Gaussian random fields on Riemannian manifolds: Sampling and error analysis

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MINES PARIS | PSL

GEOLEARNING

GEOSTATISTICAL MODELING

Geostatistical paradigm: over the spatial domain $\mathcal{D}$

Gaussian Random Field		Observed variable
$Z : \{Z(\boldsymbol{p}) : \boldsymbol{p} \in \mathcal{D}\}$	$\xrightarrow{\text{Realization}}$	$z : \{z(\boldsymbol{p}) : \boldsymbol{p} \in \mathcal{D}\}$
High correlation		High "similarity"

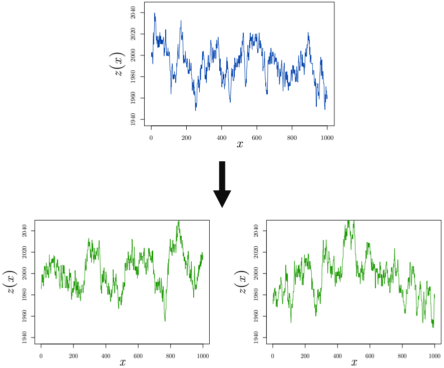
- Allows to model data which are not independent, identically distributed
- **Covariance function** C_Z:

$$\begin{array}{rcccl} C_Z & : & \mathcal{D} \times \mathcal{D} & \rightarrow & \mathbb{R} \\ & & (\boldsymbol{p}_1, \boldsymbol{p}_2) & \mapsto & C_Z(\boldsymbol{p}_1, \boldsymbol{p}_2) = \mathrm{Cov}(Z(\boldsymbol{p}_1), Z(\boldsymbol{p}_2)) \end{array}$$

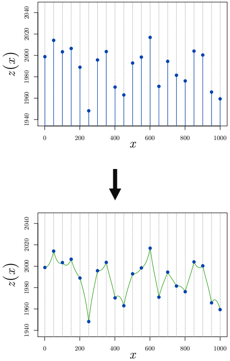
$\rightarrow$ used to model the spatial structure observed on the variable/data

CLASSICAL APPLICATIONS OF GEOSTATISTICS

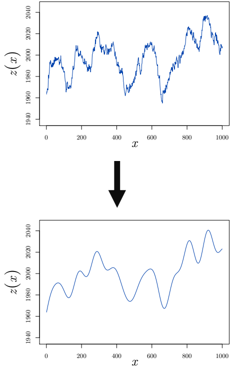
Simulation



Prediction



Filtering



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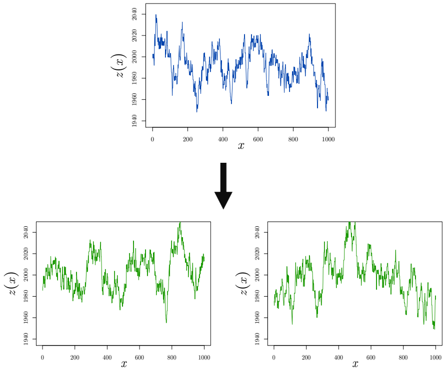

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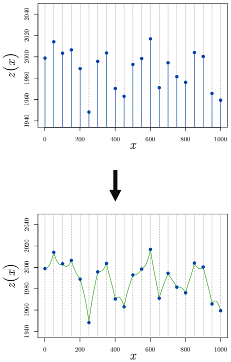

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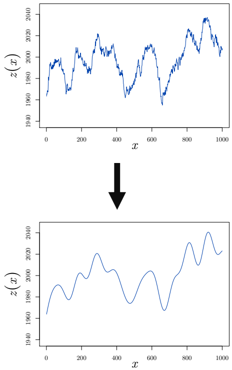

All these tasks usually require to build a covariance matrix $\boldsymbol{\Sigma}$: $\boxed{[\boldsymbol{\Sigma}]_{ij} = C_Z(\boldsymbol{p}_i, \boldsymbol{p}_j)}$

$\Rightarrow$ The covariance function C_Z must be known

EXAMPLE: (SIMPLE) KRIGING PREDICTION

Input Observations $Y(x_i)$ at some points $(x_1, \ldots, x_{N_D})$ of a spatial domain $\mathcal{D}$

$$Y(x_i) = \mathcal{Z}(x_i) + \tau\varepsilon_i, \quad i \in \{1, \ldots, k\}$$

- $\mathcal{Z}$: Underlying (non-stationary) random field
- $\varepsilon_1, \ldots, \varepsilon_{N_D} \sim \mathcal{N}(0,1)$ iid noise

Output Kriging estimates $Z^*(p_j)$ of $\mathcal{Z}$ some points $(p_1, \ldots, p_{N_T})$ of $\mathcal{D}$

Computation Solve the kriging system defined by

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$$\begin{pmatrix} \vdots \\ Z^*(p_j) \\ \vdots \end{pmatrix} = \boldsymbol{\Sigma}_{TD}\left(\boldsymbol{\Sigma}_{DD} + \tau^2 \boldsymbol{I}\right)^{-1} \begin{pmatrix} \vdots \\ Y(x_i) \\ \vdots \end{pmatrix}$$

$$\boldsymbol{\Sigma}_{TD} = \left[\mathrm{Cov}(\mathcal{Z}(p_k), \mathcal{Z}(x_l))\right]_{\substack{1 \le k \le N_T \\ 1 \le l \le N_D}} \in \mathbb{R}^{N_T \times N_D}, \quad \boldsymbol{\Sigma}_{DD} = \left[\mathrm{Cov}(\mathcal{Z}(x_k), \mathcal{Z}(x_l))\right]_{\substack{1 \le k \le N_D \\ 1 \le l \le N_D}} \in \mathbb{R}^{N_D \times N_D}$$

CHALLENGES IN PRACTICE

Non-euclidean domains

- Extensive literature for the sphere: Marinucci and Peccati (2011); Lang et al. (2015); Lantuéjoul et al. (2019); Emery and Porcu (2019)

Non-stationarity

- Examples of proposed methods: Karhunen-Loève expansions (Lindgren, 2012), Space deformation models (Sampson and Guttorp, 1992), Convolution models (Higdon et al., 1999)

Big "N" problem

- Need to restrict the choice of models to work with **sparse matrices**: Compactly-supported or tapered covariance functions (Gneiting, 2002; Furrer et al., 2006), Markovian models (Rue and Held, 2005)

THE SPDE APPROACH

Basic idea: if $\mathcal{Z}$ is an isotropic Markovian field over $\mathbb{R}^d$, then it is **equivalently** characterized by (Whittle, 1954; Rozanov, 1977):

Spectral density

$$\Gamma : \boldsymbol{\xi} \in \mathbb{R}^d \mapsto \frac{1}{P(\|\boldsymbol{\xi}\|^2)}$$

Stochastic partial differential equation (SPDE)

$$\boxed{P(-\Delta)^{1/2}\mathcal{Z} = \mathcal{W}}$$

- $\mathcal{W}$: Gaussian white noise
- $P(-\Delta)^{1/2}\mathcal{Z} := \mathscr{F}^{-1}\left[\boldsymbol{\xi} \mapsto P(\|\boldsymbol{\xi}\|^2)^{1/2} \times \mathscr{F}[\mathcal{Z}](\boldsymbol{\xi})\right]$

