Boundary adjustment methods for SPDE models

Finn Lindgren

UNIVERSITY OF BATH

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Explicit and implicit dependence specifications

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

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

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

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

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

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

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

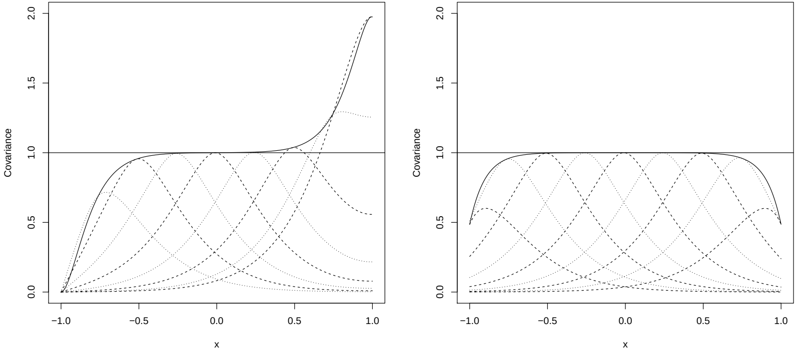
What about those *other* SPDE solutions?

If $v(\boldsymbol{s})$ is a solution to $(\kappa^2 - \Delta) v(\boldsymbol{s}) = \mathcal{W}(\boldsymbol{s}),\ \boldsymbol{s} \in \Omega$, then
$v(\boldsymbol{s}) + e(\boldsymbol{s})$ is also a solution, where $(\kappa^2 - \Delta) e(\boldsymbol{s}) = 0,\ \boldsymbol{s} \in \Omega$.
We need to eliminate the null-space solutions, e.g.
$e(\boldsymbol{s}) = \exp(\kappa \boldsymbol{s} \cdot \boldsymbol{n})$.
Problem: we can't separate between v and e!

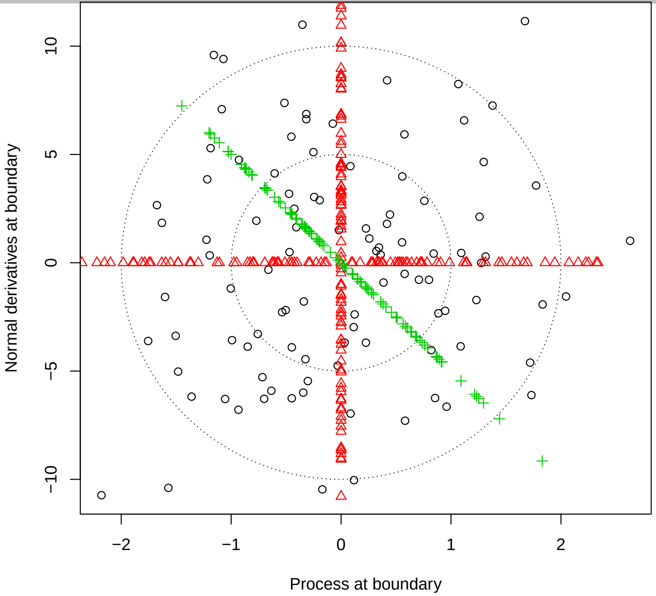
Classic approaches to constraining boundary behaviour

Deterministic boundary conditions

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



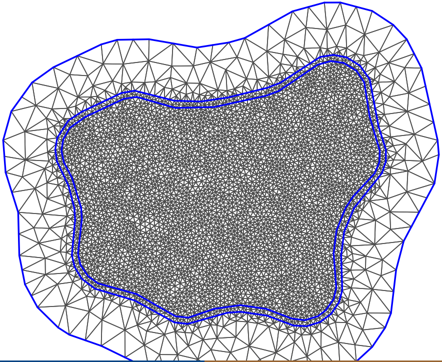
All deterministic boundary conditions are inappropriate



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)

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

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.

