An overview of the SPDE approach

Elias Teixeira Krainski

King Abdullah University of Science and Technology (KAUST)

May 2024

Outline

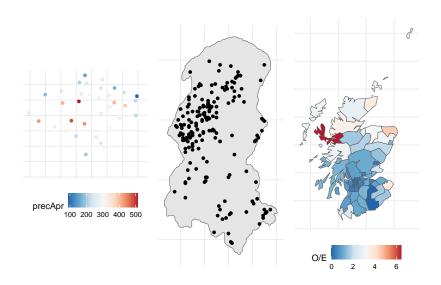
Introduction

The SPDE approach

The log Gaussian Cox process model

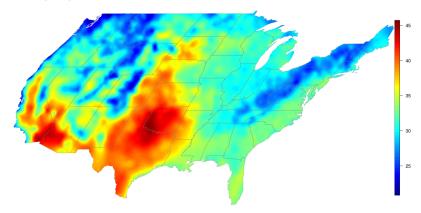


Spatial statistics data



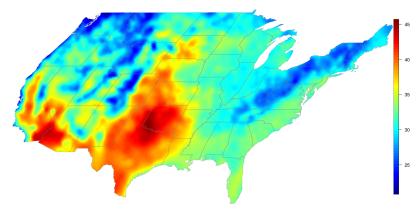
A process over space

▶ (est.) Maximum temperature in US mainland, in 2022-07-20



A process over space

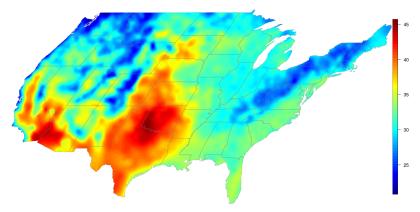
▶ (est.) Maximum temperature in US mainland, in 2022-07-20



- ▶ The spatial domain, S, is continuous.
 - ightharpoonup E.g. $S \in \mathbb{R}^2$
 - ▶ E.g. $S \in \mathbb{S}^2$ (sphere)

A process over space

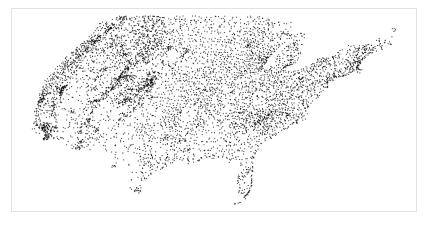
▶ (est.) Maximum temperature in US mainland, in 2022-07-20



- ▶ The spatial domain, S, is continuous.
 - ▶ E.g. $S \in \mathbb{R}^2$
 - ▶ E.g. $S \in \mathbb{S}^2$ (sphere)
- ▶ $u(\mathbf{s})$ is a stochastic process, $\mathbf{s} \in S$

Real world data: at a finite number of locations

At a finite set of n locations



$$u(\mathbf{s}_1),\ldots,u(\mathbf{s}_n)$$

Stochastic process u(I)

Covariance

$$V(\mathbf{I}, \mathbf{I}') = \operatorname{Cov}(u(\mathbf{I}), u(\mathbf{I}'))$$

Spectral density

$$u(\mathbf{I}) = \int_{-\infty}^{\infty} e^{i\mathbf{w}\mathbf{I}} du(\mathbf{w})$$

Kernel convolution

$$u(\mathbf{I}) = \int k(\mathbf{I} - \mathbf{u}) \mathcal{W}(\mathbf{I}) d\mathbf{u}$$

► Stochastic Partial Differential Equation - SPDE

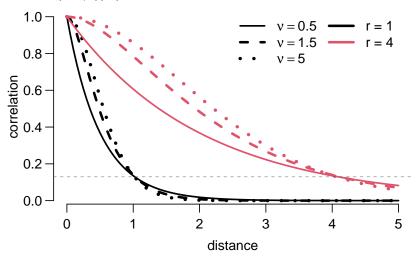
$$\mathcal{L}_1 u(\mathbf{I}) = \mathcal{L}_2 \mathcal{W}(\mathbf{I})$$

