Boundary adjustment methods for SPDE models

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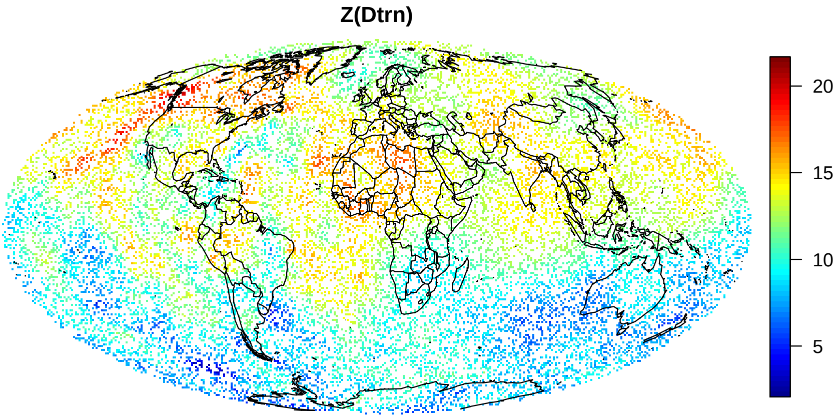
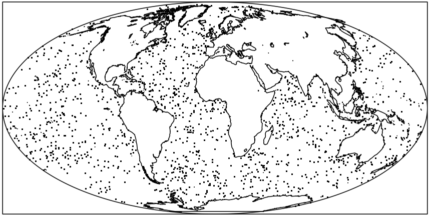
Smögen, 28 August 2014
(redacted version)

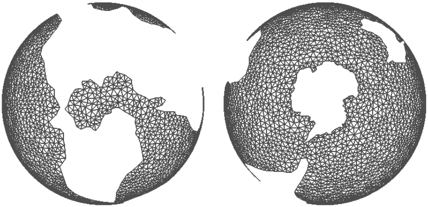
“Big” data

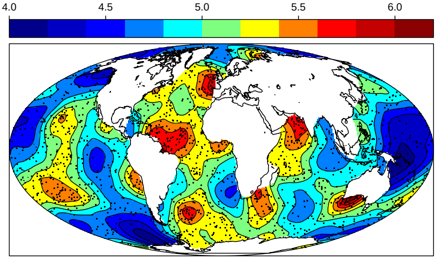


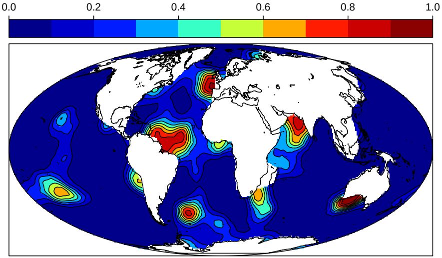
Naively implemented full likelihood/Bayesian inference is expensive for large problems, even when using Markovian stochastic PDE methods.
What are the needed boundary conditions for geographical blocks?

Inhomogeneous Poisson point process with boundary effects









Covariaces and stochastic PDEs

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

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

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

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

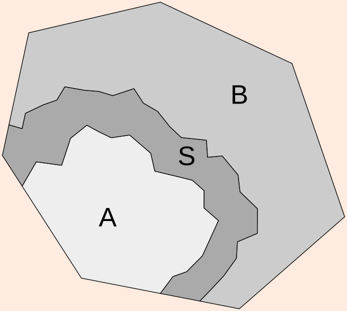
$\mathcal{W}(\cdot)$ white noise, $\nabla \cdot \nabla = \sum_{i=1}^d \frac{\partial^2}{\partial u_i^2}$, $\sigma^2 = \frac{\Gamma(\nu)}{\Gamma(\alpha)\kappa^{2\nu}(4\pi)^{d/2}}$

Important: If $v(\boldsymbol{s})$ is a solution (for $\alpha = 2$), then so is $v(\boldsymbol{s}) + \mathrm{e}^{\kappa \boldsymbol{s}\cdot\boldsymbol{n}}$, for all unit vectors $\boldsymbol{n}$. We need to handle the null-space solutions $\mathrm{e}^{\kappa \boldsymbol{s}\cdot\boldsymbol{n}}$ in a useful way.

