Physics-informed Gaussian process priors

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Workshop on Gaussian processes and related topics
IMT, Toulouse

July 9^{th}, 2025

Plan

1. Introduction
   - Generalities on GP modelling
   - Two simple examples of PDEs
2. PDE constrained random fields
   - Theorem
   - Examples
3. Sobolev regularity of the samples of a GP
   - Motivation : Sobolev spaces and PDEs
   - Gaussian measures and processes on L^2
   - Sobolev regularity of the samples of a GP
4. Application to the 3D wave equation
   - Covariance kernels for the wave equation
   - Estimation of initial data and physical parameters
5. Conclusion and perspectives

“Old” PhD work with...

Figure 1: Pascal Noble (IMT, PDEs)

Figure 2: O. Roustant (IMT, ML/UQ)

What's on the agenda?

Topic for today:

- Discuss/motivate the use of GP models for tackling PDE driven problems.
- Focus on the mathematical aspects of GP modelling w.r.t. certain specificities of (linear) PDEs :

  $\rightarrow$comply with the distributional formulation of a linear PDE ($\simeq$ weak formulation)

  $\rightarrow$adapted smoothness/"energy" spaces : Sobolev spaces
- Describe some practical applications.

Plan

Gaussian process regression (GPR)[1]

- Unknown function $u : \mathcal{D} \to \mathbb{R}$, obs. $\mathcal{B} = \{u(z_1), ..., u(z_n)\}$
- Bayesian approach : model u as a sample U_ω of a Gaussian process :

$$(U(z))_{z \in \mathcal{D}} \sim GP(m, k) \quad (\textit{prior} \text{ GP})$$

- Condition U on obs. $\mathcal{B}$: "$V(z) = [U(z) | U(z_i) = u(z_i), 1 \leq i \leq n]$".

$$(V(z))_{z \in \mathcal{D}} \sim GP(\tilde{m}, \tilde{k}) \quad (\textit{posterior} \text{ GP})$$

- Estimation : $\forall z \in \mathcal{D}$, we estimate $u(z)$ with $\tilde{m}(z)$:

$$\hat{u}(z) = \tilde{m}(z) \simeq u(z), \quad \text{uncertainty} \quad \tilde{k}(z, z) = \text{Var}(V(z))$$

If $m = 0$, then $\tilde{m}(z) = k(z, Z)^T K^{-1} Y$ (similar for $\tilde{k}$).

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Modelling of the prior GP $U \sim GP(0, k)$ and choice of k

Regularity : if $k \in C^{N,N}(\mathcal{D} \times \mathcal{D})$ with Lipschitz derivatives of order N, then

$$\mathbb{P}(U \in C^N(\mathcal{D})) = 1. \text{ In particular } \widetilde{m} \in C^N(\mathcal{D}).$$

Linear invariance : if L is a linear operator and $\forall z \in \mathcal{D},\ L(k(z,\cdot)) = 0$ then (under suitable assumptions...)

$$\mathbb{P}(LU = 0) = 1. \text{ In particular, } L\widetilde{m} = 0.$$

"Proof" of $\forall z \in \mathcal{D},\ L(k(z,\cdot)) = 0 \implies \mathbb{P}(LU = 0) = 1$

For all z, z',

$$\text{Cov}((LU)(z),(LU)(z')) = [(L_z L_{z'})k](z,z') = L_z(L_{z'}(z' \mapsto k(z,z'))) = 0.$$

Set $z' = z$: $\text{Var}(LU(z)) = 0$ hence $LU(z) = \mathbb{E}[U(z)] = 0$ a.s. !

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Periodic kernels $\implies$ periodic samples

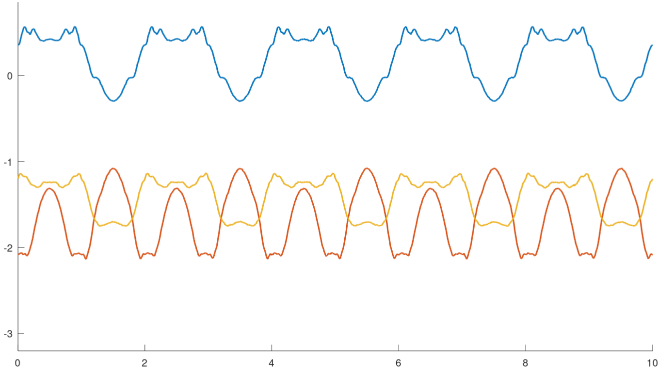


Figure 3: GP samples with a periodic Matérn 3/2 kernel

$$k(x, y) = (1 + |\sin(\pi x) - \sin(\pi y)|)\exp(-|\sin(\pi x) - \sin(\pi y)|)$$

Plan

GPR and PDEs

- GPR can take into account prior info. on u via the choice of the kernel k;
- This choice helps restrain the function space H such that $\mathbb{P}(U \in H) = 1 \rightarrow$ dimension reduction.

