PDE-constrained random fields: application to GPR for the 3D wave equation
ANR GAP

Iain Henderson, Pascal Noble, Olivier Roustant

INSA Toulouse
henderso@insa-toulouse.fr

5 Octobre 2022

Academic context

- PhD at the Institut de Mathématiques de Toulouse/INSA Toulouse, supervised by Pascal Noble and Olivier Roustant.
- Funded by the SHOM (Service Hydrographique et Océanographique de la Marine), contact : Remy Baraille

A physics informed machine learning problem

General problem :

A physics informed machine learning problem

General problem :

- unknown function $u : z \longmapsto u(z), \ z \in \mathcal{D}$

A physics informed machine learning problem

General problem :

- unknown function $u : z \longmapsto u(z), \; z \in \mathcal{D}$
- small database of values $B = \{u(z_1), ..., u(z_n)\}$

A physics informed machine learning problem

General problem :

- unknown function $u : z \longmapsto u(z),\ z \in \mathcal{D}$
- small database of values $B = \{u(z_1), ..., u(z_n)\}$
- u is a solution to a linear Partial Differential Equation (PDE) over $\mathcal{D}$:

A physics informed machine learning problem

General problem :

- unknown function $u : z \longmapsto u(z),\ z \in \mathcal{D}$
- small database of values $B = \{u(z_1), ..., u(z_n)\}$
- u is a solution to a linear Partial Differential Equation (PDE) over $\mathcal{D}$:

$$Lu = 0 \tag{1}$$

A physics informed machine learning problem

General problem :

- unknown function $u : z \longmapsto u(z), \ z \in \mathcal{D}$
- small database of values $B = \{u(z_1), ..., u(z_n)\}$
- u is a solution to a linear Partial Differential Equation (PDE) over $\mathcal{D}$:

$$Lu = 0 \tag{1}$$

Objective : reconstruct u from the knowledge of B and L.

A physics informed machine learning problem

General problem :

- unknown function $u : z \longmapsto u(z),\ z \in \mathcal{D}$
- small database of values $B = \{u(z_1), ..., u(z_n)\}$
- u is a solution to a linear Partial Differential Equation (PDE) over $\mathcal{D}$:

$$Lu = 0 \tag{1}$$

Objective : reconstruct u from the knowledge of B and L.

Possible solution : perform GPR on B, with a GP $(U(z))_{z\in\mathcal{D}}$ tailored to L,

A physics informed machine learning problem

General problem :

- unknown function $u : z \longmapsto u(z),\ z \in \mathcal{D}$
- small database of values $B = \{u(z_1), ..., u(z_n)\}$
- u is a solution to a linear Partial Differential Equation (PDE) over $\mathcal{D}$:

$$Lu = 0 \tag{1}$$

Objective : reconstruct u from the knowledge of B and L.

Possible solution : perform GPR on B, with a GP $(U(z))_{z \in \mathcal{D}}$ tailored to L, i.e. such that

1. the corresponding Kriging means $\tilde{m}$ verify $L\tilde{m} = 0$

A physics informed machine learning problem

General problem :

- unknown function $u : z \longmapsto u(z),\ z \in \mathcal{D}$
- small database of values $B = \{u(z_1), ..., u(z_n)\}$
- u is a solution to a linear Partial Differential Equation (PDE) over $\mathcal{D}$:

$$Lu = 0 \tag{1}$$

Objective : reconstruct u from the knowledge of B and L.

Possible solution : perform GPR on B, with a GP $(U(z))_{z\in\mathcal{D}}$ tailored to L, i.e. such that

1. the corresponding Kriging means $\tilde{m}$ verify $L\tilde{m} = 0$
2. the sample paths $\tilde{u}$ of U verify $L\tilde{u} = 0$

Linear constraints on the Kriging means (1)

Why impose linear constraints on the Kriging means ?

Linear constraints on the Kriging means (1)

Why impose linear constraints on the Kriging means ?

Approximate $u : \mathcal{D} \to \mathbb{R}$, i.e. $u \in \mathcal{F}(\mathcal{D}, \mathbb{R}) = E$

Linear constraints on the Kriging means (1)

Why impose linear constraints on the Kriging means ?

Approximate $u : \mathcal{D} \to \mathbb{R}$, i.e. $u \in \mathcal{F}(\mathcal{D}, \mathbb{R}) = E$

Prior knowledge : in fact, $u \in \ker L = F$:

Look for an interpolant of u directly in F rather than in E !

Linear constraints on the Kriging means (1)

Why impose linear constraints on the Kriging means ?

Approximate $u : \mathcal{D} \to \mathbb{R}$, i.e. $u \in \mathcal{F}(\mathcal{D}, \mathbb{R}) = E$

Prior knowledge : in fact, $u \in \ker L = F$:

Look for an interpolant of u directly in F rather than in E !

$F \subsetneq E \to$ "$\dim F < \dim E$" : "dimension reduction".

Why impose linear constraints on the Kriging means ?

Approximate $u : \mathcal{D} \to \mathbb{R}$, i.e. $u \in \mathcal{F}(\mathcal{D}, \mathbb{R}) = E$

Prior knowledge : in fact, $u \in \ker L = F$:

Look for an interpolant of u directly in F rather than in E !

$F \subsetneq E \to$ "$\dim F < \dim E$" : "dimension reduction".

Linear constraints on the Kriging means (2)

- Unknown function $u : z \longmapsto u(z),\ z \in \mathcal{D}$.

Linear constraints on the Kriging means (2)

- Unknown function $u : z \longmapsto u(z),\ z \in \mathcal{D}$.
- $Z = (z_1, ..., z_n)^T$ a set of locations and $Y = (y_1, ..., y_n)^T$ a set of observations of u at Z

Linear constraints on the Kriging means (2)

- Unknown function $u : z \longmapsto u(z),\ z \in \mathcal{D}$.
- $Z = (z_1, ..., z_n)^T$ a set of locations and $Y = (y_1, ..., y_n)^T$ a set of observations of u at Z

Let $(U(z))_{z \in \mathcal{D}} \sim GP(0, k(z, z'))$.

Linear constraints on the Kriging means (2)

- Unknown function $u : z \longmapsto u(z),\ z \in \mathcal{D}$.
- $Z = (z_1, ..., z_n)^T$ a set of locations and $Y = (y_1, ..., y_n)^T$ a set of observations of u at Z

Let $(U(z))_{z\in\mathcal{D}} \sim GP(0, k(z, z'))$. Kriging mean :

$$\begin{aligned}\tilde{m}(z) &= k(z, Z)k(Z, Z)^{-1}Y \\ &= \sum_{i=1}^{n} \alpha_i k(z, z_i)\end{aligned}$$

$$\rightarrow \tilde{m} \in \text{Span}(k(\cdot, z_1), ..., k(\cdot, z_n))$$

Linear constraints on the Kriging means (2)

- Unknown function $u : z \longmapsto u(z), \; z \in \mathcal{D}$.
- $Z = (z_1, ..., z_n)^T$ a set of locations and $Y = (y_1, ..., y_n)^T$ a set of observations of u at Z

Let $(U(z))_{z\in\mathcal{D}} \sim GP(0, k(z, z'))$. Kriging mean :

$$\tilde{m}(z) = k(z, Z)k(Z, Z)^{-1}Y$$
$$= \sum_{i=1}^{n} \alpha_i k(z, z_i)$$

$$\rightarrow \tilde{m} \in \text{Span}(k(\cdot, z_1), ..., k(\cdot, z_n))$$

$L(k(\cdot, z)) = 0 \; \forall z$ ensures that $L\tilde{m} = 0$.

