Spatial statistics using Markov properties

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Covariance functions and stochastic PDEs

The Matérn covariance family on $\mathbb{R}^d$

$$\text{Cov}(u(\mathbf{0}), u(\boldsymbol{s})) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} (\kappa\|\boldsymbol{s}\|)^\nu K_\nu(\kappa\|\boldsymbol{s}\|)$$

Scale $\kappa > 0$, smoothness $\nu > 0$, variance $\sigma^2 > 0$

Whittle (1954, 1963): Matérn as SPDE solution

Matérn fields are the stationary solutions to the SPDE

$$\left(\kappa^2 - \nabla \cdot \nabla\right)^{\alpha/2} u(\boldsymbol{s}) = \mathcal{W}(\boldsymbol{s}), \quad \alpha = \nu + d/2$$

$\mathcal{W}(\cdot)$ white noise, $\nabla \cdot \nabla = \sum_{i=1}^d \frac{\partial^2}{\partial s_i^2}$, $\sigma^2 = \frac{\Gamma(\nu)}{\Gamma(\alpha)\kappa^{2\nu}(4\pi)^{d/2}}$

Basis function representations for Gaussian Matérn fields

Basis definitions

	Finite basis set ($k = 1, \dots, n$)
Karhunen-Loève	$(\kappa^2 - \nabla\cdot\nabla)^{-\alpha} e_k(\boldsymbol{s}) = \lambda_k e_k(\boldsymbol{s})$
Fourier	$-\nabla\cdot\nabla e_k(\boldsymbol{s}) = \lambda_k e_k(\boldsymbol{s})$
Convolution	$(\kappa^2 - \nabla\cdot\nabla)^{\alpha/2} g(\boldsymbol{s}) = \delta(\boldsymbol{s})$
General/GMRF	$\psi_k(\boldsymbol{s})$

Field representations

	Field $u(\boldsymbol{s})$	Weights
Karhunen-Loève	$\propto \sum_k e_k(\boldsymbol{s}) z_k$	$z_k \sim \mathcal{N}(0, \lambda_k)$
Fourier	$\propto \sum_k e_k(\boldsymbol{s}) z_k$	$z_k \sim \mathcal{N}(0, (\kappa^2 + \lambda_k)^{-\alpha})$
Convolution	$\propto \sum_k g(\boldsymbol{s} - \boldsymbol{s}_k) z_k$	$\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$
General/GMRF	$\propto \sum_k \psi_k(\boldsymbol{s}) u_k$	$\boldsymbol{u} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}^{-1})$

Continuous domain Markov approximations

Continuous Markovian spatial models (Lindgren et al, 2011)

Local basis: $u(\boldsymbol{s}) = \sum_k \psi_k(\boldsymbol{s}) u_k$, (compact, piecewise linear)

Basis weights: $\boldsymbol{u} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}^{-1})$, sparse $\boldsymbol{Q}$ based on an SPDE

Special case: $(\kappa^2 - \nabla \cdot \nabla) u(\boldsymbol{s}) = \mathcal{W}(\boldsymbol{s})$, $\boldsymbol{s} \in \Omega$

Precision: $\boldsymbol{Q} = \kappa^4 \boldsymbol{C} + 2\kappa^2 \boldsymbol{G} + \boldsymbol{G}_2$

Conditional distribution in a Gaussian model

$$\boldsymbol{u} \sim \mathcal{N}(\boldsymbol{\mu}_u, \boldsymbol{Q}_u^{-1}), \quad \boldsymbol{y}|\boldsymbol{u} \sim \mathcal{N}(\boldsymbol{A}\boldsymbol{u}, \boldsymbol{Q}_{y|u}^{-1}) \qquad (A_{ij} = \psi_j(\boldsymbol{s}_i))$$

$$\boldsymbol{u}|\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{\mu}_{u|y}, \boldsymbol{Q}_{u|y}^{-1})$$

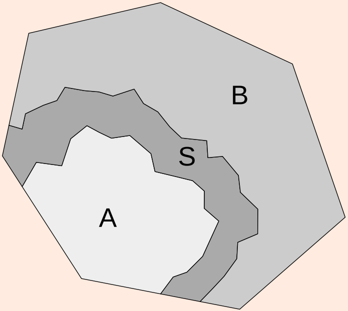
$$\boldsymbol{Q}_{u|y} = \boldsymbol{Q}_u + \boldsymbol{A}^T \boldsymbol{Q}_{y|u} \boldsymbol{A}$$ (∼"Sparse iff ψ_k have compact support")

$$\boldsymbol{\mu}_{u|y} = \boldsymbol{\mu}_u + \boldsymbol{Q}_{u|y}^{-1} \boldsymbol{A}^T \boldsymbol{Q}_{y|u} (\boldsymbol{y} - \boldsymbol{A}\boldsymbol{\mu}_u)$$

Continuous and discrete Markov properties

Markov properties

S is a separating set for A and B: $u(A) \perp u(B) \mid u(S)$



Solutions to

$$\left(\kappa^2 - \nabla \cdot \nabla\right)^{\alpha/2} u(\boldsymbol{s}) = \mathcal{W}(\boldsymbol{s})$$

are Markov when α is an integer.
(Rozanov, 1977)

