

Gaussian Markov Random Field / SPDE method

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Key concepts in Spatial statistics:

- The spatial domain is D , or if we can spatio-temporal observations $D \times T, T \subset \mathcal{R}$
- We call 'spatial random field' $u(\mathbf{s}), \mathbf{s} \in D$, or $(\mathbf{s}, t) \in D \times T$ for spatiotemporal observations.
- The observations y_i can be modelling setting: $y_i = u(\mathbf{s}_i) + \epsilon_i$. Here $u(\cdot)$ is a structured random effect.

Introduction

Gaussian distribution for $\mathbf{u} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$:

- Density function:

$$d(\mathbf{u}) = \frac{1}{(2\pi)^{N/2} |\boldsymbol{\Sigma}|^{1/2}} \exp \left(-\frac{1}{2} (\mathbf{u} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{u} - \boldsymbol{\mu}) \right) \quad (1)$$

- Covariance:

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \boldsymbol{\mu}_{u_1} \\ \boldsymbol{\mu}_{u_2} \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{u_1, u_1} & \boldsymbol{\Sigma}_{u_1, u_2} \\ \boldsymbol{\Sigma}_{u_2, u_1} & \boldsymbol{\Sigma}_{u_2, u_2} \end{bmatrix} \right) \quad (2)$$

- Conditional distribution for each random effect u :

$$u_1 \mid u_2 \sim \mathcal{N} \left(\boldsymbol{\mu}_{u_1} + \boldsymbol{\Sigma}_{u_1, u_2} \boldsymbol{\Sigma}_{u_2, u_2}^{-1} (u_2 - \boldsymbol{\mu}_{u_2}), \boldsymbol{\Sigma}_{u_1, u_1} - \boldsymbol{\Sigma}_{u_1, u_2} \boldsymbol{\Sigma}_{u_2, u_2}^{-1} \boldsymbol{\Sigma}_{u_2, u_1} \right) \quad (3)$$

What is the problem? $\boldsymbol{\Sigma}$ is a large dense matrix.

The precision matrix

The precision matrix

The precision matrix is the inverse of the covariance matrix: Σ^{-1} , so:

$$\mathbf{Q} = \Sigma^{-1} \quad (4)$$

- Density function:

$$d(\mathbf{u}) = \frac{|\mathbf{Q}|^{1/2}}{(2\pi)^{N/2}} \exp\left(-\frac{1}{2}(\mathbf{u} - \boldsymbol{\mu})^T \mathbf{Q}(\mathbf{u} - \boldsymbol{\mu})\right) \quad (5)$$

- Precision Matrix:

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_{u_1} \\ \mu_{u_2} \end{bmatrix}, \begin{bmatrix} \mathbf{Q}_{u_1, u_1} & \mathbf{Q}_{u_1, u_2} \\ \mathbf{Q}_{u_2, u_1} & \mathbf{Q}_{u_2, u_2} \end{bmatrix}^{-1}\right) \quad (6)$$

- Conditional distribution for each random effect u

$$u_1 | u_2 \sim \mathcal{N}\left(\mu_{u_1} + \mathbf{Q}_{u_1, u_1}^{-1} \mathbf{Q}_{u_1, u_2} (u_2 - \mu_{u_2}), \mathbf{Q}_{u_1, u_1}^{-1}\right) \quad (7)$$

The precision matrix

How works \mathbf{Q} ?

