An explicit link between Gaussian fields and Gaussian Markov random fields; the stochastic partial differential equation approach

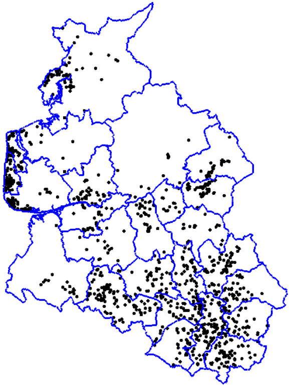
Finn Lindgren[1] Håvard Rue[1] Johan Lindström[2]

[1]Department of Mathematical Sciences
Norwegian University of Science and Technology, Trondheim, Norway

[2]Mathematical Statistics
Centre for Mathematical Sciences, Lund University, Lund, Sweden

RSS, London, 16th March 2011

Computationally efficent spatial models



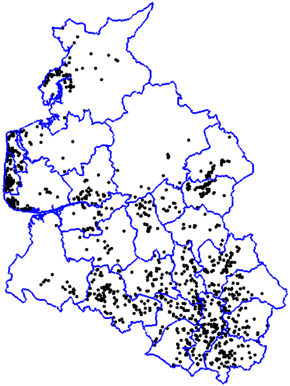
Leukaemia survival in NW England

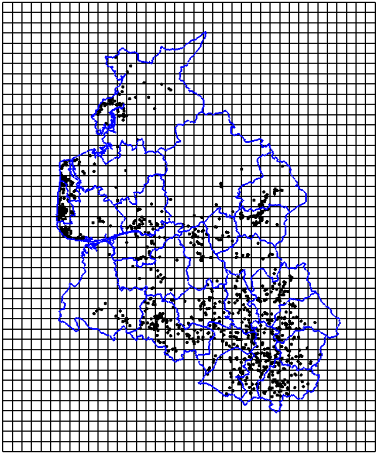
Spatial random field models

Dense covariance:
$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
$\Longrightarrow$ expensive computations

Sparse precision:
$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{Q}^{-1})$
$\Longrightarrow$ efficient computations

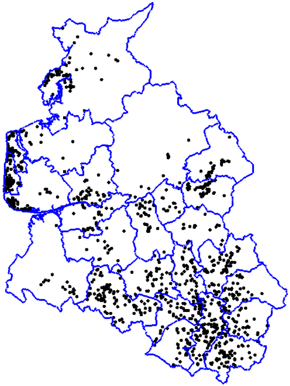
Irregular discrete data locations – lattice CAR models

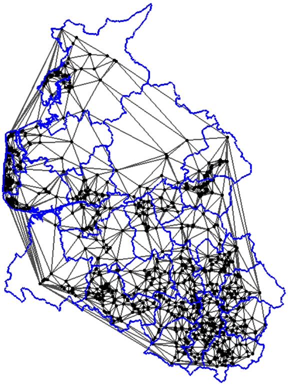




We need models with well-defined continuous interpretation

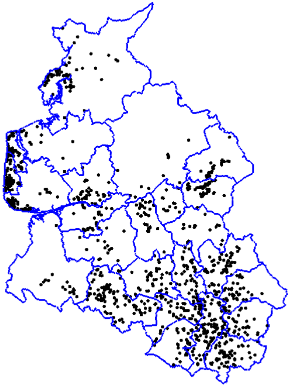
Irregular discrete data locations – triangular graph

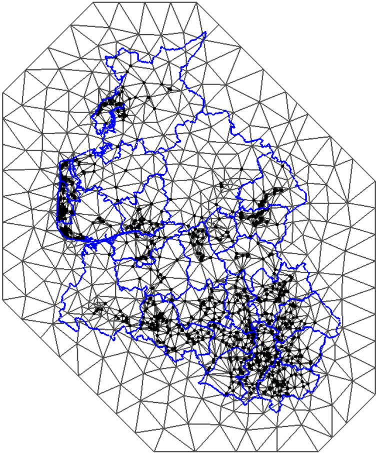




We need models with well-defined continuous interpretation

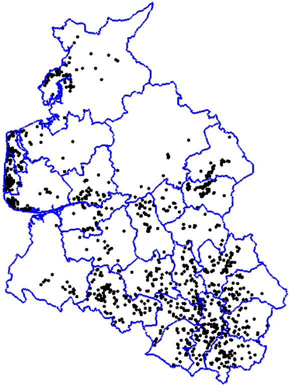
Irregular discrete data locations – refined triangulation

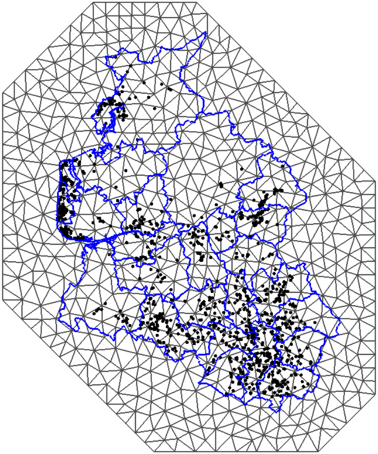




We need models with well-defined continuous interpretation

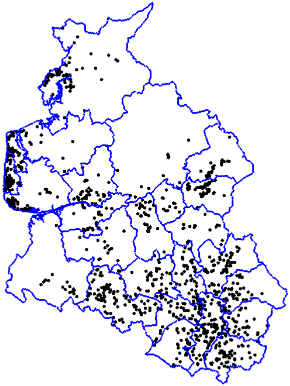
Irregular discrete data locations – smooth triangulation