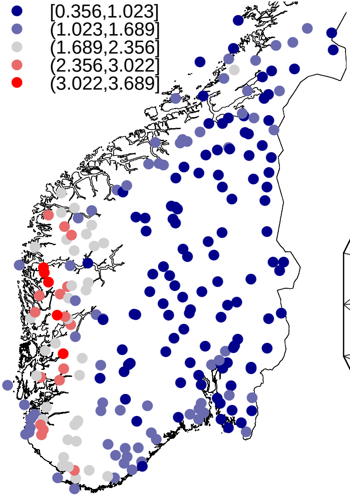
Discrete representations:

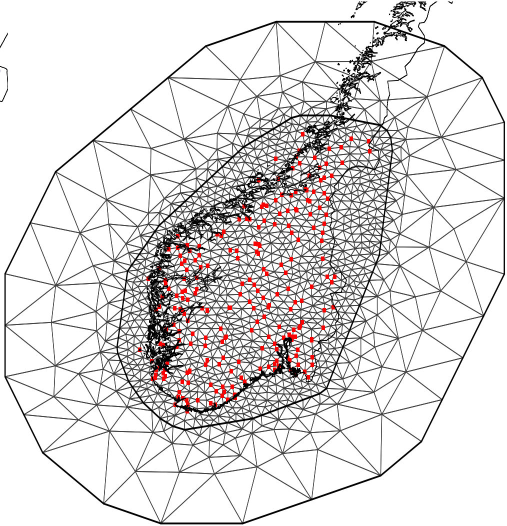
$$\boldsymbol{Q}_{AB} = \boldsymbol{0}$$

$$\boldsymbol{Q}_{A|S,B} = \boldsymbol{Q}_{AA}$$

$$\boldsymbol{\mu}_{A|S,B} = \boldsymbol{\mu}_A - \boldsymbol{Q}_{AA}^{-1}\boldsymbol{Q}_{AS}(\boldsymbol{u}_S - \boldsymbol{\mu}_S)$$

Example: Precipitation (Ingebrigtsen et al., 2013)





Non-stationary precision construction

Finite element construction of basis weight precision

Non-stationary SPDE:

$$(\kappa(\boldsymbol{s})^2 - \nabla\cdot\nabla)\,(\tau(\boldsymbol{s})u(\boldsymbol{s})) = \mathcal{W}(\boldsymbol{s})$$

The SPDE parameters are constructed via spatial covariates:

$$\log\tau(\boldsymbol{s}) = b_0^\tau(\boldsymbol{s}) + \sum_{j=1}^p b_j^\tau(\boldsymbol{s})\theta_j, \quad \log\kappa(\boldsymbol{s}) = b_0^\kappa(\boldsymbol{s}) + \sum_{j=1}^p b_j^\kappa(\boldsymbol{s})\theta_j$$

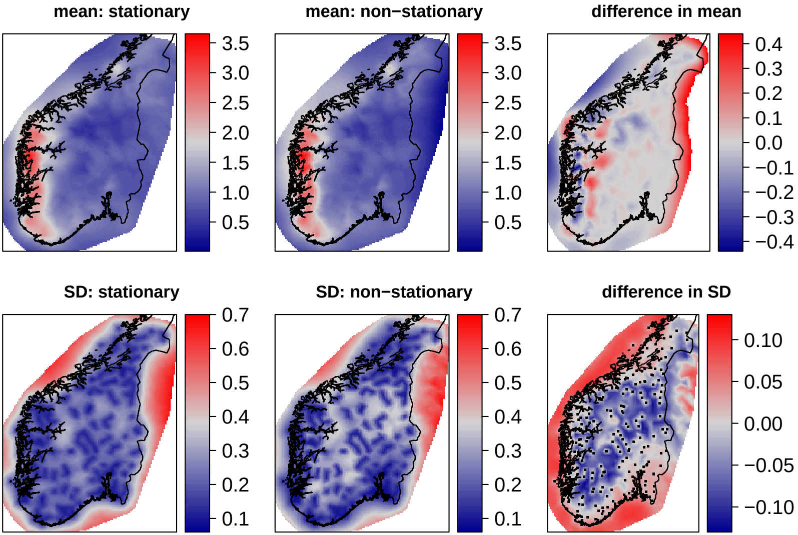
Finite element calculations give

$$\boldsymbol{T} = \operatorname{diag}(\tau(\boldsymbol{s}_i)), \quad \boldsymbol{K} = \operatorname{diag}(\kappa(\boldsymbol{s}_i))$$