► Conditional distributions (DISCRETE DOMAIN !!!)

$$u_{\mathsf{I}}|u_{\mathsf{neighbourhood}} \sim \mathbb{P}(.)$$

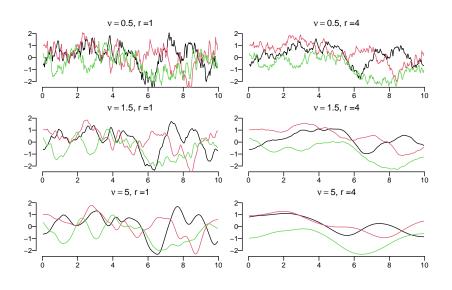
Whittle-Matérn covariance, Matérn (1960)

$$\Sigma_{ij} = \frac{\sigma^2(\kappa \|\mathbf{s}_i - \mathbf{s}_j\|)^{\nu} K_{\nu}(\kappa \|\mathbf{s}_i - \mathbf{s}_j\|)}{\Gamma(\nu + d/2)(4\pi)^{d/2} \kappa^{2\nu} 2^{\nu - 1}}. \text{ If } d = 2 \text{ and } \nu = 1: \text{ Whittle (1954)}$$

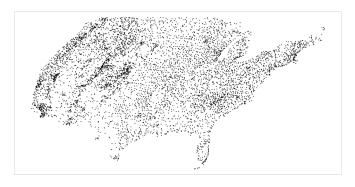


practical range = $r = \sqrt{8\nu/\kappa}$, corr(r) ≈ 0.13

Simulations, 1D, $\sigma^2 = 1$

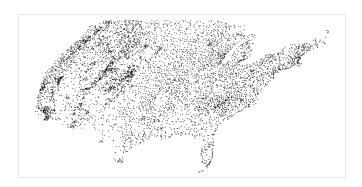


Consider a set of locations



- Consider the distribution at these locations
 - $\pi(u(s_1),...,u(s_n)|\theta) = \pi(u_1,...,u_n|\theta) = \pi(\mathbf{u}|\theta)$

Consider a set of locations

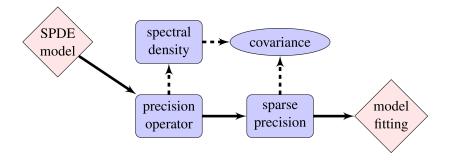


- ► Consider the distribution at these locations
 - $\pi(u(s_1),...,u(s_n)|\theta) = \pi(u_1,...,u_n|\theta) = \pi(\mathbf{u}|\theta)$
- If it is Gaussian with some covariance $\Sigma(\theta)$

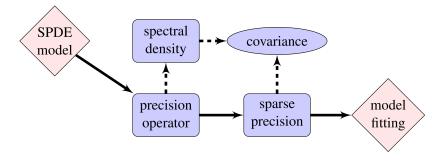
$$\pi(\mathbf{u}|\theta) = (2\pi)^{-n/2} |\Sigma(\theta)|^{-1/2} \exp\left(-\frac{1}{2}\mathbf{u}^T \Sigma(\theta)^{-1}\mathbf{u}\right)$$

The SPDE approach

SPDE framework



SPDE framework



- It avoids specifying covariance!
 - D. Simpson, Lindgren, and Rue (2011)
 - D. Simpson, Lindgren, and Rue (2012)

The Matérn's SPDE

- Whittle (1954), Whittle (1963):
 - ► Fields with Matérn covariance are solutions to the following Stochastic Partial Differential Equation (SPDE)

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

- $ightharpoonup \kappa > 0$: scale parameter
- $\sim \alpha = \nu + d/2$: smoothness
- $ightharpoonup \Delta$ is the Laplacian

$$\Delta = \sum_{i=1}^{d} \frac{\partial^2}{\partial s_i^2}$$

- Discretization
 - sparse precision matrix:
 - $\mathbf{Q}_{\alpha}(\tau,\kappa)$, for $\alpha \in \{1,2,...\}$.