Spectrum and the continuous global Markov property

Markov condition and spectral densities

Global Markov propery on a manifold:
For any separating set S 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)

Proof of the Matérn/Whittle equivalence and the Markov connection:

$$S(\boldsymbol{\omega}) = \mathcal{F}R(\cdot) = \frac{1}{(2\pi)^d(\kappa^2+\|\boldsymbol{\omega}\|^2)^\alpha}$$

Key fact: For any finite-dimensional Gaussian random field, the non-zero pattern of the precision matrix $\boldsymbol{Q} = \boldsymbol{\Sigma}^{-1}$ defines a graph on which the global Markov property holds. The reverse is also true.

Computations via Markov models on bounded domains

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: $\boldsymbol{Q} = \kappa^4 \boldsymbol{C} + 2\kappa^2 \boldsymbol{G} + \boldsymbol{G}_2$ $(\kappa^4 + 2\kappa^2 |\boldsymbol{\omega}|^2 + |\boldsymbol{\omega}|^4)$

Conditional distribution in a Gaussian model

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

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

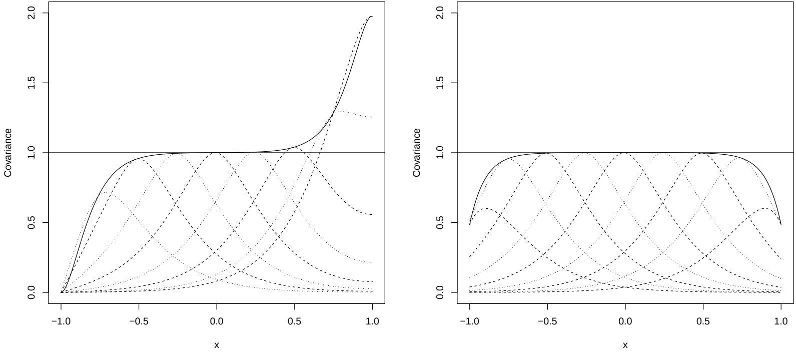
$$\boldsymbol{Q}_{u|y} = \boldsymbol{Q}_u + \boldsymbol{A}^T \boldsymbol{Q}_{y|u} \boldsymbol{A}$$ (∼"Sparse iff ψ_k have compact support")

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

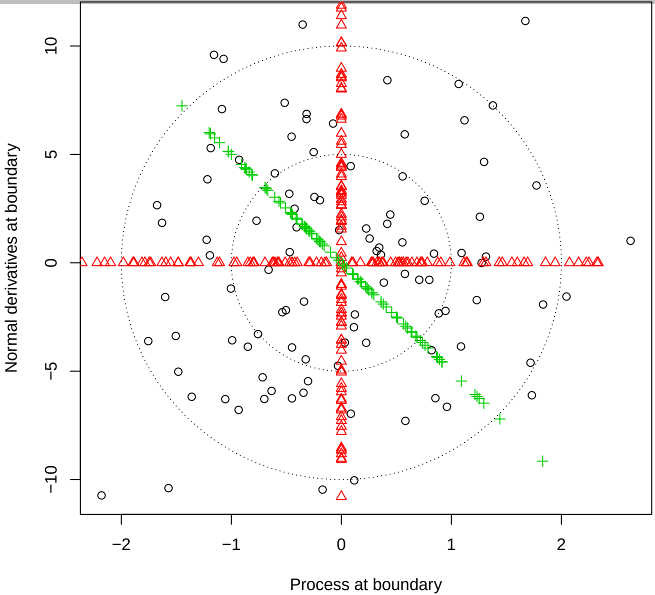
Classic approaches to constraining boundary behaviour

Deterministic boundary conditions

$$u(\boldsymbol{s}) = 0, \quad \boldsymbol{s} \in \partial\Omega \quad \text{(Dirichlet)}$$
$$\partial_{\boldsymbol{n}} u(\boldsymbol{s}) = 0, \quad \boldsymbol{s} \in \partial\Omega \quad \text{(Neumann)}$$
$$u(\boldsymbol{s}) + \gamma \partial_{\boldsymbol{n}} u(\boldsymbol{s}) = 0, \quad \boldsymbol{s} \in \partial\Omega \quad \text{(Robin)}$$



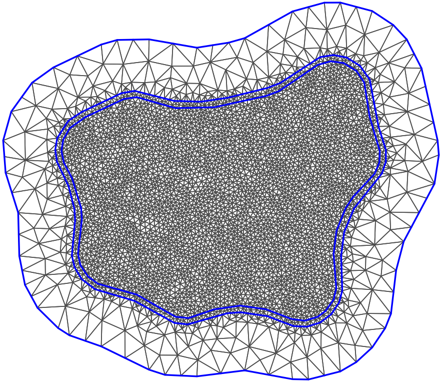
All deterministic boundary conditions are inappropriate