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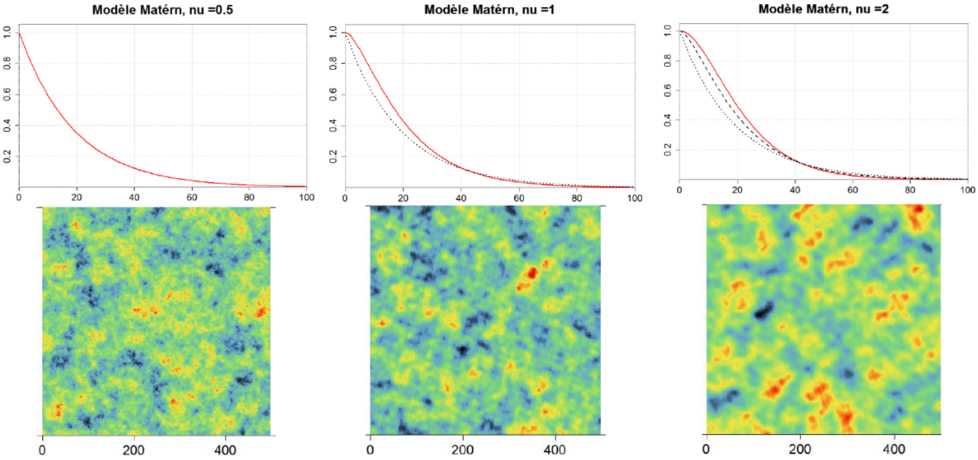
$\rightarrow$ In particular, if $P(x) = (\kappa^2 + x)^\alpha$, i.e. if we consider the SPDE

$$(\kappa^2 - \Delta)^{\alpha/2}\mathcal{Z} = \mathcal{W}$$

then Z has a Matérn covariance function

$$\operatorname{Cov}\big(\mathcal{Z}(\boldsymbol{x}+\boldsymbol{h}), \mathcal{Z}(\boldsymbol{x})\big) = C(\|h\|) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)}\big(\kappa\|h\|\big)^\nu \mathcal{K}_\nu\big(\kappa\|h\|\big), \quad \nu = \alpha - d/2$$

■ MATÉRN RANDOM FIELDS



Simulations of Gaussian random fields with a Matérn covariance

A FIRST SOLUTION: THE SPDE APPROACH

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SPDE approach: Lindgren et al. (2011) use this last characterization of isotropic Markovian fields

Problem	Solution proposed
Non-euclidean domains, Non-stationarity	Define the SPDE on manifolds or use varying parameters

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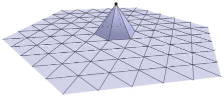
SPDE approach: Lindgren et al. (2011) use this last characterization of isotropic Markovian fields

Problem	Solution proposed
Big "N" problem	Use the finite element method to solve the SPDE

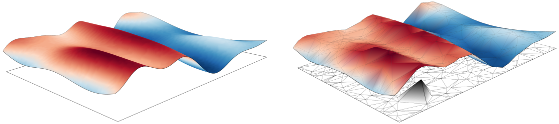
FINITE ELEMENT APPROXIMATION

$$\boxed{{\color{red}P(-\Delta)^{1/2}}\mathcal{Z} = \mathcal{W}}$$



$\mathcal{D}$

$$\to \quad \mathcal{Z}(\boldsymbol{p}) \approx \sum_{j=1}^{n} Z_j \psi_j(\boldsymbol{p}) \quad \to$$



True solution (*left*) and its finite element approximation (*right*)

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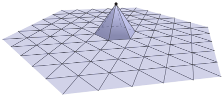

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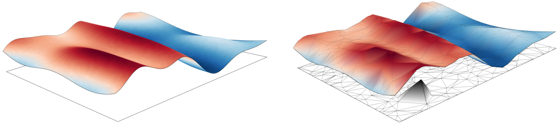


True solution (*left*) and its finite element approximation (*right*)

The weights $\boldsymbol{Z} = (Z_1, \ldots, Z_n)$ form a Gaussian vector with **precision matrix**

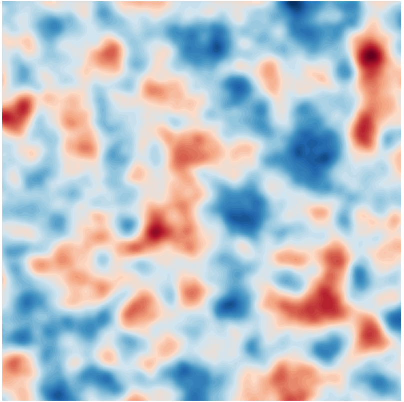
$$\boxed{\boldsymbol{Q}_Z = \boldsymbol{C}^{1/2} P(\boldsymbol{S}) \boldsymbol{C}^{1/2}} \qquad \boldsymbol{S} = \boldsymbol{C}^{-1/2} \boldsymbol{R} \boldsymbol{C}^{-1/2}$$

- $\boldsymbol{C} = [\langle \psi_i, \psi_j \rangle]$ = "Mass" matrix $\rightarrow$ Sparse (and Diagonal after approx)
- $\boldsymbol{R} = [\langle \nabla\psi_i, \nabla\psi_j \rangle]$ = "Stiffness" matrix $\rightarrow$ Sparse

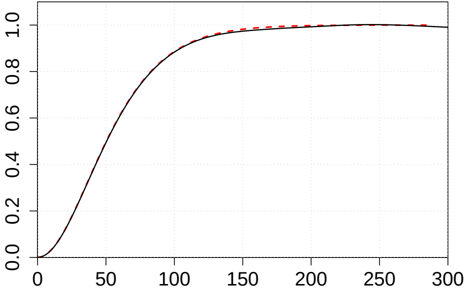
$\rightarrow$ $\boldsymbol{Q}_Z$ is sparse (when $\deg P$ is relatively small)

APPLICATION: NON-MARKOVIAN SPECTRAL DENSITIES

$$(\kappa^2 - \Delta)^{\alpha/2} \mathcal{Z} = \mathcal{W}$$



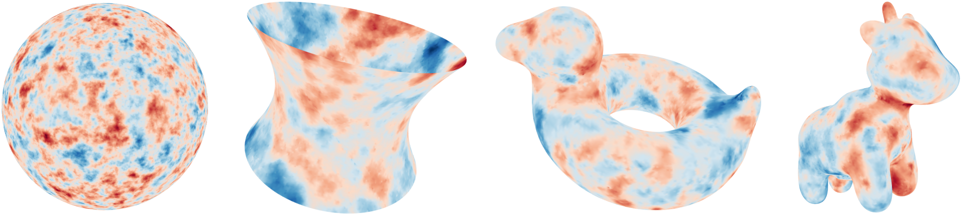
Sample



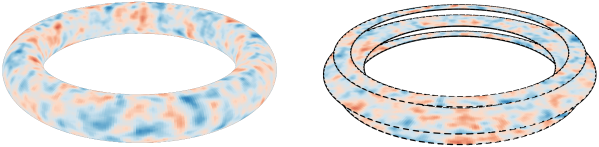
Variagram comparison with Matérn covariance

■ APPLICATION: RANDOM FIELDS ON SMOOTH MANIFOLDS

$$(\kappa^2 - \Delta)^{\alpha/2}\mathcal{Z} = \mathcal{W}$$



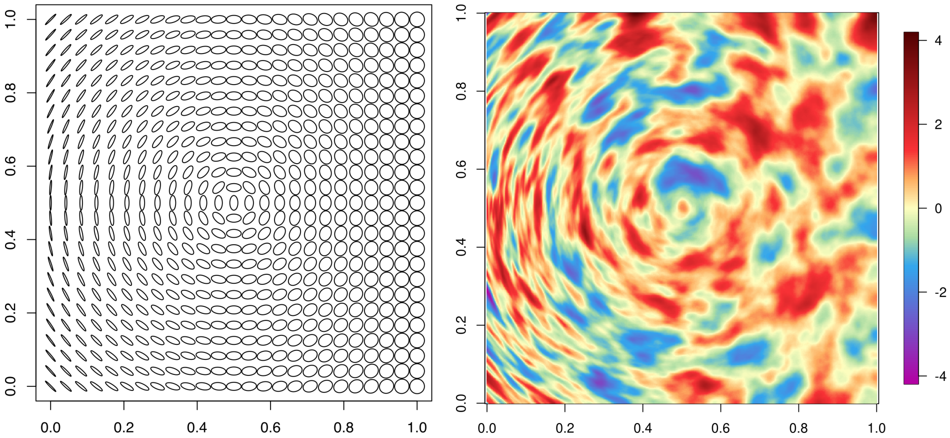
Simulations of Matérn fields on smooth two-dimensional surfaces



Simulation of a Matérn field on a “full” torus (*left*) and some selected slices (*right*)

APPLICATION: NON-STATIONARY RANDOM FIELDS

$$(\kappa^2(s) - \mathrm{div}(H(s)\nabla))^{\alpha/2}\mathcal{Z} = \mathcal{W}$$



Example of anisotropy parameters (left) and corresponding random field simulation obtained using our method (right), on the unit square.