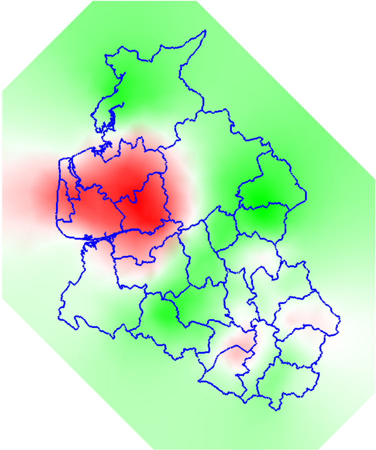




We need models with well-defined continuous interpretation

Irregular discrete data locations – continuous space

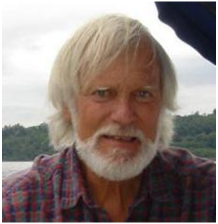




We need models with well-defined continuous interpretation

Conditional autoregression models on lattices

GMRF	Covariance	
CAR(2)	$\propto \kappa\|\mathbf{u}\| K_1(\kappa\|\mathbf{u}\|)$	Whittle (1954)
CAR(1)	$\frac{1}{2\pi} K_0(\kappa\|\mathbf{u}\|)$	Besag (1981)
ICAR(1)	$-\frac{1}{2\pi}\log(\|\mathbf{u}\|)$	Besag & Mondal (2005)



Matérn covariances (Bertil Matérn)

The Matérn covariance family

$$\mathrm{Cov}(x(\mathbf{0}), x(\mathbf{u})) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} (\kappa \|\mathbf{u}\|)^\nu K_\nu(\kappa \|\mathbf{u}\|), \quad \mathbf{u} \in \mathbb{R}^d$$

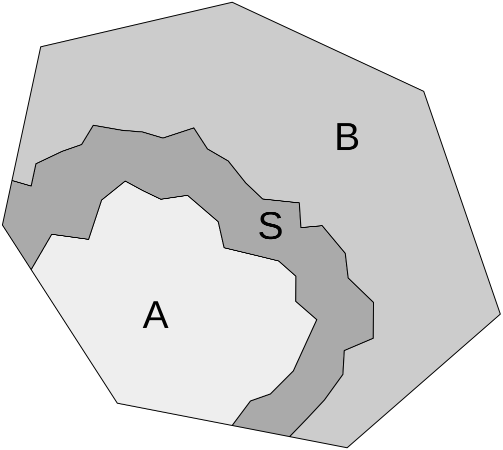
Scale $\kappa > 0$, smoothness $\nu > 0$, variance $\sigma^2 > 0$

Are any other discrete domain Markov fields close to Matérn fields?

Are any Matérn fields continuous domain Markov fields?

The continuous domain Markov property

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



Identifying a Markov field by its spectrum

Spectral representation: $x(\mathbf{u}) = \int_{\mathbb{R}^d} \exp(i\mathbf{u}\cdot\mathbf{k})\,\widehat{x}(\mathbf{k})\,\mathrm{d}\mathbf{k}$

Spectrum: $S_x(\mathbf{k}) = \mathrm{E}(|\widehat{x}(\mathbf{k})|^2)$

Rozanov (1977)

$$x(\mathbf{u}) \text{ is Markov} \iff S_x(\mathbf{k}) \propto P(\mathbf{k})^{-1}$$

where $P(\mathbf{k})$ is a non-negative symmetric polynomial

What is the spectrum of a Matérn field?

The Whittle-Matérn connection

Whittle (1954, 1963)

Matérn fields on $\mathbb{R}^d$ are stationary solutions to the SPDE

$$(\kappa^2 - \Delta)^{\alpha/2} x(\mathbf{u}) = \mathcal{W}(\mathbf{u}), \quad \alpha = \nu + d/2$$

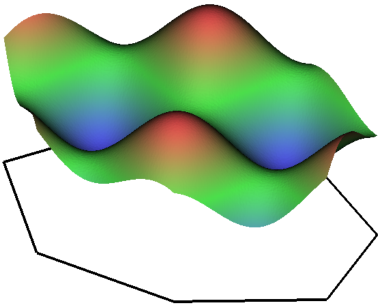
The spectrum is $S_x(\mathbf{k}) = (2\pi)^{-d}(\kappa^2 + \|\mathbf{k}\|^2)^{-\alpha}$

Therefore Matérn fields are Markov when $\nu + d/2$ is an integer.