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)

$$\begin{bmatrix} \boldsymbol{Q}_{BB} & \boldsymbol{Q}_{BD} \\ \boldsymbol{Q}_{DB} & \boldsymbol{Q}_{DD} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\Sigma}_{BB}^{-1} + \boldsymbol{Q}_{BD}\boldsymbol{Q}_{DD}^{-1}\boldsymbol{Q}_{DB} & \boldsymbol{Q}_{BD} \\ \boldsymbol{Q}_{DB} & \boldsymbol{Q}_{DD} \end{bmatrix}$$

Problem: Requires known $\boldsymbol{\Sigma}_{BB}$ and solving with $\boldsymbol{Q}_{DD}$

Extension elimination

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

Benefit: Solving with $\boldsymbol{Q}_{EE}$ is typically much cheaper.
Problem: Need to have an large enough initial extension.

Implicit stationary extension

Near-boundary precision block structure

$$Q = \begin{bmatrix} \widetilde{\widetilde{Q}}_{00} & \widetilde{Q}_{01} & Q_{02} & \mathbf{0} & \cdots \\ \widetilde{Q}_{10} & \widetilde{Q}_{00} & Q_{01} & Q_{02} & \ddots \\ Q_{20} & Q_{10} & Q_{00} & Q_{01} & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

Solve for boundary (also Discrete Algebraic Riccati Equations):

$$\begin{bmatrix} \widetilde{\widetilde{Q}}_{00} & \widetilde{Q}_{01} \\ \widetilde{Q}_{10} & \widetilde{Q}_{00} \end{bmatrix} = \begin{bmatrix} \widetilde{Q}_{00} & Q_{01} \\ Q_{10} & Q_{00} \end{bmatrix} - \begin{bmatrix} \widetilde{Q}_{10} \\ Q_{20} \end{bmatrix} \widetilde{\widetilde{Q}}_{00}^{-1} \begin{bmatrix} \widetilde{Q}_{01} & Q_{02} \end{bmatrix}$$

Hidden problem: Need $\partial\Omega$ to be a straight line.
Approximate solution: Treat curved boundaries as if they were lines!

Alternative solution: Stationary AR extension

Solve for stable matrix AR coefficients

AR(2): $\boldsymbol{A}_0\boldsymbol{u}_t + \boldsymbol{A}_1\boldsymbol{u}_{t-1} + \boldsymbol{A}_2\boldsymbol{u}_{t-2} = e_t$

$$\boldsymbol{Q}_{00} = \boldsymbol{A}_0^\top\boldsymbol{A}_0 + \boldsymbol{A}_1^\top\boldsymbol{A}_1 + \boldsymbol{A}_2^\top\boldsymbol{A}_2$$
$$\boldsymbol{Q}_{01} = \boldsymbol{A}_0^\top\boldsymbol{A}_1 + \boldsymbol{A}_1^\top\boldsymbol{A}_2, \quad \boldsymbol{Q}_{02} = \boldsymbol{A}_0^\top\boldsymbol{A}_2$$
$$\widetilde{\boldsymbol{Q}}_{00} = \boldsymbol{A}_0^\top\boldsymbol{A}_0 + \boldsymbol{A}_1^\top\boldsymbol{A}_1, \quad \widetilde{\widetilde{\boldsymbol{Q}}}_{00} = \boldsymbol{A}_0^\top\boldsymbol{A}_0, \quad \widetilde{\boldsymbol{Q}}_{01} = \boldsymbol{A}_0^\top\boldsymbol{A}_1$$

Closed form solution (in terms of matrix square roots) for 1D and 2D. Essentially equivalent to solving the Riccati equations.

No simple direct link between κ and the precision. Difficult to find good sparse approximations.

Is there a more direct way of using the SPDE model itself? Let's try to eliminate an *appropriate amount* of null-space solutions.

Stochastic boundary conditions

Stochastic null-space boundary correction

- Construct the 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:

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

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

  where $\boldsymbol{P}$ gives the projection onto the nullspace.

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

Practical construction

Let $\boldsymbol{H}^{\beta}$ be a discrete representation of $(\kappa^2 - \nabla_\partial \cdot \nabla_\partial)^{\beta}$.