- Discretization
 - sparse precision matrix:
 - $ightharpoonup \mathbf{Q}_{\alpha}(\tau,\kappa)$, for $\alpha \in \{1,2,...\}$.
- $\sim \alpha$

- Discretization
 - sparse precision matrix:
 - $ightharpoonup \mathbf{Q}_{\alpha}(\tau,\kappa)$, for $\alpha \in \{1,2,...\}$.
- $\sim \alpha$

 - $\qquad \qquad \alpha = 2, 3, 4, ...: \ \tau \mathbf{K}_1(\kappa) \mathbf{C}^{-1} \mathbf{K}_{\alpha 2}(\kappa) \mathbf{C}^{-1} \mathbf{K}_1(\kappa)$

- Discretization
 - sparse precision matrix:
 - $\mathbf{Q}_{\alpha}(\tau,\kappa)$, for $\alpha \in \{1,2,...\}$.
- a
- $\sim \alpha = 1$: $\tau \mathbf{K}_1(\kappa) = \tau(\kappa^2 \mathbf{C} + \mathbf{G})$
- $\alpha = 2, 3, 4, ...$: $\tau \mathbf{K}_1(\kappa) \mathbf{C}^{-1} \mathbf{K}_{\alpha 2}(\kappa) \mathbf{C}^{-1} \mathbf{K}_1(\kappa)$
- ▶ Equivalent models (discretized): Whittle (1954), Besag (1974), Besag (1981), Besag and Kooperberg (1995) and Besag and Mondal (2005).

$\mathbf{Q}_{\alpha}(au,\kappa)$: grid and piecewise linear basis

•
$$\alpha = 1$$
: $\tau \mathbf{K}_1(\kappa) = \tau(\kappa^2 \mathbf{C} + \mathbf{G})$
• $d=1, u_1, u_2, ..., u_n$, two neighbours

$$au^2 egin{bmatrix} 1+\kappa^2 & -1 & & & & \ -1 & 2+\kappa^2 & -1 & & & \ & & \ddots & & & \ & & -1 & 2+\kappa^2 & -1 \ & & & & -1 & 1+\kappa^2 \end{bmatrix}$$

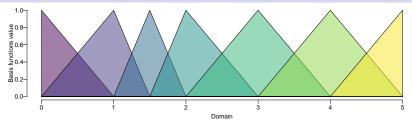
$\mathbf{Q}_{\alpha}(\tau,\kappa)$: grid and piecewise linear basis

 $\alpha = 1: \ \tau \mathbf{K}_1(\kappa) = \tau(\kappa^2 \mathbf{C} + \mathbf{G})$ $\mathbf{d} = 1, \ u_1, u_2, ..., u_n, \text{ two neighbours}$

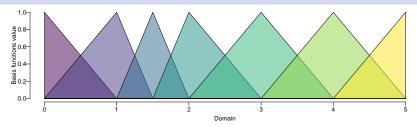
$$\tau^2 \begin{bmatrix} 1+\kappa^2 & -1 & & & \\ -1 & 2+\kappa^2 & -1 & & & \\ & & \ddots & & \\ & & -1 & 2+\kappa^2 & -1 \\ & & & -1 & 1+\kappa^2 \end{bmatrix}$$

ightharpoonup d=2, $\mathbf{C}=\mathbf{I}$, $\mathbf{G}=\mathsf{Laplacian}$ (4 neighbours)

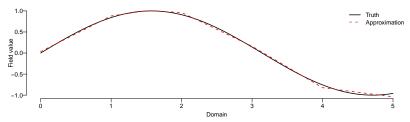
Piecewise linear basis, Finite Element Method (FEM): 1d



