

# 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 Lancaster
- ▶ 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  $\eta$ .
- ▶ 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

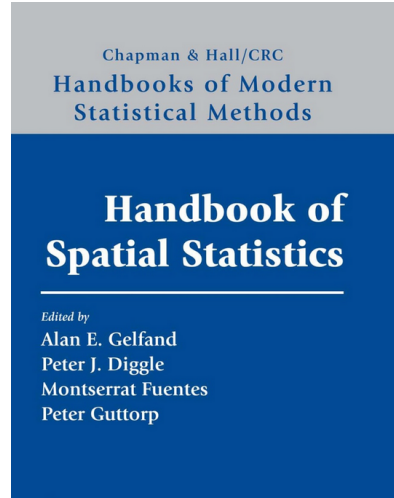
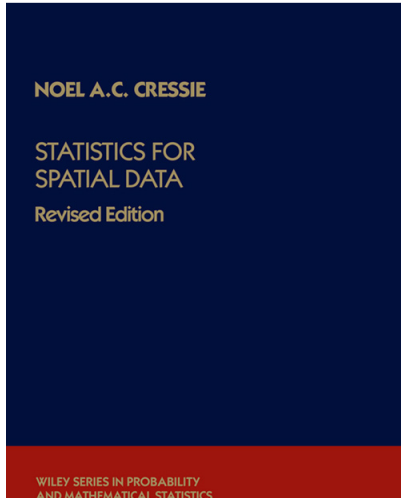
### ► **Goal:**

Account for spatial correlation to improve prediction and inference.

# Spatial Analysis



# Spatial Statistics



# Classification of spatial statistics

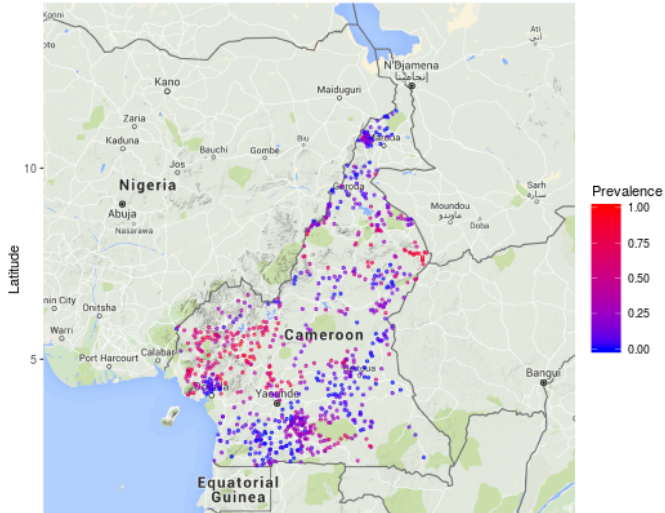
Cressie's book classifies spatial statistics according to **data format**:

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

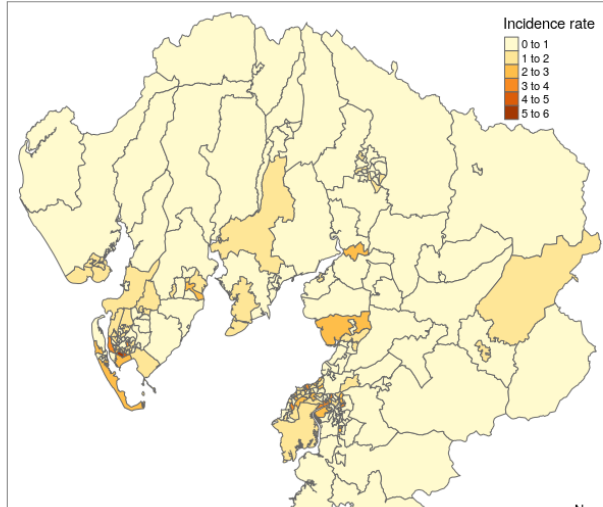
Gelfand's book classifies spatial statistics according to **spatial variation**:

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

- ▶  $\beta_0$ ,  $\beta_1$ , and  $\beta_2$  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  $\Sigma$  is