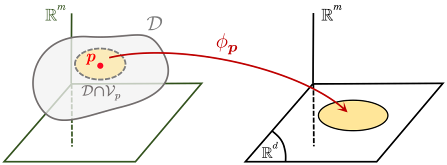
OUTLINE

■ DEFINITION: RIEMANNIAN MANIFOLDS

Let $m \geq 1$ and $1 \leq d \leq m$

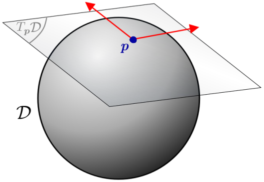
$\mathcal{M} := (\mathcal{D}, g)$ is a **compact Riemannian (sub)manifold of dimension** d

- $\mathcal{D} \subset \mathbb{R}^m$ is a **smooth (sub)manifold**
  - Locally Euclidean of dimension d
  - Can be entirely mapped by a set of smoothly *compatible* charts



Ex: Euclidean domains, smooth surfaces (eg. sphere, torus,...)

- $\mathcal{D}$ is equipped with a **Riemannian metric** g
  - $g_{\boldsymbol{p}}$: inner product on the tangent space of $\mathcal{D}$ at $\boldsymbol{p} \in \mathcal{D}$
  - $g : \boldsymbol{p} \mapsto g_{\boldsymbol{p}}$ is "smooth"



Lengths and angles of tangent vectors $\boldsymbol{u}, \boldsymbol{v}$:

$$\|\boldsymbol{u}\|_{\boldsymbol{p}} = \sqrt{g_{\boldsymbol{p}}(\boldsymbol{u}, \boldsymbol{u})}$$

$$\cos\left(\theta(\boldsymbol{u}, \boldsymbol{v})\right) = \frac{g_{\boldsymbol{p}}(\boldsymbol{u}, \boldsymbol{v})}{\|\boldsymbol{u}\|_{\boldsymbol{p}}\|\boldsymbol{v}\|_{\boldsymbol{p}}}$$

A CLASS OF GENERALIZED RANDOM FIELDS

Let $\mathcal{L}$ be a second-order self-adjoint elliptic operator with smooth coefficients, eg.

$$\mathcal{L} = -\Delta, \quad \mathcal{L} = \kappa^2(\cdot) - \mathrm{div}(H(\cdot)\nabla)$$

- **Spectral theorem on compact Riemannian manifolds** $\mathcal{M} = (\mathcal{D}, g)$:
  - $\mathcal{L}$ has discrete eigenvalues $\{\lambda_k : k \in \mathbb{N}\}$ with smooth eigenfunctions $\{e_k : k \in \mathbb{N}\}$
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- Consider the $L^2(\mathcal{M})$-valued random variables defined by

$$\boxed{\mathcal{Z} = \sum_{k\in\mathbb{N}} \gamma(\lambda_k) W_k \; e_k} \quad \text{where } \{W_k\}_{k\in\mathbb{N}} \sim \text{IID}\mathcal{N}(0,1)$$

  and $\gamma : \mathbb{R}_+ \rightarrow \mathbb{R}$ such that $|\gamma(\lambda)| = \mathcal{O}_{\lambda\rightarrow\infty}(|\lambda|^{-\beta})$ with $\beta > d/4$

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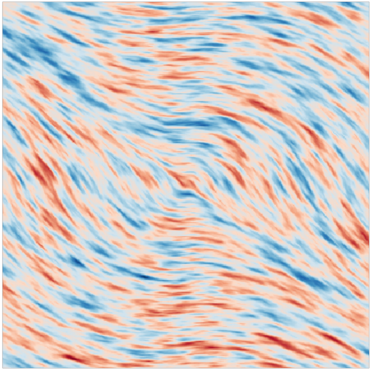
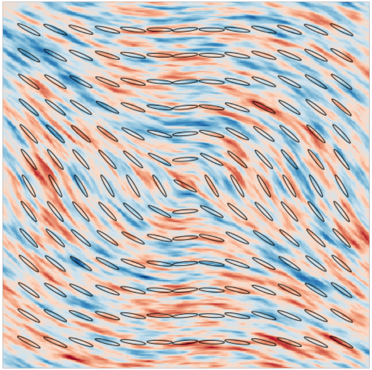
- Covariance properties (Pereira, 2019): when $(\mathcal{M}, g) = ([0,1]^d, g)$ and $\mathcal{L} = -\Delta$

$$\mathrm{Cov}\left(\mathcal{Z}(\boldsymbol{p}), \mathcal{Z}(\boldsymbol{p}+d\boldsymbol{p})\right) \approx C_0\left(\sqrt{g_{\boldsymbol{p}}(d\boldsymbol{p}, d\boldsymbol{p})}\right) \quad \text{where} \quad C_0 = \mathscr{F}^{-1}[\gamma^2]$$

ACCOUNTING FOR LOCAL ANISOTROPIES

- What about the local anisotropies?
  - $\rightarrow$ *Treat local anisotropies as a field of local deformations of the spatial domain.*





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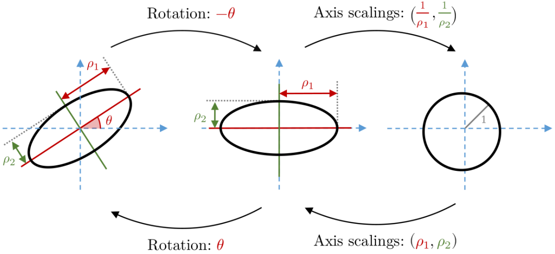


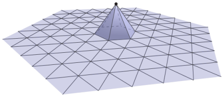
Define the metric g as

$$\boxed{g_{\boldsymbol{p}}(\boldsymbol{u}, \boldsymbol{v}) = \left(\boldsymbol{D}(\boldsymbol{p})^{-1}\boldsymbol{R}(\boldsymbol{p})^T\boldsymbol{u}\right)^T \left(\boldsymbol{D}(\boldsymbol{p})^{-1}\boldsymbol{R}(\boldsymbol{p})^T\boldsymbol{v}\right)}, \quad \boldsymbol{p} \in \mathcal{D}$$

where $\boldsymbol{R}(\boldsymbol{p})$ is the rotation matrix of angle $\theta(p)$ and $\boldsymbol{D}(\boldsymbol{p}) = \mathrm{Diag}\left(\rho_1(\boldsymbol{p}), \ldots, \rho_d(\boldsymbol{p})\right)$.