- Let W be a matrix with elements $W_{ij} = -Q_{ij}/Q_{ii}$ for $j \neq i$ and $W_{ii} = 0 \ \forall \ i$
- The conditional distribution for $u_i | \mathbf{u}$ is:

$$(u_i | u_j, j \neq i) \sim \mathcal{N} \left(\mu_i + \sum_{j \neq i} W_{ij} (u_j - \mu_j), 1/Q_{i,i} \right) \quad (8)$$

- i (row number) of W are the weights that influencing u in the conditional distribution for u_i and the conditional variance is $1/Q_{i,i}$

Gaussian Markov Random Field GMRF

A gaussian random field (GRF) is a gaussian markov random field (GMRF) if:

- $Q_{ij} = 0$
- If $Q_{ij} \neq 0$ and $i \neq j$, u_j is called neighbour of u_i
- The set of neighbours to a u_i is denoted by:

$$\mathbb{N}_i = \{j : Q_{ij} \neq 0, j \neq i\}$$

- The relation in the neighbourhood is symmetric: $j \in \mathbb{N}_i \Leftrightarrow i \in \mathbb{N}_j$ since \mathbf{Q} is symmetric too.
- The full conditional distribution for u_i depend only on the rest of random effect in the neighbourhood \mathbb{N}_i , $u_j : j \in \mathbb{N}_i$. This is the Markov property for a spatial random field

Generally in geostatistical situations, the prior and the posterior field have sparse precisions. What means that?

- If \mathbf{u} is a Markov field the precision matrix \mathbf{Q} is sparse
- If we applying a Cholesky factorization $\mathbf{Q} = \mathbf{R}^T \mathbf{R}$ it will be sparse if \mathbf{Q} is sparse.

A GMRF it would be computationally feasible if we replace operations what use Σ with operations usgin \mathbf{Q} or \mathbf{R}

The idea is use the GRF instead of full covarian useful, sparse and positive definite \mathbf{Q} -matrices

Exist general methods for estimate precision values for a given neighbourhood structures, but are inefficient for large neighbourhood. Another method is the proposal by Rue and Tjelmeland (2002) but also is computationally demanding numerical optimisation.

Stochastic partial differential equations (SPDE)

Matérn family (covariance)

We come back to definition of gaussian random field but now formally:

Let s a location in a particular area D and $u(s)$ is the random effect (spatial) at that location. $\mathbf{u}(s)$ is a stochastic process with $\mathbf{s} \in \mathbf{D}$ and $\mathbf{D} \subset \mathbb{R}^d$ is the spatial domain where are measured the observations. $u(s_i)$ is a realization of $u(s)$ where $i = 1, \dots, n$ locations. We assume that $u(s)$ has a multivariate Gaussian distribution (GRF), continuous over the space indexed by \mathbf{s} and defined by the mean and the covariance ([Cressie, 1993])

Matérn family (covariance)

Continuous domain spatial

- Matérn covariance family on $\mathbf{s} \in \mathbb{R}^d$:

$$\begin{aligned} r_M(\mathbf{s}_1, \mathbf{s}_2) &= C(u(\mathbf{s}_1), u(\mathbf{s}_2)) \\ &= \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} (\kappa \|\mathbf{s}_2 - \mathbf{s}_1\|)^\nu K_\nu(\kappa \|\mathbf{s}_2 - \mathbf{s}_1\|) \end{aligned}$$

with scale $\kappa > 0$, shape/smoothness $\nu > 0$ and K_ν a modified Bessel function.

Fields with Matérn covariances are solutions of the SPDE method (Whittle, 1954,1963) based on the Laplacian $\Delta = \nabla^T \nabla$:

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

where $\mathcal{W}(\mathbf{s})$ is the spatial white noise, $\alpha = \nu + d/2$ and

$$\sigma^2 = \frac{\Gamma(\nu)}{\Gamma(\alpha)(4\pi)^{d/2}\kappa^{2\nu}\tau^2}$$

Hilbert space approximation

A finite Hilbert space uses a set of N basis functions $\{\psi_k\}$ and weights $\{w_k\}$ for that:

$$\mathbf{u}(\mathbf{s}) = \sum_{k=1}^n \psi_k(\mathbf{s}) w_k$$

where $\psi(\cdot)$ are deterministic basis functions and $\{u_1, \dots, u_n\}$ is a vector of weights that is chosen so that the distribution of the functions $\mathbf{u}(\mathbf{s})$ approximates the distribution of solutions to the SPDE on the domain