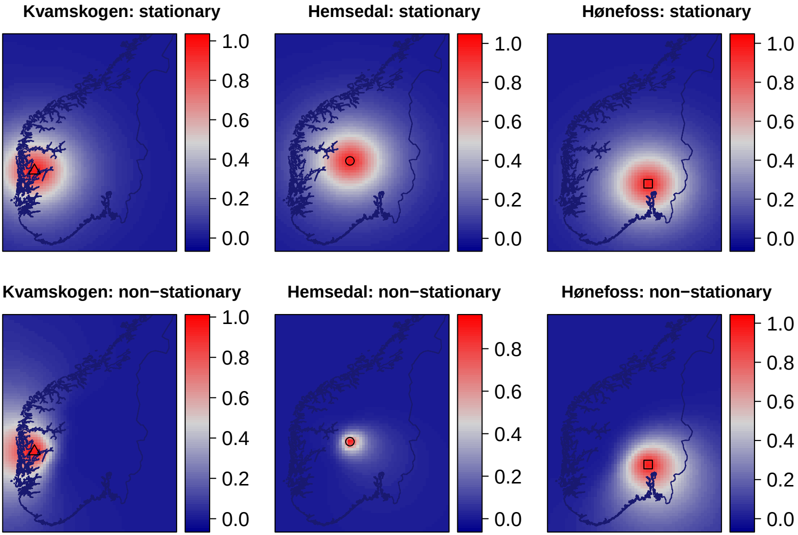
$$C_{ii} = \int \psi_i(\boldsymbol{s})\,d\boldsymbol{s}, \quad G_{ij} = \int \nabla\psi_i(\boldsymbol{s})\cdot\nabla\psi_j(\boldsymbol{s})\,d\boldsymbol{s}$$

$$\boldsymbol{Q} = \boldsymbol{T}\left(\boldsymbol{K}^2\boldsymbol{C}\boldsymbol{K}^2 + \boldsymbol{K}^2\boldsymbol{G} + \boldsymbol{G}\boldsymbol{K}^2 + \boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}\right)\boldsymbol{T}$$

Results for stationary and non-stationary models



Correlations for stationary and non-stationary models



Example: Point pattern data

Log-Gaussian Cox processes

Point intensity:

$$\lambda(\boldsymbol{s}) = \exp\left(\sum_i b_i(\boldsymbol{s})\beta_i + u(\boldsymbol{s})\right)$$

Inhomogeneous Poisson process log-likelihood:

$$\ln p(\{\boldsymbol{y}_k\} \mid \boldsymbol{\lambda}) = |\Omega| - \int_\Omega \lambda(\boldsymbol{s})\, d\boldsymbol{s} + \sum_{k=1}^n \ln \lambda(\boldsymbol{y}_k)$$

The likelihood can be approximated numerically, e.g.

$$\int_\Omega \lambda(\boldsymbol{s})\, d\boldsymbol{s} \approx \sum_{k=1}^n \lambda(\boldsymbol{s}_k) w_k$$

Laplace approximations

Quadratic posterior log-likelihood approximation

$$p(\boldsymbol{u} \mid \boldsymbol{\theta}) \sim \mathcal{N}(\boldsymbol{\mu}_u, \boldsymbol{Q}_u^{-1}), \quad \boldsymbol{y} \mid \boldsymbol{u}, \boldsymbol{\theta} \sim p(\boldsymbol{y} \mid \boldsymbol{u})$$

$$p_G(\boldsymbol{u} \mid \boldsymbol{y}, \boldsymbol{\theta}) \sim \mathcal{N}(\widetilde{\boldsymbol{\mu}}, \widetilde{\boldsymbol{Q}}^{-1})$$

$$\boldsymbol{0} = \nabla_{\boldsymbol{u}} \left\{\ln p(\boldsymbol{u} \mid \boldsymbol{\theta}) + \ln p(\boldsymbol{y} \mid \boldsymbol{u})\right\}\big|_{\boldsymbol{u}=\widetilde{\boldsymbol{\mu}}}$$

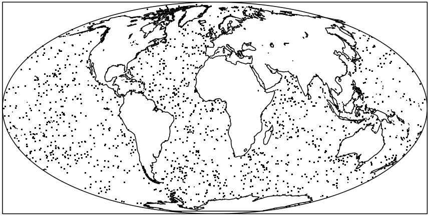
$$\widetilde{\boldsymbol{Q}} = \boldsymbol{Q}_u - \nabla_{\boldsymbol{u}}^2 \ln p(\boldsymbol{y} \mid \boldsymbol{u})\big|_{\boldsymbol{u}=\widetilde{\boldsymbol{\mu}}}$$

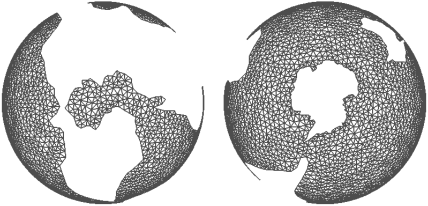
Direct Bayesian inference with INLA (`r-inla.org`)

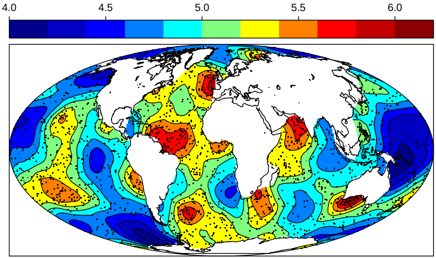
$$\widetilde{p}(\boldsymbol{\theta} \mid \boldsymbol{y}) \propto \left.\frac{p(\boldsymbol{\theta}) p(\boldsymbol{u} \mid \boldsymbol{\theta}) p(\boldsymbol{y} \mid \boldsymbol{u}, \boldsymbol{\theta})}{p_G(\boldsymbol{u} \mid \boldsymbol{y}, \boldsymbol{\theta})}\right|_{\boldsymbol{u}=\widetilde{\boldsymbol{\mu}}}$$