Implicit stationary extension

Near-boundary precision block structure

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

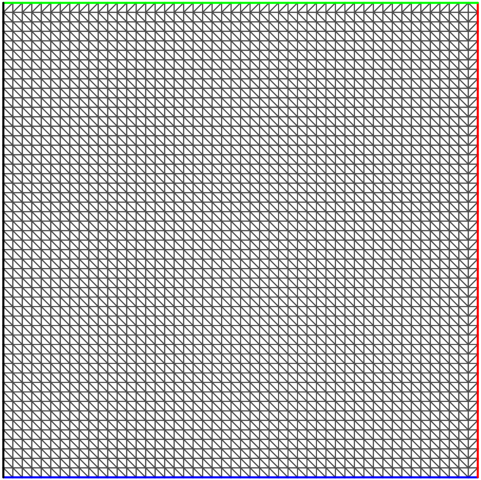
Solve for boundary (also Discrete Algebraic Riccati Equations):

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

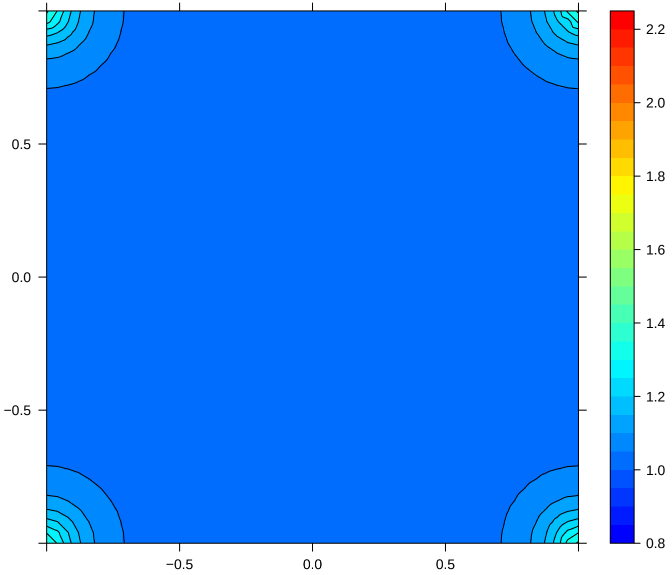
Hidden problem: Need $\partial\Omega$ to be a straight line.

Approximate solution: Treat curved boundaries as if they were lines!

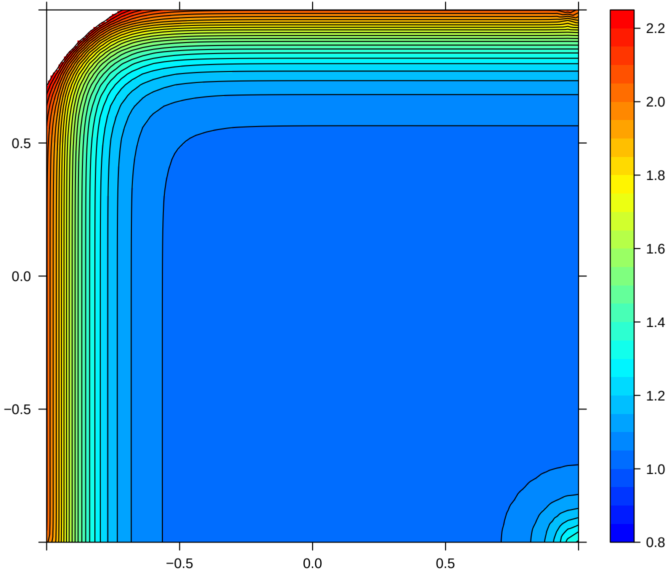
Square domain, basis triangulation



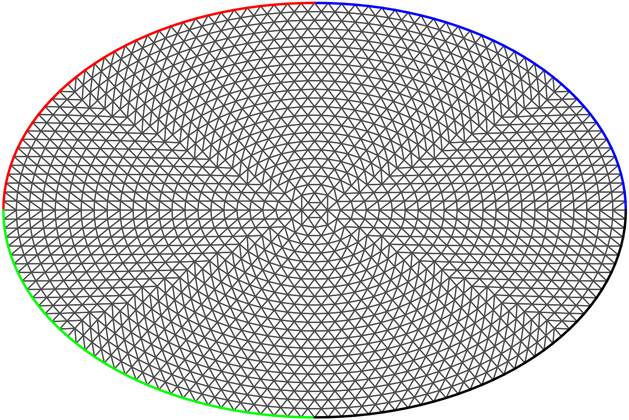
Square domain, stochastic boundary variances