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

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

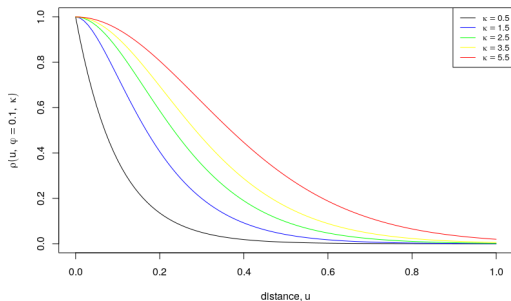
# The Matérn correlation function

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

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

## Matérn correlation function – $\nu$

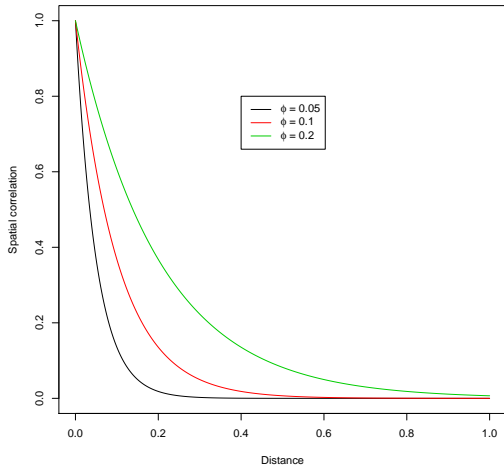
$$r(u; \rho, \nu) = \frac{1}{2^{\nu-1} \Gamma(\nu)} \left( \frac{u}{\rho} \right)^{\nu} K_{\nu} \left( \frac{u}{\rho} \right),$$



Exponential correlation functions  $\nu(\psi = 0.5)$

$\{\psi = 0.5\}$

## The scale of the spatial correlation – $\rho$



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

$$S(s_i) + Z_i$$

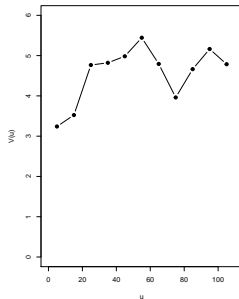
# The variogram

## ► Empirical variogram

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

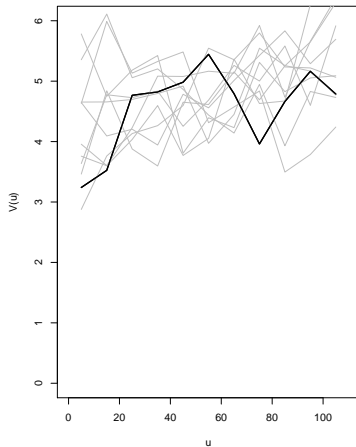
## ► where

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



## 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

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

- $D$ : 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  $\beta$  (e.g. using ordinary least squares)
2. Initialise  $\theta$  (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:**

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

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

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

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:

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

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)**:

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

where

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

# 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:

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

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:

- ▶  $\theta$  is low-dimensional  $\rightarrow$  numerical optimisation is feasible

## Stage 2: Latent field given $\theta$

- Conditional on  $\theta$ , 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  $s_1, \dots, s_n$ :
  - ▶ 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

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

with covariance function:

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

- ▶ 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:

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

where:

- ▶  $\Delta$  is the Laplacian operator
- ▶  $\mathcal{W}(s)$  is Gaussian white noise
- ▶ Parameters  $(\kappa, \alpha)$  control range and smoothness

## Matérn parameters vs SPDE parameters

We often describe a Matérn GRF using:

- ▶ **Range**  $\rho$ : distance where correlation becomes small
- ▶ **Marginal standard deviation**  $\sigma$
- ▶ **Smoothness**  $\nu$

INLA/SPDE uses a different (equivalent) parameterisation:

- ▶  $\kappa$ : controls the range
- ▶  $\tau$ : 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**

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

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**  $\rho$
- ▶ **Stdev**  $\sigma$
- ▶ **Nugget / observation noise**  $\tau_\epsilon$  (depending on model)

Even if the underlying SPDE uses  $(\kappa, \tau)$ , 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)    #  $P(\text{range} < r0) = p$ 
prior.sigma = c(s0, p)    #  $P(\text{sigma} > s0) = p$ 
```

## 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`

# Navigation

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# 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.