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Geostatistical Modelling Using Non-Gaussian Matérn Fields

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Motivation

- Underlying latent field may not be Gaussian
- Typical approach is to transform a Gaussian field
- Transformations do not allow much flexibility
- Goal to provide framework for modelling non-Gaussian fields

Gaussian Matérn fields

- Matérn covariance function:

$$C(\mathbf{h}) = \frac{2^{1-\nu}\phi^2}{(4\pi)^{\frac{d}{2}}\Gamma(\nu + \frac{d}{2})\kappa^{2\nu}}(\kappa\|\mathbf{h}\|)^{\nu}K_{\nu}(\kappa\|\mathbf{h}\|)$$

- Here $\|\mathbf{h}\| = \|\mathbf{s} - \mathbf{s}'\|$ is a Euclidean distance, d is the dimension of the domain, ν is a shape parameter, κ is a scale parameter, ϕ^2 is a variance parameter, and K is a modified Bessel function of the second kind.
- Stationary and isotropic
- Flexible and widely used

Convolution approach for Gaussian Matérn fields

- An alternative way to express a Gaussian field on $\mathbb{R}^d$ is as a process convolution

$$X(\mathbf{s}) = \int_{\mathbb{R}^d} k(\mathbf{s}, \mathbf{u}) \mathcal{B}(\mathrm{d}\mathbf{u}),$$

- where k is a deterministic kernel function and $\mathcal{B}$ is a Brownian sheet (Higdon, 2002).
- The covariance function for X is $C(\mathbf{h}) = \int k(\mathbf{u} - \mathbf{h}) k(\mathbf{u}) \mathrm{d}\mathbf{u}$.
- The covariance function C, the spectrum S, and the kernel k are related through

$$(2\pi)^d |\mathcal{F}(k)|^2 = \mathcal{F}(C) = S,$$

- where $\mathcal{F}(\cdot)$ denotes the Fourier transform
- The symmetric non-negative kernel for the Matérn field is a Matérn covariance function with parameters $\nu_k = \nu/2 - d/4$, $\phi_k = \sqrt{\phi}$, and $\kappa_k = \kappa$

SPDE approach for Gaussian fields

- A Gaussian Matérn field $X(\mathbf{s})$ is the solution to the following stochastic partial differential equation (SPDE):

$$\left(\kappa^2 - \Delta\right)^{\frac{\alpha}{2}} X(\mathbf{s}) = \phi \mathcal{W}(\mathbf{s})$$

- where $\mathcal{W}(\mathbf{s})$ is a spatial white noise process with unit variance, ϕ is a variance parameter, $\alpha = \nu + d/2$, and

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

is the Laplacian operator.

SPDE approach for Gaussian fields

- Define the inner product $\langle f, g \rangle = \int f(\mathbf{u}) g(\mathbf{u}) \mathrm{d}\mathbf{u}$
- Then the stochastic weak solution of the SPDE is found by requiring

$$\left\{ \langle \psi_j, (\kappa^2 - \Delta)^{\alpha/2} X \rangle, j = 1, \ldots, m \right\} \stackrel{d}{=} \{ \langle \psi_j, \mathcal{W} \rangle, j = 1, \ldots, m \}$$

for every finite set of test functions $\{\psi_j(\mathbf{u}), j = 1, \ldots, m\}$

SPDE approach for Gaussian fields

- Let Ω be the space of all possible solutions to the SPDE.
- Let $\{\varphi_i; i = 1, \dots, n\}$ be a set of basis functions for some subspace $\tilde{\Omega} \subset \Omega$.
- Then a finite element representation of the solution is constructed as

$$\tilde{X}(\mathbf{s}) = \sum_{i=1}^{n} w_i \varphi_i(\mathbf{s})$$

  where w_i are a set of stochastic weights.
- The basis functions and weights are associated with discrete locations i on some spatial grid.