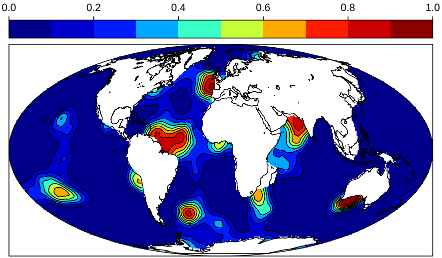
$$\widetilde{p}(\boldsymbol{u}_i \mid \boldsymbol{y}) \propto \int p_{GG}(\boldsymbol{u}_i \mid \boldsymbol{y}, \boldsymbol{\theta}) \widetilde{p}(\boldsymbol{\theta} \mid \boldsymbol{y}) \, d\boldsymbol{\theta}$$

log-Gaussian Cox point process on a manifold

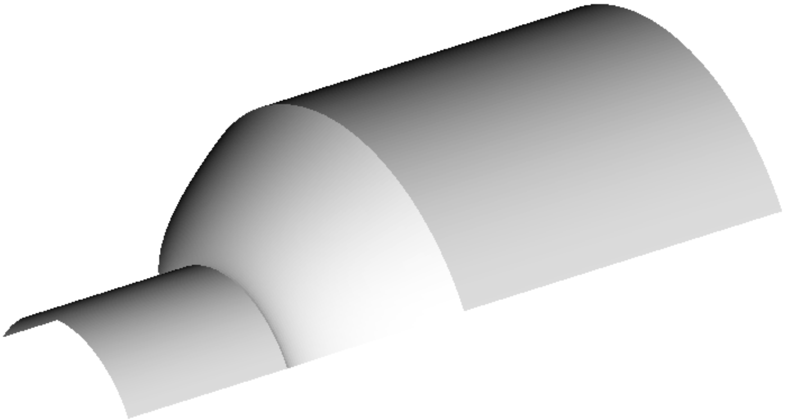




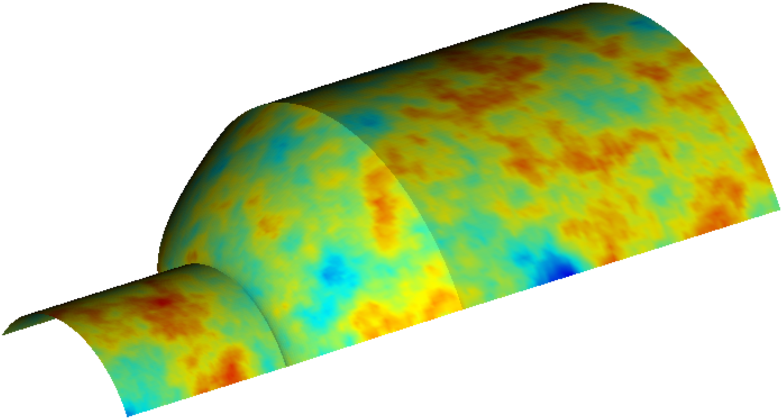




Connection with the deformation method for non-stationarity

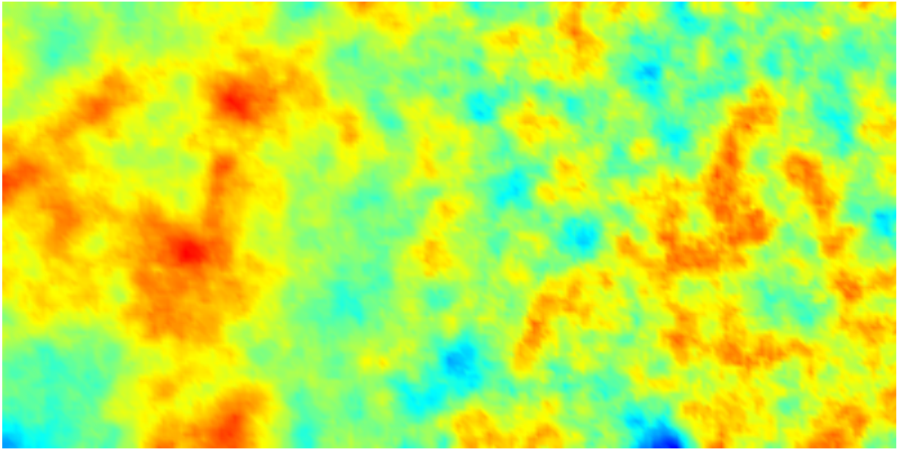


“Stationary” field on deformed manifold



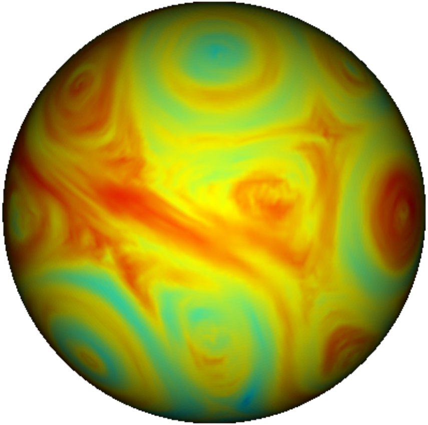
$$(1 - \widetilde{\nabla} \cdot \widetilde{\nabla})\widetilde{u}(\widetilde{\boldsymbol{s}}) = \widetilde{\mathcal{W}}(\widetilde{\boldsymbol{s}}), \quad \widetilde{\boldsymbol{s}} \in \widetilde{\Omega}$$