Construction of the $\mathbf{Q} = \Sigma^{-1}$

To obtain a Markov structure we use piecewise polynomial basis functions with compact support (essentially it's a Finite Element method)

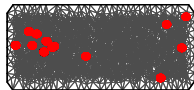
For a domain two dimensional we use piecewise linear basis functions defined by a triangulation of the domain of interest

$$\mathbf{Q} = \tau^2 (\kappa^4 \mathbf{C} + 2\kappa^2 \mathbf{G}_1 + \mathbf{G}_2)$$

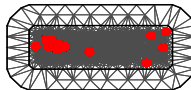
where by default $\alpha = 2$ so that the elements of \mathbf{Q} have explicit expressions as functions of κ and τ . Assigning the Gaussian distribution $\mathbf{u} \sim \mathcal{N}(\mathbf{0}, \mathbf{Q})$ now this is approximate solutions to the SPDE (in a stochastically weak sense) [Lindgren et al., 2015]

More references: [Rue and Held, 2005], [Lindgren et al., 2011], [Blangiardo and Cameletti, 2015],

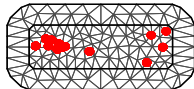
Constrained refined Delaunay triangulation



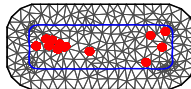
Constrained refined Delaunay triangulation



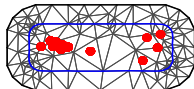
Constrained refined Delaunay triangulation



Constrained refined Delaunay triangulation



Constrained refined Delaunay triangulation



Constrained refined Delaunay triangulation

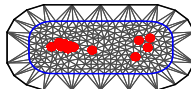


Figure: Different SPDE/GMRf triangulations

Hierarchical Models

Hierarchical Bayesian Model in INLA ([Rue et al., 2009], [Bakka et al., 2018])

- We need three principal components:
 - Parameters $\Rightarrow \boldsymbol{\theta}$
 - Spatial field ("latent field" or "gaussian field" or "gaussian random field") $\Rightarrow \boldsymbol{u}$
 - Data $\Rightarrow \boldsymbol{y}$
- Priors for the parameters: $\pi(\boldsymbol{\theta})$
- The spatial field is generally a Gaussian process (GP) or Gaussian Markov Random Field (GMRF) and the density function is $\pi(\boldsymbol{u} \mid \boldsymbol{\theta})$ (conditionally on the parameters $\boldsymbol{\theta}$)
- The data are independent for a set of locations with density function: $\pi(\boldsymbol{y} \mid \boldsymbol{u}, \boldsymbol{\theta})$
- We want estimate $\pi(\boldsymbol{\theta} \mid \boldsymbol{y})$ and $\pi(\boldsymbol{u} \mid \boldsymbol{y})$ (without MCMC method)

Hierarchical Models

Hierarchical model (Bayesian)

$$\boldsymbol{\theta} \sim \boldsymbol{\theta} \quad \text{Hyperparameters} \quad (9)$$





$$\mathbf{u} \mid \boldsymbol{\theta} \sim \mathcal{N}(\mathbf{0}, \mathbf{Q}(\boldsymbol{\theta})^{-1}) \quad \text{Latent gaussian field} \quad (10)$$

$$\eta_i = \sum_j c_{ij} x_j$$

$$y_i \mid \mathbf{u}, \boldsymbol{\theta} \sim \prod_i \pi(y_i \mid \eta_i, \boldsymbol{\theta}) \quad \text{Observations} \quad (11)$$

where $\mathbf{Q}(\boldsymbol{\theta})$ is the precision matrix, \mathbf{u} is the latent gaussian field and $\eta(\mathbf{u}) = \mathbf{A} \mathbf{u}$, where the matrix \mathbf{A} maps the latent variable vector \mathbf{u} to the predictors $\eta_i = \eta_i(\mathbf{u})$ associated to the observations y_i

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