SPDE approach for Gaussian fields

- The selected basis functions are piecewise linear functions.
- Let $s_1 < s_2 < \cdots < s_n$ be a set of discretization points.
- For a one-dimensional process, a set of basis functions is given by

$$\varphi_i(s) = \begin{cases} 0, & s < s_{i-1} \\ \frac{s-s_{i-1}}{h_{i-1}}, & s_{i-1} < s < s_i \\ 1 - \frac{s-s_i}{h_i}, & s_i < s < s_{i+1} \\ 0, & s_{i+1} < s \end{cases}$$

SPDE approach for Gaussian fields

- Define $n \times n$ matrices $\mathbf{C}$, $\mathbf{G}$, and $\mathbf{K}$ with entries
  - $C_{ij} = \langle \varphi_i, \varphi_j \rangle$
  - $G_{ij} = \langle \nabla\varphi_i, \nabla\varphi_j \rangle$
  - $(\mathbf{K}_{\kappa^2})_{ij} = \kappa^2 C_{ij} + G_{ij}$
- Let $\mathbf{Q}_{\alpha,\kappa^2}$ be the precision matrix for the Gaussian weights $\mathbf{w}$ for $\alpha = 1, 2, \ldots$.
- Then the finite dimensional representations of the solutions have precisions:
  - $\mathbf{Q}_{1,\kappa^2} = \mathbf{K}_{\kappa^2}$
  - $\mathbf{Q}_{2,\kappa^2} = \mathbf{K}_{\kappa^2}\mathbf{C}^{-1}\mathbf{K}_{\kappa^2}$
  - $\mathbf{Q}_{\alpha,\kappa^2} = \mathbf{K}_{\kappa^2}\mathbf{C}^{-1}\mathbf{Q}_{\alpha-2,\kappa^2}\mathbf{C}^{-1}\mathbf{K}_{\kappa^2}$, for $\alpha = 3, 4, \ldots$.

SPDE approach for Gaussian fields

- The dense matrix $\mathbf{C}^{-1}$ makes the precision matrices dense.
- If we approximate $\mathbf{C}$ with a diagonal matrix $\tilde{\mathbf{C}}$, where $\tilde{C}_{ii} = \langle \varphi_i, 1 \rangle$, then the weights $\mathbf{w}$ follow a GMRF (computational benefits).

Connection between SPDE and convolution

- The connection between the SPDE and the convolution is through Green's function of the differential operator in the SPDE

$$G_\alpha(\mathbf{s},\mathbf{t}) = \frac{2^{1-\frac{\alpha-d}{2}}}{(4\pi)^{\frac{d}{2}}\Gamma(\frac{\alpha}{2})\kappa^{\alpha-d}}(\kappa\|\mathbf{s}-\mathbf{t}\|)^{\frac{\alpha-d}{2}}K_{\frac{\alpha-d}{2}}(\kappa\|\mathbf{s}-\mathbf{t}\|)$$

- which serves as the kernel in the convolution

SPDE approach for non-Gaussian fields

- The SPDE for a non-Gaussian Matérn field is

$$\left(\kappa^2 - \Delta\right)^{\frac{\alpha}{2}} X(\mathbf{s}) = \dot{M}$$

  where $\dot{M}$ is non-Gaussian noise process.
- We restrict focus to the case where $M(\mathbf{s})$ is a type G Lévy process.
- Note that for the models we investigate, $\dot{M} = \phi(\mathbf{s})\mathcal{W}(\mathbf{s})$, where $\phi(\mathbf{s})$ follows a distribution.

Lévy processes

- A type G Lévy process has increments that can be written as a scale mixture of Gaussian variables $V^{1/2}Z$.
- V is a non-negative and infinitely divisible random variable, and Z is standard Gaussian.
- For infinitely divisible V, there exists a non-decreasing Lévy process $V(\mathbf{s})$ with increments distributed the same as V.
- The generalized hyperbolic distributions are a subtype of type G Lévy process.
- We restrict class to those closed under convolution so that V_i has known distribution for any increment area.
- This restricts to the normal inverse Gaussian (NIG) and gerneralized asymmetric Laplace (GAL) distributions.

