Further SPDE topics:
Fractional operators
Non-stationary models
Boundary corrections
Space-time models

Finn Lindgren

UNIVERSITY OF BATH

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Fractional SPDE operator

The spectrum for a Matérn/Whittle SPDE is

$$S(\boldsymbol{\omega};\alpha,\kappa)=\frac{1}{(2\pi)^d}\left(\kappa^2+\|\boldsymbol{\omega}\|^2\right)^{-\alpha}$$

For integer α we can write

$$S(\boldsymbol{\omega};\alpha,\kappa)^{-1}=(2\pi)^d\sum_{k=0}^{\alpha}b_k(\alpha,\kappa)\|\boldsymbol{\omega}\|^{2k},$$

$$\begin{aligned}\boldsymbol{b}(0,\kappa)&=\{1\}\\ \boldsymbol{b}(1,\kappa)&=\{\kappa^2,1\}\\ \boldsymbol{b}(2,\kappa)&=\{\kappa^4,2\kappa^2,1\}\\ \boldsymbol{b}(3,\kappa)&=\{\kappa^6,3\kappa^4,3\kappa^2,1\}\end{aligned}$$

$$Q_{\alpha,\kappa}=\sum_{k=0}^{\alpha}b_k(\alpha,\kappa)\boldsymbol{C}^{1/2}(\boldsymbol{C}^{-1/2}\boldsymbol{G}\boldsymbol{C}^{-1/2})^k\boldsymbol{C}^{1/2}$$

Fractional SPDE operator

Find coefficient vectors $\boldsymbol{b}(\alpha, \kappa)$ for polynomials

$$P(\boldsymbol{\omega}; \alpha, \kappa) = \sum_{k=0}^{p} b_k(\alpha, \kappa) \|\boldsymbol{\omega}\|^{2k}, \quad p = \lceil \alpha \rceil$$

such that $\widetilde{S}(\boldsymbol{\omega}; \alpha, \kappa)^{-1} = (2\pi)^d P(\boldsymbol{\omega}; \alpha, \kappa)$ approximates $S(\boldsymbol{\omega}; \alpha, \kappa)^{-1}$ in some useful sense. Minimise

$$\int_{\mathbb{R}^d} (\widetilde{S}(\boldsymbol{\omega}) - S(\boldsymbol{\omega}))^2 w_\lambda(\boldsymbol{\omega}) \, \mathrm{d}\boldsymbol{\omega} = \int_{\kappa^2}^{\infty} \left(z^\alpha - \sum_{k=0}^{p} b_k(\alpha, \kappa)(z - \kappa^2)^k \right)^2 z^{-2p-1-\lambda} \, \mathrm{d}z$$

for suitably chosen λ. Matching derivatives for $S(\boldsymbol{\omega})$ and $\widetilde{S}(\boldsymbol{\omega})$ at $\boldsymbol{\omega} = \boldsymbol{0}$ is obtained for $\lambda \to \infty$.

Fractional SPDE operator

The resulting approximation for any $\alpha > 2$ is the same as the approximation for $\alpha - 2\lfloor\alpha/2\rfloor$ fed recursively through $(\kappa^2 - \nabla\cdot\nabla)u_\alpha(\boldsymbol{s}) = u_{\alpha-2}(\boldsymbol{s})$, so we only need to consider $0 \leq \alpha \leq 2$. Choose $\lambda = \infty$ or $\lambda = \alpha - \lfloor\alpha\rfloor$ (the latter shown only for half-integers):

$$
\begin{aligned}
\boldsymbol{b}(0,\kappa) &= \{1\} & \\
\boldsymbol{b}(\alpha,\kappa) &= \{\kappa^2, \alpha\}\kappa^{2\alpha-2} & \{\kappa^2, 1/2\}\kappa^{-1}3/4 \\
\boldsymbol{b}(1,\kappa) &= \{\kappa^2, 1\} & \\
\boldsymbol{b}(\alpha,\kappa) &= \{\kappa^4, \alpha\kappa^2, \alpha(\alpha-1)/2\}\kappa^{2\alpha-4} & \{\kappa^4, 2\kappa^2, 1/8\}\kappa^{-1}15/16 \\
\boldsymbol{b}(2,\kappa) &= \{\kappa^4, 2\kappa^2, 1\} &
\end{aligned}
$$

The choice $\lambda = \infty$ gives accurate large region integration properties.
The choice $\lambda = \alpha - \lfloor\alpha\rfloor$ gives accurate overall "$\nu = 1/2$-properties".

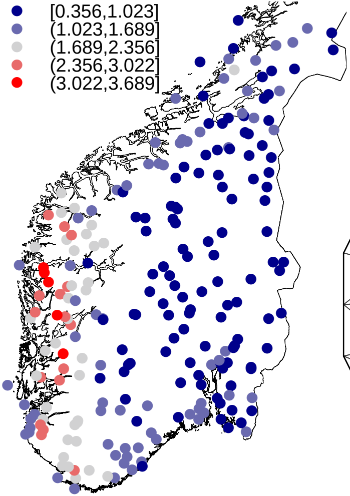
Alternative, more general spectrum approximation

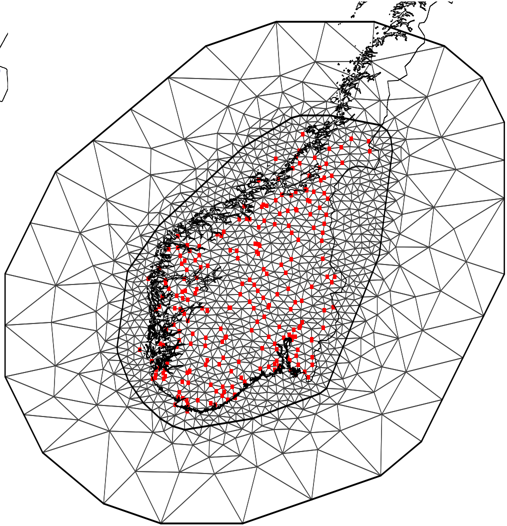
The LatticeKrig approach (`latticekrig` on CRAN; Nychka et al) essentially constructs random field models as $(K+1)$-level multiscale sum of independent fields with coupled parameters controlling Markov basis function weights, with resulting approximate spectrum

$$S(\boldsymbol{\omega}) = \frac{1}{(2\pi)^d} \sum_{k=0}^{K} \frac{a_k}{((2^k\kappa_0)^2 + \|\omega\|^2)^2}$$

The sequence $\{a_0, a_1, \ldots, a_K\}$ can be chosen generally, or so that $S(\boldsymbol{\omega})$ approximates a Matérn field spectrum with (almost) arbitrary ν. K can be kept small.