Some examples of GPR for differential operators

Given L, find a kernel k_L s.t. $L(k_L(\cdot, z)) = 0 \ \forall z$;

Some examples of GPR for differential operators

Given L, find a kernel k_L s.t. $L(k_L(\cdot, z)) = 0\ \forall z$; $\Delta = \sum_{i=1}^{d} \partial^2_{x_i x_i}$:

Some examples of GPR for differential operators

Given L, find a kernel k_L s.t. $L(k_L(\cdot, z)) = 0 \ \forall z$; $\Delta = \sum_{i=1}^{d} \partial^2_{x_i x_i}$:

- Laplace : $\Delta u = 0$ Mendes and da Costa Júnior [2012], Ginsbourger et al. [2016]

Some examples of GPR for differential operators

Given L, find a kernel k_L s.t. $L(k_L(\cdot, z)) = 0 \ \forall z$; $\Delta = \sum_{i=1}^{d} \partial^2_{x_i x_i}$:

- Laplace : $\Delta u = 0$ Mendes and da Costa Júnior [2012], Ginsbourger et al. [2016]
- Heat : $\partial_t - D\Delta u = 0$ Albert and Rath [2020]

Some examples of GPR for differential operators

Given L, find a kernel k_L s.t. $L(k_L(\cdot, z)) = 0 \; \forall z$; $\Delta = \sum_{i=1}^{d} \partial^2_{x_i x_i}$:

- Laplace : $\Delta u = 0$ Mendes and da Costa Júnior [2012], Ginsbourger et al. [2016]
- Heat : $\partial_t - D\Delta u = 0$ Albert and Rath [2020]
- Div/Curl : $\nabla \cdot u = 0$, $\nabla \times u = 0$ Scheuerer and Schlather [2012]

Some examples of GPR for differential operators

Given L, find a kernel k_L s.t. $L(k_L(\cdot, z)) = 0 \; \forall z$; $\Delta = \sum_{i=1}^{d} \partial^2_{x_i x_i}$:

- Laplace : $\Delta u = 0$ Mendes and da Costa Júnior [2012], Ginsbourger et al. [2016]
- Heat : $\partial_t - D\Delta u = 0$ Albert and Rath [2020]
- Div/Curl : $\nabla \cdot u = 0$, $\nabla \times u = 0$ Scheuerer and Schlather [2012]
- Continuum mechanics : Jidling et al. [2018]

Some examples of GPR for differential operators

Given L, find a kernel k_L s.t. $L(k_L(\cdot, z)) = 0\ \forall z$; $\Delta = \sum_{i=1}^{d} \partial^2_{x_i x_i}$:

- Laplace : $\Delta u = 0$ Mendes and da Costa Júnior [2012], Ginsbourger et al. [2016]
- Heat : $\partial_t - D\Delta u = 0$ Albert and Rath [2020]
- Div/Curl : $\nabla \cdot u = 0$, $\nabla \times u = 0$ Scheuerer and Schlather [2012]
- Continuum mechanics : Jidling et al. [2018]
- Helmholtz : $-\Delta u = \lambda u$ Albert and Rath [2020]

Some examples of GPR for differential operators

Given L, find a kernel k_L s.t. $L(k_L(\cdot, z)) = 0 \; \forall z$; $\Delta = \sum_{i=1}^{d} \partial^2_{x_i x_i}$:

- Laplace : $\Delta u = 0$ Mendes and da Costa Júnior [2012], Ginsbourger et al. [2016]
- Heat : $\partial_t - D\Delta u = 0$ Albert and Rath [2020]
- Div/Curl : $\nabla \cdot u = 0$, $\nabla \times u = 0$ Scheuerer and Schlather [2012]
- Continuum mechanics : Jidling et al. [2018]
- Helmholtz : $-\Delta u = \lambda u$ Albert and Rath [2020]
- Stationary Maxwell : Wahlstrom et al. [2013], Jidling et al. [2017],Lange-Hegermann [2018]

Some examples of GPR for differential operators

Given L, find a kernel k_L s.t. $L(k_L(\cdot, z)) = 0 \ \forall z$; $\Delta = \sum_{i=1}^d \partial^2_{x_i x_i}$:

- Laplace : $\Delta u = 0$ Mendes and da Costa Júnior [2012], Ginsbourger et al. [2016]
- Heat : $\partial_t - D\Delta u = 0$ Albert and Rath [2020]
- Div/Curl : $\nabla \cdot u = 0$, $\nabla \times u = 0$ Scheuerer and Schlather [2012]
- Continuum mechanics : Jidling et al. [2018]
- Helmholtz : $-\Delta u = \lambda u$ Albert and Rath [2020]
- Stationary Maxwell : Wahlstrom et al. [2013], Jidling et al. [2017],Lange-Hegermann [2018]
- See also latent forces : Álvarez et al. [2009], López-Lopera et al. [2021]

Some examples of GPR for differential operators

Given L, find a kernel k_L s.t. $L(k_L(\cdot, z)) = 0 \ \forall z$; $\Delta = \sum_{i=1}^{d} \partial^2_{x_i x_i}$:

- Laplace : $\Delta u = 0$ Mendes and da Costa Júnior [2012], Ginsbourger et al. [2016]
- Heat : $\partial_t - D\Delta u = 0$ Albert and Rath [2020]
- Div/Curl : $\nabla \cdot u = 0$, $\nabla \times u = 0$ Scheuerer and Schlather [2012]
- Continuum mechanics : Jidling et al. [2018]
- Helmholtz : $-\Delta u = \lambda u$ Albert and Rath [2020]
- Stationary Maxwell : Wahlstrom et al. [2013], Jidling et al. [2017],Lange-Hegermann [2018]
- See also latent forces : Álvarez et al. [2009], López-Lopera et al. [2021]

Uses representations of solutions of $Lu = 0$ as

$$u = Gf \tag{2}$$

Some examples of GPR for differential operators

Given L, find a kernel k_L s.t. $L(k_L(\cdot, z)) = 0 \ \forall z$; $\Delta = \sum_{i=1}^{d} \partial^2_{x_i x_i}$:

- Laplace : $\Delta u = 0$ Mendes and da Costa Júnior [2012], Ginsbourger et al. [2016]
- Heat : $\partial_t - D\Delta u = 0$ Albert and Rath [2020]
- Div/Curl : $\nabla \cdot u = 0$, $\nabla \times u = 0$ Scheuerer and Schlather [2012]
- Continuum mechanics : Jidling et al. [2018]
- Helmholtz : $-\Delta u = \lambda u$ Albert and Rath [2020]
- Stationary Maxwell : Wahlstrom et al. [2013], Jidling et al. [2017],Lange-Hegermann [2018]
- See also latent forces : Álvarez et al. [2009], López-Lopera et al. [2021]

Uses representations of solutions of $Lu = 0$ as

$$u = Gf \tag{2}$$

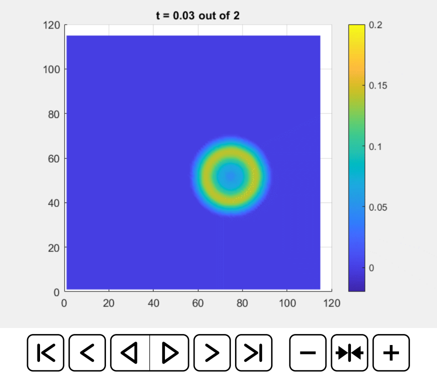
Then $k_L = (G \otimes G)k$ yields suitable Kriging means.

GPR for the wave equation

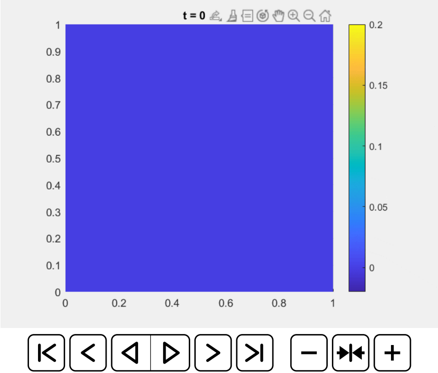
Use explicit formulas for solving $(\partial_{tt}^2 - c^2\Delta)u = \Box u = 0$...

Build a kernel k s.t. $\Box k(\cdot,(x,t)) = 0 \; \forall (x,t)$.

Direct numerical simulation



Reconstruction with GPR



Linear constraints on the sample paths (Ginsbourger et al. [2016])

Let $U = (U(z))_{z\in\mathcal{D}} \sim GP(0, k(z, z'))$.

