Statistical modeling of spatio-temporal data distributed over surfaces

Charlie Sire¹, Mike Pereira¹, Thomas Romary¹, Julien Cotton²

¹Centre for geosciences and geoengineering, Mines Paris, PSL University

²ANDRA

April 1, 2025













Spatio-temporal

Content



Splines on surfaces

- Mathematical framework
- Applications on the cylinder surface
- Future work

³ Spatio-temporal

Spatio-temporal

Cigeo project



CIGEO GEOLOGICAL DISPOSAL PROJECT

Objectives

Predict the evolution of the gallery during its operational phase based on measurements taken by sensors

2 quantities of interest:

- Temperature
- Deformation

Multiple sensors in the zone of interest, provide data everyday since 2017



Deformations

The sensors collects measurements of the 3 components of the deformation:

Radial deformation
 Orthoradial deformation
 Longitudinal deformation
 z

Here, focus and radial deformation and temperature

Spatio-temporal

Sensors position

One deformation sensor \Leftrightarrow One temperature sensor



Charlie SIRE

Introduction

Splines on surfaces

Spatio-temporal

Signals



Spatio-temporal

Trend estimation



Charlie SIRE

Spatio-temporal

Different trends



Spatio-temporal

Trend modeling for deformation

Every trend can be expressed

$$\mu_{\mathsf{Defo}}(t,\mathbf{s}) = \beta_0(\mathbf{s}) + \beta_1(\mathbf{s})\exp\left(-\beta_2(\mathbf{s})t\right) + \beta_3(\mathbf{s})\sin\left(\frac{2\pi}{365}t + \beta_4(\mathbf{s})\right)$$

Problem: Seek for linear relation in $\beta(\mathbf{s}) = (\beta_0(\mathbf{s}), \beta_1(\mathbf{s}), \beta_2(\mathbf{s}), \beta_3(\mathbf{s}), \beta_4(\mathbf{s}))$

Idea: Express trend as

$$\begin{split} \mu_{\mathsf{Defo}}(t,\mathbf{s}) &= \beta_0(\mathbf{s}) \\ &+ \beta_1(\mathbf{s}) \exp\left(-c_1 t\right) + \beta_2(\mathbf{s}) \exp\left(-c_2 t\right) \\ &+ \beta_3(\mathbf{s}) \sin\left(\frac{2\pi}{365}t + c_3\right) + \beta_4(\mathbf{s}) \sin\left(\frac{2\pi}{365}t + c_4\right) \end{split}$$

where c_1, c_2, c_3 and c_4 do not depend on **s**

Introduction 00000000000

Spatio-temporal

Trend modeling for temperature



$$\mu_{\mathsf{Temp}}(t,\mathbf{s}) = lpha_0(\mathbf{s}) + lpha_1(\mathbf{s})\sin\left(rac{2\pi}{365}t + c_5
ight)$$

Estimating the coefficients

Question : How to define functions $\beta_j(\mathbf{s})$ and $\alpha_j(\mathbf{s})$

Idea :

- Denote $(\mathbf{s}_i)_{i=1}^n$ the positions of the sensors
- Compute $\beta_j(\mathbf{s}_i)$ and $\alpha_j(\mathbf{s}_i)$, $1 \le i \le n$ with linear regression
- Use interpolation method to get β_j(s) and α_j(s) on the surface of the cylinder

Specific study: Work with interpolating splines on Riemannian manifold

 Spatio-temporal

Content





Splines on surfaces

- Mathematical framework
- Applications on the cylinder surface
- Future work



Splines in $\ensuremath{\mathbb{R}}$

Considering points $(x_i)_{i=1}^n$ in \mathbb{R} and observations $(y_i)_{i=1}^n$ at these points

The interpolation spline problem is to minimize

$$E(u) = \int_{\mathbb{R}} \left[u''(x) \right]^2 dx$$

given the constraint $u(x_i) = y_i, \ 1 \leq i \leq n$

Solution: $u^{*}(x) = a_0 + a_1 x + \sum_{i=1}^{n} b_i |x - x_i|^3$ [1] with

$$\begin{cases} \sum_i b_i = 0\\ \sum_i b_i x_i = 0\\ u(x_i) = y_i \quad \text{for } 1 \le i \le n. \end{cases}$$

Spatio-temporal

Splines 1D





Interpretation

Why the form $u^{*}(x) = a_0 + a_1 x + \sum_{i=1}^{n} b_i |x - x_i|^3$?