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:

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

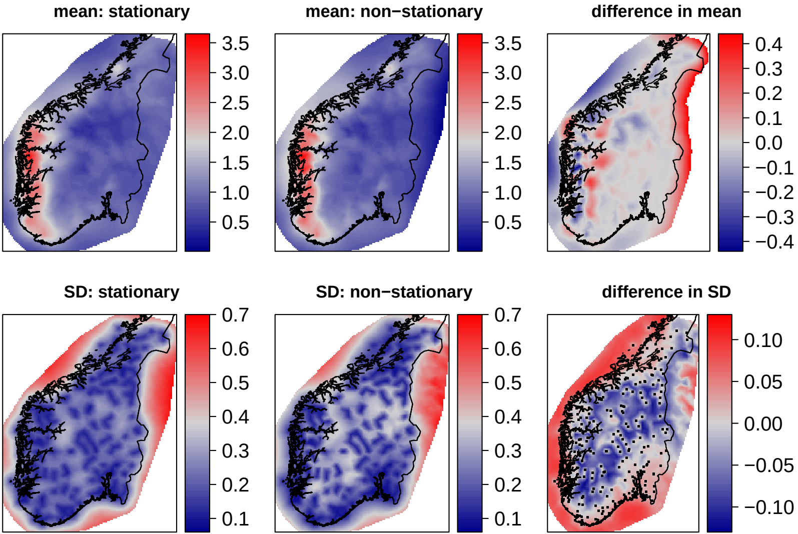
Finite element calculations give

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

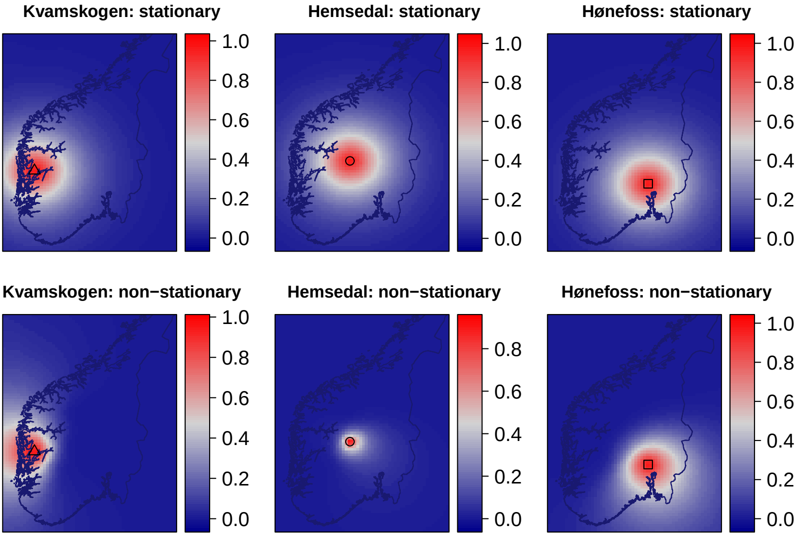
$$C_{ii} = \int \psi_i(\boldsymbol{s})\,d\boldsymbol{s}, \quad G_{ij} = \int \nabla\psi_i(\boldsymbol{s})\cdot\nabla\psi_j(\boldsymbol{s})\,d\boldsymbol{s}$$

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

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.

$$\int_\Omega \lambda(\boldsymbol{s})\,d\boldsymbol{s} \approx \sum_{j=1}^{N} \lambda(\boldsymbol{s}_j) w_j$$

Laplace approximations

Quadratic posterior log-likelihood approximation

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

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

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

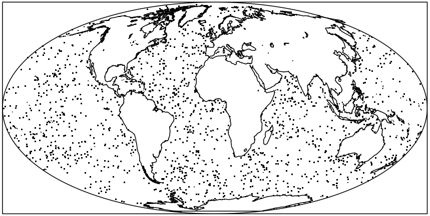
$$\widetilde{\boldsymbol{Q}} = \boldsymbol{Q}_u - \nabla_{\boldsymbol{u}}^2 \ln p(\boldsymbol{y} \mid \boldsymbol{u})\Big|_{\boldsymbol{u}=\widetilde{\boldsymbol{\mu}}}$$

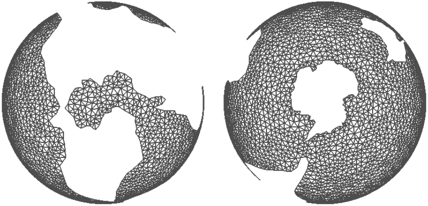
Direct Bayesian inference with INLA (`r-inla.org`)

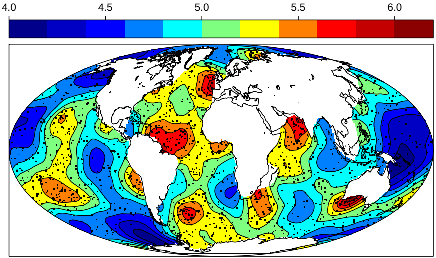
$$\widetilde{p}(\boldsymbol{\theta} \mid \boldsymbol{y}) \propto \left.\frac{p(\boldsymbol{\theta})p(\boldsymbol{u} \mid \boldsymbol{\theta})p(\boldsymbol{y} \mid \boldsymbol{u}, \boldsymbol{\theta})}{p_G(\boldsymbol{u} \mid \boldsymbol{y}, \boldsymbol{\theta})}\right|_{\boldsymbol{u}=\widetilde{\boldsymbol{\mu}}}$$