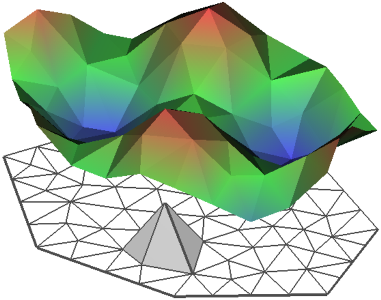
Laplacian: $\Delta = \sum_{i=1}^{d} \frac{\partial^2}{\partial u_i^2}$

Piecewise linear representations

$x(\mathbf{u}) = \cos(u_1) + \sin(u_2)$



$x(\mathbf{u}) = \sum_k \psi_k(\mathbf{u})\, x_k$



Guiding principle

Attack the SPDE with local finite dimensional representations instead of covariances or kernels (subsets of Green's functions)!

The best piecewise linear approximation $\sum_k \psi_k(\mathbf{u})\, x_k$

Projection of the SPDE: Linear systems of equations ($\alpha = 2$)

$$\sum_j \Big(\kappa^2 \underbrace{\langle \psi_i,\, \psi_j \rangle}_{\mathbf{C}_{ij}} + \underbrace{\langle \psi_i,\, -\Delta \psi_j \rangle}_{\mathbf{G}_{ij}}\Big) x_j \overset{D}{=} \langle \psi_i,\, \mathcal{W} \rangle \quad \text{jointly for all } i.$$

$\mathbf{C}$ and $\mathbf{G}$ are as sparse as the triangulation neighbourhood

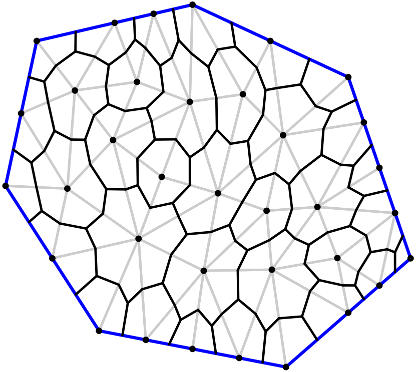
Constructing the precision matrices

$\mathbf{K} = \kappa^2 \mathbf{C} + \mathbf{G}$	$\alpha = 1$	$\alpha = 2$	$\alpha = 3, 4, \ldots$
$\mathbf{K}\mathbf{x}$	$\mathcal{N}(\mathbf{0}, \mathbf{K})$	$\mathcal{N}(\mathbf{0}, \mathbf{C})$	$\mathcal{N}\left(\mathbf{0}, \mathbf{C}\mathbf{Q}_{\mathbf{x},\alpha-2}^{-1}\mathbf{C}\right)$
$\mathbf{Q}_{\mathbf{x},\alpha}$	$\mathbf{K}$	$\mathbf{K}^{\mathsf{T}}\mathbf{C}^{-1}\mathbf{K}$	$\mathbf{K}^{\mathsf{T}}\mathbf{C}^{-1}\mathbf{Q}_{\mathbf{x},\alpha-2}\mathbf{C}^{-1}\mathbf{K}$

Markov approximation

$\mathbf{C}^{-1}$ is dense, which leads to non-Markov models!

The diagonal matrix $\widetilde{\mathbf{C}}$, $\widetilde{\mathbf{C}}_{i,i} = \langle \psi_i, 1 \rangle =$ the local cell area, gives a sparse precision with the total energy preserved.



Lattice on $\mathbb{R}^2$, node distance h, regular triangulation

Order $\alpha = 1$: generalised covariance $\frac{1}{2\pi} K_0(\kappa\|\mathbf{u}\|)$

$$\kappa^2 h^2 \begin{bmatrix} & & \\ & 1 & \\ & & \end{bmatrix} + \begin{bmatrix} & -1 & \\ -1 & 4 & -1 \\ & -1 & \end{bmatrix}$$

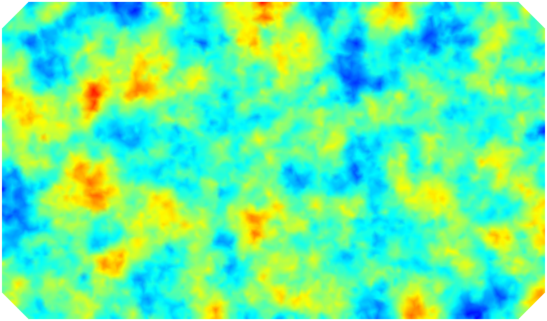
Order $\alpha = 2$: covariance $\frac{1}{4\pi\kappa^2} \kappa\|\mathbf{u}\| \, K_1(\kappa\|\mathbf{u}\|)$

$$\kappa^4 h^2 \begin{bmatrix} & & \\ & 1 & \\ & & \end{bmatrix} + 2\kappa^2 \begin{bmatrix} & -1 & \\ -1 & 4 & -1 \\ & -1 & \end{bmatrix} + \frac{1}{h^2} \begin{bmatrix} & & 1 & & \\ & 2 & -8 & 2 & \\ 1 & -8 & 20 & -8 & 1 \\ & 2 & -8 & 2 & \\ & & 1 & & \end{bmatrix}$$

Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

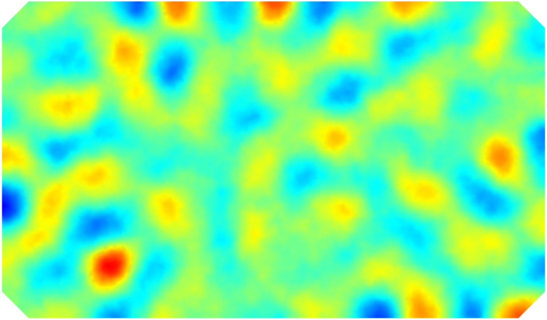
$$(\kappa^2 - \Delta)^{\alpha/2}(\tau\, x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^d$$



Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

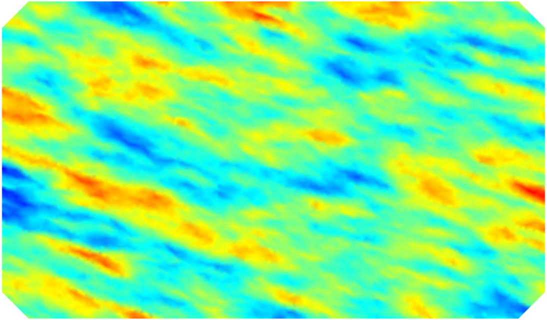
$$(\kappa^2 e^{i\pi\theta} - \Delta)^{\alpha/2}(\tau\, x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^d$$



Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

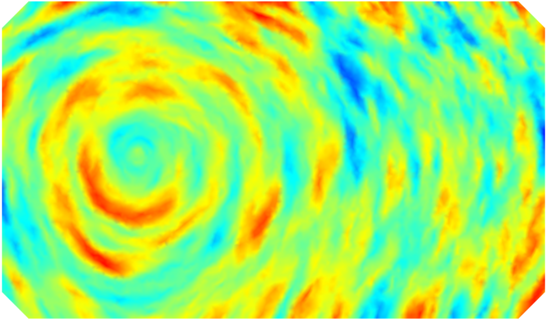
$$(\kappa^2 + \nabla \cdot \mathbf{m} - \nabla \cdot \mathbf{M}\nabla)^{\alpha/2}(\tau x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^d$$



Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

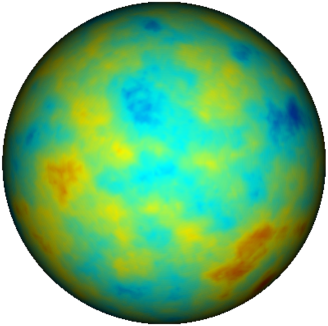
$$(\kappa_{\mathbf{u}}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u}} - \nabla \cdot \mathbf{M}_{\mathbf{u}} \nabla)^{\alpha/2} (\tau_{\mathbf{u}} x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^d$$

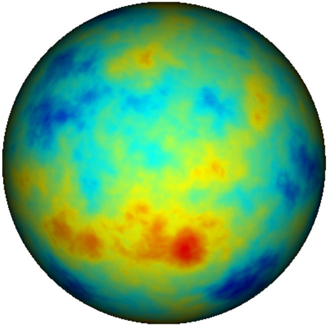


Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

$$(\kappa_{\mathbf{u}}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u}} - \nabla \cdot \mathbf{M}_{\mathbf{u}} \nabla)^{\alpha/2} (\tau_{\mathbf{u}} x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \Omega$$

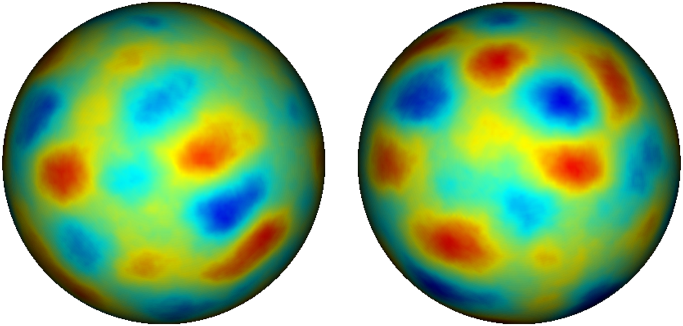




Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

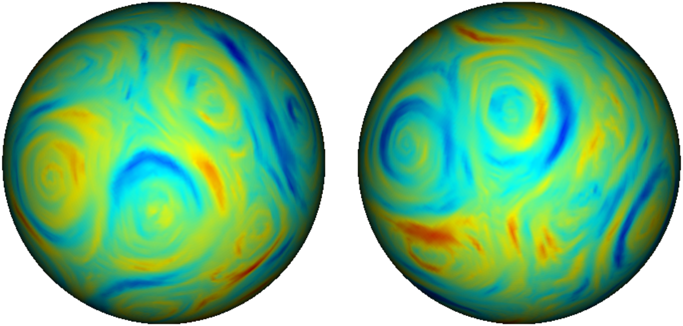
$$(\kappa_{\mathbf{u}}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u}} - \nabla \cdot \mathbf{M}_{\mathbf{u}} \nabla)^{\alpha/2} (\tau_{\mathbf{u}} x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \Omega$$



Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

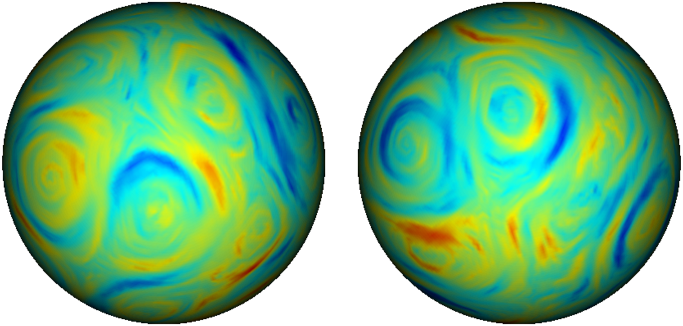
$$(\kappa_{\mathbf{u}}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u}} - \nabla \cdot \mathbf{M}_{\mathbf{u}} \nabla)^{\alpha/2} (\tau_{\mathbf{u}} x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \Omega$$



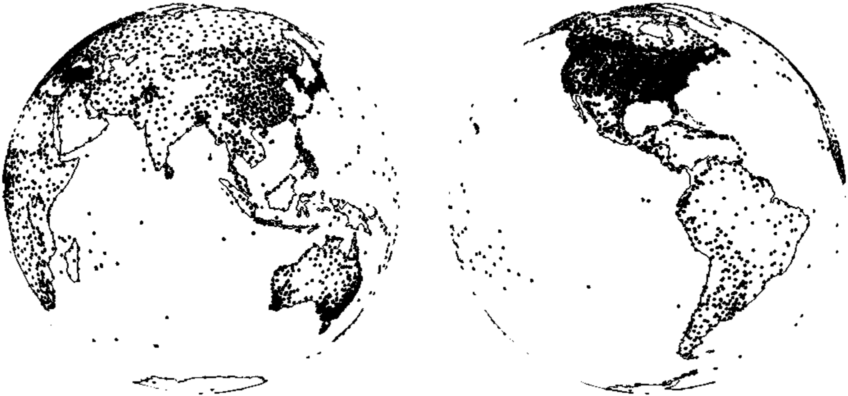
Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

$$\left(\frac{\partial}{\partial t} + \kappa_{\mathbf{u},t}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u},t} - \nabla \cdot \mathbf{M}_{\mathbf{u},t} \nabla\right) (\tau_{\mathbf{u},t} x(\mathbf{u},t)) = \mathcal{E}(\mathbf{u},t), \quad (\mathbf{u},t) \in \Omega \times \mathbb{R}$$



Large spatial problems: covariances are impractical



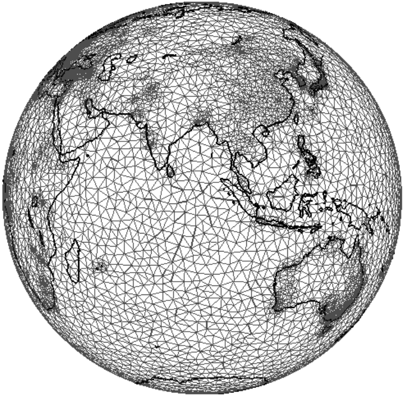
Data points $n \approx 2500 \cdot 20$ Kriging locations $m \approx 15000 \cdot 20$

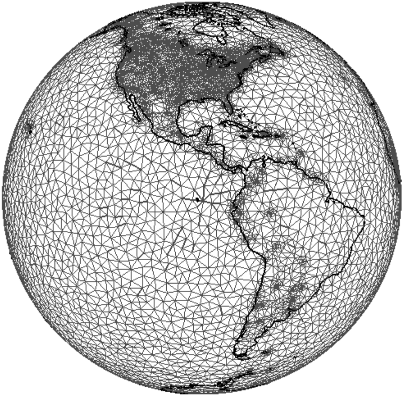
Estimation: time $\mathcal{O}(n^3)$, storage $\mathcal{O}(n^2) \sim 20\,Gbytes$

Kriging: time $\mathcal{O}(mn + n^3)$, storage $\mathcal{O}(mn + n^2) \sim 130\,Gbytes$

This is *not* a “huge” data set.

Practical triangulation based GMRFs





Data points $n \approx 2500 \cdot 20$ Basis functions $m \approx 15000 \cdot 20$

Estimation+Kriging: time $\mathcal{O}(m^{3/2})$, storage $\mathcal{O}(m+n) \sim 50 Mbytes$

Global temperature analysis

- http://www.ncdc.noaa.gov/ghcn/ghcn.html
- Monthly average temperatures
- On average 2500 locations per year
- Covariate data (elevation, land use, etc.) for 7000 stations

Model for yearly mean temperatures

Observations : temperature $\sim$ elevation + climate + anomaly

Climate : $\mu_{\mathbf{u}},\ \tau_{\mathbf{u}},\ \kappa_{\mathbf{u}}^2 = \sum_k \psi_k^{\cdot}(\mathbf{u})\theta_k^{\cdot}$

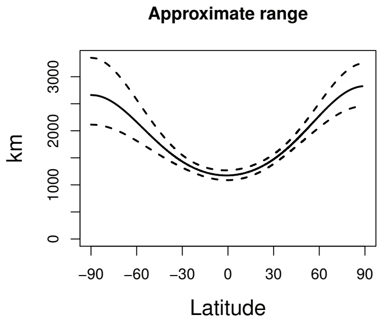
Anomaly : $\left(\kappa_{\mathbf{u}}^2 - \Delta\right)\left(\tau_{\mathbf{u}} x_t(\mathbf{u})\right) = \mathcal{W}(\mathbf{u})$