Projection and precision matrices

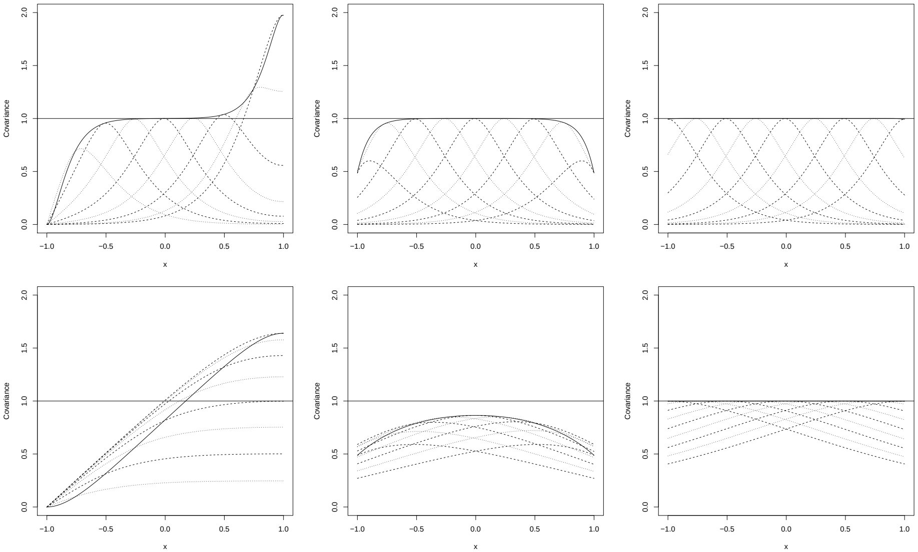
$$\boldsymbol{P} = \begin{bmatrix} \boldsymbol{H}^{1} & \boldsymbol{H}^{1/2} \end{bmatrix}$$

$$\boldsymbol{Q}_w = 4 \begin{bmatrix} \boldsymbol{H}^{3/2} & 0 \\ 0 & \boldsymbol{H}^{1/2} \end{bmatrix}$$

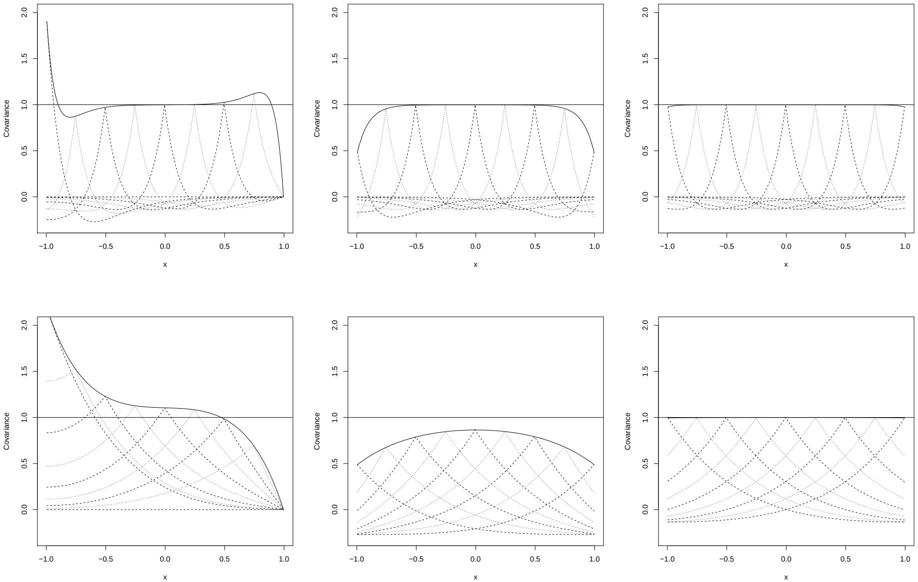
$$\boldsymbol{P}^\top (\boldsymbol{P} \boldsymbol{Q}_w^{-1} \boldsymbol{P}^\top)^{-1} \boldsymbol{P} = 2 \begin{bmatrix} \boldsymbol{H}^{3/2} & \boldsymbol{H}^{1} \\ \boldsymbol{H}^{1} & \boldsymbol{H}^{1/2} \end{bmatrix}$$

This looks promising, and with potential for extensions!
Direct sparse approximations are within reach via spectral fractional-to-Markov approximation methods, e.g. Lindgren (2011, Authors' discussion response)