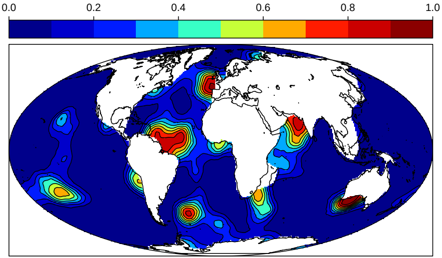
$$\widetilde{p}(\boldsymbol{u}_i \mid \boldsymbol{y}) \propto \int p_{GG}(\boldsymbol{u}_i \mid \boldsymbol{y}, \boldsymbol{\theta})\widetilde{p}(\boldsymbol{\theta} \mid \boldsymbol{y})\, d\boldsymbol{\theta}$$

log-Gaussian Cox point process on a manifold

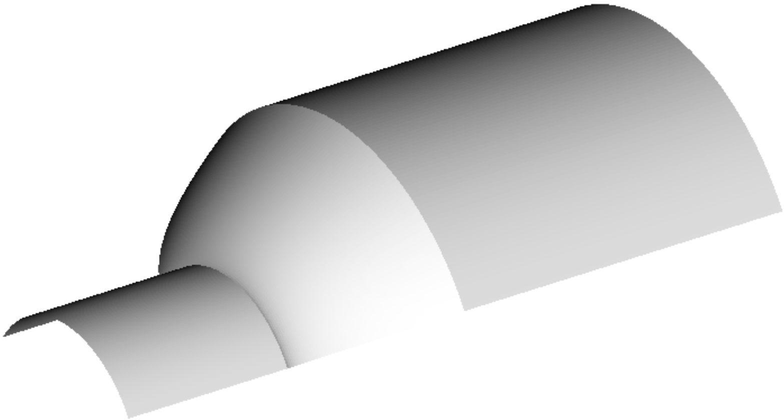




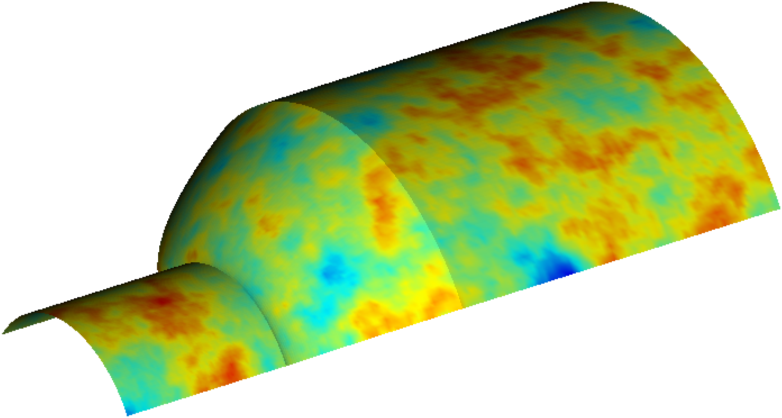




Connection with the deformation method for non-stationarity

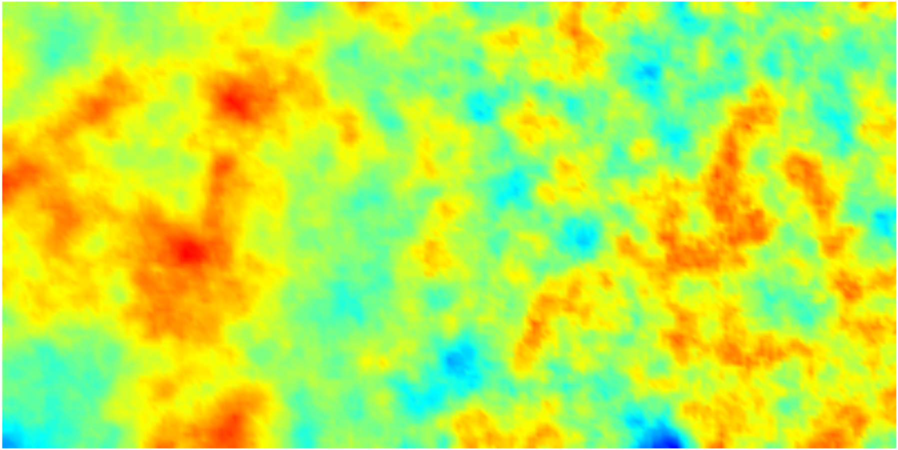


“Stationary” field on deformed manifold



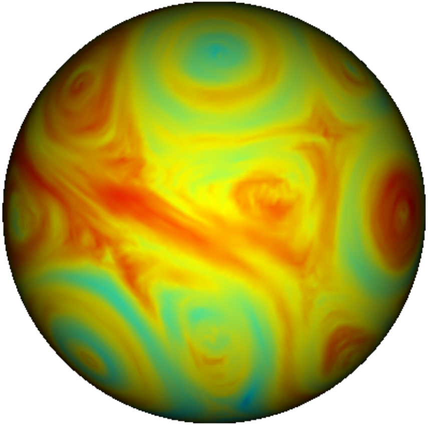
$$(1 - \widetilde{\nabla} \cdot \widetilde{\nabla})\widetilde{u}(\widetilde{\boldsymbol{s}}) = \widetilde{\mathcal{W}}(\widetilde{\boldsymbol{s}}), \quad \widetilde{\boldsymbol{s}} \in \widetilde{\Omega}$$