SPDE approach for non-Gaussian fields

- We use the same type of finite element representation with basis functions and stochastic weights as Gaussian case.
- The distribution of the stochastic weights conditional on the variance process V is

$$\mathbf{w} \mid V \sim \mathrm{N}\left(\mathbf{K}_\alpha^{-1}\mathbf{m},\ \mathbf{K}_\alpha^{-1}\boldsymbol{\Sigma}\mathbf{K}_\alpha^{-1}\right)$$

- Here $\mathbf{K}_\alpha^{-1} = \mathbf{C}\left(\mathbf{C}^{-1}\mathbf{K}\right)^{\alpha/2}$
- The matrices **K** **C**, and **Σ** have elements
  - $C_{ij} = \langle \varphi_i, \varphi_j \rangle$
  - $K_{ij} = \kappa^2 \langle \varphi_i, \varphi_j \rangle + \langle \nabla\varphi_i, \nabla\varphi_j \rangle$
  - $\Sigma_{ij} = \int \varphi_i(\mathbf{s})\varphi_j(\mathbf{s}) V(\mathrm{d}\mathbf{s})$
- and $m_i = \int \varphi_i(\mathbf{s}) V(\mathrm{d}\mathbf{s})$

SPDE approach for non-Gaussian fields

- For GAL and NIG distributions $\mathbf{m}$ and $\mathbf{\Sigma}$ can be written as

$$m_i = \gamma\tau h_i + \mu V_i$$

$$\mathbf{\Sigma} = \mathrm{diag}(V_1, \dots, V_n)$$

- $h_i = \int \varphi_i(\mathbf{s})\mathrm{d}\mathbf{s}$ is the area associated with φ_i.
- $V_i = \int_{h_i} V(\mathrm{d}\mathbf{s})$
    - For GAL, $V(s)$ is gamma process: $V_i \sim \Gamma(h_i\tau, 1)$.
    - For NIG, $V(s)$ is inverse-Gaussian process: $V_i \sim \mathrm{IG}(2, (h_i\nu)^2)$.

Sampling from a GAL process

- Want to sample process at locations $\mathbf{s} = (\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_n)$. Let $\mathbf{\Phi}$ be a matrix with elements $\Phi_{ij} = \varphi_j(\mathbf{s}_i)$.

1. Generate two independent random vectors $\mathbf{\Gamma}$ and $\mathbf{Z}$, where $\Gamma_i \sim \Gamma(\tau h_i, 1)$ and $Z_i \sim \mathrm{N}(0, 1)$
2. Let $\mathbf{\Lambda} = \gamma\tau\mathbf{h} + \mu\mathbf{\Gamma} + \sigma\mathrm{diag}(\sqrt{\mathbf{\Gamma}})\mathbf{Z}$ and calculate $\mathbf{w} = \mathbf{C}^{-1}\mathbf{\Lambda}$.
3. $\mathbf{X} = \mathbf{\Phi}\mathbf{K}_\alpha^{-1}\mathbf{w}$ is now a sample of the random field at locations $\mathbf{s}$.