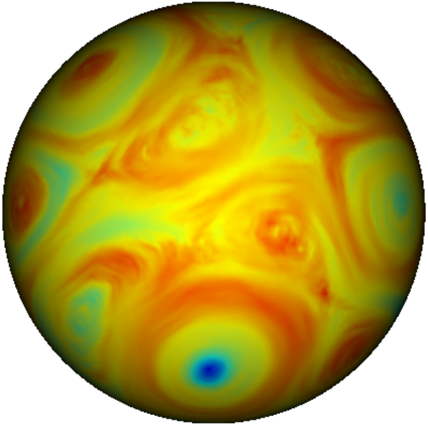
Non-stationary field on original manifold



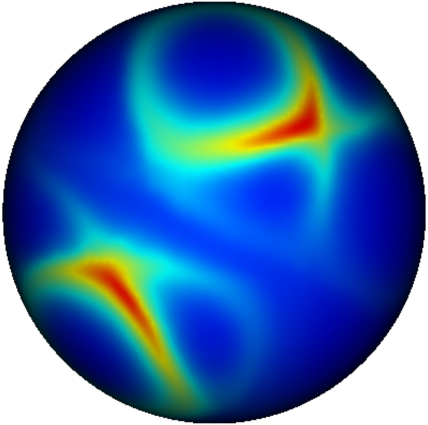
$$(\kappa(\boldsymbol{s})^2 - \nabla \cdot \nabla) u(\boldsymbol{s}) = \kappa(\boldsymbol{s}) \mathcal{W}(\boldsymbol{s}), \quad \boldsymbol{s} \in \Omega$$

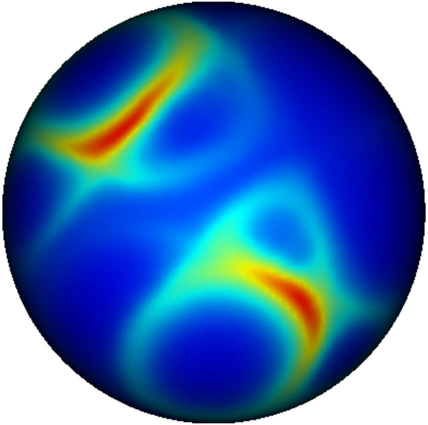
Anisotropic field on a globe via change of manifold metric



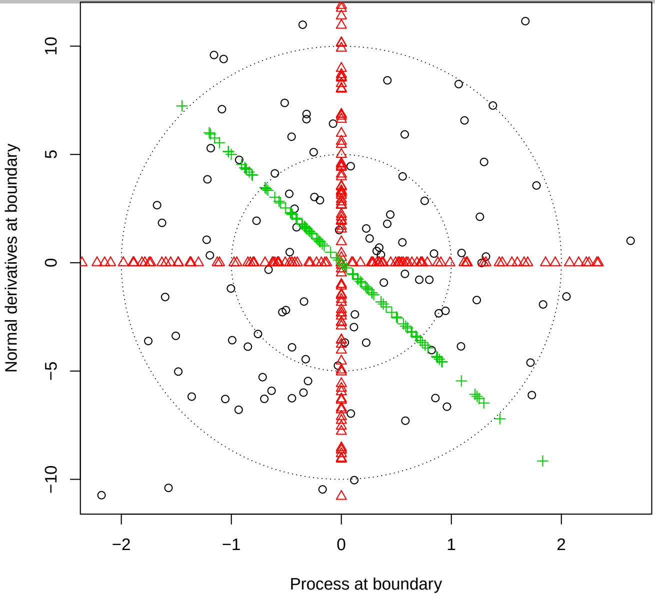


Four covariance functions





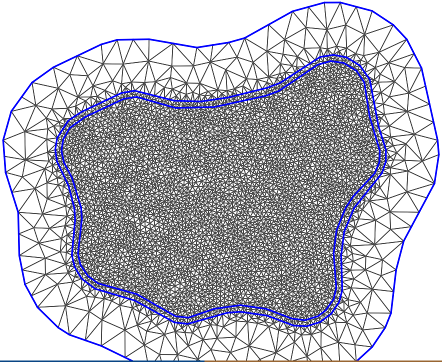
All deterministic boundary conditions are ‘inappropriate’