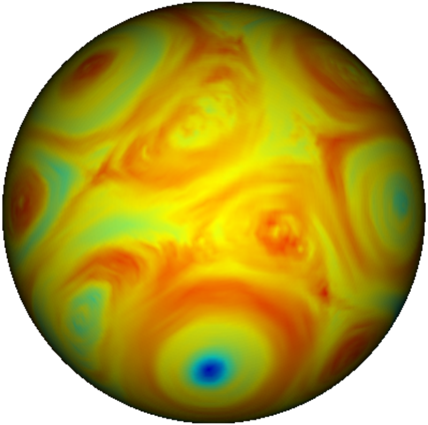
Non-stationary field on original manifold



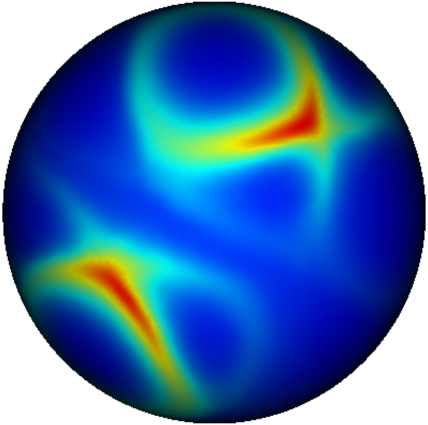
$$(\kappa(\boldsymbol{s})^2 - \nabla \cdot \nabla)u(\boldsymbol{s}) = \kappa(\boldsymbol{s})\mathcal{W}(\boldsymbol{s}), \quad \boldsymbol{s} \in \Omega$$

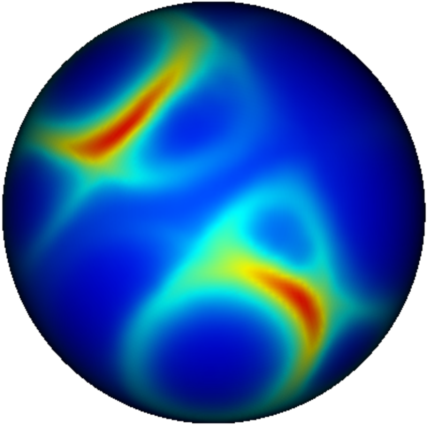
Anisotropic field on a globe via change of manifold metric





Four covariance functions





Stationary models on bounded domains

We want to approximate stationary solutions to

$$(\kappa^2 - \nabla \cdot \nabla)^{\alpha/2} u(\boldsymbol{s}) = W(\boldsymbol{s}), \quad \boldsymbol{s} \in \mathbb{R}^d$$

We actually approximate solutions to

$$\begin{cases} (\kappa^2 - \nabla \cdot \nabla)^{\alpha/2} u(\boldsymbol{s}) = W(\boldsymbol{s}), & \boldsymbol{s} \in \Omega \subset \mathbb{R}^d \\ \partial_{\boldsymbol{n}} (\kappa^2 - \nabla \cdot \nabla)^{k} u(\boldsymbol{s}) = 0, & \boldsymbol{s} \in \partial\Omega,\ k = 0, 1, \ldots, \lfloor (\alpha - 1)/2 \rfloor . \end{cases}$$

For a stationary field, the spectrum for $(u(\cdot), \partial_{\boldsymbol{n}} u(\cdot))$ for some unit vector $\boldsymbol{n}$ is

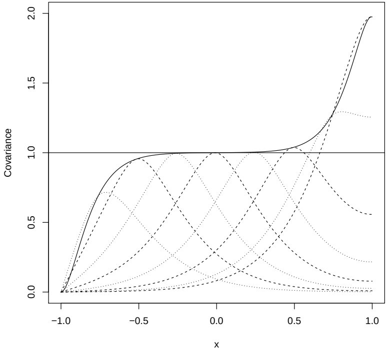
$$S_u(\boldsymbol{\omega}) \begin{bmatrix} 1 & -i\boldsymbol{n} \cdot \boldsymbol{\omega} \\ i\boldsymbol{n} \cdot \boldsymbol{\omega} & (\boldsymbol{n} \cdot \boldsymbol{\omega})^2 \end{bmatrix}$$

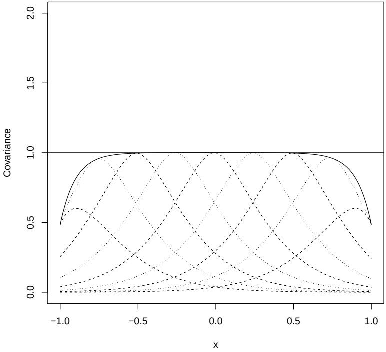
showing that $u(\cdot)$ and $\partial_{\boldsymbol{n}} u(\cdot)$ should be independent along lines perpendicular to $\boldsymbol{n}$.

Classic approaches to constraining boundary behaviour

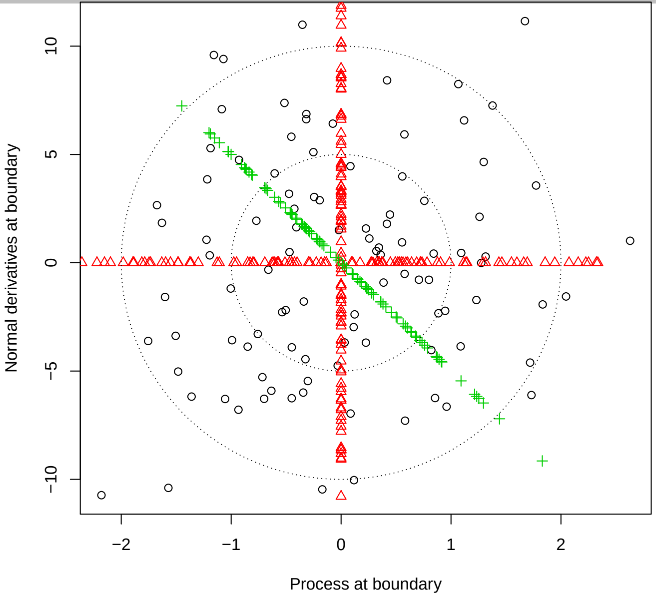
Deterministic boundary conditions

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





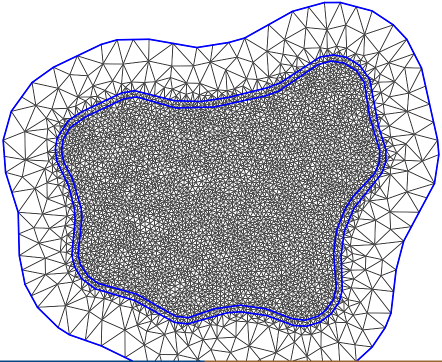
All deterministic boundary conditions are 'inappropriate'