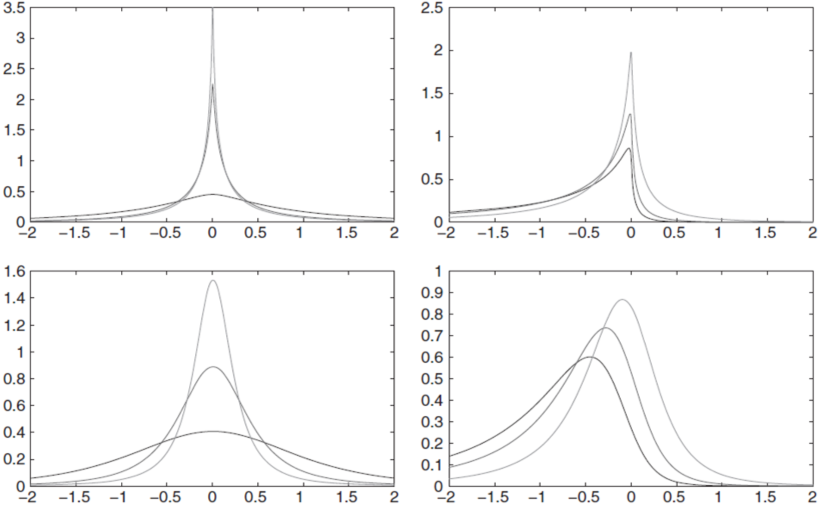

Fig. 1. Examples of marginal probability density functions (pdfs) for a stationary Matérn field $X(\mathbf{s})$ from (3), where $\dot{M}$ is either NIG (top row) or GAL noise (bottom row). The left panels show pdfs with different values of τ or ν^2, and the right panels shows pdfs with different values of μ. For all examples, $X(\mathbf{s})$ has a Matérn covariance function with shape parameter $\alpha = 2$.

from Bolin 2014

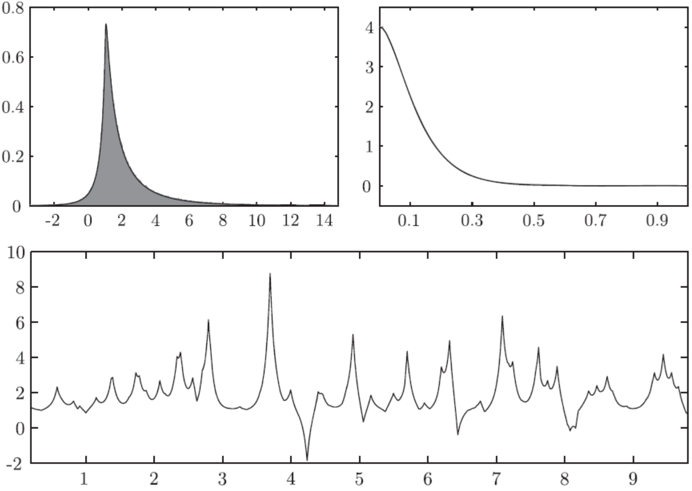

Fig. 2. The lower panel shows a simulation of the Laplace-driven stochastic partial differential equation (9) on $\mathbb{R}$ with parameters $\mu = \gamma = \sigma = 1$, $\tau = 2$, $\kappa = 15$ and $\alpha = 2$. The upper left panel shows a histogram of the samples from 1000 simulations together with the true density. The upper right panel shows the empirical covariance function for the samples (grey curve) together with the true Matérn covariance function (black curve). It is difficult to see the grey curve because the two curves are very similar.

from Bolin 2014

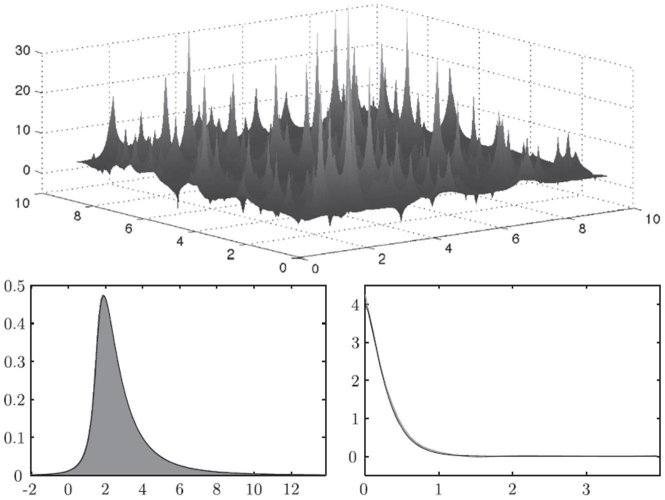

Fig. 4. The top panel shows a simulation of an asymmetric model (9) in $\mathbb{R}^2$ where the parameters are $\kappa = 5, \sigma = \mu = \gamma = 1, \tau = 2$ and $\alpha = 2$. The bottom left panel shows the histogram of samples from 1000 simulations together with the true density. The bottom right panel shows the empirical covariance function for the samples (grey curve) together with the true Matérn covariance function (black curve).