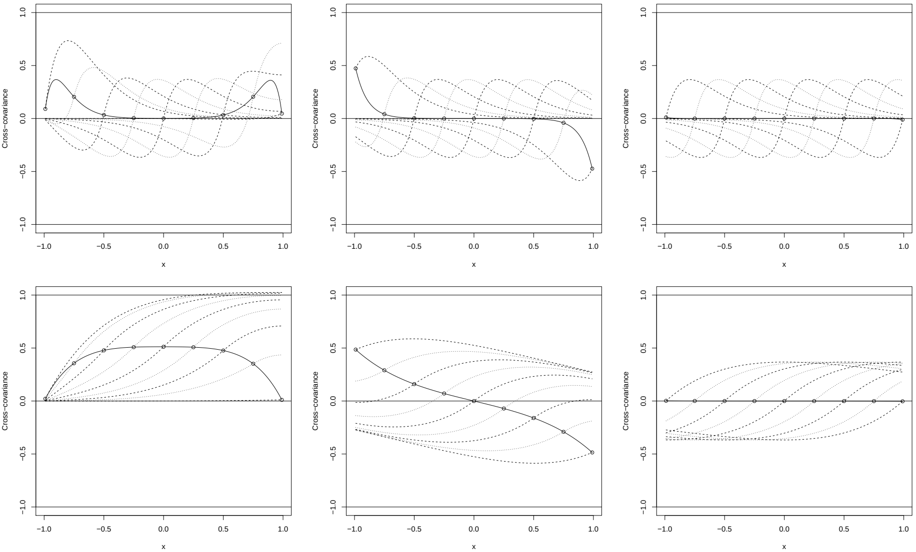
Covariances (D&N, Robin, Stoch) for $\kappa = 5$ and 1



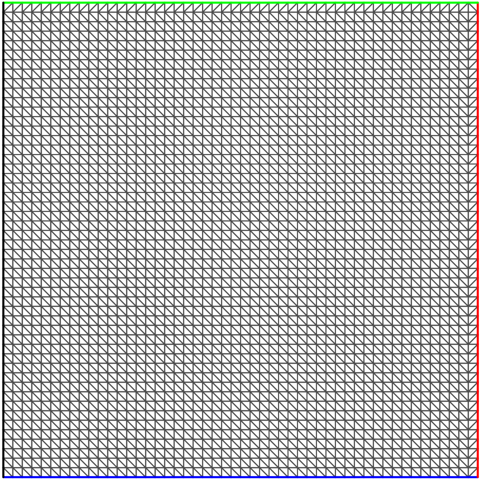
Derivative covariances (D&N, Robin, Stoch) for $\kappa = 5$ and 1



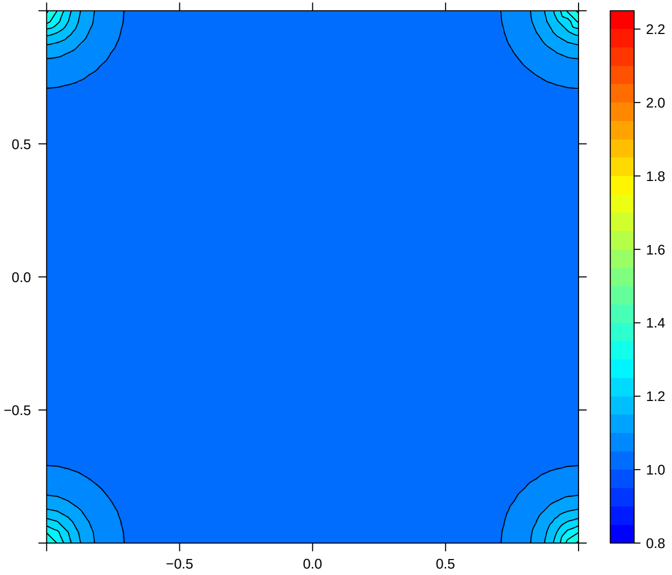
Process-derivative cross-covariances (D&N, Robin, Stoch)