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:

$$w = \begin{bmatrix} u \\ \partial_{\boldsymbol{n}} u \end{bmatrix}$$

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

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

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

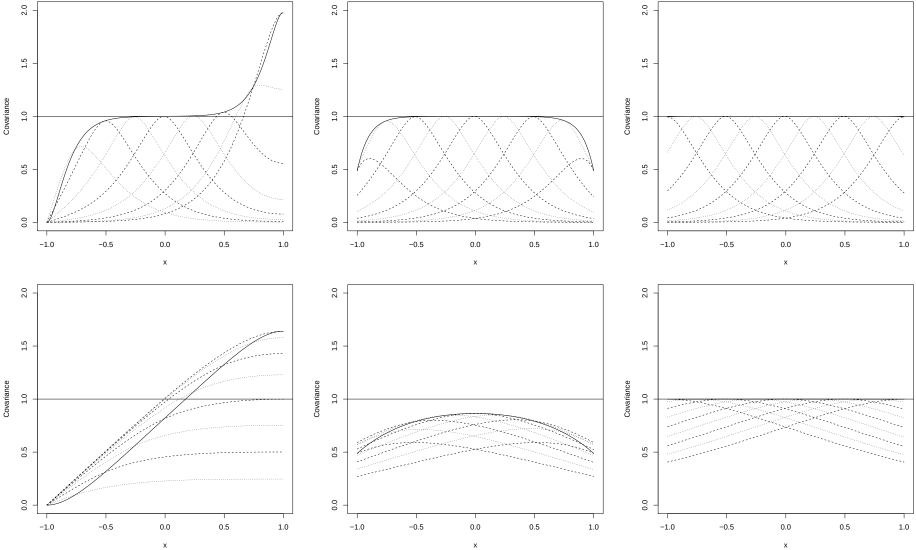
Scalar product for projection:

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

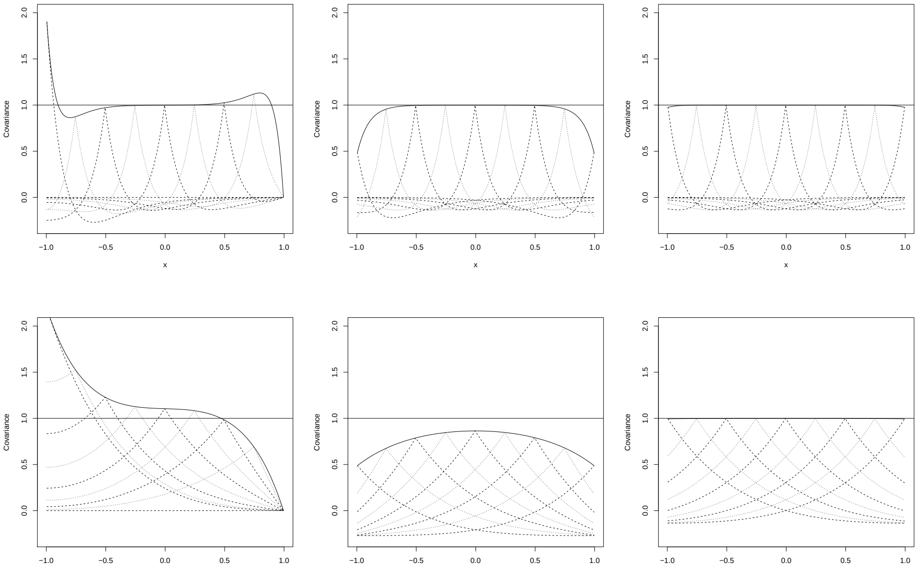
Spectral characterisation of stationary solutions

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

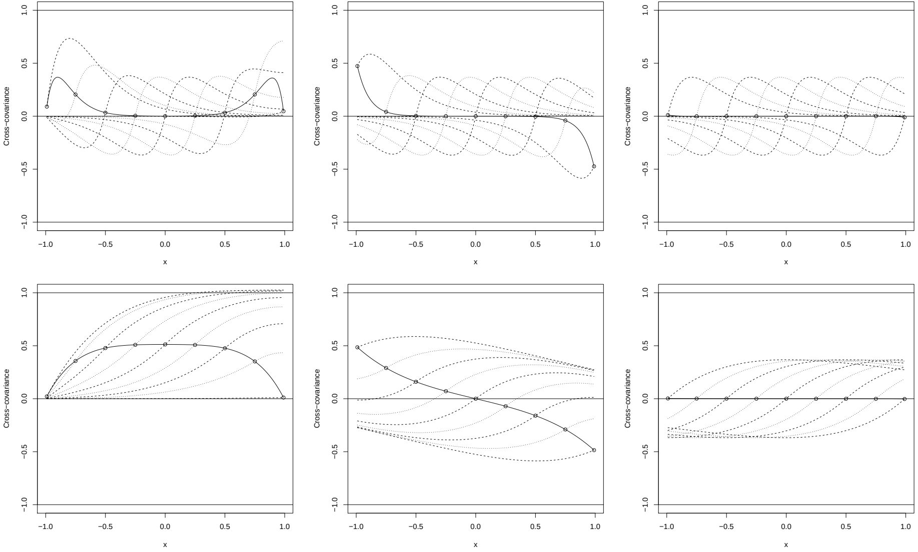
Covariances (D&N, Robin, Stoch) for $\kappa = 5$ and 1