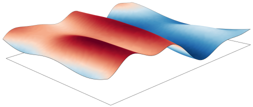
FINITE ELEMENT APPROXIMATION

Principle: $\mathcal{Z} = \sum_{k\in\mathbb{N}} \gamma(\lambda_k) W_k \; e_k \quad \approx \quad \mathcal{Z}_h = \sum_{i=1}^{N_h} Z_i \psi_i \in V_h.$



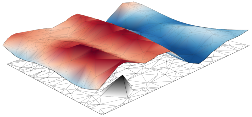
Mesh size h

$\rightarrow \quad \mathcal{Z}_h(p) = \sum_{i=1}^{N_h} Z_i \psi_i(p) \quad \rightarrow$



$\mathcal{Z}$

$\approx$



$\mathcal{Z}_n$

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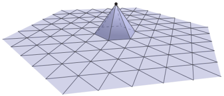

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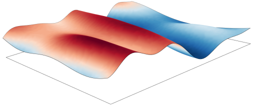

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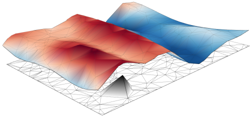

$\mathcal{Z}$ $\qquad$ $\mathcal{Z}_n$

$\to$ **How?** Galerkin approximation $\mathcal{L}_h : V_h = \text{span}\{\psi_1, \dots, \psi_{N_h}\} \to V_h$ such that, for any $\phi \in V_h$

$\mathcal{L}_h\phi \in V_h$ satisfies $\boxed{\langle \mathcal{L}_h\phi, f\rangle = \langle \mathcal{L}\phi, f\rangle} \quad \forall f \in V_h$

$$\mathcal{Z} = \sum_{k=1}^{\infty} \gamma(\lambda_k) W_k e_k$$

Eigendecomposition of the Laplace-Beltrami operator

$\approx$

$$\mathcal{Z}_n = \sum_{k=1}^{N_h} \gamma(\lambda_k^{(h)}) W_k e_k^{(h)} \in V_h$$

Eigendecomposition of the "Galerkin Laplacian"

EXPLICIT COMPUTATION OF THE APPROXIMATION

$$\mathcal{Z} = \sum_{k=1}^{\infty} \gamma(\lambda_k) W_k e_k \quad \rightarrow \quad \mathcal{Z}_h = \sum_{k=1}^{N_h} \gamma(\lambda_k^{(h)}) W_k e_k^{(h)} = \sum_{i=1}^{N_h} Z_i \psi_i \in V_h$$

Introduce:

Mass matrix

$$\boldsymbol{C} = [\langle \psi_k, \psi_l \rangle]_{1 \leq k,l \leq N_h}$$

Stiffness matrix

$$\boldsymbol{R} = [\langle \mathcal{L}\psi_k, \psi_l \rangle]_{1 \leq k,l \leq N_h}$$

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Stiffness matrix

$$\boldsymbol{R} = [\langle \mathcal{L}\psi_k, \psi_l \rangle]_{1 \leq k,l \leq N_h}$$

The weights $\boldsymbol{Z} = (Z_1, \ldots, Z_{N_h})$ can be computed through the relation (Lang and Pereira, 2023)

$$\boxed{\boldsymbol{Z} = \boldsymbol{C}^{-1/2} \gamma(\boldsymbol{S}) \boldsymbol{W}}, \quad \text{with } \boldsymbol{W} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

where $\boldsymbol{C}^{1/2}$ is a symmetric matrix satisfying $\left(\boldsymbol{C}^{1/2}\right)^2 = \boldsymbol{C}$ and $\boldsymbol{S} = \boldsymbol{C}^{-1/2} \boldsymbol{R} \boldsymbol{C}^{-1/2}$ with

$$\boldsymbol{S} = \boldsymbol{V} \begin{pmatrix} \lambda_1^{(h)} & & \\ & \ddots & \\ & & \lambda_{N_h}^{(h)} \end{pmatrix} \boldsymbol{V}^T \quad \Rightarrow \quad \gamma(\boldsymbol{S}) := \boldsymbol{V} \begin{pmatrix} \gamma(\lambda_1^{(h)}) & & \\ & \ddots & \\ & & \gamma(\lambda_{N_h}^{(h)}) \end{pmatrix} \boldsymbol{V}^T$$

■ QUICK COMPARISON WITH THE SPDE APPROACH

We have a direct generalization!

SPDE approach (Lindgren et al., 2011)

Field

$$(\kappa^2 - \Delta)^{\alpha/2}\mathcal{Z} = \mathcal{W}$$

where $\alpha \in \mathbb{N}$

Approximation

$$\mathcal{Z}_h = \sum_{i=1}^{N_h} Z_i \psi_i$$

Weights of the approximation

$$\boldsymbol{Z} = \boldsymbol{C}^{-1/2}\left(\kappa^2 \boldsymbol{I} + \boldsymbol{S}\right)^{-\alpha/2}\boldsymbol{W}$$

Generalized random fields approach

Field

$$\mathcal{Z} = \gamma(\mathcal{L})\mathcal{W},$$

where $|\gamma(\lambda)| = \mathcal{O}_{\lambda\to\infty}(|\lambda|^{-\beta})$ with $\beta > d/4$

Approximation

$$\mathcal{Z}_h = \sum_{i=1}^{N_h} Z_i \psi_i$$

Weights of the approximation

$$\boldsymbol{Z} = \boldsymbol{C}^{-1/2}\gamma(\boldsymbol{S})\boldsymbol{W}$$

RANDOM FIELDS ON RIEMANNIAN MANIFOLDS: RECAP

$L^2(\mathcal{M})$

$\downarrow$

Spectral theorem: $\{(\lambda_k, e_k) : k \in \mathbb{N}\}$
eigenvalues/functions of $\mathcal{L}$

$\downarrow$

$L^2(\mathcal{M})$-valued random variables

$$\mathcal{Z} = \sum_{k\in\mathbb{N}} \underbrace{\gamma(\lambda_k)W_k}_{\substack{\text{independent}\\ \text{Gaussian weights}}} \; e_k$$

$V_{N_h} = \operatorname{span}\{\psi_1, \dots, \psi_{N_h}\} \subset L^2(\mathcal{M})$ FEM basis

$\downarrow$

"Spectral theorem": $\left\{(\lambda_k^{(h)}, e_k^{(h)}) : k \in [\![1, N_h]\!]\right\}$
eigenvalues/functions of $\mathcal{L}_h$

$\downarrow$

V_{N_h}-valued random variables

$$\mathcal{Z}_h = \sum_{k=1}^{N_h} \underbrace{\gamma(\lambda_k^{(h)})W_k^{(h)}}_{\substack{\text{independent}\\ \text{Gaussian weights}}} e_k^{(h)} = \sum_{i=1}^{N_h} Z_i \psi_i$$

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$$\mathcal{Z} = \sum_{k\in\mathbb{N}} \underbrace{\gamma(\lambda_k) W_k}_{\substack{\text{independent}\\ \text{Gaussian weights}}} e_k$$

$\downarrow$

✓ Local definition of covariance:

$$\mathrm{Cov}\left(\mathcal{Z}(\boldsymbol{p}), \mathcal{Z}(\boldsymbol{p}+d\boldsymbol{p})\right) \approx C_0\left(\sqrt{g_{\boldsymbol{p}}(d\boldsymbol{p}, d\boldsymbol{p})}\right)$$

where $C_0 = \mathscr{F}^{-1}[\gamma^2]$

✓ Local anisotropy modeling:

$$g_{\boldsymbol{p}}(\boldsymbol{u}, \boldsymbol{v}) = \left(\boldsymbol{D}(\boldsymbol{p})^{-1}\boldsymbol{R}(\boldsymbol{p})^T\boldsymbol{u}\right)^T\left(\boldsymbol{D}(\boldsymbol{p})^{-1}\boldsymbol{R}(\boldsymbol{p})^T\boldsymbol{v}\right)$$

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✓ Explicit computation:

$$\boxed{\boldsymbol{Z} = \boldsymbol{C}^{-1/2}\gamma(\boldsymbol{S})\boldsymbol{W}, \quad \boldsymbol{W} \sim \mathcal{N}(0, \boldsymbol{I})}$$

where $\boldsymbol{S} = \boldsymbol{C}^{-1/2}\boldsymbol{R}\boldsymbol{C}^{-1/2}$,
$\boldsymbol{C} = [\langle\psi_i, \psi_j\rangle]$, $\boldsymbol{R} = [\langle\mathcal{L}\psi_i, \psi_j\rangle]$

$\rightarrow$ **sparse matrices**

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$L^2(\mathcal{M})$

$\downarrow$

Spectral theorem: $\{(\lambda_k, e_k) : k \in \mathbb{N}\}$
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$\downarrow$