In search of practical stochastic boundary conditions

Separate the domain into the interior D, the boundary region B and an optional exterior extension E:

$$\boldsymbol{Q} = \begin{bmatrix} \boldsymbol{Q}_{EE} & \boldsymbol{Q}_{EB} & \boldsymbol{0} \\ \boldsymbol{Q}_{BE} & \boldsymbol{Q}_{BB} & \boldsymbol{Q}_{BD} \\ \boldsymbol{0} & \boldsymbol{Q}_{DB} & \boldsymbol{Q}_{DD} \end{bmatrix}$$



In search of practical stochastic boundary conditions

Classical approach (see e.g. Rue & Held, 2005)

$$\begin{bmatrix} Q_{BB} & Q_{BD} \\ Q_{DB} & Q_{DD} \end{bmatrix} = \begin{bmatrix} \Sigma_{BB}^{-1} + Q_{BD} Q_{DD}^{-1} Q_{DB} & Q_{BD} \\ Q_{DB} & Q_{DD} \end{bmatrix}$$

Problem: Requires known Σ_{BB} and solving with Q_{DD}

Extension elimination

$$\begin{bmatrix} \widetilde{Q}_{BB} & Q_{BD} \\ Q_{DB} & Q_{DD} \end{bmatrix} = \begin{bmatrix} Q_{BB} - Q_{BE} Q_{EE}^{-1} Q_{EB} & Q_{BD} \\ Q_{DB} & Q_{DD} \end{bmatrix}$$

Benefit: Solving with Q_{EE} is typically much cheaper.
Problem: Need to have an large enough initial extension.

Stochastic boundary conditions

Stochastic null-space boundary correction

- Construct an unconstrained model, with singular precision $\boldsymbol{Q}_0$.
- Find the desired joint distribution for the field and its normal derivatives along the boundary of Ω expressed via a bivariate SPDE model with precision $\boldsymbol{Q}_w$.
- Remove the extra bits generated by the null space by modifying the boundary precisions:

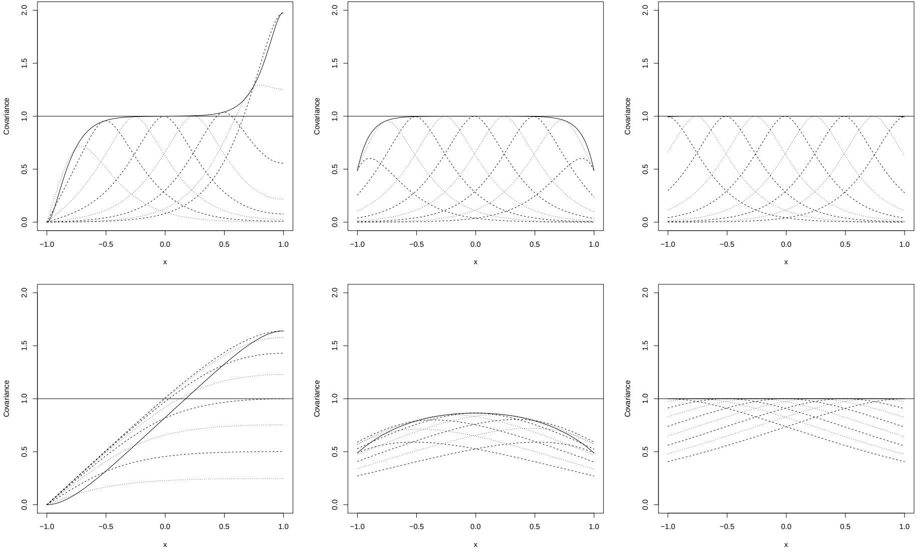
$$w = \begin{bmatrix} u \\ \partial_n u \end{bmatrix}$$

$$u^* \boldsymbol{Q} u = u^* \boldsymbol{Q}_0 u + w^* \mathcal{P}^* (\mathcal{P} \boldsymbol{Q}_w^{-1} \mathcal{P}^*)^{-1} \mathcal{P} w$$

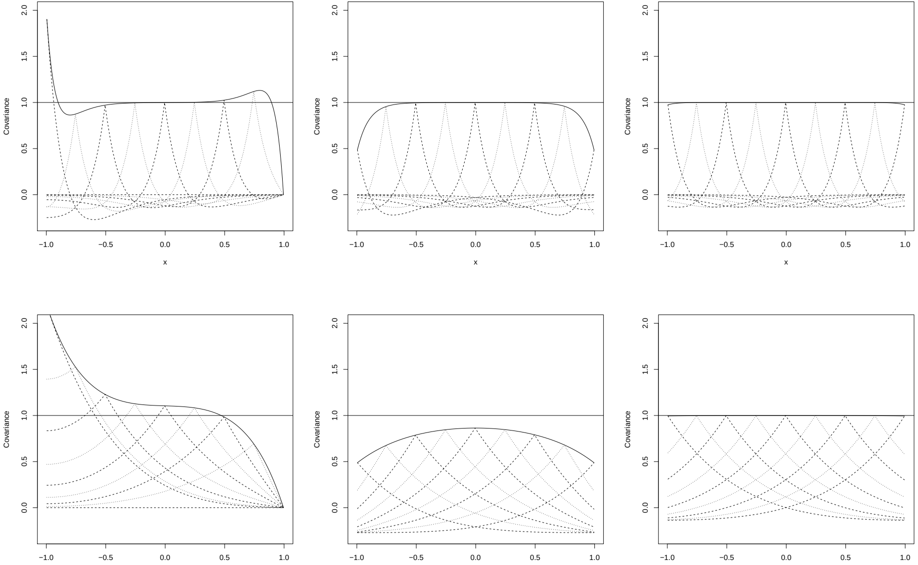
where $\mathcal{P}$ is a specific projection onto the nullspace.

