)

A **Gaussian Markov Random Field (GMRF)** is a Gaussian random vector with **conditional independence** structure.

Let

$$\mathbf{S} = (S_1, \dots, S_n)^\top \sim \mathcal{N}(0, Q^{-1})$$

where:

- Q is the **precision matrix**
- **Zeros in** Q encode conditional independence

Markov property (key idea)

For a GMRF:

$$Q_{ij} = 0 \quad \Longleftrightarrow \quad S_i \perp\!\!\!\perp S_j \mid \mathbf{S}_{-ij}$$

Interpretation:

- Each location depends **only on its neighbours**
- No long-range conditional dependence

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:

$$\pi(S_i \mid y), \qquad \pi(\theta_j \mid y)$$

INLA computes:

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

- 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 $s_1, \dots, s_n$:
  - 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

$$S(s) \sim \mathsf{GRF}(0, C(\cdot))$$

with covariance function:

$$\mathsf{Cov}\{S(s), S(s')\} = C(\|s - s'\|)$$

- 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:

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

where:

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

Matérn parameters vs SPDE parameters

We often describe a Matérn GRF using:

- **Range** ρ: distance where correlation becomes small
- **Marginal standard deviation** σ
- **Smoothness** ν

INLA/SPDE uses a different (equivalent) parameterisation:

- κ: controls the range
- τ: controls the marginal variance
- $\alpha = \nu + d/2$ (with spatial dimension $d = 2$)

From SPDE parameters to range and variance

Key relationships (common INLA convention):

- **Practical range**

$$\rho \approx \frac{\sqrt{8\nu}}{\kappa}$$

- **Marginal variance**

$$\mathrm{Var}\{S(s)\} = \sigma^2 \propto \frac{1}{\tau^2 \kappa^{2\nu}}$$

Interpretation:

- larger $\kappa \Rightarrow$ shorter range (rougher field)
- larger $\tau \Rightarrow$ smaller marginal variance

What INLA reports (hyperparameters)

In INLA output you will often see hyperparameters related to:

- **Range** ρ
- **Stdev** σ
- **Nugget / observation noise** τ_ϵ (depending on model)

Even if the underlying SPDE uses (κ, τ), INLA/inlabru often provides summaries in the more interpretable scale:

- range (km or m)
- marginal sd

PC priors in practice (what you set in code)

In `inla.spde2.pcmatern()` you specify:

```
prior.range = c(r0, p)    # P(range < r0) = p
prior.sigma = c(s0, p)    # P(sigma > s0) = p
```

Discretising the SPDE

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

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

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.

Diggle, Peter, Jonathan Tawn, and Rana Moyeed. 1998. "Model-Based Geostatistics." *Journal of the Royal Statistical Society: Series C* 47: 299–350.

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.