Parameterization of Nonstationarity in Stochastic PDE Models

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Describing spatial dependence

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

Computations via piecewise linear Markov models

Continuous Markovian spatial models (Lindgren et al, 2011)

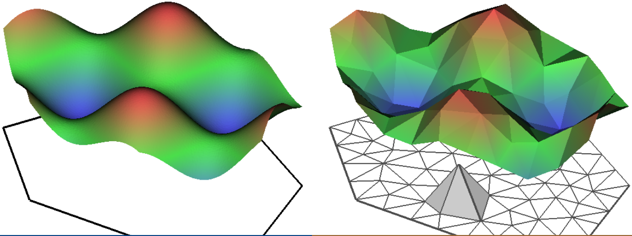
Local basis: $u(\boldsymbol{s}) = \sum_k \psi_k(\boldsymbol{s}) u_k$

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

Measurements: $\boldsymbol{y} = \boldsymbol{B}\boldsymbol{\beta} + \boldsymbol{A}\boldsymbol{u} + \boldsymbol{\epsilon}$, $\boldsymbol{\epsilon}|\boldsymbol{u} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}_{y|u}^{-1})$

Posterior: Local observations $\Longrightarrow$ Markovian posterior for $\boldsymbol{u}$

$\boldsymbol{Q}$ chosen to give best approximation to an SPDE



Non-stationary models via deformations

Deformations (Sampson & Guttorp, 1992)

- Random field $\{u(\boldsymbol{s});\ \boldsymbol{s} \in \mathbb{R}^n\}$
- Deformation function $\widetilde{\boldsymbol{s}} = f(\boldsymbol{s}) : \mathbb{R}^n \mapsto \mathbb{R}^m, m \geq n$
- Stationary covariance $\{\widetilde{r}(\widetilde{\boldsymbol{s}}, \widetilde{\boldsymbol{t}});\ \widetilde{\boldsymbol{s}}, \widetilde{\boldsymbol{t}} \in \mathbb{R}^m\}$
- Resulting covariance $\text{Cov}(u(\boldsymbol{s}), u(\boldsymbol{t})) = \widetilde{r}(f(\boldsymbol{s}), f(\boldsymbol{t}))$

- Allows separation between modelling variances and correlations: $v(\boldsymbol{s}) := \sigma(\boldsymbol{s})u(\boldsymbol{s})$
- Euclidean distances in the deformation space, which may be of higher dimension than the model domain.
- Inference: Find a suitable deformation f and correlation $\widetilde{r}$.

Non-stationary SPDE models via deformations

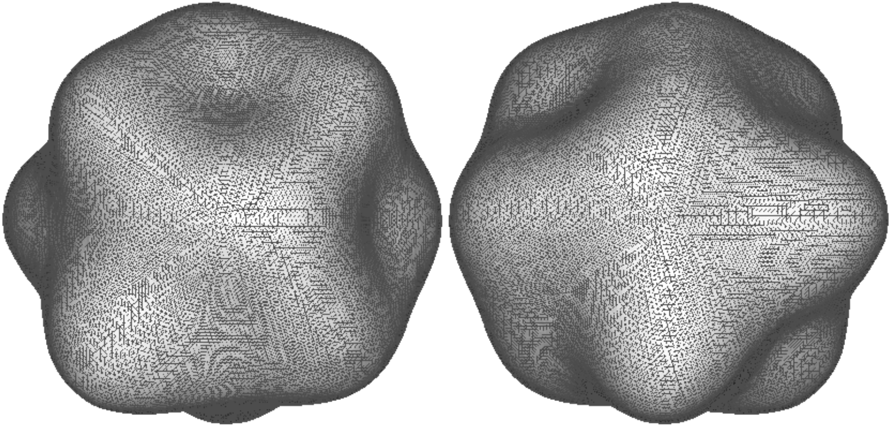
Deformation of manifolds

- Let $\Omega \subseteq \mathbb{R}^n$ and $\Omega \subseteq \mathbb{R}^m$ be d-manifolds, $d \leq n, m$, with metrics induced by the embedding Euclidean spaces.
- Deformation function $\widetilde{\boldsymbol{s}} = f(\boldsymbol{s}) : \Omega \mapsto \widetilde{\Omega}$
- "Stationary" SPDE on $\widetilde{\Omega}$: $(1 - \widetilde{\nabla} \cdot \widetilde{\nabla})^{\alpha/2} \widetilde{u}(\widetilde{\boldsymbol{s}}) = \widetilde{\mathcal{W}}(\widetilde{\boldsymbol{s}})$
- Define random field by mapping back to Ω: $u(\boldsymbol{s}) := \widetilde{u}(f(\boldsymbol{s}))$

- Distances are measured *within* the deformed manifold.
- When $\widetilde{\Omega} = \mathbb{R}^d$ or $\mathbb{S}^d$, $\widetilde{u}(\widetilde{\boldsymbol{s}})$ is a stationary (Matérn) field, and we have a special case of the classical deformation method.
- What happens when $\widetilde{\Omega}$ has non-constant curvature?
- Can we rewrite the model using a non-stationary SPDE operator on Ω itself?