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$\longleftrightarrow$ **FEM convergence result**

$V_{N_h} = \mathrm{span}\,\{\psi_1, \dots, \psi_{N_h}\} \subset L^2(\mathcal{M})$ FEM basis

$\downarrow$

"Spectral theorem": $\left\{(\lambda_k^{(h)}, e_k^{(h)}) : k \in [\![1, N_h]\!]\right\}$
eigenvalues/functions of $\mathcal{L}_h$

$\downarrow$

V_{N_h}-valued random variables

$$\mathcal{Z}_h = \sum_{k=1}^{N_h} \underbrace{\gamma(\lambda_k^{(h)})W_k^{(h)}}_{\text{independent Gaussian weights}} e_k^{(h)} = \sum_{i=1}^{N_h} Z_i\psi_i$$

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$$\boxed{\boldsymbol{Z} = \boldsymbol{C}^{-1/2}\gamma(\boldsymbol{S})\boldsymbol{W}, \quad \boldsymbol{W} \sim \mathcal{N}(0, \boldsymbol{I})}$$

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$\boldsymbol{C} = [\langle\psi_i, \psi_j\rangle], \boldsymbol{R} = [\langle\mathcal{L}\psi_i, \psi_j\rangle]$
$\rightarrow$ **sparse matrices**

FEM CONVERGENCE: SKETCH OF PROOF

- Let $\Pi_h : L^2(\mathcal{M}) \to V_h$ orthogonal projection and define the action of the operator $\gamma(\mathcal{L})$ (and by analogy $\gamma(\mathcal{L}_h)$) as
$$\gamma(\mathcal{L})f = \sum_i \gamma(\lambda_i)\langle f, e_i\rangle e_i$$

- Then,

$$\mathcal{Z} = \sum_{k\in\mathbb{N}} \gamma(\lambda_k) W_k e_k = \gamma(\mathcal{L})\mathcal{W}$$

where $\mathcal{W} = \sum_{k\in\mathbb{N}} W_k e_k$

$$\mathcal{Z}_h = \sum_{k=1}^{N_h} \gamma(\lambda_k^{(h)}) W_k^{(h)} e_k^{(h)} = \gamma(\mathcal{L}_h)\mathcal{W}_h$$

where $\mathcal{W}_h = \sum_{k=1}^{N_h} W_k^{(h)} e_k^{(h)} = \Pi_h \mathcal{W}$

- Goal: Bound the following so-called strong error by the mesh size h
$$\|\mathcal{Z} - \mathcal{Z}_h\|_{L^2(\Omega;L^2(\mathcal{M}))} = \mathbb{E}[\|\mathcal{Z} - \mathcal{Z}_h\|^2]^{1/2} = \|\gamma(\mathcal{L})\mathcal{W} - \gamma(\mathcal{L}_h)(\Pi_h\mathcal{W})\|_{L^2(\Omega;L^2(\mathcal{M}))}$$

FEM CONVERGENCE: SKETCH OF PROOF

- Start with the deterministic case : $f \in L^2(\mathcal{M})$,
$$\|\gamma(\mathcal{L})f - \gamma(\mathcal{L}_h)(\Pi_h f)\|$$
- Classical FEM results give estimates for the error $\|u - u_h\|$ between the solutions of problems
$$\mathcal{L}u = f \quad \text{and} \quad \mathcal{L}u_h = \Pi_h f$$
i.e. bounds for
$$\|\mathcal{L}^{-1}f - \mathcal{L}_h^{-1}(\Pi_h f)\|$$
$\rightarrow$ Find a way to use this estimate (or something close)
- $\gamma : \mathbb{C} \rightarrow \mathbb{R}$ such that if $\mathrm{Re}(z) \geq 0$, $|\gamma(z)| = \mathcal{O}_{|\infty| \rightarrow \infty}(|\lambda|^{-\beta})$ with $\beta > d/4$ and γ is smooth

FEM CONVERGENCE: SKETCH OF PROOF

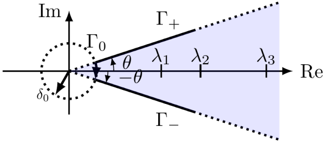
- Idea: Functional calcul and Cauchy theorem : If γ is holomorphic around $\lambda \in \mathbb{C}$,

$$\gamma(\lambda) = \int_\Gamma \gamma(z)(z-\lambda)^{-1}dz$$

where Γ is a closed curve containing $\lambda \in \mathbb{C}$ and in the region where γ is holomorphic

- We build a contour Γ containing all the eigenvalues of $\mathcal{L}$ so that we can write

$$\begin{aligned}
\gamma(\mathcal{L})f &= \sum_{i=1}^{\infty} \left(\int_\Gamma \gamma(z)(z-\lambda_i)^{-1}dz \right) \langle f, e_i \rangle e_i \\
&= \int_\Gamma \gamma(z) \left(\sum_{i=1}^{\infty} (z-\lambda_i)^{-1} \langle f, e_i \rangle e_i \right) dz \\
&= \int_\Gamma \gamma(z)(z-\mathcal{L})^{-1} f dz
\end{aligned}$$



FEM CONVERGENCE: SKETCH OF PROOF

- Hence,

$$\|\gamma(\mathcal{L})f - \gamma(\mathcal{L}_h)(\Pi_h f)\| = \| \int_\Gamma \gamma(z)(z-\mathcal{L})^{-1} f dz - \int_\Gamma \gamma(z)(z-\mathcal{L}_h)^{-1}\Pi_h f dz\|$$
$$\leq \int_\Gamma |\gamma(z)| \, \|(z-\mathcal{L})^{-1} f - (z-\mathcal{L}_h)^{-1}\Pi_h f\| dz$$

$\rightarrow$ Error $\|u - u_h\|$ between the solutions of the finite element problems

$$zu - \mathcal{L}u = f \text{ and } zu_h - \mathcal{L}u_h = \Pi_h f$$

Computed using classical FEM estimate for $\|\mathcal{L}^{-1} f - \mathcal{L}_h^{-1}(\Pi_h f)\|$

- **Deterministic error**: for $p \in [0,1]$, if $\|\mathcal{L}^p f\| < \infty$,

$$\|\gamma(\mathcal{L}_h)\Pi_h f - \gamma(\mathcal{L})f\| \leq C_{\alpha+p}(h) h^{2\min\{\beta+p;1\}} \|\mathcal{L}^p f\|,$$

where $C_{\alpha+p}(h)$ is a logarithmic term

FEM CONVERGENCE: SKETCH OF PROOF

- Direct generalization to $f = \mathcal{W}$ is not possible since $\mathcal{W} \notin L^2(\mathcal{M})$
- Case $\beta < 1$: We write

$$\begin{aligned}\|\gamma(\mathcal{L}_h)\Pi_h\mathcal{W}-\gamma(\mathcal{L})\mathcal{W}\|_{L^2(\Omega;L^2(\mathcal{M}))} \\ \leq \underbrace{\|\gamma(\mathcal{L})\mathcal{W}-\gamma(\mathcal{L})\Pi_h\mathcal{W}\|_{L^2(\Omega;L^2(\mathcal{M}))}}_{:=S_1} + \underbrace{\|\gamma(\mathcal{L})\Pi_h\mathcal{W}-\gamma(\mathcal{L}_h)\Pi_h\mathcal{W}\|_{L^2(\Omega;L^2(\mathcal{M}))}}_{:=S_2}\end{aligned}$$

where S_2 is bounded using the deterministic bound since $\Pi_h\mathcal{W} \in L^2(\mathcal{M})$, and

$$S_1^2 = \|\sum_{i\in\mathbb{N}} \gamma(\lambda_i)W_i(e_i - \Pi_h e_i)\|^2_{L^2(\Omega;L^2(\mathcal{M}))} = \sum_{i\in\mathbb{N}} \gamma(\lambda_i)^2\|e_i - \Pi_h e_i\|^2,$$