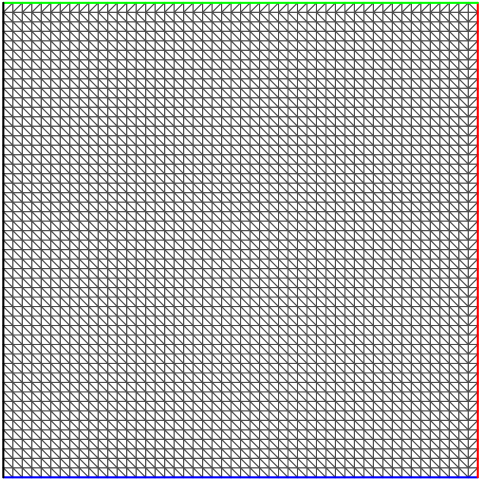
Derivative covariances (D&N, Robin, Stoch) for $\kappa = 5$ and 1



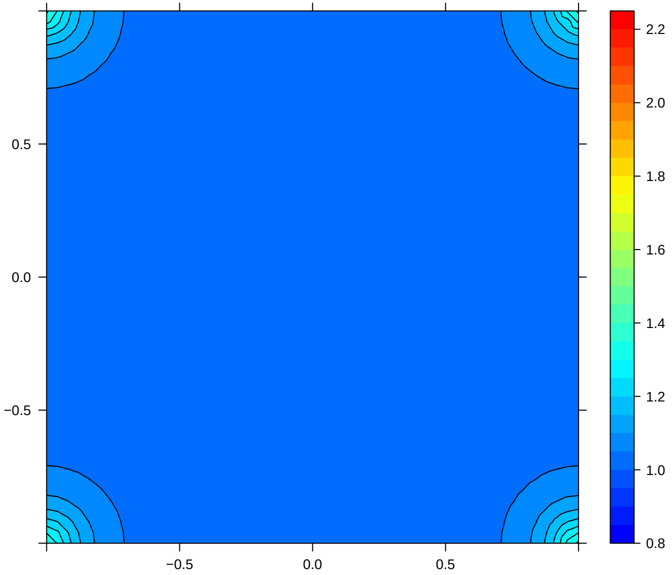
Process-derivative cross-covariances (D&N, Robin, Stoch)



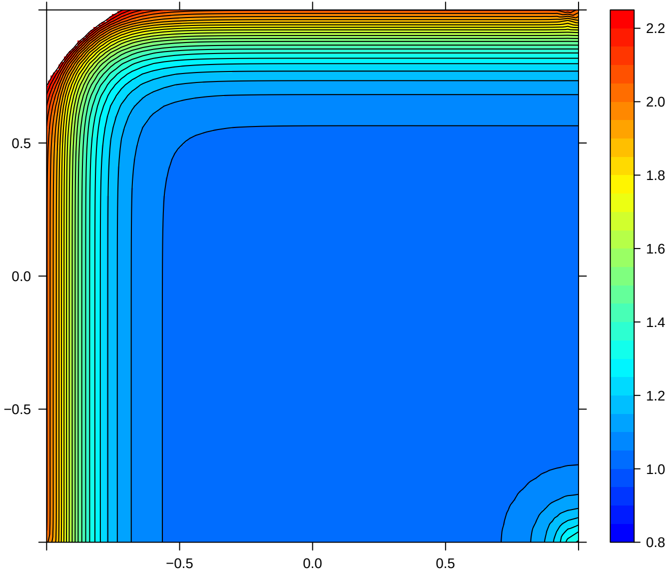
Square domain, basis triangulation



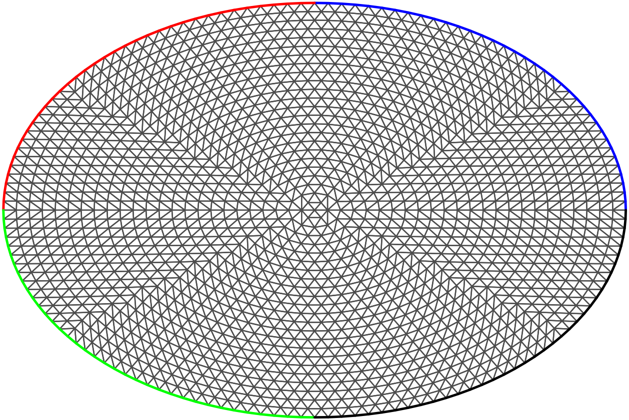
Square domain, stochastic boundary (variances)



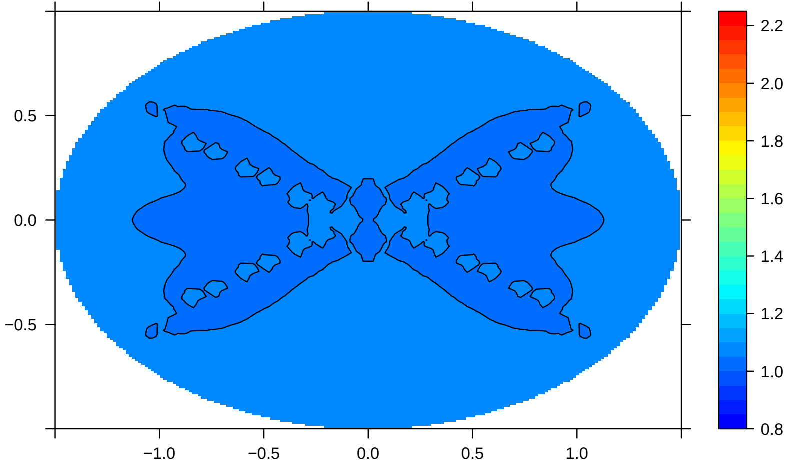
Square domain, mixed boundary (variances)