Manifold example: Radially deformed sphere

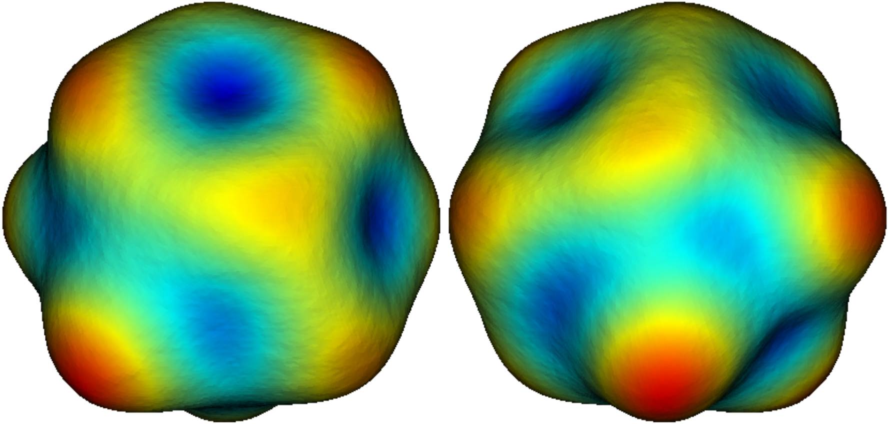
Deformation generated by an oscillating SPDE model



(25002 mesh nodes, sample generated in 1.75 seconds)

Manifold example: Radially deformed sphere

Deformation generated by an oscillating SPDE model



(25002 mesh nodes, sample generated in 1.75 seconds)

Deformation

For simplicity, only consider $\alpha = 2$ and notation for $\Omega = \mathbb{R}^d$.

Manifold deformation

Deformation function ($f : \Omega \mapsto \widetilde{\Omega} \subseteq \mathbb{R}^m$), Jacobian, metric tensor:

$$f(\boldsymbol{s}) = \left[f(\boldsymbol{s})_i\right], \quad Df(\boldsymbol{s}) = \left[\frac{\partial f(\boldsymbol{s})_i}{\partial s_j}\right], \quad g(\boldsymbol{s}) = Df(\boldsymbol{s})^\top \cdot Df(\boldsymbol{s})$$

Change of variables in an SPDE

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

is equivalent to

$$H(\boldsymbol{s}) = g^{-1}(\boldsymbol{s}) \det(g)^{1/2}$$
$$(\det(g)^{1/2} - \nabla \cdot H\nabla)u(\boldsymbol{s}) = \det(g)^{1/4}\mathcal{W}(\boldsymbol{s})$$

Stationary deformation

Simple scaling

Deformation, Jacobian, metric tensor, assume $\det \boldsymbol{A} = 1$:

$$f(\boldsymbol{s}) = \kappa \boldsymbol{A}\boldsymbol{s}, \qquad Df(\boldsymbol{s}) = \kappa \boldsymbol{A}, \qquad g(\boldsymbol{s}) = \kappa^2 \boldsymbol{A}^\top \boldsymbol{A},$$

Resulting SPDE:

$$\det(g)^{1/2} = \kappa^d$$

$$H(\boldsymbol{s}) = \kappa^{d-2} (\boldsymbol{A}^\top \boldsymbol{A})^{-1}$$

$$(\kappa^d - \nabla \cdot \kappa^{d-2} (\boldsymbol{A}^\top \boldsymbol{A})^{-1} \nabla) u(\boldsymbol{s}) = \kappa^{d/2} \mathcal{W}(\boldsymbol{s})$$

or

$$(\kappa^2 - \nabla \cdot (\boldsymbol{A}^\top \boldsymbol{A})^{-1} \nabla) u(\boldsymbol{s}) = \kappa^{2-d/2} \mathcal{W}(\boldsymbol{s})$$

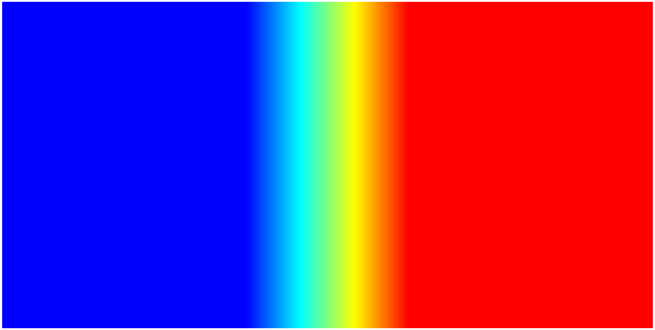
Note: Because $\det(H) = \det(g)^{d/2} / \det(g) = \det(g)^{d/2-1}$, the determinant of H is 1 when $d = 2$, for *all* g!