is bounded using the FEM projection estimate (Bramble-–Hilbert lemma)

$$\|(I-\Pi_h)f\| \lesssim h^t\|\mathcal{L}^{t/2}f\|, \text{for } t \in (0,2)$$

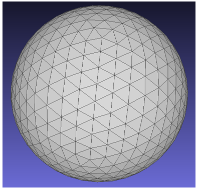
FEM CONVERGENCE: SKETCH OF PROOF

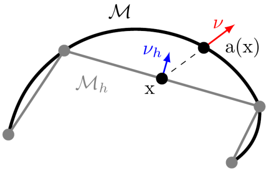
- We proceed similarly for $\beta \geq 1$
- Final error estimate: (for $\beta > d/4$)

$$\|\mathcal{Z} - \mathcal{Z}_h\|_{L^2(\Omega;L^2(\mathcal{M}))} = \|\gamma(\mathcal{L})\mathcal{W} - \gamma(\mathcal{L}_h)\Pi_h\mathcal{W}\|_{L^2(\Omega;L^2(\mathcal{M}))} \leq C_\alpha(h)h^{2\min\{\beta-d/4;1\}},$$

where $C_\alpha(h)$ is a logarithmic term

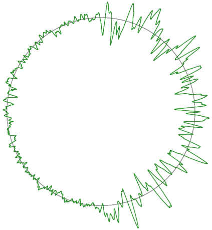
- When working on surfaces: FEM defined on a polyhedral approximation of the surface and not on the real ideal surface

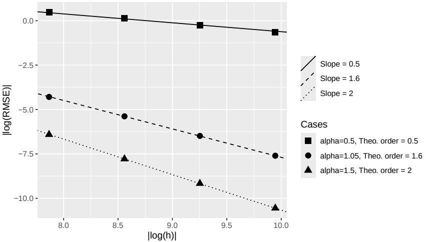


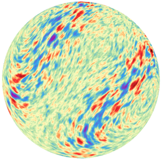


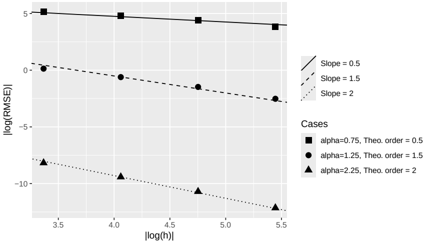
$\rightarrow$ Additional error term for geomertic consistency, but of the same order (or higher)

■ CONFIRMING THE CONVERGENCE RATES









OUTLINE

I. Random fields on Riemannian manifolds

II. Sampling and prediction

III. Conclusion

■ COMPUTING THE DISCRETIZED RANDOM FIELDS

Finite element approximation of GRF: $\mathcal{Z}_h = \sum_{i=1}^{N_h} Z_i \psi_i$ where $\boldsymbol{Z} = (Z_1, \dots, Z_n)^T$ is obtained by

$$\boxed{\boldsymbol{Z} = \boldsymbol{C}^{-1/2}\gamma(\boldsymbol{S})\boldsymbol{W}} \quad \text{with} \quad \boldsymbol{W} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

$\rightarrow$ How to compute $\gamma(\boldsymbol{S})\boldsymbol{W}$?

- Direct computation?

$$\boldsymbol{S} = \boldsymbol{V} \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_{N_h} \end{pmatrix} \boldsymbol{V}^T \Rightarrow \gamma(\boldsymbol{S})\boldsymbol{W} = \underline{\boldsymbol{V} \underline{\begin{pmatrix} \gamma(\lambda_1) & & \\ & \ddots & \\ & & \gamma(\lambda_{N_h}) \end{pmatrix} \underline{\boldsymbol{V}^T \boldsymbol{W}}}}$$

$\Rightarrow$ Diagonalization + Storage : Expensive!!

■ COMPUTING THE DISCRETIZED RANDOM FIELDS

Finite element approximation of GRF: $\mathcal{Z}_h = \sum_{i=1}^{N_h} Z_i \psi_i$ where $\boldsymbol{Z} = (Z_1, \dots, Z_n)^T$ is obtained by

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$\rightarrow$ How to compute $\gamma(\boldsymbol{S})\boldsymbol{W}$?

- **Idea: use the polynomial case**

$$\text{For } P(X) = \sum a_k X^k, \quad P(\boldsymbol{S})\boldsymbol{w} = \boldsymbol{V} \begin{pmatrix} P(\lambda_1) & & \\ & \ddots & \\ & & P(\lambda_n) \end{pmatrix} \boldsymbol{V}^T \boldsymbol{w} = \sum a_k \boldsymbol{S}^k \boldsymbol{w}$$

$\Rightarrow$ $P(\boldsymbol{S})\boldsymbol{w}$ is computable iteratively: only involves matrix-vector multiplications!

Compute $P(\boldsymbol{S})\boldsymbol{w}$ where P **is an approximation of** γ over an interval containing $\{\lambda_1, \dots, \lambda_n\}$

$$\Rightarrow P(\boldsymbol{S})\boldsymbol{w} \approx \gamma(\boldsymbol{S})\boldsymbol{w} \quad \text{since} \quad \forall i \in \{1, \dots, N_h\}, \quad P(\lambda_i) \approx \gamma(\lambda_i)$$

GALERKIN–CHEBYSHEV APPROXIMATION

Finite element approximation: $\mathcal{Z}_h = \sum_{i=1}^{N_h} Z_i \psi_i$ where $\boldsymbol{Z} = (Z_1, \dots, Z_n)^T$ is obtained by:

$$\boxed{\boldsymbol{Z} = \boldsymbol{C}^{-1/2}\gamma(\boldsymbol{S})\boldsymbol{W}} \quad \text{with} \quad \boldsymbol{W} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

Galerkin–Chebyshev approximation: $\widehat{\mathcal{Z}}_n = \sum_{i=1}^{n} \widehat{Z}_i \psi_i$ where $\widehat{\boldsymbol{Z}} = (\widehat{Z}_1, \dots, \widehat{Z}_n)$is obtained by:

$$\boxed{\widehat{\boldsymbol{Z}} = \boldsymbol{C}^{-1/2} P_\gamma(\boldsymbol{S})\boldsymbol{W}} \quad \text{with } \boldsymbol{W} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

and P_γ **is a Chebyshev polynomial approximation of** γ

$\rightarrow$ **No need to compute any matrix decomposition!**

$\rightarrow$ Additional polynomial approximation error decreasing with the degree of P_γ

BACK TO KRIGING PREDICTION

Input Observations $Y(x_i)$ at some points $(x_1, \dots, x_{N_D})$ of a spatial domain $\mathcal{D}$

$$Y(x_i) = \mathcal{Z}(x_i) + \tau\varepsilon_i, \quad i \in \{1, \dots, k\}$$

- $\mathcal{Z}$: Underlying (non-stationary) random field $\rightarrow$ Galerkin–Chebyshev approach
- $\varepsilon_1, \dots, \varepsilon_{N_D} \sim \mathcal{N}(0, 1)$ iid noise

Output Kriging estimates $Z^*(p_j)$ of $\mathcal{Z}$ some points $(p_1, \dots, p_{N_T})$ of $\mathcal{D}$

BACK TO KRIGING PREDICTION

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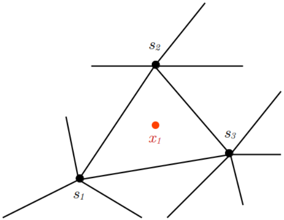
Model: Observations $\boldsymbol{Y} = (Y(\boldsymbol{x}_1), \dots, Y(\boldsymbol{x}_{N_D}))^T$ are given by

$$\boxed{\boldsymbol{Y} = \boldsymbol{M}_D\boldsymbol{Z} + \tau\boldsymbol{\epsilon}}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

where $\boldsymbol{Z} = (Z(\boldsymbol{s}_1), \dots, Z(\boldsymbol{s}_n))^T$ contains the weights of the Galerkin–Chebyshev approximation of $\mathcal{Z}$ and $\boldsymbol{M}_D$ is a projection matrix