Linear constraints on the sample paths (Ginsbourger et al. [2016])

Let $U = (U(z))_{z \in \mathcal{D}} \sim GP(0, k(z, z'))$.

- $U(z) : (\Omega, \mathcal{F}, \mathbb{P}) \longrightarrow \mathbb{R}$ is a (Gaussian) random variable.

Linear constraints on the sample paths (Ginsbourger et al. [2016])

Let $U = (U(z))_{z\in\mathcal{D}} \sim GP(0, k(z, z'))$.

- $U(z) : (\Omega, \mathcal{F}, \mathbb{P}) \longrightarrow \mathbb{R}$ is a (Gaussian) random variable.
- Forall $\omega \in \Omega,\ z \longmapsto U(z)(\omega)$ is a sample path.

Linear constraints on the sample paths (Ginsbourger et al. [2016])

Let $U = (U(z))_{z\in\mathcal{D}} \sim GP(0, k(z, z'))$.

- $U(z) : (\Omega, \mathcal{F}, \mathbb{P}) \longrightarrow \mathbb{R}$ is a (Gaussian) random variable.
- Forall $\omega \in \Omega,\ z \longmapsto U(z)(\omega)$ is a sample path.

let L be a linear operator acting on a suitable space of functions.

Linear constraints on the sample paths (Ginsbourger et al. [2016])

Let $U = (U(z))_{z\in\mathcal{D}} \sim GP(0, k(z, z'))$.

- $U(z) : (\Omega, \mathcal{F}, \mathbb{P}) \longrightarrow \mathbb{R}$ is a (Gaussian) random variable.
- Forall $\omega \in \Omega,\ z \longmapsto U(z)(\omega)$ is a sample path.

let L be a linear operator acting on a suitable space of functions.

General property : bilinearity of the covariance yields

$$\mathbb{P}(L(U) = 0) = 1 \iff \forall z \in \mathcal{D}, \quad L(k(\cdot, z)) = 0$$

Linear constraints on the sample paths (Ginsbourger et al. [2016])

Let $U = (U(z))_{z\in\mathcal{D}} \sim GP(0, k(z, z'))$.

- $U(z) : (\Omega, \mathcal{F}, \mathbb{P}) \longrightarrow \mathbb{R}$ is a (Gaussian) random variable.
- Forall $\omega \in \Omega,\ z \longmapsto U(z)(\omega)$ is a sample path.

let L be a linear operator acting on a suitable space of functions.

General property : bilinearity of the covariance yields

$$\mathbb{P}(L(U) = 0) = 1 \iff \forall z \in \mathcal{D}, \quad L(k(\cdot, z)) = 0$$

Rigorous proof : case-by-case depending on L.

Linear constraints on the sample paths (Ginsbourger et al. [2016])

Let $U = (U(z))_{z\in\mathcal{D}} \sim GP(0, k(z, z'))$.

- $U(z) : (\Omega, \mathcal{F}, \mathbb{P}) \longrightarrow \mathbb{R}$ is a (Gaussian) random variable.
- Forall $\omega \in \Omega,\ z \longmapsto U(z)(\omega)$ is a sample path.

let L be a linear operator acting on a suitable space of functions.

General property : bilinearity of the covariance yields

$$\mathbb{P}(L(U) = 0) = 1 \iff \forall z \in \mathcal{D},\quad L(k(\cdot, z)) = 0$$

Rigorous proof : case-by-case depending on L.
Previous linear PDEs are elliptic or parabolic :

Linear constraints on the sample paths (Ginsbourger et al. [2016])

Let $U = (U(z))_{z\in\mathcal{D}} \sim GP(0, k(z, z'))$.

- $U(z) : (\Omega, \mathcal{F}, \mathbb{P}) \longrightarrow \mathbb{R}$ is a (Gaussian) random variable.
- Forall $\omega \in \Omega,\ z \longmapsto U(z)(\omega)$ is a sample path.

let L be a linear operator acting on a suitable space of functions.

General property : bilinearity of the covariance yields

$$\mathbb{P}(L(U) = 0) = 1 \iff \forall z \in \mathcal{D}, \quad L(k(\cdot, z)) = 0$$

Rigorous proof : case-by-case depending on L.
Previous linear PDEs are elliptic or parabolic :

- Regular solutions (C^k or C^∞ solutions)

Linear constraints on the sample paths (Ginsbourger et al. [2016])

Let $U = (U(z))_{z\in\mathcal{D}} \sim GP(0, k(z, z'))$.

- $U(z) : (\Omega, \mathcal{F}, \mathbb{P}) \longrightarrow \mathbb{R}$ is a (Gaussian) random variable.
- Forall $\omega \in \Omega,\ z \longmapsto U(z)(\omega)$ is a sample path.

let L be a linear operator acting on a suitable space of functions.

General property : bilinearity of the covariance yields

$$\mathbb{P}(L(U) = 0) = 1 \iff \forall z \in \mathcal{D}, \quad L(k(\cdot, z)) = 0$$

Rigorous proof : case-by-case depending on L.
Previous linear PDEs are elliptic or parabolic :

- Regular solutions (C^k or C^∞ solutions)
- PDE $Lu = 0$ can be understood using classical derivatives

Linear constraints on the sample paths (Ginsbourger et al. [2016])

Let $U = (U(z))_{z\in\mathcal{D}} \sim GP(0, k(z, z'))$.

- $U(z) : (\Omega, \mathcal{F}, \mathbb{P}) \longrightarrow \mathbb{R}$ is a (Gaussian) random variable.
- Forall $\omega \in \Omega,\ z \longmapsto U(z)(\omega)$ is a sample path.

let L be a linear operator acting on a suitable space of functions.

General property : bilinearity of the covariance yields

$$\mathbb{P}(L(U) = 0) = 1 \iff \forall z \in \mathcal{D}, \quad L(k(\cdot, z)) = 0$$

Rigorous proof : case-by-case depending on L.
Previous linear PDEs are elliptic or parabolic :

- Regular solutions (C^k or C^∞ solutions)
- PDE $Lu = 0$ can be understood using classical derivatives

Prototype for hyperbolic PDEs : the wave equation

3D free space wave eq. : consider $\Delta = \partial_{xx}^2 + \partial_{yy}^2 + \partial_{zz}^2$ and the PDE

$$\begin{cases} Lu &= \frac{1}{c^2}\partial_{tt}^2 u - \Delta u = \Box u = 0, \quad (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ u(x,0) &= u_0(x), \quad \partial_t u(x,0) = v_0(x) \end{cases} \tag{3}$$

Prototype for hyperbolic PDEs : the wave equation

3D free space wave eq. : consider $\Delta = \partial^2_{xx} + \partial^2_{yy} + \partial^2_{zz}$ and the PDE

$$\begin{cases} Lu &= \frac{1}{c^2}\partial^2_{tt}u - \Delta u = \square u = 0, \quad (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ u(x,0) &= u_0(x), \qquad \partial_t u(x,0) = v_0(x) \end{cases} \tag{3}$$

Solution representation formula :

$$u(x,t) = (F_t * v_0)(x) + (\dot{F}_t * u_0)(x) = G(u_0, v_0)(x,t) \tag{4}$$

Prototype for hyperbolic PDEs : the wave equation

3D free space wave eq. : consider $\Delta = \partial^2_{xx} + \partial^2_{yy} + \partial^2_{zz}$ and the PDE

$$\begin{cases} Lu & = \frac{1}{c^2}\partial^2_{tt}u - \Delta u = \Box u = 0, \quad (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ u(x,0) & = u_0(x), \qquad \partial_t u(x,0) = v_0(x) \end{cases} \tag{3}$$

Solution representation formula :

$$u(x,t) = (F_t * v_0)(x) + (\dot{F}_t * u_0)(x) = G(u_0, v_0)(x,t) \tag{4}$$

Contrarily to previous examples, F_t and $\dot{F}_t$ are "singular" :

Prototype for hyperbolic PDEs : the wave equation

3D free space wave eq. : consider $\Delta = \partial^2_{xx} + \partial^2_{yy} + \partial^2_{zz}$ and the PDE

$$\begin{cases} Lu & = \frac{1}{c^2}\partial^2_{tt}u - \Delta u = \Box u = 0, \quad (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ u(x,0) & = u_0(x), \quad \partial_t u(x,0) = v_0(x) \end{cases} \tag{3}$$