Deformation from non-stationary SPDE

Given a non-stationary SPDE

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

can we find a corresponding deformation representation?
Domain $\Omega = [0, 4] \times [-1, 1]$, κ varying between $2\sqrt{8}$ and $4\sqrt{8}$:



Deformation from non-stationary SPDE

Deformation structure

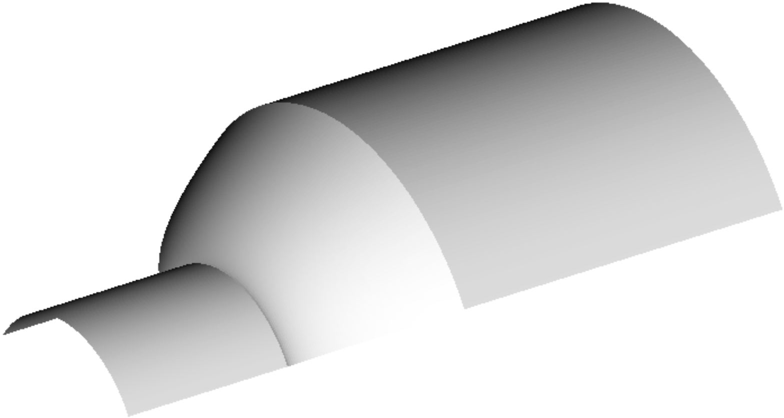
$$f(\boldsymbol{s}) = \begin{bmatrix} h(x) \\ \kappa(x)\sin(y) \\ \kappa(x)\cos(y) \end{bmatrix}, \quad Df(\boldsymbol{s}) = \begin{bmatrix} h'(x) & 0 \\ \kappa'(x)\sin(y) & \kappa(x)\cos(y) \\ \kappa'(x)\cos(y) & -\kappa(x)\sin(y) \end{bmatrix}$$

$$g(\boldsymbol{s}) = Df^\top \cdot Df = \begin{bmatrix} h'(x)^2 + \kappa'(x)^2 & 0 \\ 0 & \kappa(x)^2 \end{bmatrix}$$

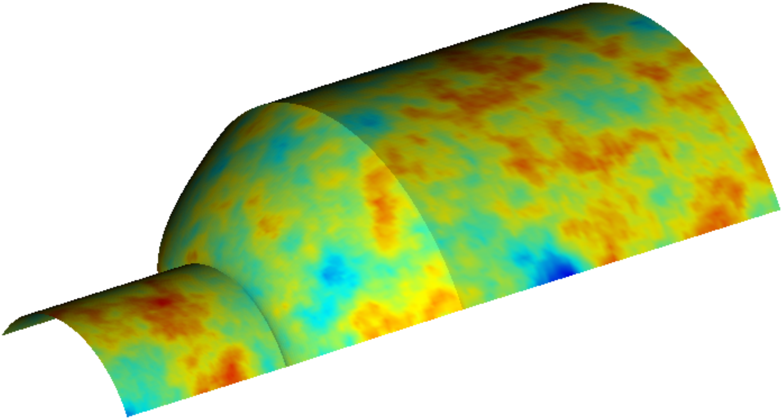
We need $\det(g)^{1/2} = \kappa(x)^2$ and $\boldsymbol{H} = \boldsymbol{I}_2$. Solution:

$$h(x) = \int_0^x \sqrt{\kappa(t)^2 - \kappa'(t)^2} \mathrm{d}t$$

Deformed manifold

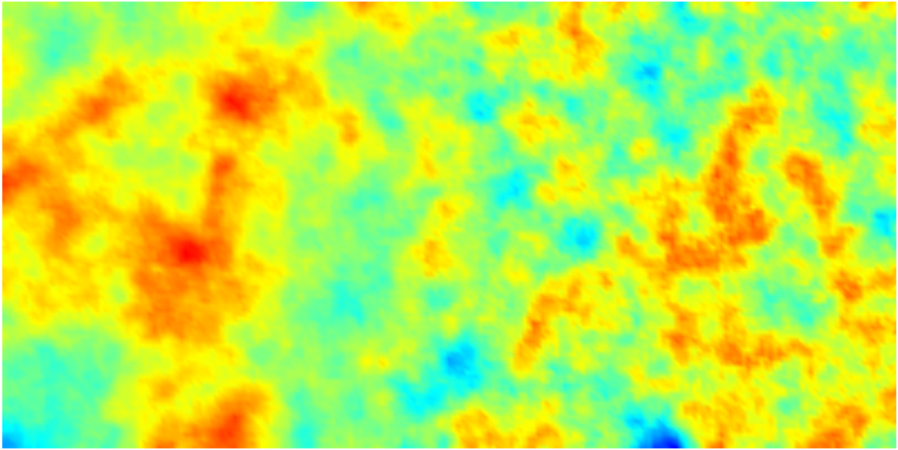


"Stationary" field on deformed manifold



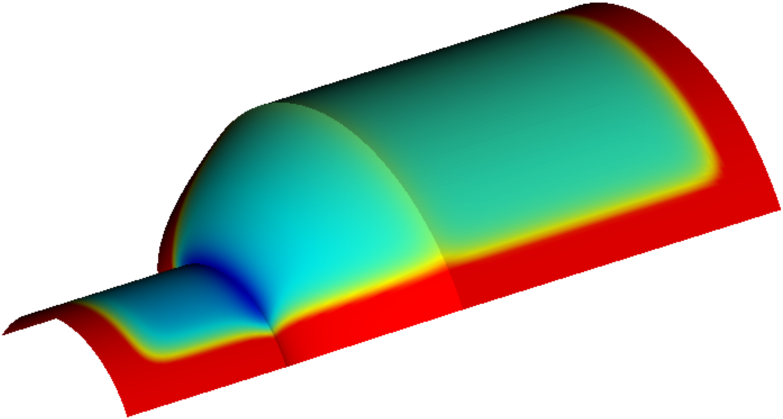
$$(1 - \widetilde{\nabla} \cdot \widetilde{\nabla})\widetilde{u}(\widetilde{\boldsymbol{s}}) = \widetilde{\mathcal{W}}(\widetilde{\boldsymbol{s}}), \quad \widetilde{\boldsymbol{s}} \in \widetilde{\Omega}$$

Non-stationary field on original manifold



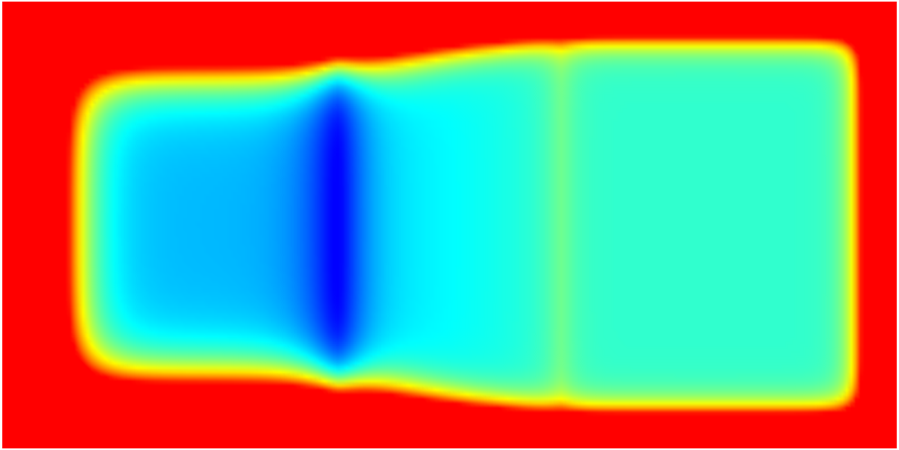
$$(\kappa(\boldsymbol{s})^2 - \nabla \cdot \nabla)u(\boldsymbol{s}) = \kappa(\boldsymbol{s})\mathcal{W}(\boldsymbol{s}), \quad \boldsymbol{s} \in \Omega$$

Standard deviations on deformed manifold



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

Standard deviations on original manifold



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

Vertical displacement deformations

Deformation structure

$$f(\boldsymbol{s}) = \kappa_0 \begin{bmatrix} x \\ y \\ h(x,y) \end{bmatrix}, \quad Df(\boldsymbol{s}) = \kappa_0 \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ v_x & v_y \end{bmatrix}, \quad \boldsymbol{v} = \nabla h$$

$$g(\boldsymbol{s}) = Df^\top \cdot Df = \kappa_0^2 \begin{bmatrix} 1+v_x^2 & v_x v_y \\ v_x v_y & 1+v_y^2 \end{bmatrix} = \kappa_0^2(\boldsymbol{I} + \boldsymbol{v}\boldsymbol{v}^\top)$$