from Bolin 2014

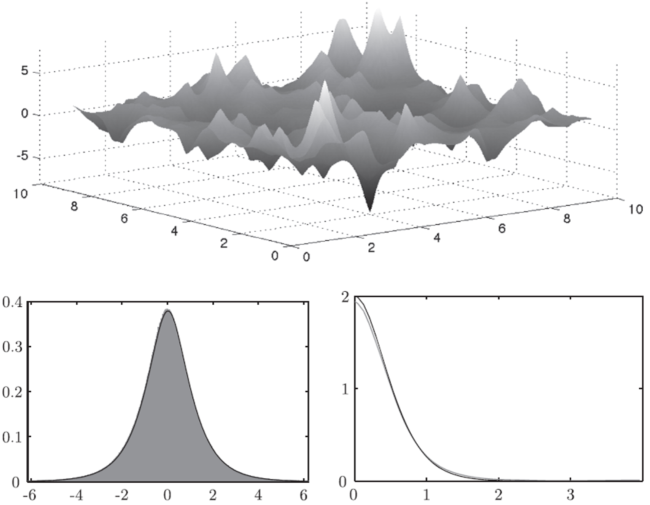

Fig. 5. The top panel shows a simulation of a symmetric model (9) in $\mathbb{R}^2$ with parameters $\kappa = 5, \sigma = 1, \mu = \gamma = 0, \tau = 2$ and $\alpha = 4$. The bottom left panel shows the histogram of samples from 1000 simulations together with the true density. The bottom right panel shows the empirical covariance function for the samples (grey curve) together with the true Matérn covariance function (black curve).

A geostatistical model

- Assume field $X(\mathbf{s})$ is observed at some locations $\mathbf{s}_1, \ldots, \mathbf{s}_N$ generating observations $y_1, \ldots, y_N$.
- Assume $X(\mathbf{s})$ is of the form

$$X(\mathbf{s}) = \sum_{i=1}^{n_x} B_i(\mathbf{s})\beta_i + \xi(\mathbf{s})$$

where $\xi(\mathbf{s})$ is an SPDE field, and $\{B_1, \ldots, B_{n_x}\}$ are known covariates.

A geostatistical model

- Using the finite element representation, the hierarchical model expressed in terms of the weights $\mathbf{w}$ and the basis expansion for $\xi(\mathbf{s})$ is

$$\mathbf{y} = \mathbf{B}\boldsymbol{\beta} + \mathbf{A}\mathbf{w} + \boldsymbol{\epsilon}$$

$$\mathbf{w} = \mathbf{K}_{\alpha}^{-1}\left(\tau\mathbf{a}\gamma + \mathbf{V}\mu + \sigma\sqrt{\mathbf{V}} \circ \mathbf{Z}\right)$$

- Here $\mathbf{A}$ is $N \times n$ with elements $A_{ji} = \varphi_i(\mathbf{s}_j)$
- ϵ is a vector of iid $\mathrm{N}(0, \sigma_\epsilon^2)$ variables
- $\mathbf{a}$ is vector with elements $a_i = h_i = \int \varphi_i(\mathbf{s})\mathrm{d}\mathbf{s}$
- $\mathbf{V}$ contains independent variables V_i
- $\mathbf{Z}$ is iid standard Gaussian variables

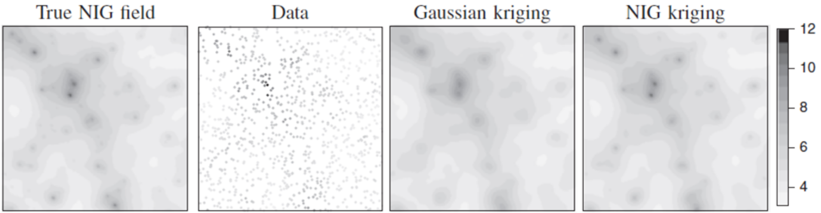

Fig. 3. The two leftmost panels show a simulated normal inverse Gaussian (NIG) field and measurements of that field under Gaussian noise. The two rightmost panels show Kriging predictions based on the data, assuming the correct normal inverse Gaussian model and a Gaussian model.