• $x \mapsto a_0 + a_1 x$: Space of function with null energy *E*

•
$$\sum_{i=1}^{n} b_i |x - x_i|^3 = \sum_{i=1}^{n} b_i K(x_i - x)$$
 with $K(h) = |h|^3$

Where this Kernel comes from ?

Fourier integral of a function u:

$$u(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{u}(\omega) e^{i\omega x} d\omega, \ \hat{u}$$
 the Fourier transform of u .

Functions $\phi_{\omega}(x) = e^{i\omega x}$ the eigenvectors of the second derivative operator.

Fourier transform of $K(h) \propto rac{1}{\omega^4}$, and ω^2 is the eigenvalue associated to $\phi_\omega(x)$

Generalization on Riemannian manifold

- \mathcal{M} a *d*-dimensional compact Riemannian manifold
- Δ the Laplace-Beltrami operator on ${\mathcal M}$

 $(\phi_k)_k$ eigen functions of Δ is a complete orthonormal basis for $L^2(\mathcal{M})$. Eigvenvalues λ_k with $\lambda_0 = 0$ and $\lambda_k \leq \lambda_{k+1}$

•
$$\forall u \in L^2(\mathcal{M}), u = \sum_k u_k \phi_k$$

•
$$\forall u \in L^2(\mathcal{M}), \Delta u = \sum_k \lambda_k u_k \phi_k$$

We define

$$H(\mathcal{M})=H_0(\mathcal{M})\oplus H_1(\mathcal{M}), \;\; {
m where}$$

• $H_0(\mathcal{M}) = \mathcal{E}_0$

- $H_1(\mathcal{M}) = \bigoplus_{k \neq 0} \mathcal{E}_k$
- \mathcal{E}_k eigenspace associated with λ_k

Generalization on Riemannian manifold

 $H_0(\mathcal{M}), H_1(\mathcal{M}) \text{ and } H(\mathcal{M})$ are RKHS with scalar products

- $\langle u, v \rangle_0 = u_0 \bar{v_0}$
- $\langle u, v \rangle_1 = \sum_{k \neq 0} \lambda_k^2 u_k \bar{v}_k$
- $\langle u, v \rangle = \langle u, v \rangle_0 + \langle u, v \rangle_1$

and reproducing kernels

•
$$K_0(\mathbf{s}_1, \mathbf{s}_2) = \phi_0(\mathbf{s}_1)\bar{\phi_0}(\mathbf{s}_2)$$

• $K_1(\mathbf{s}_1, \mathbf{s}_2) = \sum_{k \neq 0} \frac{1}{\lambda_k^2} \phi_k(\mathbf{s}_1) \bar{\phi_k}(\mathbf{s}_2)$
• $K(\mathbf{s}_1, \mathbf{s}_2) = K_0(\mathbf{s}_1, \mathbf{s}_2) + K_1(\mathbf{s}_1, \mathbf{s}_2)$



Generalization on Riemannian manifold

Interpolation problem is to minimize the norm in $H_1(\mathcal{M})$:

$$\|u\|_{H_1(\mathcal{M})} = \sum_k \lambda_k^2 |u_k|^2 = \int_M |\Delta u|^2$$

subject to the constraint $u(\mathbf{s}_i) = y_i$, with $s_i \in \mathcal{M}, 1 \leq i \leq n$,

Solution [3]

$$u^{\star}(\mathbf{s}) = a_0 \Phi_0(\mathbf{s}) + \sum_{i=1}^n b_i K_1(\mathbf{s}, \mathbf{s}_i)$$
 with

•
$$\forall 1 \le j \le n, \sum_{i=1}^{n} b_i K_1(s_j, s_i) + a_0 \Phi_0(\mathbf{s}_i) = y_j$$

• $\sum_{i=1}^{n} b_i \Phi_0(\mathbf{s}_i) = 0$

Analogy with case 1D

When $\mathcal{X}=\mathcal{M},$ compact manifold we have

- $u = \sum_{k} u_k \phi_k$
- $\Delta u = \sum_k \lambda_k u_k \phi_k$
- $H_0 = \{a_0\phi_0\}$
- $\mathcal{K}_1(\mathbf{s}_1, \mathbf{s}_2) = \sum_{k \neq 0} \frac{1}{\lambda_k^2} \phi_k(\mathbf{s}_1) \overline{\phi_k}(\mathbf{s}_2)$