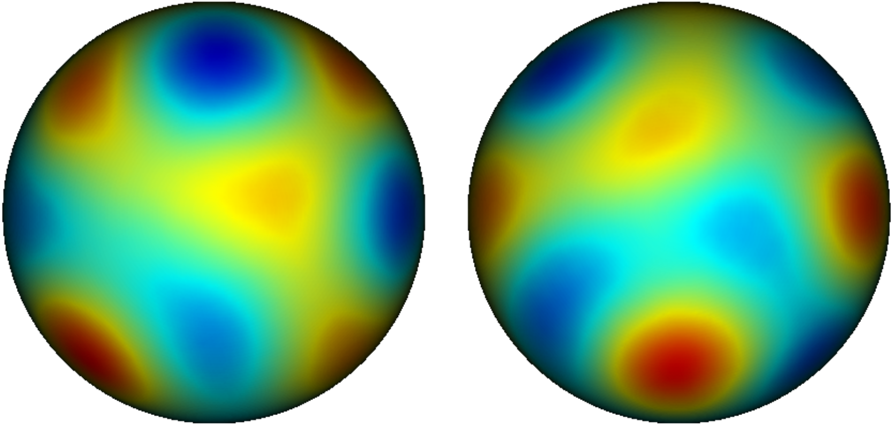
With $\boldsymbol{v}_\perp \cdot \boldsymbol{v} = 0$, $\|\boldsymbol{v}_\perp\| = \|\boldsymbol{v}\|$, we get

$$\kappa(\boldsymbol{s})^2 = \kappa_0^2 \sqrt{1 + \|\boldsymbol{v}_\perp\|^2},$$

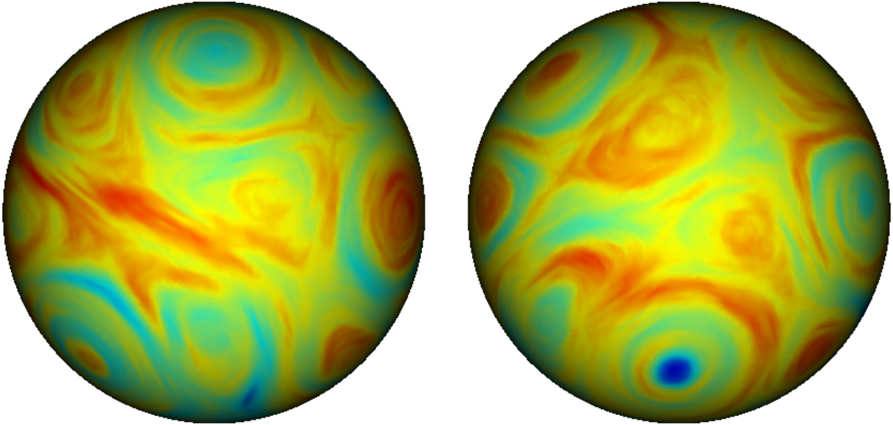
$$\boldsymbol{H}(\boldsymbol{s}) = (\boldsymbol{I} + \boldsymbol{v}_\perp \boldsymbol{v}_\perp^\top) / \sqrt{1 + \|\boldsymbol{v}_\perp\|^2}$$