Solution representation formula :

$$u(x,t) = (F_t * v_0)(x) + (\dot{F}_t * u_0)(x) = G(u_0, v_0)(x,t) \tag{4}$$

Contrarily to previous examples, F_t and $\dot{F}_t$ are "singular" :

$$F_t = \frac{\sigma_{ct}}{4\pi c^2 t} \text{ (singular measure) and } \dot{F}_t = \partial_t F_t \tag{5}$$

Prototype for hyperbolic PDEs : the wave equation

3D free space wave eq. : consider $\Delta = \partial^2_{xx} + \partial^2_{yy} + \partial^2_{zz}$ and the PDE

$$\begin{cases} Lu &= \frac{1}{c^2}\partial^2_{tt}u - \Delta u = \Box u = 0, \quad (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ u(x,0) &= u_0(x), \quad \partial_t u(x,0) = v_0(x) \end{cases} \tag{3}$$

Solution representation formula :

$$u(x,t) = (F_t * v_0)(x) + (\dot{F}_t * u_0)(x) = G(u_0, v_0)(x,t) \tag{4}$$

Contrarily to previous examples, F_t and $\dot{F}_t$ are "singular" :

$$F_t = \frac{\sigma_{ct}}{4\pi c^2 t} \text{ (singular measure) and } \dot{F}_t = \partial_t F_t \tag{5}$$

In some cases (e.g. u_0 and/or v_0 only C^1), u is well defined but not of class C^2 !

Prototype for hyperbolic PDEs : the wave equation

3D free space wave eq. : consider $\Delta = \partial^2_{xx} + \partial^2_{yy} + \partial^2_{zz}$ and the PDE

$$\begin{cases} Lu &= \frac{1}{c^2}\partial^2_{tt} u - \Delta u = \Box u = 0, \quad (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ u(x,0) &= u_0(x), \quad \partial_t u(x,0) = v_0(x) \end{cases} \tag{3}$$

Solution representation formula :

$$u(x,t) = (F_t * v_0)(x) + (\dot{F}_t * u_0)(x) = G(u_0, v_0)(x,t) \tag{4}$$

Contrarily to previous examples, F_t and $\dot{F}_t$ are "singular" :

$$F_t = \frac{\sigma_{ct}}{4\pi c^2 t} \text{ (singular measure) and } \dot{F}_t = \partial_t F_t \tag{5}$$

In some cases (e.g. u_0 and/or v_0 only C^1), u is well defined but not of class C^2 !

$\longrightarrow$ Link between L, k_L and underlying GP U not obvious anymore.

Distributional formulation of PDEs

Let $\mathcal{D}$ be an open set of $\mathbb{R}$.

Distributional formulation of PDEs

Let $\mathcal{D}$ be an open set of $\mathbb{R}$. Note D the single derivative operator.

Distributional formulation of PDEs

Let $\mathcal{D}$ be an open set of $\mathbb{R}$. Note D the single derivative operator. Linear differential operator L :

$$Lu = \sum_{k=1}^{n} a_k D^k u$$

Distributional formulation of PDEs

Let $\mathcal{D}$ be an open set of $\mathbb{R}$. Note D the single derivative operator. Linear differential operator L :

$$Lu = \sum_{k=1}^{n} a_k D^k u$$

Suppose u is a classical solution to $Lu = 0$: u is of class C^n and verifies

$$\forall x \in \mathcal{D}, (Lu)(x) = 0 \tag{6}$$

Distributional formulation of PDEs

Let $\mathcal{D}$ be an open set of $\mathbb{R}$. Note D the single derivative operator. Linear differential operator L :

$$Lu = \sum_{k=1}^{n} a_k D^k u$$

Suppose u is a classical solution to $Lu = 0$: u is of class C^n and verifies

$$\forall x \in \mathcal{D}, (Lu)(x) = 0 \tag{6}$$

Multiply (6) by $\varphi \in C_0^\infty(\mathcal{D})$ and integrate over $\mathcal{D}$:

$$\forall \varphi \in C_0^\infty(\mathcal{D}), \int_{\mathcal{D}} Lu(x)\varphi(x)dx = 0 \tag{7}$$

Distributional formulation of PDEs

IBP on (7) :

$$\int_{\mathcal{D}} D^k u(x)\varphi(x)dx = (-1)^k \int_{\mathcal{D}} u(x)D^k(\varphi(x))dx$$

Distributional formulation of PDEs

IBP on (7) :

$$\int_{\mathcal{D}} D^k u(x)\varphi(x)dx = (-1)^k \int_{\mathcal{D}} u(x)D^k(\varphi(x))dx$$

Define $L^* v = \sum_{k=1}^{n} a_k(-1)^k D^k v$.

Distributional formulation of PDEs

IBP on (7) :

$$\int_{\mathcal{D}} D^k u(x)\varphi(x)dx = (-1)^k \int_{\mathcal{D}} u(x)D^k(\varphi(x))dx$$

Define $L^* v = \sum_{k=1}^n a_k(-1)^k D^k v$. Then,

$$\forall \varphi \in C_0^\infty(\mathcal{D}), \int_{\mathcal{D}} Lu(x)\varphi(x)dx = \int_{\mathcal{D}} u(x)L^*\varphi(x)dx = 0$$

Distributional formulation of PDEs

IBP on (7) :

$$\int_{\mathcal{D}} D^k u(x)\varphi(x)dx = (-1)^k \int_{\mathcal{D}} u(x)D^k(\varphi(x))dx$$

Define $L^* v = \sum_{k=1}^{n} a_k(-1)^k D^k v$. Then,

$$\forall \varphi \in C_0^\infty(\mathcal{D}), \int_{\mathcal{D}} Lu(x)\varphi(x)dx = \int_{\mathcal{D}} u(x)L^*\varphi(x)dx = 0$$

A function u is a solution to the PDE $Lu = 0$ in the distributional sense if

$$\forall \varphi \in C_0^\infty(\mathcal{D}), \int_{\mathcal{D}} u(x)L^*\varphi(x)dx = 0 \tag{8}$$

Distributional formulation of PDEs

IBP on (7) :

$$\int_{\mathcal{D}} D^k u(x)\varphi(x)dx = (-1)^k \int_{\mathcal{D}} u(x)D^k(\varphi(x))dx$$

Define $L^* v = \sum_{k=1}^n a_k(-1)^k D^k v$. Then,

$$\forall \varphi \in C_0^\infty(\mathcal{D}), \int_{\mathcal{D}} Lu(x)\varphi(x)dx = \int_{\mathcal{D}} u(x)L^*\varphi(x)dx = 0$$

A function u is a solution to the PDE $Lu = 0$ in the distributional sense if

$$\forall \varphi \in C_0^\infty(\mathcal{D}), \int_{\mathcal{D}} u(x)L^*\varphi(x)dx = 0 \tag{8}$$

The standard hypothesis for (8) to make sense is $u \in L^1_{loc}(\mathcal{D})$:

$$\int_K |u| < +\infty \quad \text{for all compact set} \quad K \subset \mathcal{D}$$

Can we have something like

Imposing distributional diff. constraints on sample paths

Can we have something like

$$\mathbb{P}(L(U) = 0 \text{ in the sense of distribs}) = 1$$
$$\Longleftrightarrow$$
$$\forall z \in \mathcal{D}, \quad L(k(\cdot, z)) = 0 \text{ in the sense of distribs}$$

Can we have something like

$$\mathbb{P}(L(U) = 0 \text{ in the sense of distribs}) = 1$$
$$\iff$$
$$\forall z \in \mathcal{D}, \quad L(k(\cdot, z)) = 0 \text{ in the sense of distribs}$$

Answer :

Imposing distributional diff. constraints on sample paths

Can we have something like

$$\mathbb{P}(L(U) = 0 \text{ in the sense of distribs}) = 1$$
$$\iff$$
$$\forall z \in \mathcal{D}, \quad L(k(\cdot, z)) = 0 \text{ in the sense of distribs}$$

Answer : yes.