Need to find $\boldsymbol{Q}_w$ and evaluate $\mathcal{P}^* (\mathcal{P} \boldsymbol{Q}_w^{-1} \mathcal{P}^*)^{-1} \mathcal{P}$.

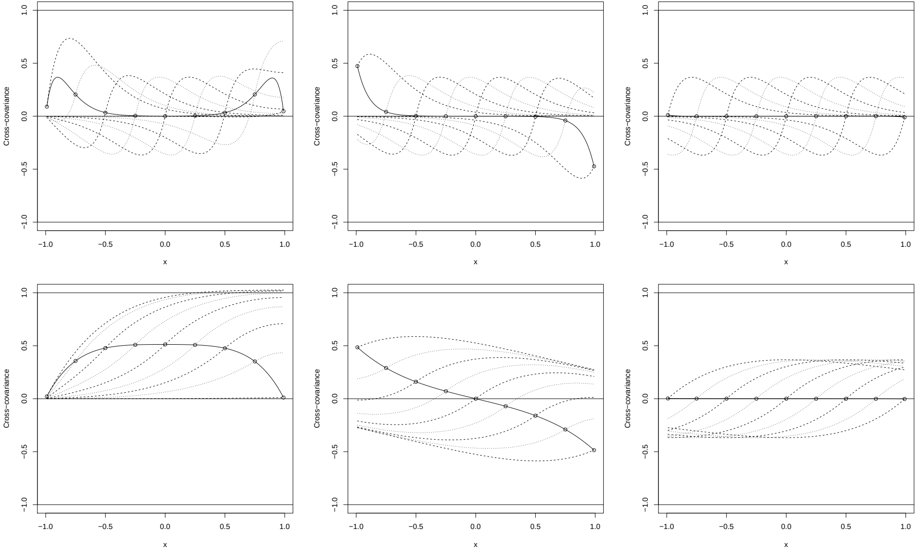
Covariances (D&N, Robin, Stoch) for $\kappa = 5$ and 1



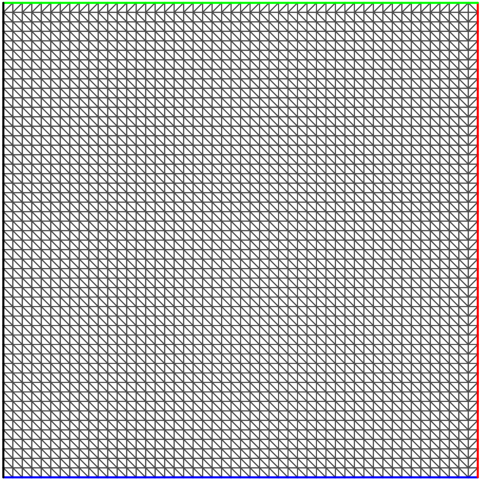
Derivative covariances (D&N, Robin, Stoch) for $\kappa = 5$ and 1



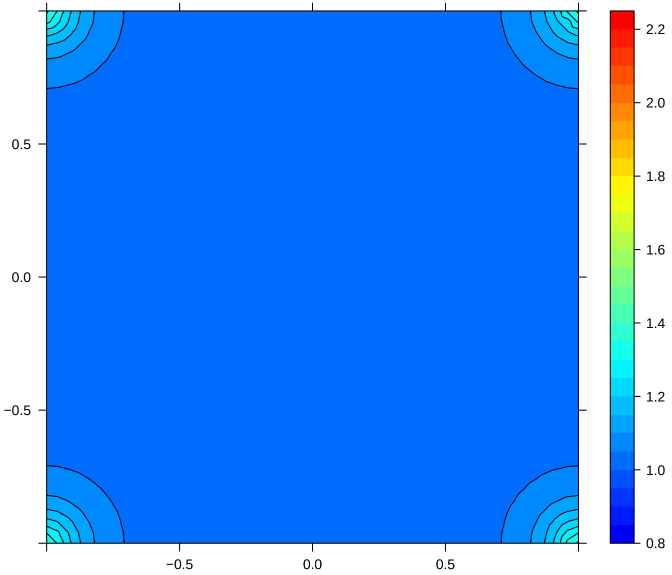
Process-derivative cross-covariances (D&N, Robin, Stoch)