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

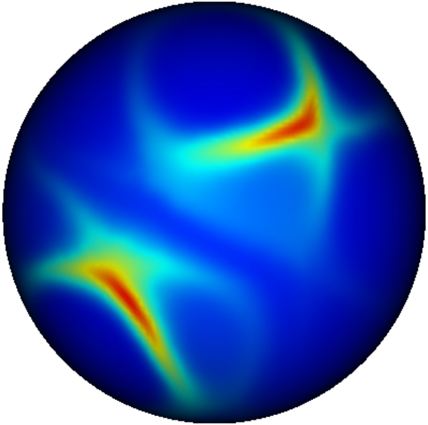
Displacement field

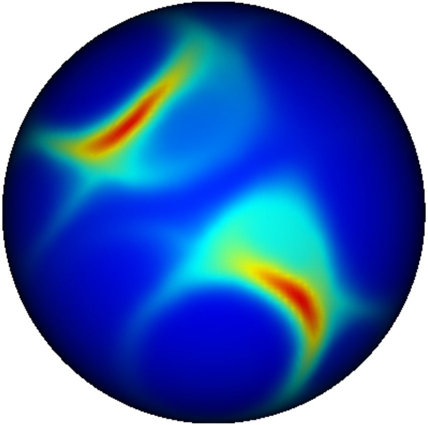


Simulated non-stationary field

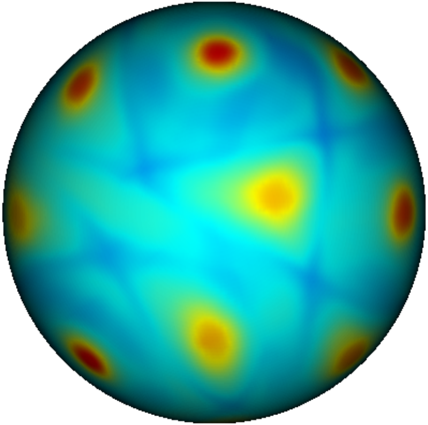


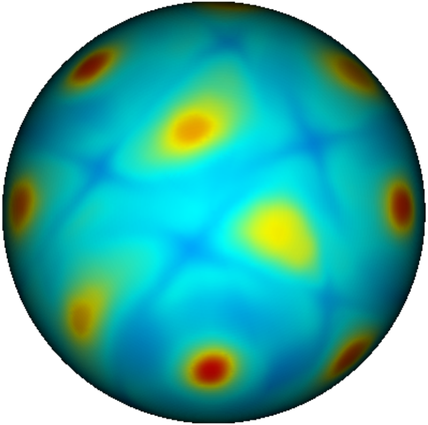
Four covariance functions





Standard deviations





The variance varies by almost a factor 4, so it is now clearly not constant. We've partially lost the separation between correlation and variance allowed by the classical deformation method.

Interpretation and direct metric parameterisation

Subtractive parameterisation (like displacement model)

Baseline range $\sqrt{8}/\kappa_0$, the model *removes* dependence orthogonal to the vector field.

$$\kappa(\boldsymbol{s})^2 = \kappa_0^2\sqrt{1+\|\boldsymbol{v}\|^2}$$

Additive parameterisation

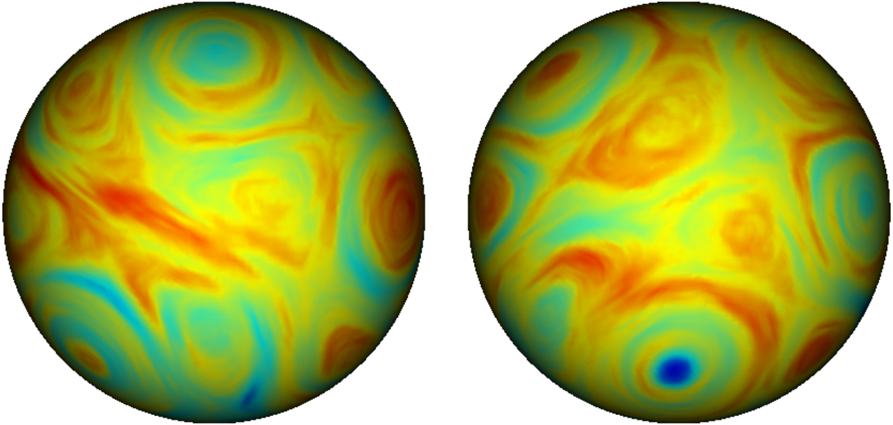
Baseline range $\sqrt{8}/\kappa_0$, the model *adds* dependence along the vector field.

$$\kappa(\boldsymbol{s})^2 = \kappa_0^2/\sqrt{1+\|\boldsymbol{v}\|^2}$$

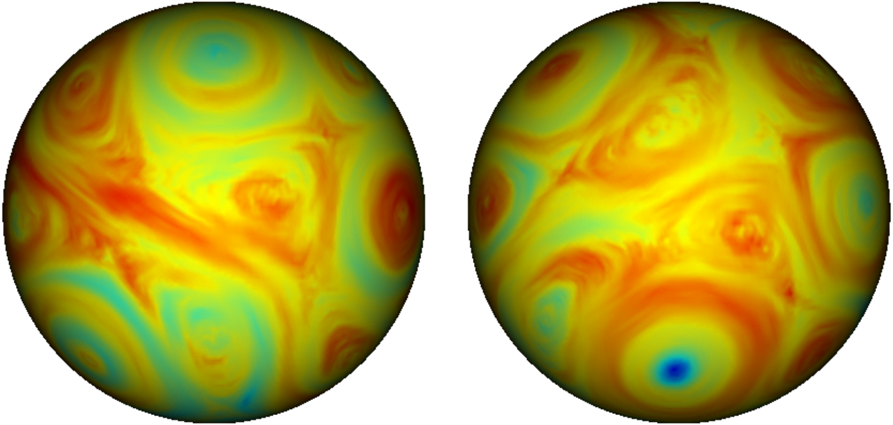
$$\boldsymbol{H}(\boldsymbol{s}) = (\boldsymbol{I}+\boldsymbol{v}\boldsymbol{v}^\top)/\sqrt{1+\|\boldsymbol{v}\|^2}$$