Random fields under distributional diff. constraints

Proposition 1 (H. et al. [2022])

Let $\mathcal{D} \subset \mathbb{R}^d$ be an open set and let $L = \sum_{|k| \leq n} a_k(x)\partial^k$ be a linear differential operator with coefficients $a_k(x) \in \mathcal{C}^{|k|}(\mathcal{D})$. Let $U = (U(x))_{x \in \mathcal{D}}$ be a measurable centered second order random field with covariance kernel $k(x, x')$. Suppose that its standard deviation function $\sigma : x \longmapsto \sqrt{k(x,x)}$ lies in $L^1_{loc}(\mathcal{D})$.

1) Then on a set of probability 1, the trajectories of U lie in $L^1_{loc}(\mathcal{D})$ as well as the functions $k(\cdot, x)$ for all $x \in \mathcal{D}$.

2) The following statements are equivalent :

- $\mathbb{P}(L(U) = 0$ *in the sense of distributions*$) = 1$
- $\forall x \in \mathcal{D}, L(k_x) = 0$ *in the sense of distributions.*

Random fields under distributional diff. constraints

Proposition 1 (H. et al. [2022])

Let $\mathcal{D} \subset \mathbb{R}^d$ be an open set and let $L = \sum_{|k|\leq n} a_k(x)\partial^k$ be a linear differential operator with coefficients $a_k(x) \in \mathcal{C}^{|k|}(\mathcal{D})$. Let $U = (U(x))_{x\in\mathcal{D}}$ be a measurable centered second order random field with covariance kernel $k(x,x')$. Suppose that its standard deviation function $\sigma : x \longmapsto \sqrt{k(x,x)}$ lies in $L^1_{loc}(\mathcal{D})$.

1) Then on a set of probability 1, the trajectories of U lie in $L^1_{loc}(\mathcal{D})$ as well as the functions $k(\cdot,x)$ for all $x \in \mathcal{D}$.

2) The following statements are equivalent :

- $\mathbb{P}(L(U) = 0$ *in the sense of distributions*$) = 1$
- $\forall x \in \mathcal{D}, L(k_x) = 0$ *in the sense of distributions.*

Extends results from Ginsbourger et al. [2016]. to linear distributional diff. constraints. Application to GPR : this property is inherited to conditioned GPs and the Kriging means.

GP modelling for the 3D wave equation

3D free space wave equation :

$$\begin{cases} Lu & = \frac{1}{c^2}\partial_{tt}^2 u - \Delta u = \Box u = 0, \quad (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ u(x,0) & = u_0(x) \\ \partial_t u(x,0) & = v_0(x) \end{cases} \tag{9}$$

GP modelling for the 3D wave equation

3D free space wave equation :

$$\begin{cases} Lu & = \frac{1}{c^2}\partial_{tt}^2 u - \Delta u = \Box u = 0, \quad (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ u(x,0) & = u_0(x) \\ \partial_t u(x,0) & = v_0(x) \end{cases} \tag{9}$$

Fourier in the space variable on (9)

$$u(x,t) = (F_t * v_0)(x) + (\dot{F}_t * u_0)(x) \qquad \forall (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \tag{10}$$

GP modelling for the 3D wave equation

3D free space wave equation :

$$\begin{cases} Lu & = \frac{1}{c^2}\partial_{tt}^2 u - \Delta u = \Box u = 0, \quad (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ u(x,0) & = u_0(x) \\ \partial_t u(x,0) & = v_0(x) \end{cases} \tag{9}$$

Fourier in the space variable on (9)

$$u(x,t) = (F_t * v_0)(x) + (\dot{F}_t * u_0)(x) \qquad \forall (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \tag{10}$$

with

$$F_t = \frac{\sigma_{ct}}{4\pi c^2 t} \qquad \text{and} \qquad \dot{F}_t = \partial_t F_t \tag{11}$$

Details on F_t and $\dot{F}_t$

$\longrightarrow F_t = \frac{\sigma_{ct}}{4\pi c^2 t}$ means that

Details on F_t and $\dot{F}_t$

$\longrightarrow F_t = \frac{\sigma_{ct}}{4\pi c^2 t}$ means that

$$\int_{\mathbb{R}^3} f(x) F_t(dx) = \frac{t}{4\pi} \int_0^{2\pi} \int_0^{\pi} f(ct\gamma) \sin\theta d\theta d\varphi = \frac{t}{4\pi} \int_{S(0,1)} f(ct\gamma) d\Omega$$

where γ is the unit length vector $\gamma = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)^T$.

Details on F_t and $\dot{F}_t$

$\longrightarrow$ $F_t = \frac{\sigma_{ct}}{4\pi c^2 t}$ means that

$$\int_{\mathbb{R}^3} f(x)F_t(dx) = \frac{t}{4\pi}\int_0^{2\pi}\int_0^{\pi} f(ct\gamma)\sin\theta d\theta d\varphi = \frac{t}{4\pi}\int_{S(0,1)} f(ct\gamma)d\Omega$$

where γ is the unit length vector $\gamma = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)^T$.

$\longrightarrow$ Convolution between functions and measures :

$$(f * g)(x) = \int_{\mathbb{R}^3} g(x-y)f(y)dy \quad (\mu * g)(x) = \int_{\mathbb{R}^3} g(x-y)\mu(dy)$$

Details on F_t and $\dot{F}_t$

$\longrightarrow F_t = \frac{\sigma_{ct}}{4\pi c^2 t}$ means that

$$\int_{\mathbb{R}^3} f(x)F_t(dx) = \frac{t}{4\pi}\int_0^{2\pi}\int_0^{\pi} f(ct\gamma)\sin\theta d\theta d\varphi = \frac{t}{4\pi}\int_{S(0,1)} f(ct\gamma)d\Omega$$

where γ is the unit length vector $\gamma = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)^T$.

$\longrightarrow$ Convolution between functions and measures :

$$(f * g)(x) = \int_{\mathbb{R}^3} g(x-y)f(y)dy \qquad (\mu * g)(x) = \int_{\mathbb{R}^3} g(x-y)\mu(dy)$$

$\longrightarrow \dot{F}_t = \partial_t F_t$ means that

$$\begin{aligned}\langle \dot{F}_t, f\rangle &= \partial_t \int f(x)dF_t(x)\\ &= \frac{1}{4\pi}\int_{S(0,1)} f(ct\gamma)d\Omega + \frac{c}{4\pi}\int_{S(0,1)} \nabla f(ct\gamma)\cdot\gamma d\Omega\end{aligned}$$

GP modelling for the 3D wave equation

Suppose that u_0 and v_0 are unknown.

GP modelling for the 3D wave equation

Suppose that u_0 and v_0 are unknown.

$\longrightarrow$ model them as random functions.

GP modelling for the 3D wave equation

Suppose that u_0 and v_0 are unknown.

$\longrightarrow$ model them as random functions.

Let $(U_0(x))_{x\in\mathbb{R}^3} \sim GP(0, k_u)$ and $(V_0(x))_{x\in\mathbb{R}^3} \sim GP(0, k_v)$ be two independent GPs.

GP modelling for the 3D wave equation

Suppose that u_0 and v_0 are unknown.

$\longrightarrow$ model them as random functions.

Let $(U_0(x))_{x\in\mathbb{R}^3} \sim GP(0, k_u)$ and $(V_0(x))_{x\in\mathbb{R}^3} \sim GP(0, k_v)$ be two independent GPs.

Model u_0 and v_0 as sample paths drawn from U_0 and V_0 respectively : $\exists\omega \in \Omega, u_0(\cdot) = U_0(\cdot)(\omega)$ and $v_0(\cdot) = V_0(\cdot)(\omega)$.

GP modelling for the 3D wave equation

Suppose that u_0 and v_0 are unknown.

$\longrightarrow$ model them as random functions.

Let $(U_0(x))_{x\in\mathbb{R}^3} \sim GP(0, k_u)$ and $(V_0(x))_{x\in\mathbb{R}^3} \sim GP(0, k_v)$ be two independent GPs.