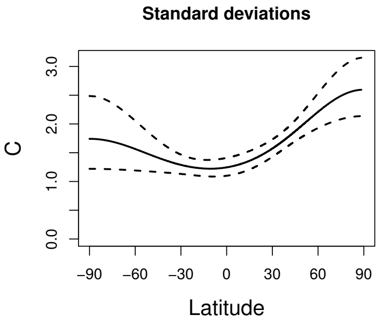
Weather : $\mu(\mathbf{u}) + x_t(\mathbf{u})$

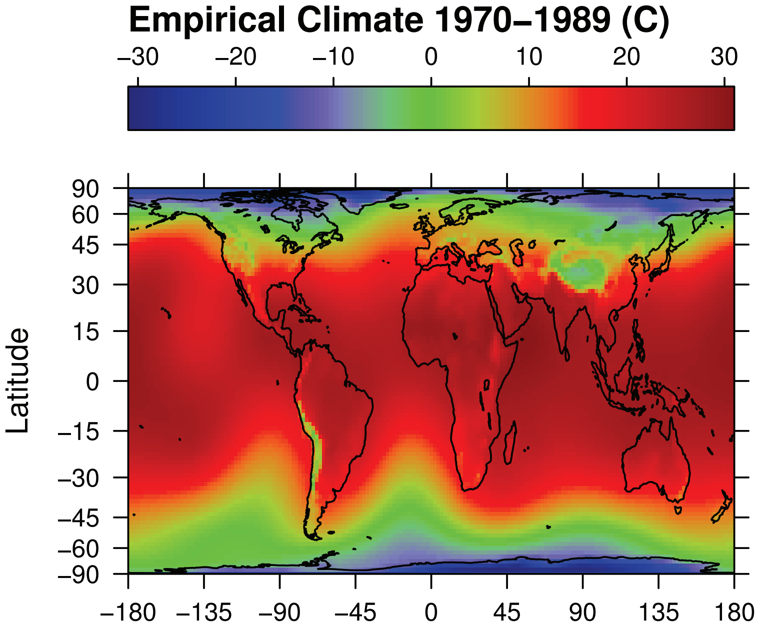
Code outline for Bayesian inference with R-INLA

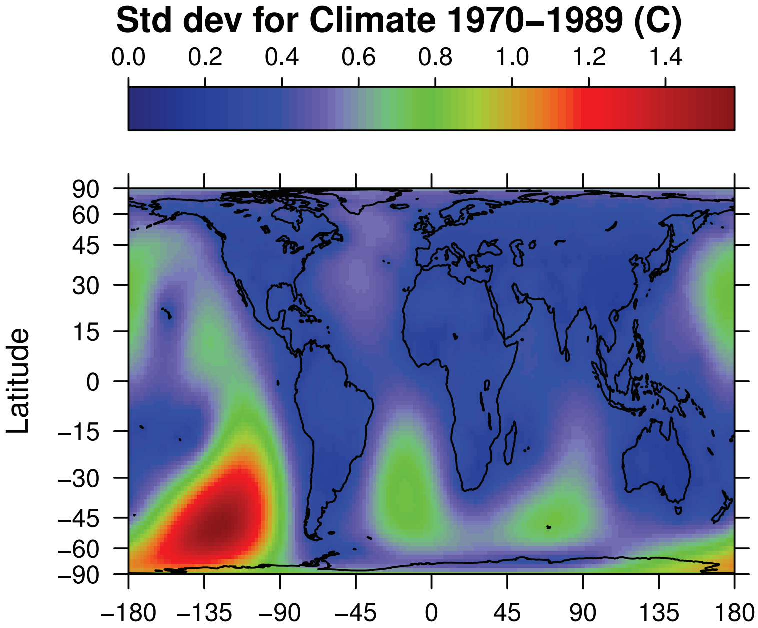
```
mesh = inla.mesh(loc=station.locations, ## optional
                 cutoff=10/earth.radius,
                 refine=list(max.edge=500/earth.radius))
...
spde = inla.spde(mesh, model="matern", ...
                 param=list(basis.T=B.tau, ...))
...
formula = temperature ~ elevation + climate.mu +
                        f(anomaly, model=spde,
                          replicate=year)
...
result = inla(formula, data, family="gaussian", ...)
```