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

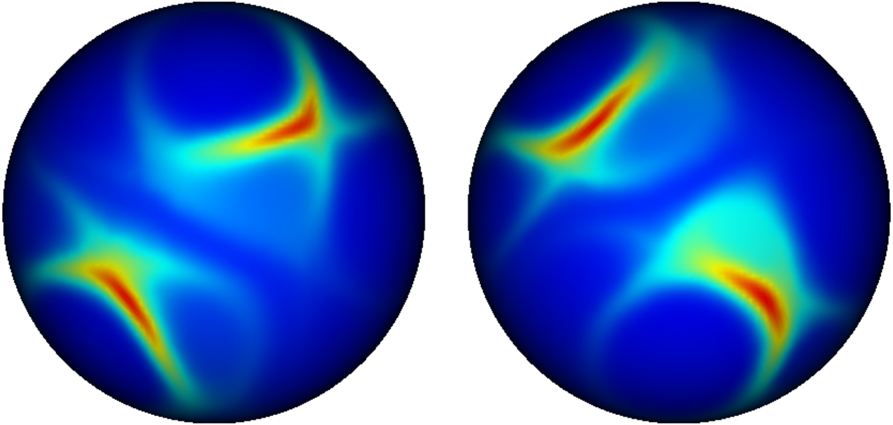
Simulated non-stationary field (subtractive)



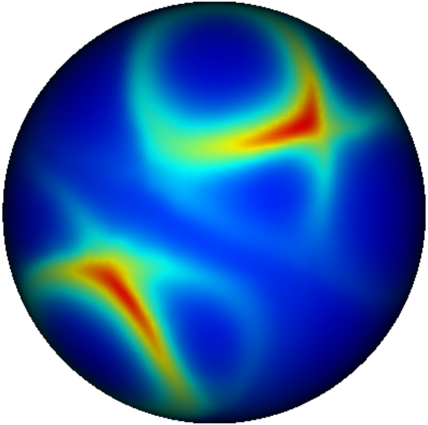
Simulated non-stationary field (additive)

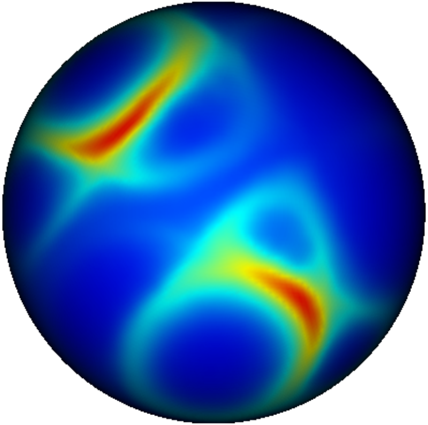


Four covariance functions (subtractive)

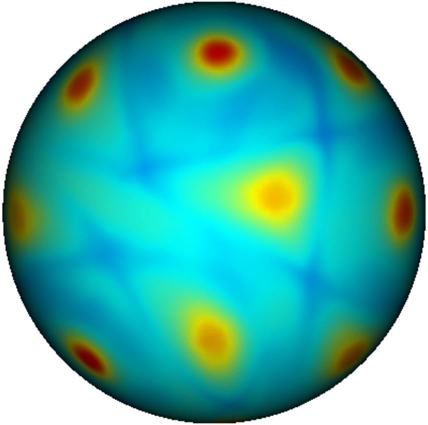


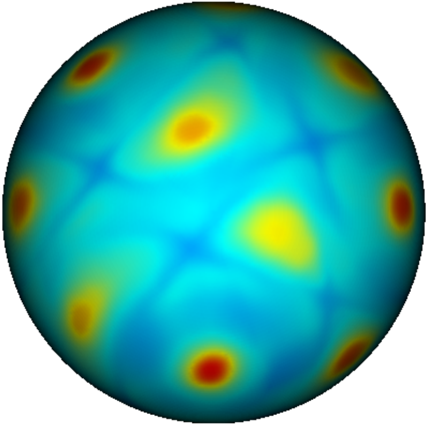
Four covariance functions (additive)