Model u_0 and v_0 as sample paths drawn from U_0 and V_0 respectively : $\exists \omega \in \Omega, u_0(\cdot) = U_0(\cdot)(\omega)$ and $v_0(\cdot) = V_0(\cdot)(\omega)$.

For fixed (x, t), define the random variables $V(x,t)$, $U(x,t)$ and $W(x,t)$ by

$$V(x,t) : \omega \longmapsto (F_t * V_0(\cdot)(\omega))(x) \tag{12}$$

$$U(x,t) : \omega \longmapsto (\dot{F}_t * U_0(\cdot)(\omega))(x) \tag{13}$$

$$W(x,t) := V(x,t) + U(x,t) \tag{14}$$

GP modelling for the 3D wave equation

Proposition 2

Note $\mathcal{D} = \mathbb{R}^3 \times \mathbb{R}$. *Define the functions*

$$\forall z, z' \in \mathcal{D}, \quad k_v^{\mathrm{wave}}(z, z') = [(F_t \otimes F_{t'}) * k_v](x, x') \tag{15}$$

$$k_u^{\mathrm{wave}}(z, z') = [(\dot{F}_t \otimes \dot{F}_{t'}) * k_u](x, x') \tag{16}$$

1) Then $(U(z))_{z \in \mathcal{D}}$,$(V(z))_{z \in \mathcal{D}}$ *and* $(W(z))_{z \in \mathcal{D}}$ *are centered GPs.*

2) The covariance kernels of $(U(z))_{z \in \mathcal{D}}$,$(V(z))_{z \in \mathcal{D}}$ *and* $(W(z))_{z \in \mathcal{D}}$ *are given by* k_u^{wave}, k_v^{wave} *and* $k_u^{\mathrm{wave}} + k_v^{\mathrm{wave}}$ *respectively.*

Sketch of proof : bilinearity of the covariance + technical details...

Solving inverse problems

For all $z \in \mathcal{D}$, $\Box k_u^{\mathrm{wave}}(\cdot, z) = \Box k_v^{\mathrm{wave}}(\cdot, z) = 0\,!$

For all $z \in \mathcal{D}$, $\Box k_u^{\mathrm{wave}}(\cdot, z) = \Box k_v^{\mathrm{wave}}(\cdot, z) = 0\,!$

Proposition 1 $\implies$ any random field with either of the covariance kernels above has its sample paths solutions to the wave equation.

Solving inverse problems

For all $z \in \mathcal{D}$, $\Box k_u^{\mathrm{wave}}(\cdot, z) = \Box k_v^{\mathrm{wave}}(\cdot, z) = 0\,!$

Proposition 1 $\implies$ any random field with either of the covariance kernels above has its sample paths solutions to the wave equation.

Objective now : perform GPR with either of these covariance kernels.

Solving inverse problems

For all $z \in \mathcal{D}$, $\Box k_u^{\mathrm{wave}}(\cdot, z) = \Box k_v^{\mathrm{wave}}(\cdot, z) = 0\,!$

Proposition 1 $\implies$ any random field with either of the covariance kernels above has its sample paths solutions to the wave equation.

Objective now : perform GPR with either of these covariance kernels.

$\rightarrow$ Parameter estimation (marginal likelihood)

Solving inverse problems

For all $z \in \mathcal{D}$, $\Box k_u^{\text{wave}}(\cdot, z) = \Box k_v^{\text{wave}}(\cdot, z) = 0\,!$

Proposition 1 $\implies$ any random field with either of the covariance kernels above has its sample paths solutions to the wave equation.

Objective now : perform GPR with either of these covariance kernels.

$\rightarrow$ Parameter estimation (marginal likelihood)

$\rightarrow$ function prediction/reconstruction (Kriging mean/covariance)

Localization of point sources

Truncated kernel for v_0, around $x_0 \in \mathbb{R}^3$, radius R :

Localization of point sources

Truncated kernel for v_0, around $x_0 \in \mathbb{R}^3$, radius R :

$$k_v^R(x,x') = k_v(x,x')\frac{\mathbb{1}_{B(x_0,R)}(x)}{4\pi R^3/3}\frac{\mathbb{1}_{B(x_0,R)}}{4\pi R^3/3}$$

$$k_v^{wave}((x,t),(x',t')) = [(F_t \otimes F_{t'}) * k_v^R](x,x')$$

Localization of point sources

Truncated kernel for v_0, around $x_0 \in \mathbb{R}^3$, radius R :

$$k_v^R(x,x') = k_v(x,x')\frac{\mathbb{1}_{B(x_0,R)}(x)}{4\pi R^3/3}\frac{\mathbb{1}_{B(x_0,R)}}{4\pi R^3/3}$$

$$k_v^{wave}((x,t),(x',t')) = [(F_t \otimes F_{t'}) * k_v^R](x,x')$$

(x_0, R, c) are hyperparameters of k_V^{wave}. Limit $R \to 0$: point source.

Localization of point sources

Truncated kernel for v_0, around $x_0 \in \mathbb{R}^3$, radius R :

$$k_v^R(x,x') = k_v(x,x')\frac{\mathbb{1}_{B(x_0,R)}(x)}{4\pi R^3/3}\frac{\mathbb{1}_{B(x_0,R)}}{4\pi R^3/3}$$

$$k_v^{wave}((x,t),(x',t')) = [(F_t \otimes F_{t'}) * k_v^R](x,x')$$

(x_0, R, c) are hyperparameters of k_V^{wave}. Limit $R \to 0$: point source.

Objective : recover x_0^*, the true source position, given sensor data w.r.t. $u(x,t)$.

Localization of point sources

Truncated kernel for v_0, around $x_0 \in \mathbb{R}^3$, radius R :

$$k_v^R(x,x') = k_v(x,x') \frac{\mathbb{1}_{B(x_0,R)}(x)}{4\pi R^3/3} \frac{\mathbb{1}_{B(x_0,R)}}{4\pi R^3/3}$$

$$k_v^{wave}((x,t),(x',t')) = [(F_t \otimes F_{t'}) * k_v^{R}](x,x')$$

(x_0, R, c) are hyperparameters of k_V^{wave}. Limit $R \to 0$: point source.

Objective : recover x_0^*, the true source position, given sensor data w.r.t. $u(x,t)$.Suppose that all the hyperparameters are set to the correct value except x_0. Solve :

$$x_0^* = \underset{x_0 \in \mathbb{R}^3}{\arg\min}\, u_{obs}^T (K_{x_0} + \lambda I)^{-1} u_{obs} + \log\det(K_{x_0} + \lambda I) =: L(x_0)$$

Minimize negative marginal likelihood ≡ GPS localization

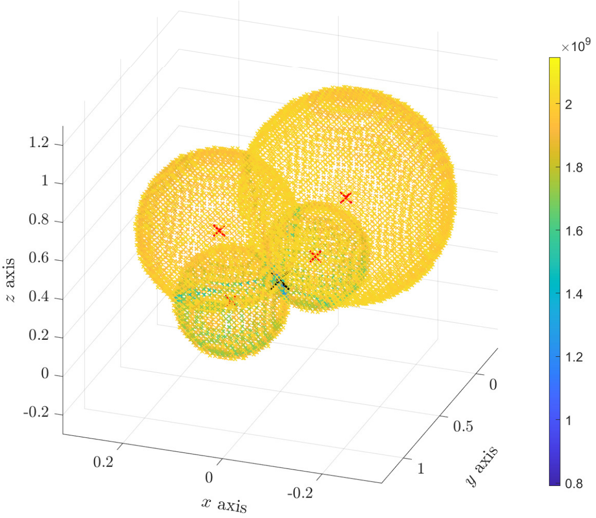


Figure : negative log marginal likelihood.

Display values : less than 2.035×10^9.

× : sensor locations.

× : source location.

See H. et al. [2021] for study/proofs.