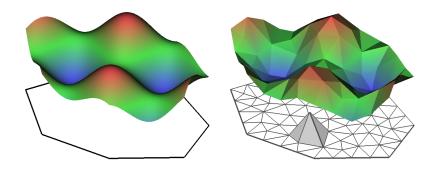
Piecewise linear basis, Finite Element Method (FEM): 1d



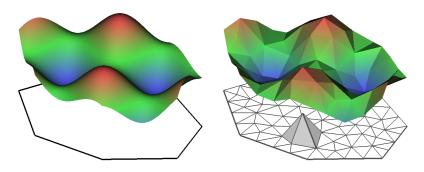
- $\triangleright u(\mathbf{s}) \approx \sum_{k=1}^{m} \psi_k(\mathbf{s}) u_k = \mathbf{A}(\mathbf{s}, \mathbf{s}_0) u(\mathbf{s}_0),$
 - ψ_k : basis functions evaluated at data locations **s**
 - $ightharpoonup u_k$: the process at the discretization points \mathbf{s}_0



Piecewise linear basis, Finite Element Method: 2d

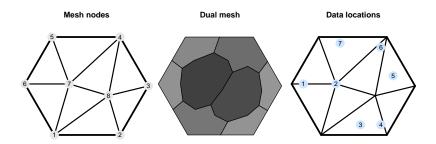


Piecewise linear basis, Finite Element Method: 2d

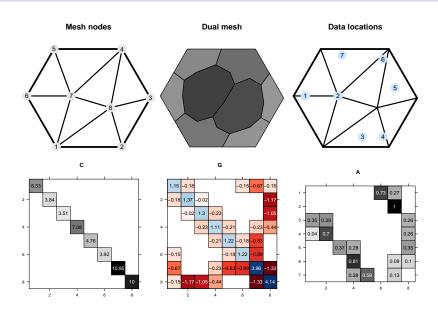


- $\triangleright u(\mathbf{s}) \approx \sum_{k=1}^{m} \psi_k(\mathbf{s}) u_k = \mathbf{A}(\mathbf{s}, \mathbf{s}_0) u(\mathbf{s}_0),$
 - ψ_k : basis functions evaluated at data locations **s**
 - \triangleright u_k : the process at the discretization points \mathbf{s}_0

Piecewise linear basis, FEM matrices



Piecewise linear basis, FEM matrices



The log Gaussian Cox process model

- ightharpoonup Given a set of locations on a domain ${\cal D}$
- One interest is to estimate the intensity function
 - $\lambda(\mathbf{I}), \ \lambda(\mathbf{I}) \geq 0, \ \mathbf{I} \in \mathcal{D}.$

- lacktriangle Given a set of locations on a domain ${\cal D}$
- ▶ One interest is to estimate the intensity function
 - $\lambda(\mathbf{I}), \lambda(\mathbf{I}) \geq 0, \mathbf{I} \in \mathcal{D}.$
 - ▶ number of events in $\mathcal{R} \subset \mathcal{D}$: $y_{\mathcal{R}} \sim \mathsf{Poisson}(n_{\mathcal{R}})$

- lacktriangle Given a set of locations on a domain ${\cal D}$
- ▶ One interest is to estimate the intensity function
 - $\lambda(\mathbf{I}), \lambda(\mathbf{I}) \geq 0, \mathbf{I} \in \mathcal{D}.$
 - ▶ number of events in $\mathcal{R} \subset \mathcal{D}$: $y_{\mathcal{R}} \sim \mathsf{Poisson}(n_{\mathcal{R}})$
- \blacktriangleright Cox process (CP): $\lambda(.)$ is assumed to be a random function
 - $\triangleright \lambda(\mathbf{I})$ is a random variable