When $\mathcal{X} = \mathbb{R}$, we have

• $u(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{u}(\omega) e^{i\omega x} d\omega$ • $u''(x) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} w^2 \hat{u}(\omega) e^{i\omega x} d\omega$ • $H_0 = \{x \mapsto a_0 + a_1 x\}$ • $K_1(x_1, x_2) \propto \int_{\mathbb{R}} \frac{1}{\omega^4} e^{-i\omega(x_2 - x_1)} d\omega$ inverse Fourier transform of $\omega \mapsto \frac{1}{\omega^4}$

Splines vs Gaussian process regression

Challenge: The eigenvalues and eigenvectors (λ_k, ϕ_k) are unknwon

Idea: Equivalence between Splines interpolation and GP Regression [2]

The solution u^* of the interpolation problem is

$$u^{\star}(\mathbf{s}) = \mathbb{E}\left(Y(\mathbf{s}) \mid y(\mathbf{s}_1), \dots, y(\mathbf{s}_n)\right)$$

where $Y(\mathbf{s})$ is a Gaussian process of

- Prior mean $a_0\phi_0(\mathbf{s})$, with unknown a_0
- Covariance kernel K_1

Can we simulate $Y(\mathbf{s})$ on Riemannian manifold ?

Introduction 00000000000 Splines on surfaces

Spatio-temporal

Expansion on $(\phi_k)_k$

Consider centered GRF Z through the expansion [5]

$$Z=\sum_k f^{1/2}(\lambda_k)W_k\phi_k,$$

with $f^{1/2}$ such that $(f^{1/2})^2 = f$ and $(W_k)_k$ independant Gaussian variables

Z has covariance function

$$C(\mathbf{s}_1,\mathbf{s}_2) = \sum_k f(\lambda_k)\phi_k(\mathbf{s}_1)\phi_k(\mathbf{s}_2)$$

Then, here we define

$$f(\lambda) = egin{cases} 0, & ext{if } \lambda = 0 \ rac{1}{\lambda^2}, & ext{else.} \end{cases}$$

Galerkin approximation

Consider triangulation T of \mathcal{M} :

- m nodes $(\mathbf{c}_1, \ldots, \mathbf{c}_m)$
- Compact support functions ψ₁,..., ψ_m: ψ_i piecewise linear equal to 1 at c_i and 0 at all other nodes to define approximation

$$Z_{\mathrm{T}}(\mathbf{s}) = \sum_{i=1}^{m} Z(\mathbf{c}_i) \psi_i(\mathbf{s})$$

Objective :

$$Z_{
m T}({f s}) = \sum_{k=1}^m f^{1/2}(\lambda_k^{(m)}) W_k \phi_k^{(m)}$$

with $\lambda_k^{(m)}$ and $\phi_k^{(m)}$ the eigenvalues and eigenvectors of the discretization Δ_m of the Laplace-Beltrami operator.

Galerkin approximation

- Mass matrix $\mathbf{M} = [\langle \psi_i, \psi_j \rangle]$ and stiffness matrix $\mathbf{G} = [\langle \nabla \psi_i, \nabla \psi_j \rangle]$
- Matrix $\mathbf{S} = (\sqrt{\mathbf{M}})^{-1} \mathbf{G} (\sqrt{\mathbf{M}})^{-T}$ with \mathbf{M} such that $\sqrt{\mathbf{M}} (\sqrt{\mathbf{M}})^{T} = \mathbf{M}$

Then, $(\lambda_k^{(m)})_{k=1}^m$ are the eigenvalues of **S**

From [4], **S** is diagonalizable:

$$\mathbf{S} = \mathbf{V} \mathsf{Diag}(\lambda_1^{(m)}, \dots, \lambda_m^{(m)}) \mathbf{V}^{\mathcal{T}}$$