Initial condition reconstruction

The Kriging means are also solutions to the wave equation : $\Box \tilde{m} = 0$

Initial condition reconstruction

The Kriging means are also solutions to the wave equation : $\Box\tilde{m} = 0$

$\longrightarrow$ if we observe values of a function u that is solution to $\Box u = 0$, then $\tilde{m}$ provides approximations for u_0 and v_0 with :

Initial condition reconstruction

The Kriging means are also solutions to the wave equation : $\Box\tilde{m} = 0$

$\longrightarrow$ if we observe values of a function u that is solution to $\Box u = 0$, then $\tilde{m}$ provides approximations for u_0 and v_0 with :

$$\tilde{m}(x,0) \simeq u(x,0) = u_0(x)$$
$$\partial_t \tilde{m}(x,0) \simeq \partial_t u(x,0) = v_0(x)$$

- Test case : radial symmetry around some x_0, source size R.

Initial condition reconstruction

The Kriging means are also solutions to the wave equation : $\Box\tilde{m} = 0$

$\longrightarrow$ if we observe values of a function u that is solution to $\Box u = 0$, then $\tilde{m}$ provides approximations for u_0 and v_0 with :

$$\tilde{m}(x,0) \simeq u(x,0) = u_0(x)$$
$$\partial_t \tilde{m}(x,0) \simeq \partial_t u(x,0) = v_0(x)$$

- Test case : radial symmetry around some x_0, source size R.
- Estimate (x_0, R, c)

Initial condition reconstruction

The Kriging means are also solutions to the wave equation : $\Box \tilde{m} = 0$

$\longrightarrow$ if we observe values of a function u that is solution to $\Box u = 0$, then $\tilde{m}$ provides approximations for u_0 and v_0 with :

$$\tilde{m}(x,0) \simeq u(x,0) = u_0(x)$$
$$\partial_t \tilde{m}(x,0) \simeq \partial_t u(x,0) = v_0(x)$$

- Test case : radial symmetry around some x_0, source size R.
- Estimate (x_0, R, c)

Test case : v_0 only : use k_v^{wave} for GPR ; Matérn kernel for k_v.

$$\begin{cases} u_0(x) & = 0 \\ v_0(x) & = A\mathbb{1}_{[R_1,R_2]}(|x-x_0|)\left(1+\cos\left(\frac{2\pi(|x-x_0|-\frac{R_1+R_2}{2})}{R_2-R_1}\right)\right) \end{cases}$$

Initial condition reconstruction

The Kriging means are also solutions to the wave equation : $\Box\tilde{m} = 0$

$\longrightarrow$ if we observe values of a function u that is solution to $\Box u = 0$, then $\tilde{m}$ provides approximations for u_0 and v_0 with :

$$\tilde{m}(x,0) \simeq u(x,0) = u_0(x)$$
$$\partial_t\tilde{m}(x,0) \simeq \partial_t u(x,0) = v_0(x)$$

- Test case : radial symmetry around some x_0, source size R.
- Estimate (x_0, R, c)

Test case : v_0 only : use k_v^{wave} for GPR ; Matérn kernel for k_v.

$$\begin{cases} u_0(x) &= 0 \\ v_0(x) &= A\mathbb{1}_{[R_1,R_2]}(|x-x_0|)\left(1+\cos\left(\frac{2\pi(|x-x_0|-\frac{R_1+R_2}{2})}{R_2-R_1}\right)\right) \end{cases}$$

$\longrightarrow$ Simulate numerically the corresponding solution $u(x,t)$.

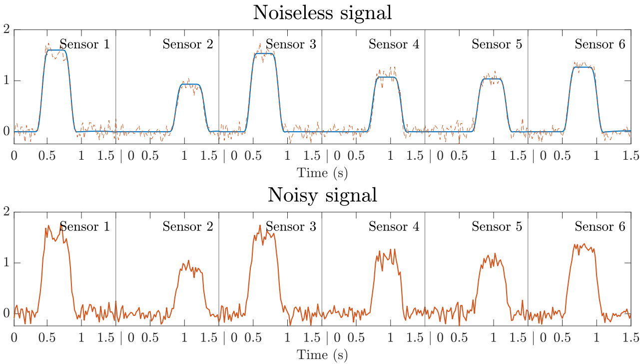
Initial condition reconstruction

- Kriging data : $B = \{u(x_i, t_j), 1 \leq i \leq N_C, 1 \leq j \leq N_T\}$ + noisy data

Initial condition reconstruction

- Kriging data : $B = \{u(x_i, t_j), 1 \leq i \leq N_C, 1 \leq j \leq N_T\}$ + noisy data
- $N_C = 30$ sensors scattered over $[0, 1]^3$ (Latin hypercube), $N_T = 75$.

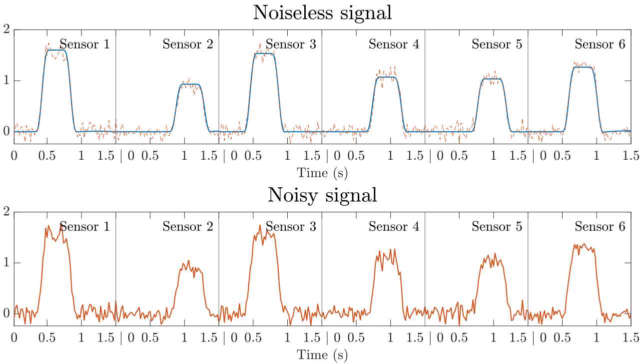
- Kriging data : $B = \{u(x_i, t_j), 1 \le i \le N_C, 1 \le j \le N_T\}$ + noisy data
- $N_C = 30$ sensors scattered over $[0,1]^3$ (Latin hypercube), $N_T = 75$.



Goals

Initial condition reconstruction

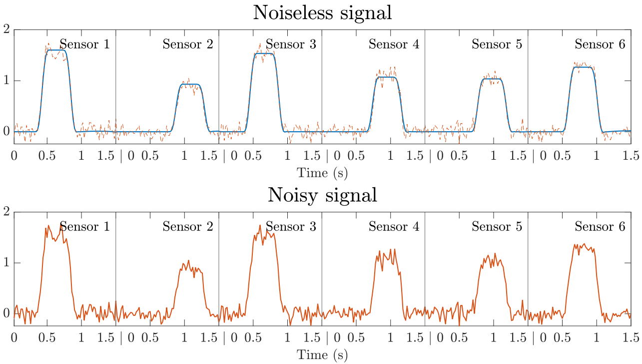
- Kriging data : $B = \{u(x_i, t_j), 1 \leq i \leq N_C, 1 \leq j \leq N_T\}$ + noisy data
- $N_C = 30$ sensors scattered over $[0,1]^3$ (Latin hypercube), $N_T = 75$.



Goals $\longrightarrow$ Physical parameter estimation/recovery : (x_0, R, c)

Initial condition reconstruction

- Kriging data : $B = \{u(x_i, t_j), 1 \leq i \leq N_C, 1 \leq j \leq N_T\}$ + noisy data
- $N_C = 30$ sensors scattered over $[0,1]^3$ (Latin hypercube), $N_T = 75$.



Goals $\longrightarrow$ Physical parameter estimation/recovery : (x_0, R, c)

$\longrightarrow$ initial condition reconstruction

Physical parameter recovery

Perform Log-marginal likelihood maximization with

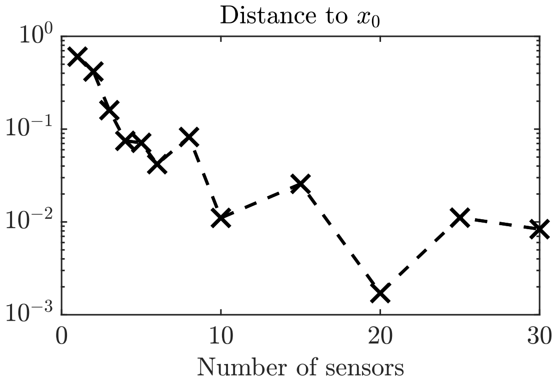
$$\theta = (c, R, x_0, \theta_{matern})$$

Physical parameter recovery

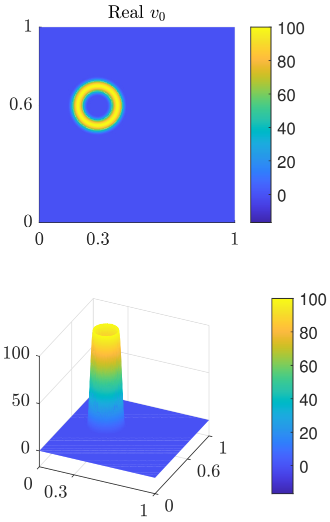
Perform Log-marginal likelihood maximization with

$$\theta = (c, R, x_0, \theta_{matern})$$

Example for $|c - c^*|$:



Initial condition reconstruction



Future perspectives : Sobolev regularity of GPs

Natural generalization of distributional formulation of PDEs : replace $C_c^\infty(\mathcal{D})$ with larger space of test functions, e.g. $H^1(\mathcal{D})$.