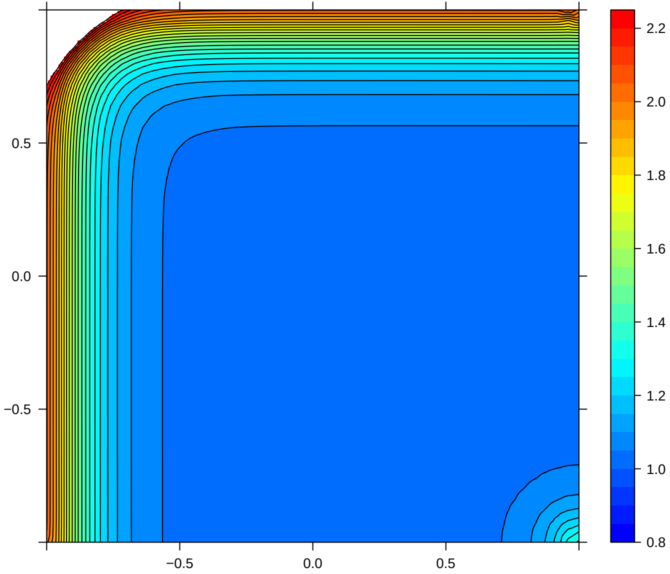
Square domain, basis triangulation



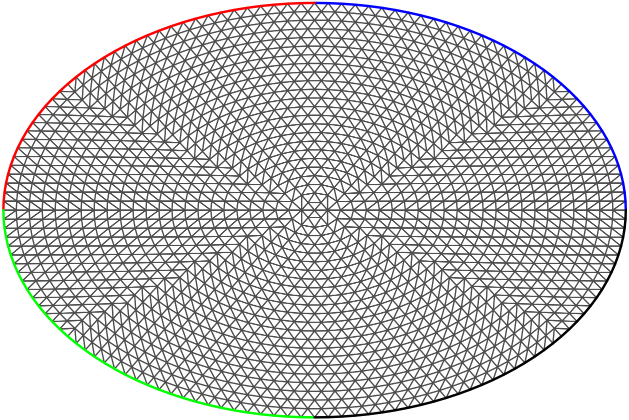
Square domain, stochastic boundary (variances)



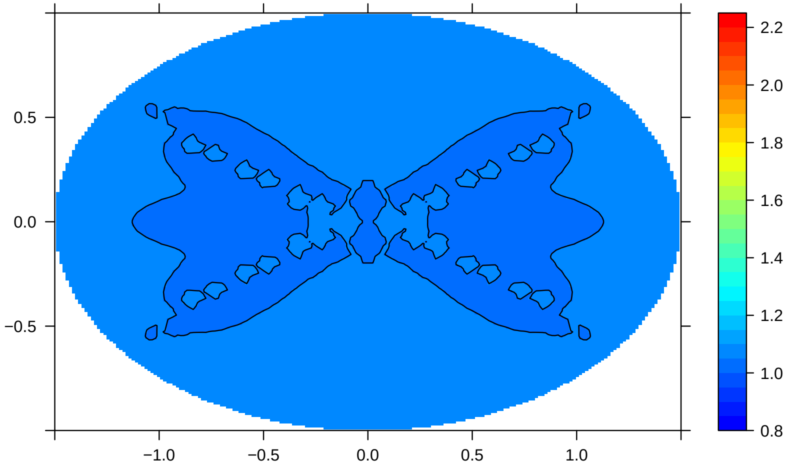
Square domain, mixed boundary (variances)



Elliptical domain, basis triangulation



Elliptical domain, stochastic boundary (variances)



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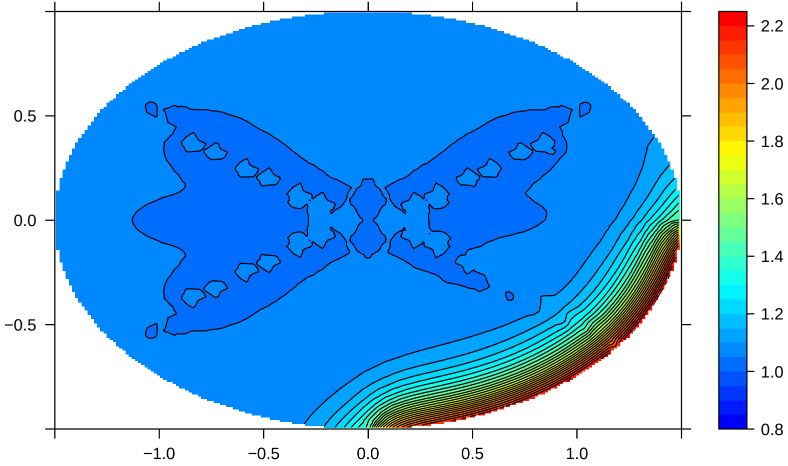

References

References (see also `r-inla.org`)

- F. Lindgren, 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)*, JRSSB, 73(4), 423–498.
- R. Ingebrigtsen, F. Lindgren, I. Steinsland (2013), *Spatial models with explanatory variables in the dependence structure*, Spatial Statistics, In Press (available online).
- G-A. Fuglstad, F. Lindgren, D. Simpson, H. Rue (2013), *Exploring a new class of non-stationary spatial Gaussian random fields with varying local anisotropy*, arXiv:1304.6949
- D. Bolin, F. Lindgren (2013), *Excursion and contour uncertainty regions for latent Gaussian models*, JRSSB, in press. Accepted version at arXiv:1211.3946. CRAN package: `excursions`