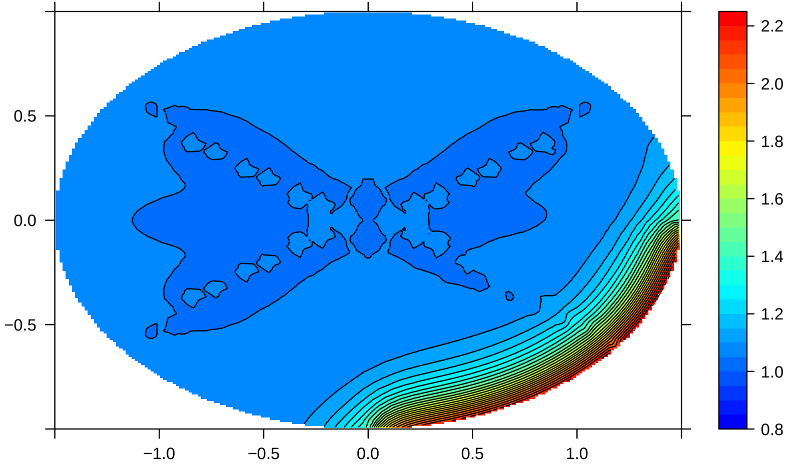
Elliptical domain, basis triangulation



Elliptical domain, stochastic boundary (variances)



Elliptical domain, mixed boundary (variances)



Linear model for weather observations

Weather = Climate + Anomaly

$$\mathbf{z} \sim \mathsf{N}(\mathbf{0}, \mathbf{Q}_z^{-1}) \quad \text{(climate: space-time model)}$$

$$z(t, \mathbf{s}) = \sum_k B_k(t)\mathbf{z}_k(\mathbf{s}) \quad \text{(basis function representation)}$$

$$\mathbf{a} \sim \mathsf{N}(\mathbf{0}, \mathbf{I} \otimes \mathbf{Q}_a^{-1}) \quad \text{(anomaly: spatial model, indep. in time)}$$

$$w(t, \mathbf{s}) = a(t, \mathbf{s}) + z(t, \mathbf{s}) \quad \text{(weather)}$$

$$y_i = \text{altitude effect } + w(t_i, \mathbf{s}_i) + \epsilon_i \quad \text{(observations)}$$

$$\epsilon \sim \mathsf{N}(0, \mathbf{Q}_\epsilon^{-1})$$

$$\mathbf{y} = \mathbf{A}(\mathbf{a} + (\mathbf{B} \otimes \mathbf{I})\mathbf{z}) + \epsilon$$

Stochastic weather anomaly model

Non-stationary spatial SPDE

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

$$\log \kappa(\mathbf{s}) = \sum B_k^\kappa(\mathbf{s})\theta_k$$

$$\log \tau(\mathbf{s}) = \sum B_k^\tau(\mathbf{s})\theta_k$$

Precision

$$\boldsymbol{K}_{ii} = \kappa(\mathbf{s}_i) \quad \boldsymbol{T}_{ii} = \tau(\mathbf{s}_i)$$

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

Stochastic climate model

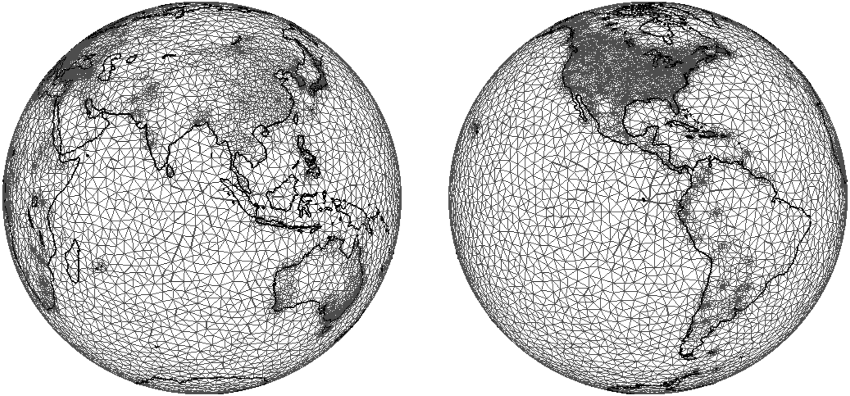
Simplified heat equation with spatially correlated noise

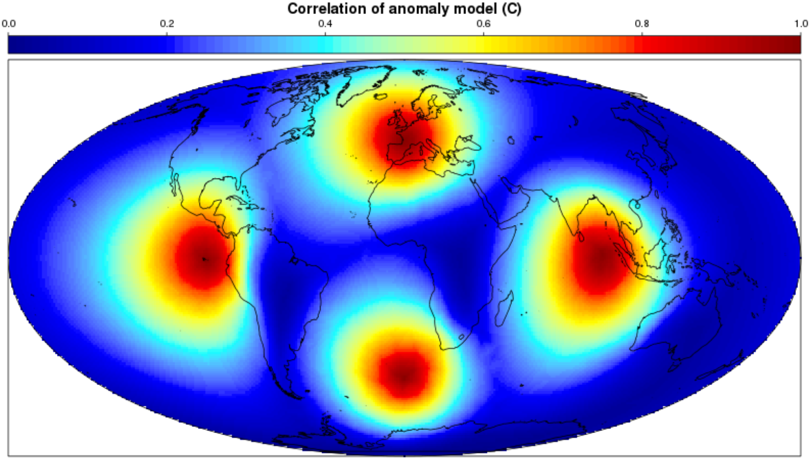
$$\gamma_t \dot{z}(\mathbf{s}, t) - \Delta z(\mathbf{s}, t) = \gamma_s^{-1/2} \mathcal{E}(\mathbf{s}, t)$$
$$\mathcal{E}(\mathbf{s}, \delta t) - \gamma_{\mathcal{E}} \Delta \mathcal{E}(\mathbf{s}, \delta t) = \mathcal{W}_{\mathcal{E}}(\mathbf{s}, \delta t)$$