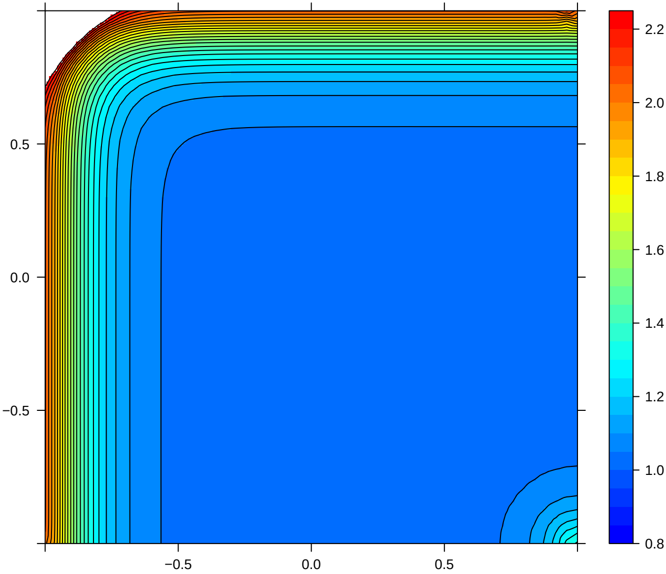
Square domain, basis triangulation



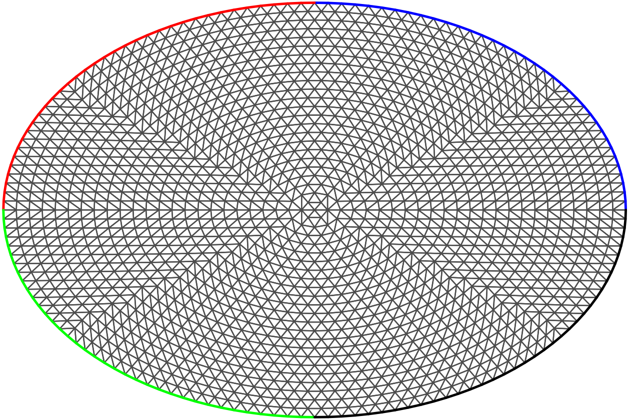
Square domain, stochastic boundary (variances)



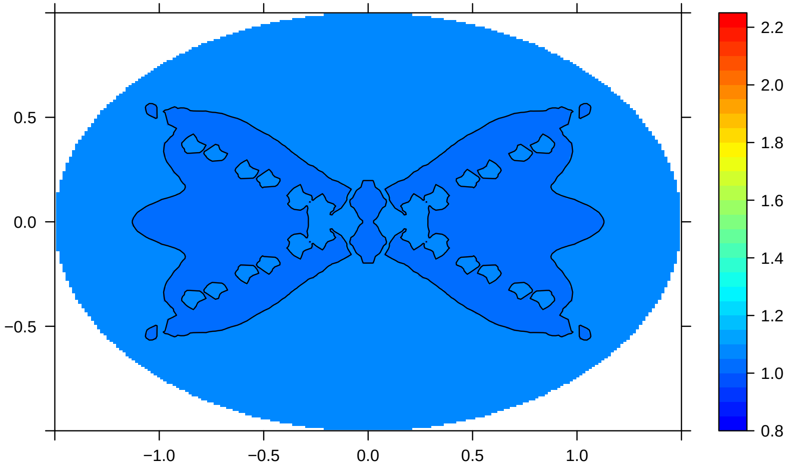
Square domain, mixed boundary (variances)



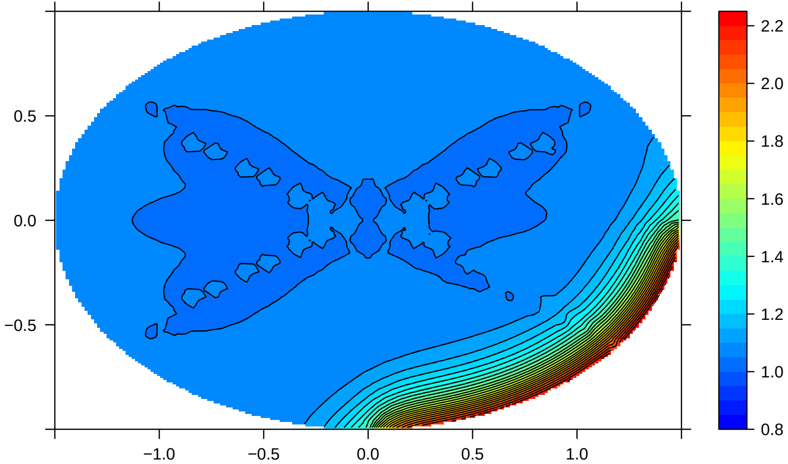
Elliptical domain, basis triangulation



Elliptical domain, stochastic boundary (variances)



Elliptical domain, mixed boundary (variances)



References

References

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