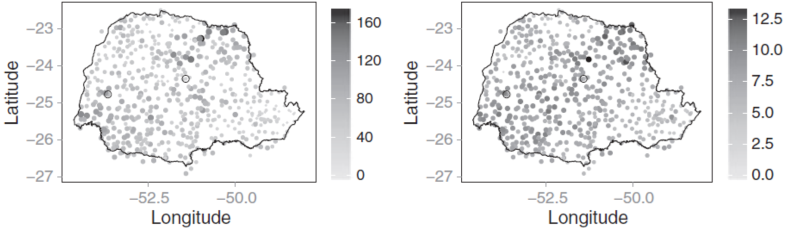

Fig. 4. The panels display precipitation data from the state of Paraná in Brazil for October 2012. To the left is the maximum daily precipitation of the month and to the right is monthly average. The two encircled locations are the locations where the predictive distributions are studied in Figure 5; the left location is denoted $\mathbf{s}_2$ and the right $\mathbf{s}_1$.

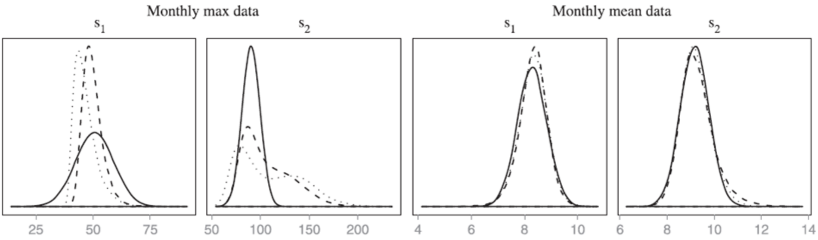

Fig. 5. The posterior densities of $\mathbf{X}$ for the Gaussian model (solid), the normal inverse Gaussian model (dashed), and the generalized asymmetric Laplace model (dotted) at the locations $\mathbf{s}_1$ and $\mathbf{s}_2$ for the monthly maximum data and the monthly mean data. The locations of $\mathbf{s}_1$ and $\mathbf{s}_2$ are displayed in Figure 4.

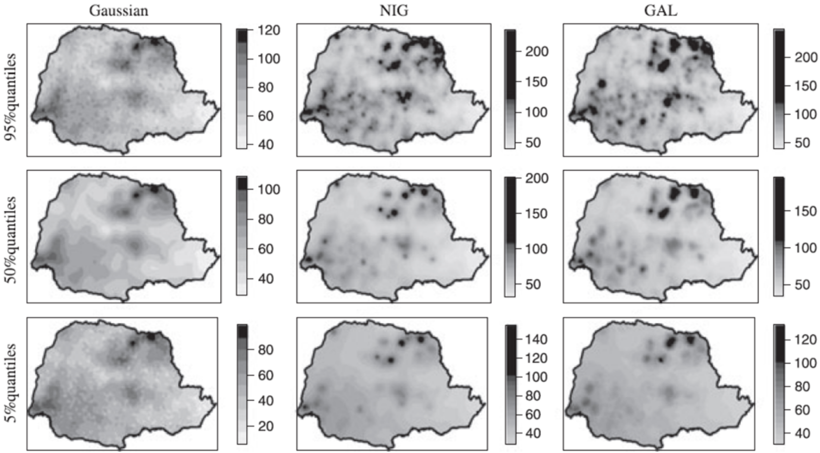

Fig. 6. Marginal quantiles of the posterior distribution for the Gaussian, normal inverse Gaussian (NIG), and generalized asymmetric Laplace (GAL) models for the maximum daily precipitation data. The colour scale of the NIG and GAL estimates have been selected to match the Gaussian model for each quantile, so all values above the largest value of the Gaussian model are shown in black.

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