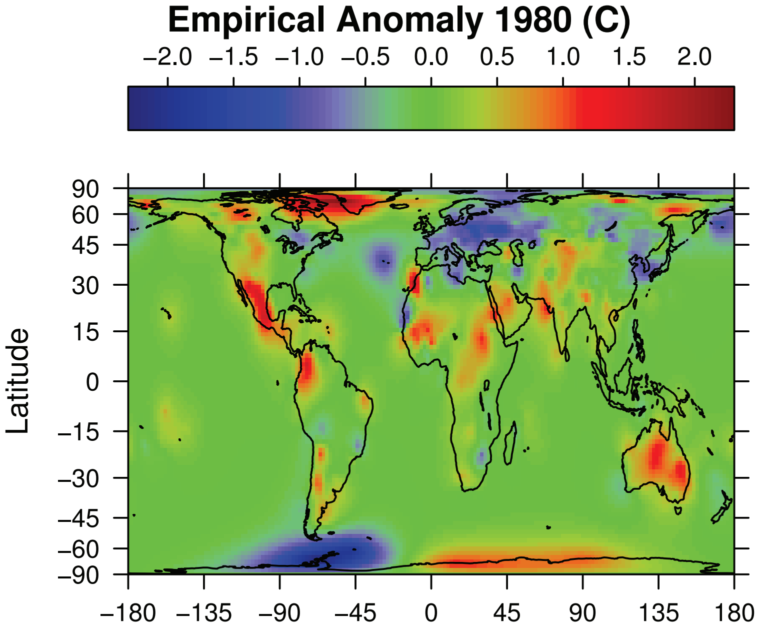
Estimated climate covariance properties 1970-1989

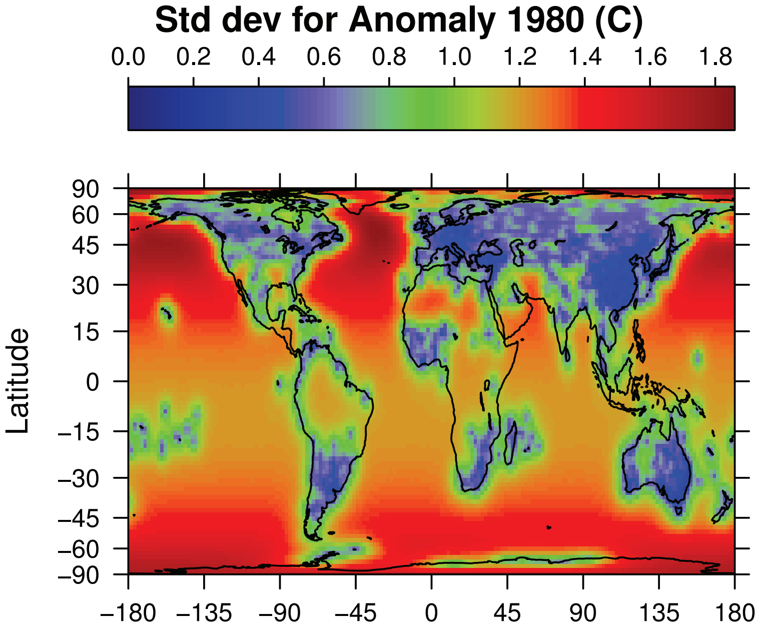





Empirical Climate 1970–1989 (C)
–30 –20 –10 0 10 20 30
Latitude
90 60 45 30 15 0 –15 –30 –45 –60 –90
–180 –135 –90 –45 0 45 90 135 180


Std dev for Climate 1970–1989 (C)
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4
Latitude
90 60 45 30 15 0 –15 –30 –45 –60 –90
–180 –135 –90 –45 0 45 90 135 180


Empirical Anomaly 1980 (C)
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2.0
Latitude
90 60 45 30 15 0 −15 −30 −45 −60 −90
−180 −135 −90 −45 0 45 90 135 180


Std dev for Anomaly 1980 (C)
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8
Latitude
90 60 45 30 15 0 –15 –30 –45 –60 –90
–180 –135 –90 –45 0 45 90 135 180

Conclusion

SPDE/GMRF

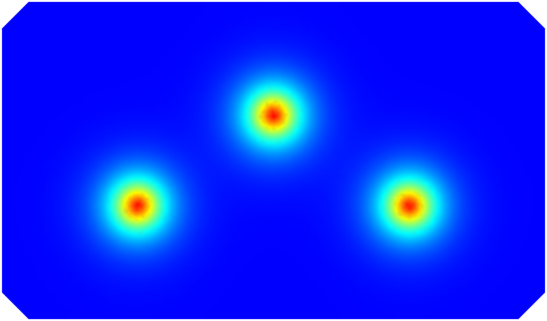
The connection allows for consistent local specifications of general spatio-temporal models that allow efficient practical computations.

- Unavoidably beyond the traditional computational statistics toolbox
- Combines standard concepts from different areas in applied mathematics and engineering
- Detailed knowledge of SPDEs is not needed for practical use
- Open source software available: `http://www.r-inla.org/`

Covariances for Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

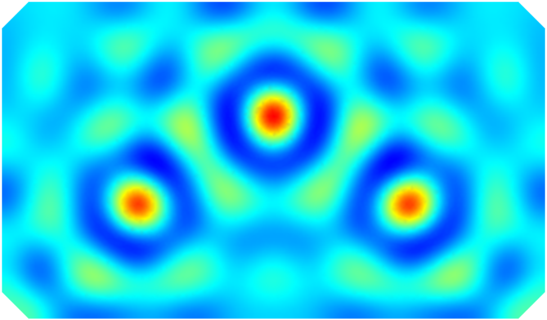
$$(\kappa^2 - \Delta)^{\alpha/2}(\tau\, x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^d$$