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Output Kriging estimates $Z^*(p_j)$ of $\mathcal{Z}$ at some points $(p_1, \dots, p_{N_T})$ of $\mathcal{D}$

Computation Solve the kriging system defined by

$$\begin{pmatrix} \vdots \\ Z^*(p_j) \\ \vdots \end{pmatrix} = \boldsymbol{M}_T \boldsymbol{\Sigma} \boldsymbol{M}_D^T (\boldsymbol{M}_D \boldsymbol{\Sigma} \boldsymbol{M}_D^T + \tau^2 \boldsymbol{I}_p)^{-1} \boldsymbol{Y} = \boldsymbol{M}_T (\tau^2 \boldsymbol{Q} + \boldsymbol{M}_D^T \boldsymbol{M}_D)^{-1} \boldsymbol{M}_D^T \boldsymbol{Y}$$

where $\boldsymbol{\Sigma}$ is the covariance matrix of the Galerkin–Chebyshev weights, $\boldsymbol{Q}$ its precision matrix, and $\boldsymbol{M}_T$ is a projection matrix

BACK TO KRIGING PREDICTION

Goal Solve the kriging system defined by

$$\begin{pmatrix} \vdots \\ Z^*(p_j) \\ \vdots \end{pmatrix} = \boldsymbol{M}_T \boldsymbol{\Sigma} \boldsymbol{M}_D^T (\boldsymbol{M}_D \boldsymbol{\Sigma} \boldsymbol{M}_D^T + \tau^2 \boldsymbol{I}_p)^{-1} \boldsymbol{Y} = \boldsymbol{M}_T (\tau^2 \boldsymbol{Q} + \boldsymbol{M}_D^T \boldsymbol{M}_D)^{-1} \boldsymbol{M}_D^T \boldsymbol{Y}$$

Challenges

- Defining the covariance matrices
- The big "N" problem

BACK TO KRIGING PREDICTION

Goal Solve the kriging system defined by

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Challenges

- Defining the covariance matrices ✓
- The big "N" problem

Explicit formula from the Galerkin–Chebyshev approach for the covariance matrix

$$\boldsymbol{\Sigma} = \boldsymbol{C}^{-1/2} P_\gamma^2(\boldsymbol{S}) \boldsymbol{C}^{-1/2}$$

or for the precision matrix

$$\boldsymbol{Q} = \boldsymbol{C}^{1/2} P_{1/\gamma}^2(\boldsymbol{S}) \boldsymbol{C}^{1/2}$$

BACK TO KRIGING PREDICTION

Goal Solve the kriging system defined by

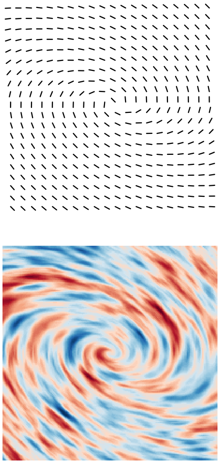
$$\begin{pmatrix} \vdots \\ Z^*(p_j) \\ \vdots \end{pmatrix} = \boldsymbol{M}_T \boldsymbol{\Sigma} \boldsymbol{M}_D^T (\boldsymbol{M}_D \boldsymbol{\Sigma} \boldsymbol{M}_D^T + \tau^2 \boldsymbol{I}_p)^{-1} \boldsymbol{Y} = \boldsymbol{M}_T (\tau^2 \boldsymbol{Q} + \boldsymbol{M}_D^T \boldsymbol{M}_D)^{-1} \boldsymbol{M}_D^T \boldsymbol{Y}$$

Challenges

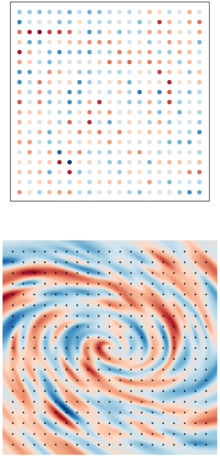
- Defining the covariance matrices ✓
- The big "N" problem ✓

The linear system is solved using a matrix-free iterative algorithm (eg. Conjugate gradient): In the end, only require products between (sparse) matrices and vectors

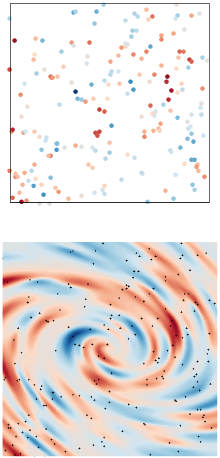
■ EXAMPLE ON SIMULATED DATA



Simulation a non-stationary field, and associated local anisotropies.

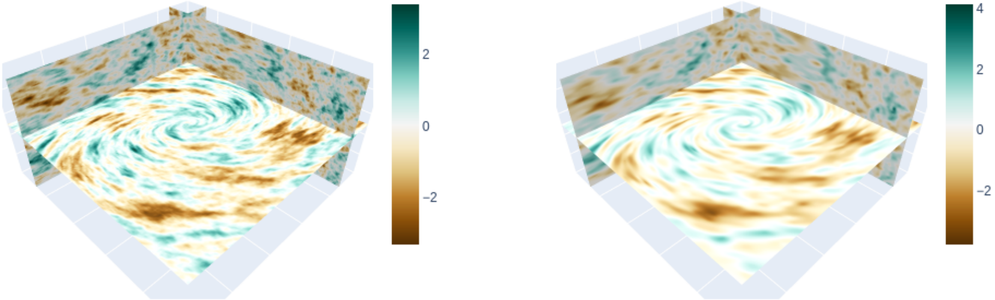


Field observations (regular sampling) and kriging estimate.



Field observations (random sampling) and kriging estimate.

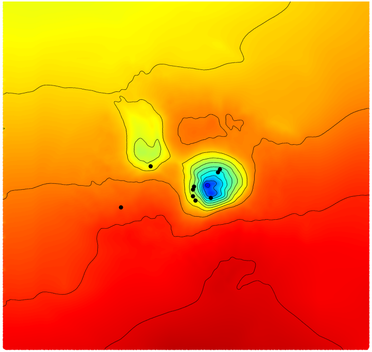
■ EXAMPLE ON SIMULATED DATA



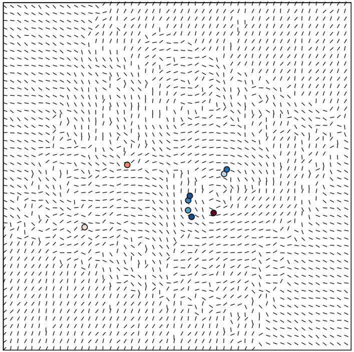
Left: 3D simulation of a GRF with varying anisotropies. Right: Kriging estimate using 10^5 randomly located samples from the simulation on the left.

■ EXAMPLE ON REAL DATA DATA: WELL CALIBRATION

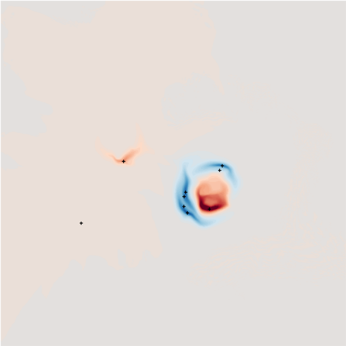
Goal: Calibrate depth estimation from seismic data using well data by kriging the residuals.



Depth map obtained from seismic data. The continuous lines represent level sets, and the black dots represent well locations.



Local anisotropies computed from the level sets, and well locations.

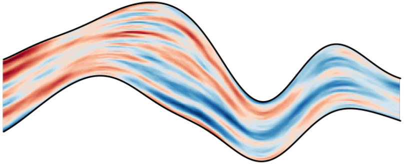


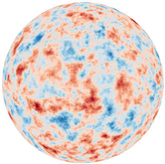
Kriging estimate of residual points between well and seismic data from the ODA field.