$\rightarrow$ variational/weak formulation

Future perspectives : Sobolev regularity of GPs

Natural generalization of distributional formulation of PDEs : replace $C_c^\infty(\mathcal{D})$ with larger space of test functions, e.g. $H^1(\mathcal{D})$.

$\rightarrow$ variational/weak formulation

Natural regularity : Sobolev $\rightarrow H^1(\mathcal{D}), W^{m,p}(\mathcal{D})$...

$$||f||_{H^1}^2 := \int_{\mathcal{D}} f(x)^2 dx + \int_{\mathcal{D}} |\nabla f(x)|^2 dx$$

Future perspectives : Sobolev regularity of GPs

Natural generalization of distributional formulation of PDEs : replace $C_c^\infty(\mathcal{D})$ with larger space of test functions, e.g. $H^1(\mathcal{D})$.

$\rightarrow$ variational/weak formulation

Natural regularity : Sobolev $\rightarrow H^1(\mathcal{D}), W^{m,p}(\mathcal{D})$...

$$||f||_{H^1}^2 := \int_{\mathcal{D}} f(x)^2 dx + \int_{\mathcal{D}} |\nabla f(x)|^2 dx$$

Natural interpretation of Sobolev norms : energy, energy balance,... Tackle physics problems with GP modelling :

$\rightarrow$ identify GPs whose sample paths enjoy a specified form of Sobolev regularity
$\rightarrow$ how to control their Sobolev norm ?
$\rightarrow$ obtain posterior convergence rates in Sobolev norm...
$\rightarrow$ see H. [2022]

Some conclusions

- random fields under linear differential constraints : solutions in the distributional sense.

Some conclusions

- random fields under linear differential constraints : solutions in the distributional sense.
- GP modelling for the wave equation : formulas for k_u^{wave} and k_v^{wave}.

Some conclusions

- random fields under linear differential constraints : solutions in the distributional sense.
- GP modelling for the wave equation : formulas for k_u^{wave} and k_v^{wave}.
- Inverse problem approach : numerical experiments.

References I

C. G. Albert and K. Rath. Gaussian process regression for data fulfilling linear differential equations with localized sources. *Entropy*, 22(2), 2020. ISSN 1099-4300. URL `https://www.mdpi.com/1099-4300/22/2/152`.

D. Ginsbourger, O. Roustant, and N. Durrande. On degeneracy and invariances of random fields paths with applications in Gaussian process modelling. *Journal of Statistical Planning and Inference*, page 170 :117 – 128, 2016.

I H. Sobolev regularity of Gaussian random fields. working paper or preprint, September 2022. URL `https://hal.archives-ouvertes.fr/hal-03769576`.

I. H., O. Roustant, and P. Noble. Stochastic processes under linear differential constraints : Application to gaussian process regression for the 3 dimensional free space wave equation. *arXiv*, 2021. URL `https://arxiv.org/abs/2111.12035`.

References II

I H., Pascal Noble, and Olivier Roustant. Characterization of the second order random fields subject to linear distributional PDE constraints. working paper or preprint, September 2022. URL `https://hal.archives-ouvertes.fr/hal-03770715`.

C. Jidling, N. Wahlström, A. Wills, and T. B. Schön. Linearly constrained Gaussian processes. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017. URL `https://proceedings.neurips.cc/paper/2017/file/71ad16ad2c4d81f348082ff6c4b20768-Paper.pdf`.

C. Jidling, J. Hendriks, N. Wahlstrom, A. Gregg, T. Schon, C. Wensrich, and A. Wills. Probabilistic modelling and reconstruction of strain. *Nuclear Instruments & Methods in Physics Research Section B-beam Interactions With Materials and Atoms*, 436 :141–155, 2018.

References III

M. Lange-Hegermann. Algorithmic linearly constrained Gaussian processes. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 31. Curran Associates, Inc., 2018. URL `https://proceedings.neurips.cc/paper/2018/file/68b1fbe7f16e4ae3024973f12f3cb313-Paper.pdf`.

A. F. López-Lopera, N. Durrande, and M. Álvarez. Physically-inspired Gaussian process models for post-transcriptional regulation in drosophila. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, 18 :656–666, 2021.

Fábio Macêdo Mendes and Edson Alves da Costa Júnior. Bayesian inference in the numerical solution of Laplace's equation. *AIP Conference Proceedings*, 1443(1) :72–79, 2012. doi : 10.1063/1.3703622. URL `https://aip.scitation.org/doi/abs/10.1063/1.3703622`.

M. Scheuerer and M. Schlather. Covariance models for divergence-free and curl-free random vector fields. *Stochastic Models*, 28 :433 – 451, 2012.

N. Wahlstrom, M. Kok, T. B. Schön, and F. Gustafsson. Modeling magnetic fields using Gaussian processes. *2013 IEEE International Conference on Acoustics, Speech and Signal Processing*, pages 3522–3526, 2013.

M. Álvarez, D. Luengo, and N. D. Lawrence. Latent force models. In D. van Dyk and M. Welling, editors, *Proceedings of the Twelth International Conference on Artificial Intelligence and Statistics*, volume 5 of *Proceedings of Machine Learning Research*, pages 9–16, Hilton Clearwater Beach Resort, Clearwater Beach, Florida USA, 16–18 Apr 2009. PMLR. URL https://proceedings.mlr.press/v5/alvarez09a.html.

"Explicit" formulas for $(F_t \otimes F_{t'}) * k_v$ and $(\dot{F}_t \otimes \dot{F}_{t'}) * k_u$

More explicitly,

$$
\begin{aligned}
&[(F_t \otimes F_{t'}) * k_v](x, x') \\
&\qquad = tt' \int_{S(0,1)\times S(0,1)} k_v(x - ct\gamma, x' - ct'\gamma') \frac{d\Omega d\Omega'}{(4\pi)^2} \\
&[(\dot{F}_t \otimes \dot{F}_{t'}) * k_u](x, x') = \int_{S(0,1)\times S(0,1)} \Big(k_u(x - ct\gamma, x' - ct'\gamma') \\
&\qquad - ct\nabla_1 k_u(x - ct\gamma, x' - ct'\gamma') \cdot \gamma \\
&\qquad - ct'\nabla_2 k_u(x - ct\gamma, x' - ct'\gamma') \cdot \gamma' \\
&\qquad + c^2 tt' \gamma^T \nabla_1 \nabla_2 k_u(x - ct\gamma, x' - ct'\gamma')\gamma' \Big) \frac{d\Omega d\Omega'}{(4\pi)^2}
\end{aligned}
$$

Radial symmetry formulas

$$k_{\mathrm{v}}^{\mathrm{wave}}(z,z') = \frac{\mathrm{sgn}(tt')}{16c^2rr'} \sum_{\varepsilon,\varepsilon'\in\{-1,1\}} \varepsilon\varepsilon' K_{\mathrm{v}}\big((r+\varepsilon ct)^2,(r'+\varepsilon' c|t'|)^2\big)$$

$$k_{\mathrm{u}}^{\mathrm{wave}}(z,z') = \frac{1}{4rr'} \sum_{\varepsilon,\varepsilon'\in\{-1,1\}} (r+\varepsilon ct)(r'+\varepsilon' c|t'|) k_{\mathrm{u}}^0\big((r+\varepsilon ct)^2,(r'+\varepsilon' c|t'|)^2\big)$$