Covariances for Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

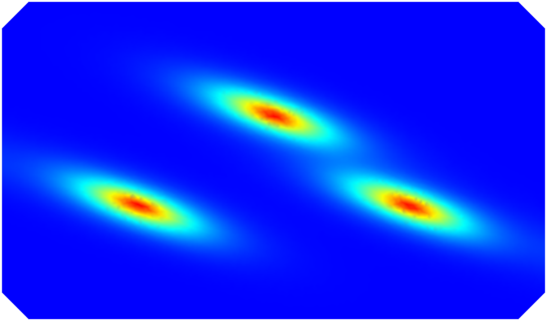
$$(\kappa^2 e^{i\pi\theta} - \Delta)^{\alpha/2}(\tau\, x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^d$$



Covariances for Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

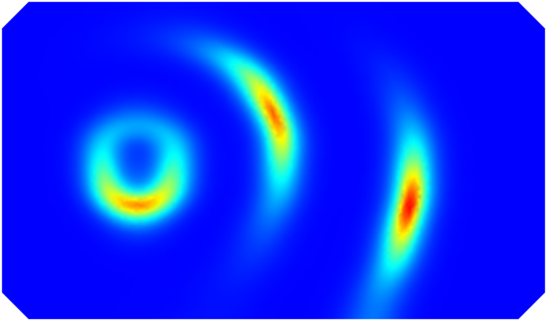
$$(\kappa^2 + \nabla \cdot \mathbf{m} - \nabla \cdot \mathbf{M}\nabla)^{\alpha/2}(\tau x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^d$$



Covariances for Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

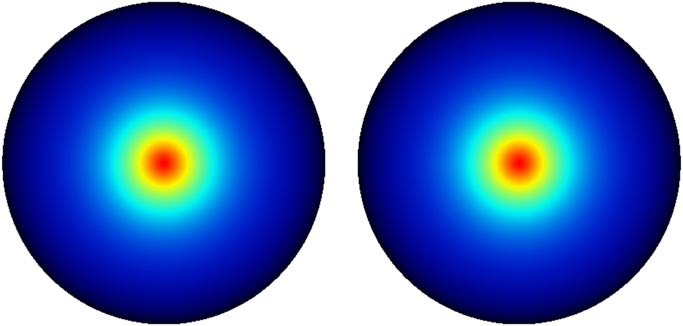
$$(\kappa_{\mathbf{u}}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u}} - \nabla \cdot \mathbf{M}_{\mathbf{u}} \nabla)^{\alpha/2}(\tau_{\mathbf{u}} x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^d$$



Covariances for Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

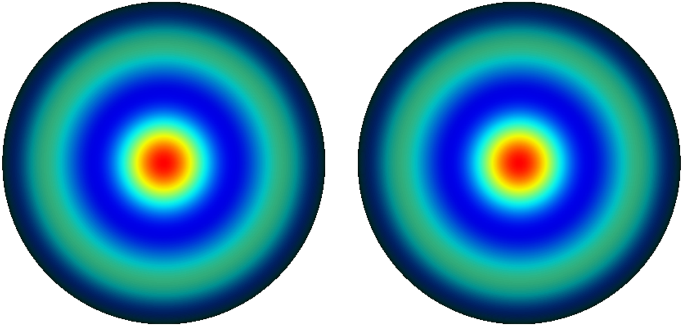
$$(\kappa_{\mathbf{u}}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u}} - \nabla \cdot \mathbf{M}_{\mathbf{u}} \nabla)^{\alpha/2} (\tau_{\mathbf{u}} x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \Omega$$



Covariances for Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

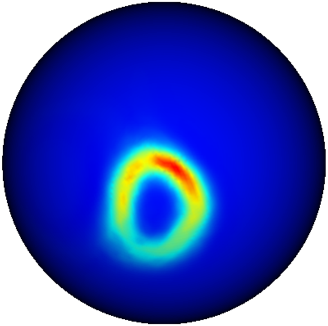
$$(\kappa_{\mathbf{u}}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u}} - \nabla \cdot \mathbf{M}_{\mathbf{u}} \nabla)^{\alpha/2} (\tau_{\mathbf{u}} x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \Omega$$

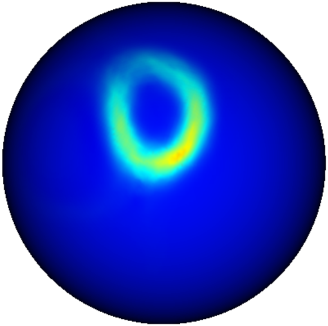


Covariances for Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

$$(\kappa_{\mathbf{u}}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u}} - \nabla \cdot \mathbf{M}_{\mathbf{u}} \nabla)^{\alpha/2} (\tau_{\mathbf{u}} x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \Omega$$





Covariances for Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

$$\left(\frac{\partial}{\partial t} + \kappa^2_{\mathbf{u},t} + \nabla\cdot\mathbf{m}_{\mathbf{u},t} - \nabla\cdot\mathbf{M}_{\mathbf{u},t}\nabla\right)(\tau_{\mathbf{u},t}x(\mathbf{u},t)) = \mathcal{E}(\mathbf{u},t), \quad (\mathbf{u},t)\in\Omega\times\mathbb{R}$$