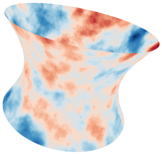
OUTLINE

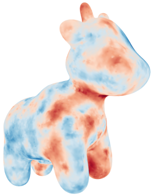
■ CONCLUDING REMARKS

- Modeling complex spatial data using Riemannian manifolds
  - Riemannian metric for local anisotropy in the data
  - Manifold for data lying on locally Euclidean domains
- Finite element method for numerical purposes
  - Explicit expression the covariance of the weights
  - Convergence linked to the mesh size
  - Sparse matrix algebra
- Change of paradigm
  - Covariance parameters $\rightarrow$ SPDE parameters
  - Possible physical interpretation of results (eg. advection, diffusion)



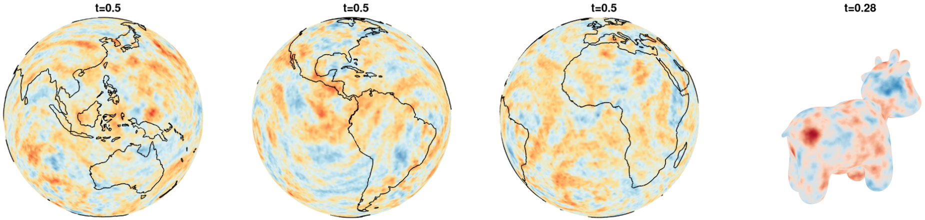






■ OUTLOOKS

- Numerically efficient inference for spatio-temporal models
  - Currently based on likelihood maximization
  - Work on neural-network based approaches (Lenzi et al., 2023; Sainsbury-Dale et al., 2023; Walchessen et al., 2023)
- (Stochastic) Analysis of spatio-temporal extension: Convergence results, Stabilization problems
- Applications: CO_2 data on the globe, Temperature and deformation fields on nuclear waste galleries



THANK YOU FOR YOUR ATTENTION!

For more on this subject

Jansson, E., Lang, A., and **P., M.** (2024). Non-stationary Gaussian random fields on hypersurfaces: Sampling and strong error analysis. *arXiv:2406.08185*.

P., M. (2023). A note on spatio-temporal random fields on meshed surfaces defined from advection-diffusion SPDEs. *hal-04132148*.

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P., M., Desassis, N., Allard D. (2022). Geostatistics for Large Datasets on Riemannian Manifolds: A Matrix-Free Approach, *Journal of Data Science, 20(4), 512-532*.

OUTLOOK: INFERENCE

Model Observations $\boldsymbol{Y} = (Y(\boldsymbol{x}_1), \dots, Y(\boldsymbol{x}_{N_D}))^T$ are given by

$$\boxed{\boldsymbol{Y} = \boldsymbol{M}_D \boldsymbol{Z} + \tau \boldsymbol{\epsilon}}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

where $\boldsymbol{Z} = (Z(\boldsymbol{s}_1), \dots, Z(\boldsymbol{s}_n))^T$ is the vector containing the weights of the Galerkin–Chebyshev approximation of $\mathcal{Z}$ and $\boldsymbol{M}_D$ is a projection matrix

Log-likelihood given by

$$\mathcal{L}(\boldsymbol{\theta}) = \log |\boldsymbol{Q}_{\boldsymbol{Y}}(\boldsymbol{\theta})| - \boldsymbol{Y}^T \boldsymbol{Q}_{\boldsymbol{Y}}(\boldsymbol{\theta}) \boldsymbol{Y} + \text{Constant},$$

where

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where

$$\boldsymbol{Y}^T \boldsymbol{Q}_{\boldsymbol{Y}}(\boldsymbol{\theta}) \boldsymbol{Y} = \tau^{-2} \left(\boldsymbol{Y}^T \boldsymbol{Y} - \boldsymbol{Y}^T \boldsymbol{M}_D \left(\tau^2 \boldsymbol{Q}(\boldsymbol{\theta}) + \boldsymbol{M}_D^T \boldsymbol{M}_D \right)^{-1} \boldsymbol{M}_D^T \boldsymbol{Y} \right),$$

$\rightarrow$ Solved again by matrix-free approach

OUTLOOK: INFERENCE

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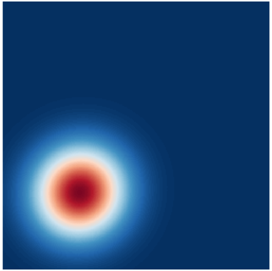
where

$$\log|\boldsymbol{Q}_{\boldsymbol{Y}}(\boldsymbol{\theta})| = \log|\boldsymbol{Q}(\boldsymbol{\theta})| + (n-p)\log\tau^2 - \log|\tau^2 \boldsymbol{Q}(\boldsymbol{\theta}) + \boldsymbol{M}_D^T \boldsymbol{M}_D|$$

$\rightarrow$ Hutchinson estimator (Hutchinson, 1989)

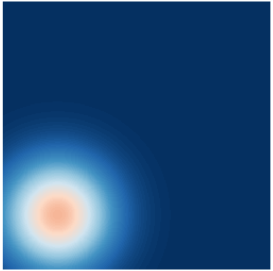
$$\log|h(\boldsymbol{B})| = \mathrm{Trace}(\log h(\boldsymbol{B})) = \mathbb{E}[\boldsymbol{W}^T \log h(\boldsymbol{B}) \boldsymbol{W}], \quad \boldsymbol{W} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$$

SOME SIMPLE TRANSPORT PHENOMENA



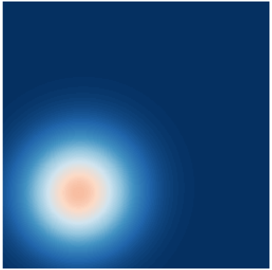
Advection

$$\frac{\partial z}{\partial t} + \vec{v} \cdot \nabla z = 0$$



Diffusion

$$\frac{\partial z}{\partial t} - \Delta z = 0$$



Advection + Diffusion

$$\frac{\partial z}{\partial t} + \vec{v} \cdot \nabla z - \Delta z = 0$$

ADVECTION-DIFFUSION SPDE ON RIEMANNIAN MANIFOLD

On a compact smooth Riemannian manifolds $(\mathcal{M}, g)$ of dimension 2, consider the SPDE (Pereira and Lang, 2023)

$$\frac{\partial \mathcal{Z}}{\partial t} + \frac{1}{c}\big((\kappa^2 - \Delta_{\mathcal{M}})^{\alpha}\mathcal{Z} + \mathrm{div}_{\mathcal{M}}(\mathcal{Z}\gamma)\big) = \frac{\tau}{\sqrt{c}}\mathcal{W}_T \otimes \mathcal{Y}_S,$$

where

- $-\Delta_{\mathcal{M}}$ is the Laplace–Beltrami operator and $\mathrm{div}_{\mathcal{M}}$ the divergence operator on $(\mathcal{M}, g)$
- $\mathcal{W}_T \otimes \mathcal{Y}_S$ is a noise white in time, colored in space
- $s \in \mathcal{M} \mapsto \gamma(s)$ is a smooth field of tangent vectors field

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- $s \in \mathcal{M} \mapsto \gamma(s)$ is a smooth field of tangent vectors field

Examples of tangent vector fields γ

$$\gamma(s) = \nabla\xi(s) \in T_s\mathcal{M}.$$

and if $\mathcal{M}$ is the 2-sphere :

$$\gamma(s) = \nabla\xi(s) + \vec{n}(s) \times \nabla\chi(s) \in T_s\mathbb{S}^2,$$

where $\xi, \chi : \mathcal{M} \to \mathbb{R}$ smooth functions, and $\vec{n}(s)$ outward normal at $s \in \mathcal{M}$

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