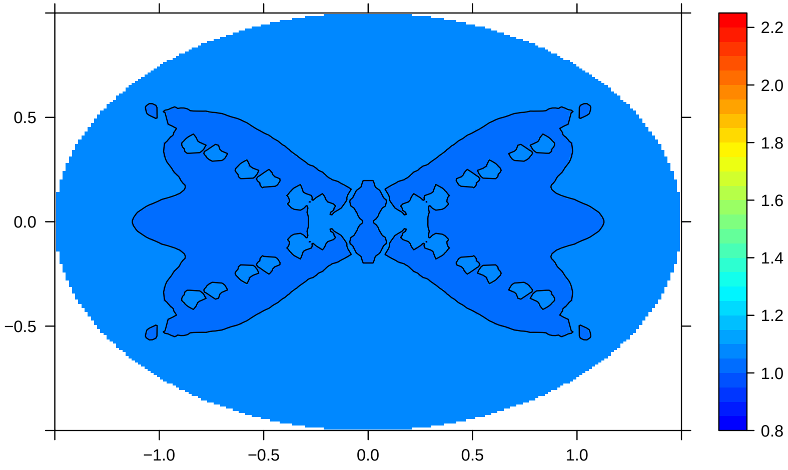
Square domain, mixed boundary variances



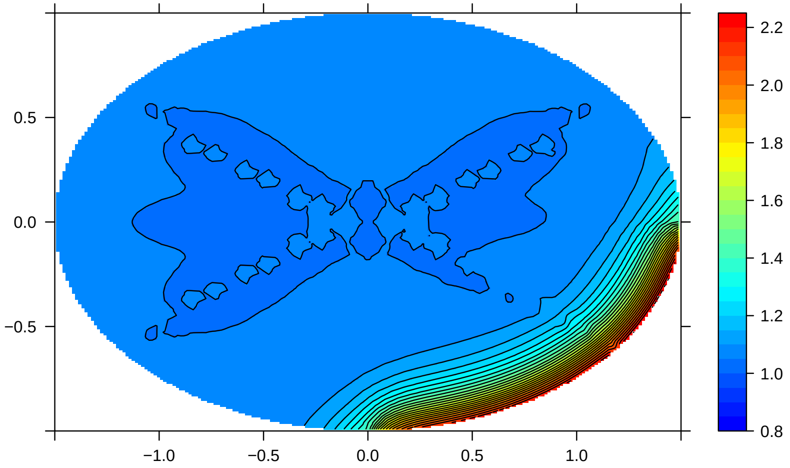
Elliptical domain, basis triangulation



Elliptical domain, stochastic boundary variances



Elliptical domain, mixed boundary variances



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:

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

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

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

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

Boundary properties

Characterisation of nullspace functions

$$\mathcal{F}_{\partial\Omega}\begin{bmatrix}\phi\\ \partial_n\phi\end{bmatrix}=\begin{bmatrix}\widehat{\phi}\\ \sqrt{\kappa^2+\omega^2}\widehat{\phi}\end{bmatrix},\quad \widehat{\phi}(\omega):=\mathcal{F}_{\partial\Omega}\phi$$

Scalar product for projection:

$$\langle f,\, g\rangle_{\mathcal{H}(\partial\Omega)}=\kappa^2\langle f,\, g\rangle_{\partial\Omega}+\langle\nabla_\partial f,\, \nabla_\partial g\rangle_{\partial\Omega}+\langle\partial_{\boldsymbol{n}} f,\, \partial_{\boldsymbol{n}} g\rangle_{\partial\Omega}$$

Spectral characterisation of stationary solutions

$$S_w(\omega)=\begin{bmatrix}\frac{1/(2\pi)}{4(\kappa^2+\omega^2)^{3/2}} & 0\\ 0 & \frac{1/(2\pi)}{4(\kappa^2+\omega^2)^{1/2}}\end{bmatrix}$$

Practical construction

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

Projection and precision matrices

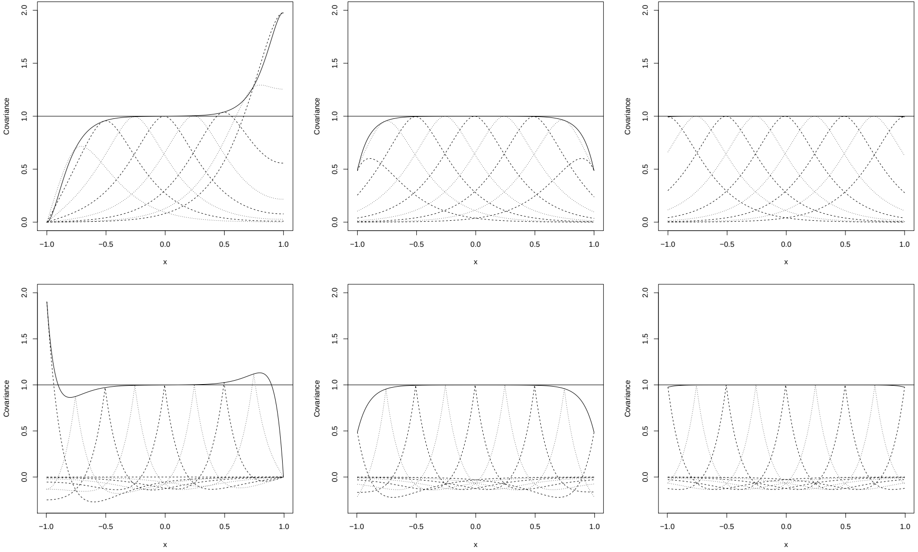
$$\mathcal{P} = \begin{bmatrix} \boldsymbol{H}^1 & \boldsymbol{H}^{1/2} \end{bmatrix}$$