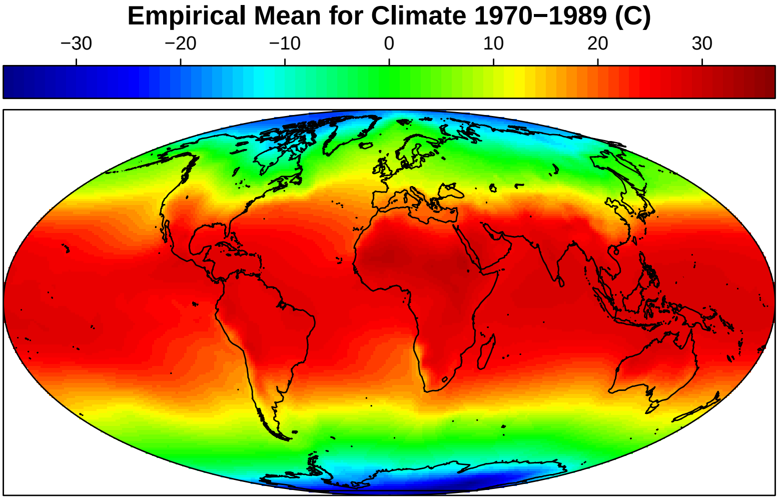
Precision

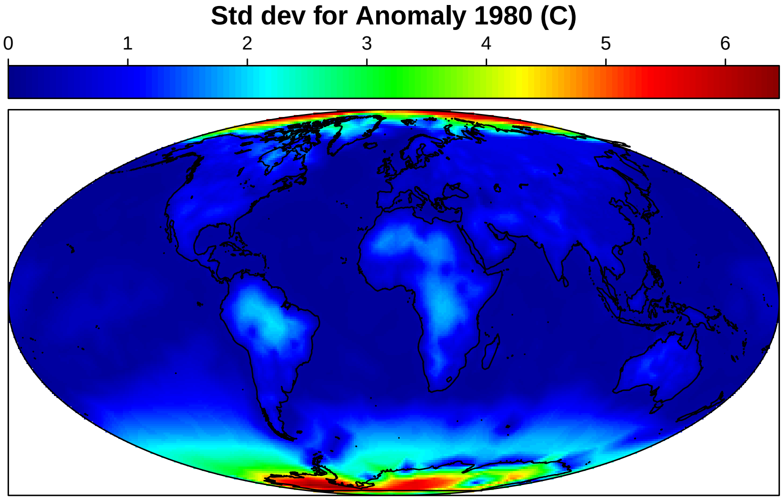
$$\mathbf{Q}_z = \gamma_s \left(\gamma_t^2 \mathbf{M}_0 + 2\gamma_t \mathbf{M}_1 + \mathbf{M}_2\right)$$
$$\mathbf{M}_0 = \mathbf{M}_2^{(t)} \otimes \mathbf{C}(\mathbf{I} + \gamma_{\mathcal{E}} \mathbf{C}^{-1}\mathbf{G})$$
$$\mathbf{M}_1 = \mathbf{M}_1^{(t)} \otimes \mathbf{G}(\mathbf{I} + \gamma_{\mathcal{E}} \mathbf{C}^{-1}\mathbf{G})$$
$$\mathbf{M}_2 = \mathbf{M}_0^{(t)} \otimes \mathbf{G}\mathbf{C}^{-1}\mathbf{G}(\mathbf{I} + \gamma_{\mathcal{E}} \mathbf{C}^{-1}\mathbf{G})$$
$$\mathbf{Q}_x = \phi^2 \mathbf{M}_0^{(t)} + 2\phi \mathbf{M}_1^{(t)} + \mathbf{M}_2^{(t)}, \quad \dot{x}(t) + \phi x(t) = \mathcal{W}(t)$$

Spherical triangulation GMRF/SPDE




Correlation of anomaly model (C)
0.0
0.2
0.4
0.6
0.8
1.0


Empirical Mean for Climate 1970−1989 (C)
−30
−20
−10
0
10
20
30


Std dev for Anomaly 1980 (C)
0
1
2
3
4
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Practical computations: Precision structure

Problem: Large, ill-conditioned precision with interlocking blocks

Reparameterisation gives a more well behaved matrix

$$\mathbf{Q}_{(\mathbf{a},\mathbf{z})|\mathbf{y}} = \begin{bmatrix} \mathbf{I}\otimes\mathbf{Q}_a & 0 \\ 0 & \mathbf{Q}_z \end{bmatrix} + \begin{bmatrix} \mathbf{A}^T \\ (\mathbf{B}^T\otimes\mathbf{I})\mathbf{A}^T \end{bmatrix} \mathbf{Q}_\varepsilon \begin{bmatrix} \mathbf{A} & \mathbf{A}(\mathbf{B}\otimes\mathbf{I}) \end{bmatrix}$$

$$\mathbf{Q}_{(\mathbf{z}+\mathbf{a},\mathbf{z})|\mathbf{y}} = \begin{bmatrix} \mathbf{I}\otimes\mathbf{Q}_a + \mathbf{A}^T\mathbf{Q}_\varepsilon\mathbf{A} & -\mathbf{B}\otimes\mathbf{Q}_a \\ -\mathbf{B}^T\otimes\mathbf{Q}_a & \mathbf{Q}_z + (\mathbf{B}^T\mathbf{B})\otimes\mathbf{Q}_a \end{bmatrix}$$

Use conditional distributions

Block-Rao-Blackwellised Monte Carlo integration

$$\mathsf{Var}(\mathbf{x}_1) \approx \mathsf{Var}(\mathbf{x}_1 \mid \mathbf{x}_2) + \frac{1}{N}\sum_{k=1}^{N}\left(\mathsf{E}(\mathbf{x}_1 \mid \mathbf{x}_2^{(k)}) - \mathsf{E}(\mathbf{x}_1)\right)^2$$

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