Spatio-temporal

Galerkin approximation

$$Z_{\rm T} = \sum_{k=1}^m f^{1/2}(\lambda_k^{(m)}) W_k \phi_k^{(m)} = \sum_{i=1}^m Z_i \psi_i$$

with $\mathbf{Z} = (Z_1, \ldots, Z_n)$ centered Gaussian vector with covariance

$$\boldsymbol{\Sigma} = (\sqrt{\mathbf{M}})^{-T} f(\mathbf{S}) (\sqrt{\mathbf{M}})^{-1}$$

with

$$f(\mathbf{S}) = \mathbf{V} \mathsf{Diag}(f(\lambda_1^{(m)}), \dots, f(\lambda_m^{(m)})) \mathbf{V}^{\mathsf{T}}$$

Galerkin approximation

\Rightarrow $Z_{\rm T}$ is a centered GRF with covariance kernel

$$\mathcal{K}_{1}^{(m)}(\mathbf{s}_{1},\mathbf{s}_{2}) = \sum_{k=1}^{m} f(\lambda_{k}^{(m)})\phi_{k}^{(m)}(\mathbf{s}_{1})\phi_{k}^{(m)}(\mathbf{s}_{2})$$

and
$$Z_{\mathrm{T}}(\mathbf{s}) = \sum_{i=1}^{m} Z_i \psi_i = \mathbf{A}(\mathbf{s}) \mathbf{Z}$$
 with $\mathbf{A}(\mathbf{s}) = (\psi_1(\mathbf{s}), \dots, \psi_m(\mathbf{s}))$

Then

$$\mathcal{K}_1^{(m)}(\mathbf{s}_1,\mathbf{s}_2) = \mathbf{A}(\mathbf{s}_1) \mathbf{\Sigma} \mathbf{A}(\mathbf{s}_2)^T$$

Summary

- **(**) We have observations $\mathbf{y} = (y_i)_{i=1}^n$ at points $(\mathbf{s}_i)_{i=1}^n$ on a manifold \mathcal{M}
- 2 Build triangulation of \mathcal{M}
- Solution Consider $Z_{\mathrm{T}}(\mathbf{s}) = \sum_{i=1}^{m} Z_i \psi_i = \mathbf{A}(\mathbf{s}) \mathbf{Z}$ with $\mathbf{Z} = (Z_1, \dots, Z_m)$ of covariance $\mathbf{\Sigma} = (\sqrt{\mathbf{M}})^{-T} f(\mathbf{S}) (\sqrt{\mathbf{M}})^{-1}$
- Get $\phi_1^{(m)}$ eigenvector of Δ_m associated with $\lambda_1^{(m)} = 0$: $\phi_1^{(m)} = \sum_{k=1}^m \left[(\sqrt{M})^{-T} \mathbf{v}_1 \right]_k \psi_k$ with \mathbf{v}_1 first column of \mathbf{V}

() Consider the GRF $Y_{\mathrm{T}}(\mathbf{s}) = a_0 \phi_1^{(m)}(\mathbf{s}) + Z_{\mathrm{T}}(\mathbf{s})$ where

$$\mathsf{a}_0 = (\mathsf{P}^{\mathsf{T}}\mathsf{K}^{-1}\mathsf{P})^{-1}\mathsf{P}^{\mathsf{T}}\mathsf{K}^{-1}oldsymbol{y}$$
 where

$$\mathbf{P} = (\phi_1^{(m)}(\mathbf{s}_1), \dots, \phi_1^{(m)}(\mathbf{s}_n))^{\mathsf{T}}$$
, $\mathbf{K} = \mathbf{A}_n \mathbf{\Sigma}(\mathbf{A}_n)^{\mathsf{T}}$, $\mathbf{A}_n = (\mathbf{A}(\mathbf{s}_j))_{j=1}^n$

Spatio-temporal

Interpolation

Back to our interpolation problem

$$u^{\star}(\mathbf{s}) = \mathbb{E}\left(Y_{\mathrm{T}}(\mathbf{s}) \mid Y_{\mathrm{T}}(\mathbf{s}_{1}) = y_{1}, \ldots, Y_{\mathrm{T}}(\mathbf{s}_{n}) = y_{n}\right)$$

and then with the classical posterior expectation formula

$$u^{\star}(\mathbf{s}) = a_0 \phi_1^{(m)}(\mathbf{s}) + \mathbf{A}(\mathbf{s}) \mathbf{\Sigma} (\mathbf{A}_n)^T \left(\mathbf{A}_n \mathbf{\Sigma} (\mathbf{A}_n)^T \right)^{-1} \left(\mathbf{y} - a_0 \mathbf{P} \right)$$