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

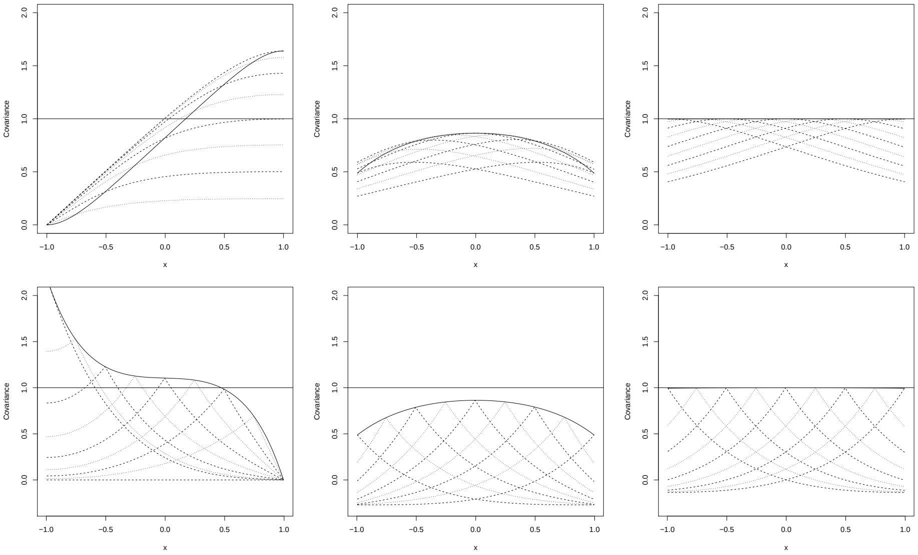
$$\mathcal{P}^*(\mathcal{P}\boldsymbol{Q}_w^{-1}\mathcal{P}^*)^{-1}\mathcal{P} = 2 \begin{bmatrix} \boldsymbol{H}^{3/2} & \boldsymbol{H}^1 \\ \boldsymbol{H}^1 & \boldsymbol{H}^{1/2} \end{bmatrix}$$

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)

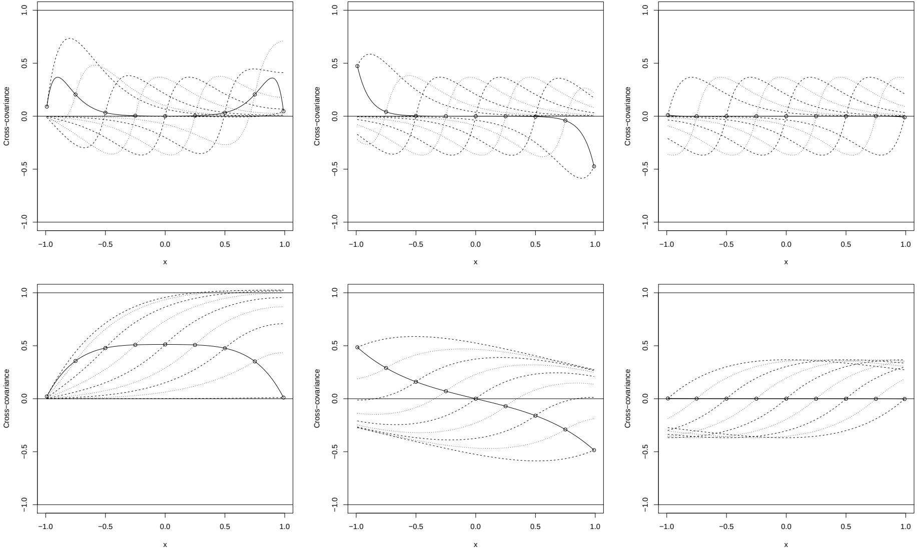
Covariances (D&N, Robin, Stoch) for $\kappa = 5$



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



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



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