- ightharpoonup Given a set of locations on a domain $\mathcal D$
- ▶ One interest is to estimate the intensity function
 - $\lambda(\mathbf{I}), \lambda(\mathbf{I}) \geq 0, \mathbf{I} \in \mathcal{D}.$
 - ▶ number of events in $\mathcal{R} \subset \mathcal{D}$: $y_{\mathcal{R}} \sim \mathsf{Poisson}(n_{\mathcal{R}})$
- \triangleright Cox process (CP): $\lambda(.)$ is assumed to be a random function
 - $\triangleright \lambda(\mathbf{I})$ is a random variable
- ► Log Gaussian Cox Process (LGCP)
 - $\log(\lambda(.)) = u(.)$ is a Gaussian process GP, Møller, Syversveen, and Waagepetersen (1998) .
 - \triangleright $u(.|\theta)$, θ are GP parameters

LGCP inference

► The log-likelihood function:

$$I(\Lambda, \theta | \mathcal{Y}) = c - \int_{\mathcal{D}} \lambda(I) \partial I + \sum_{i=1}^{n} \log(\lambda(\mathbf{I}_{i}))$$

LGCP inference

► The log-likelihood function:

$$I(\Lambda, \theta | \mathcal{Y}) = c - \int_{\mathcal{D}} \lambda(I) \partial I + \sum_{i=1}^{n} \log(\lambda(\mathbf{I}_{i}))$$

The log-likelihood function direct approximation

$$I(\Lambda, \theta | \mathcal{Y}) \approx c - \sum_{j=1}^{m} w_j \lambda(I) + \sum_{i=1}^{n} \log(\lambda(\mathbf{I}_i))$$

= $c - \sum_{j=1}^{m} w_j \exp(\eta(I)) + \sum_{i=1}^{n} \eta(\mathbf{I}_i)$

approximated with m integration points.

- ➤ SPDE approach for easier computations, D. P. Simpson et al. (2016)
- more complex Point Process models using INLA in inlabru

References

- Besag, J. 1974. "Spatial Interaction and the Statistical Analysis of Lattice Systems." JRSS-B 36 (2): 192–236.
- ——. 1981. "On a System of Two-Dimensional Recurrence Equations." JRSS-B 43 (3): 302–9.
- Besag, J., and C. Kooperberg. 1995. "On Conditional and Intrinsic Autoregression." Biometrika 82 (4): 733-46.
 Besag, J., and D. Mondal. 2005. "First-Order Intrinsic Autoregressions and the de Wijs Process." Biometrika 92 (4): 909-20.
- Lindgren, F., H. Rue, and J. Lindström. 2011. "An Explicit Link Between Gaussian Fields and Gaussian Markov Random Fields: The Stochastic Partial Differential Equation Approach (with Discussion)." JRSS-B 73 (4): 423–98.
- Matérn, B. 1960. "Spatial Variation-Stochastic Models and Their Application to Some Problems in Forest Surveys and Other Sampling Investigations. Meddelanden Fran Statens Skogsforskningsintitut, Almaenna Foerlaget, Stockholm. (1986), 49 (5)." Springer, Berlin.
- Møller, J., A. R. Syversveen, and R. P. Waagepetersen. 1998. "Log Gaussian Cox Processes." SJS 25: 451–82.
 Simpson, D. P., J. B. Illian, F. Lindren, S. H Sørbye, and H. Rue. 2016. "Going Off Grid: Computationally Efficient Inference for Log-Gaussian Cox Processes." Biometrika 103 (1): 49–70.
- Simpson, D., F. Lindgren, and H. Rue. 2011. "In Order to Make Spatial Statistics Computationally Feasible, We Need to Forget about the Covariance Function." Environmetrics, no. 23: 65–74. https://doi.org/ https://doi.org/10.1002/env.1137.
- 2012. "Think Continuous: Markovian Gaussian Models in Spatial Statistics." Spatial Statistics 1: 16–29. https://doi.org/http://dx.doi.org/10.1016/j.spasta.2012.02.003.
- Whittle, P. 1954. "On Stationary Processes in the Plane." Biometrika 41 (3/4): 434-49.
- 1963. "Stochastic-Processes in Several Dimensions." Bulletin of the International Statistical Institute 40 (2): 974–94.