with

Content





Splines on surfaces

- Mathematical framework
- Applications on the cylinder surface
- Future work



Spatio-temporal

Triangulation



Charlie SIRE

Geolearning

Spatio-temporal

Analytical test case



Spatio-temporal

Coefficients for temperature







Spatio-temporal

Coefficients for deformation



Prediction of β_2



Prediction of β₃

Prediction of β₄



Content





Splines on surfaces

- Mathematical framework
- Applications on the cylinder surface
- Future work

3 Spatio-temporal

Future work

Problem: For the moment, need to diagonalize S to work with

$$f(\mathbf{S}) = \mathbf{V} \mathsf{Diag}(f(\lambda_1^{(m)}), \dots, f(\lambda_m^{(m)})) \mathbf{V}^{\mathcal{T}}$$

Impossible in practice if very fine mesh

Question: How to work directly with precision matrix with singular Σ ?

 \Rightarrow Adapt work on intrinsic GMRF [6]



Content



Splines on surfaces

- Mathematical framework
- Applications on the cylinder surface
- Future work



Spatio-temporal model

We consider the model

$$\begin{cases} Y_{\mathsf{Defo}}(t, \mathbf{s}) = \mu_{\mathsf{Defo}}(t, \mathbf{s}) + X_{\mathsf{Defo}}(t, \mathbf{s}) + E_{\mathsf{Defo}}(t, \mathbf{s}) \\ Y_{\mathsf{Temp}}(t, \mathbf{s}) = \mu_{\mathsf{Temp}}(t, \mathbf{s}) + X_{\mathsf{Temp}}(t, \mathbf{s}) + E_{\mathsf{Temp}}(t, \mathbf{s}) \end{cases}$$

- $\mu(t, \mathbf{s})$ the deterministic trend trend
- $X(t, \mathbf{s})$ the centered random residual
- $E(t, \mathbf{s})$ the measurement white noise

Question: How to predict $X_{Defo}(t, \mathbf{s})$ and $X_{Temp}(t, \mathbf{s})$

Spatio-temporal

Account for dependency

We consider

$$\begin{bmatrix} X_{\mathsf{Temp}}(\mathbf{s},t) \\ X_{\mathsf{Defo}}(\mathbf{s},t) \end{bmatrix} = \mathbf{B} \begin{bmatrix} X_1(\mathbf{s},t) \\ X_2(\mathbf{s},t) \end{bmatrix}$$

with

•
$$\mathbf{B} = \begin{bmatrix} 1 & b_1 \\ b_2 & 1 \end{bmatrix}$$

• X₁(t, s) and X₂(t, s) independent spatio-temporal random fields solution of SPDE

Discretization:

$$egin{aligned} & X_1^{ ext{T}}(\mathbf{s},t) = \sum_{i=1}^m X_1^i(t)\psi_i(\mathbf{s})) \ & X_2^{ ext{T}}(\mathbf{s},t) = \sum_{i=1}^m X_2^i(t)\psi_i(\mathbf{s}) \end{aligned}$$

Spatio-temporal

Bibliography I



Olivier Dubrule.

Comparing splines and kriging.

Computers and Geosciences, 10(2):327–338, 1984.



Max Dunitz

Thin-plate splines on the sphere for interpolation, computing spherical averages, and solving inverse problems.

Image Processing On Line, 13:199, 2023.

P Kim.

Splines on riemannian manifolds and a proof of a conjecture by wahba. preprint (http://www. uoguelph. ca/pkim/research. html), 2001.

Bibliography II



Annika Lang and Mike Pereira.

Galerkin-chebyshev approximation of gaussian random fields on compact riemannian manifolds.

BIT Numerical Mathematics, 63(4):51, 2023.

Mike Pereira, Nicolas Desassis, and Denis Allard.

Geostatistics for large datasets on riemannian manifolds: A matrix-free approach.

Journal of Data Science, 20(4):512–532, 2022.



Daniel Peter Simpson, Ian W Turner, and Anthony N Pettitt.

Sampling from gaussian markov random fields conditioned on linear constraints.

The Proceedings of ANZIAM, 48:C1041–C1053, 2006.