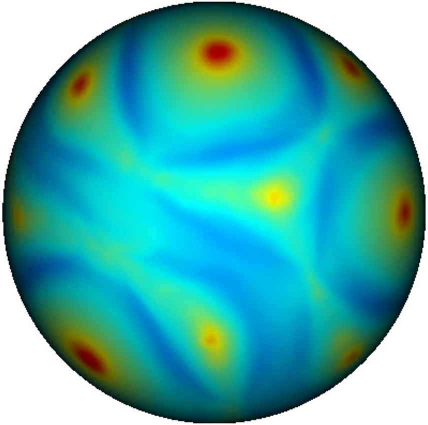


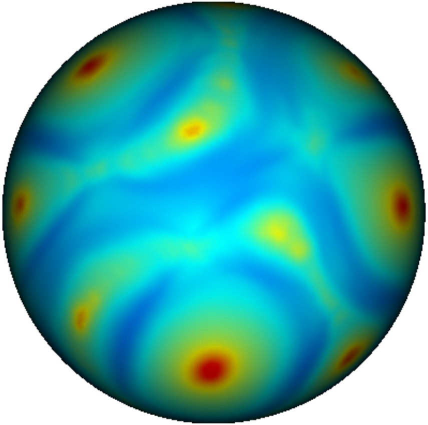
Standard deviations (subtractive)





Standard deviations (additive)





Semiparametric inference

True model, with a single realisation of $u(\boldsymbol{s})$:

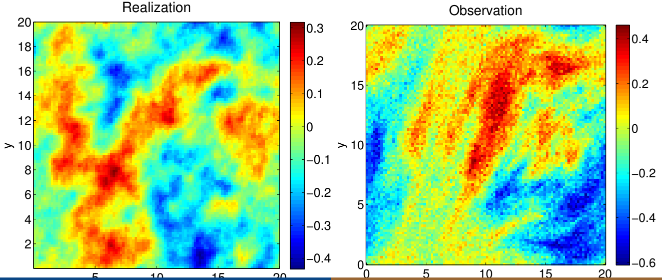
$$(1 - \nabla \cdot \boldsymbol{H}(\boldsymbol{s})\nabla)u(\boldsymbol{s}) = \mathcal{W}(\boldsymbol{s}), \quad \boldsymbol{H}(\boldsymbol{s}) = \gamma \boldsymbol{I} + \boldsymbol{v}(\boldsymbol{s})\boldsymbol{v}(\boldsymbol{s})^\top$$

Model for inference, with low order harmonic vector basis functions,

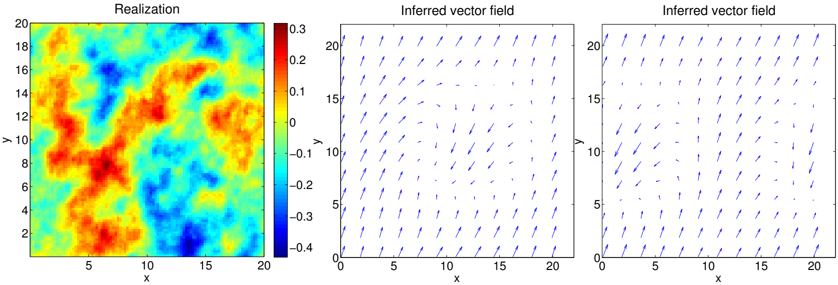
$$\boldsymbol{v}(\boldsymbol{s}) = \sum_{ij} \psi_{ij}(\boldsymbol{s})$$

with a vector-SPDE prior for regularisation.

Constant and non-constant true vector fields:

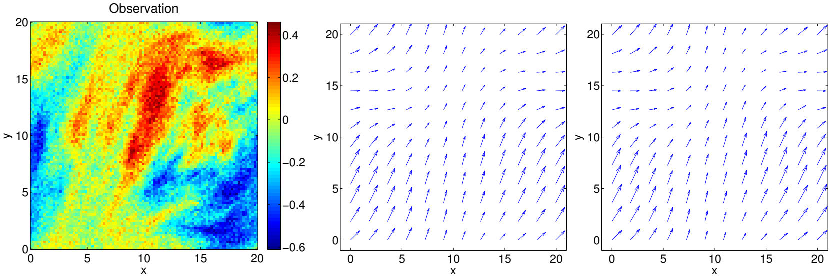


Sample and estimates



There are several local maxima, partly due to fundamental non-identifiability issues.

Sample and estimates



The inference is more stable when there is more structure (that also matches the vector field model). Covariate information would be extremely valuable.

Closing remarks

Remarks

- The connection between Matérn fields, stochastic PDEs, and Markov random fields can be extended to the classical deformation method for non-stationary models.
- Direct parameterization of the manifold metric appears more practical than parameterizing a deformation, while still keeping interpretability.
- The question should not be "*Stationary or non-stationary?*" but rather what *kind* of non-stationarity.
- The latter also applies to *separable vs. non-separable* in space-time models.

References

References

- 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
- G-A. Fuglstad, D. Simpson, F. Lindgren, H. Rue (2013), *Non-stationary spatial modelling with applications to spatial prediction of precipitation*, arXiv:1306.0408
- 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)*, Journal of the Royal Statistical Society, Series B, 73(4), 423–498.