Questions for today :

- Discuss/describe the use of kernel methods for PDEs.
- General problem: estimate $u : \mathcal{D} \rightarrow \mathbb{R}$ and θ, knowing

$$\mathcal{B} = \{u(z_1), ..., u(z_n)\} \quad \text{and} \quad L_\theta(u) = 0. \tag{1}$$

L_θ : linear partial differential operator (time-dependent or not).

$\rightarrow$ Impose PDE constraint on GP prior : $\mathbb{P}(L_\theta(U) = 0) = 1$

$\rightarrow$ Impose relevant energy space H : $\mathbb{P}(U \in H) = 1$

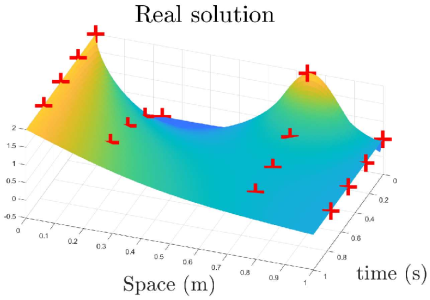
A nice parabolic PDE : the 1D heat equation

Consider the PDE with $L = \partial_t - D\partial^2_{xx}$:

$$\begin{cases} Lu = \partial_t u - D\partial^2_{xx} u = 0, \quad \forall t > 0, \quad \forall x \in \mathbb{R}. \\ u(t=0,x) = u_0(x). \end{cases} \tag{2}$$

We wish to estimate u given space-time measurements :

$$\mathcal{B} = \{u(t_i, x_j),\ 1 \leq i,j \leq 4\}, \quad \#\mathcal{B} = 16.$$



Here, $z = (t,x)$, GP model for u :

$$(U(t,x))_{(t,x)\in\mathbb{R}_+\times\mathbb{R}} \sim GP(0,k)$$
$$k(z,z') = k((t,x),(t',x')).$$

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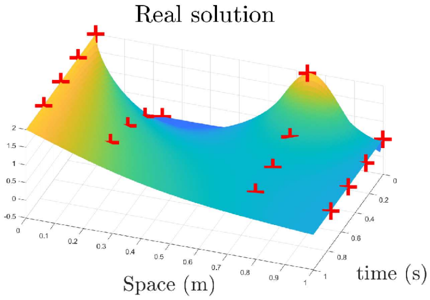

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A nice parabolic PDE : the 1D heat equation

Denote k_t = density of $\mathcal{N}(0, 2Dt)$ = *heat kernel*. Set also $k^0(x, x') = \sigma^2 \exp(-(x - x')^2/2\ell^2) = k_S(x - x')$.

Theorem 1

The function

$$k((t,x),(t',x')) = [(k_t \otimes k_{t'}) * k^0](x,x') = (k_t * k_{t'} * k_S)(x - x') \quad (3)$$

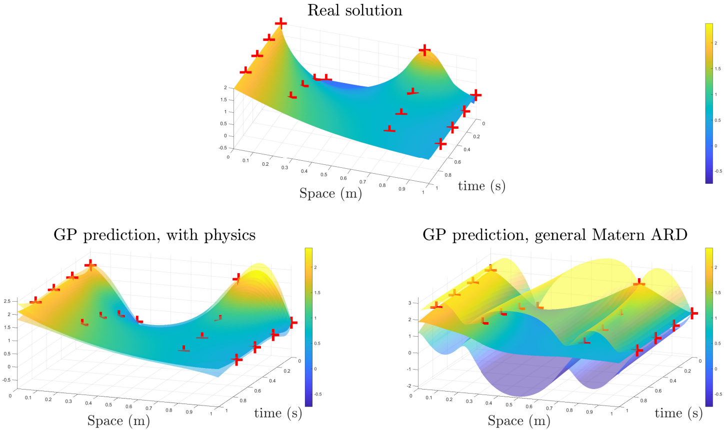
$$= \frac{\ell\sigma^2}{\sqrt{\alpha(t,t')}} \exp\left(-\frac{(x-x')^2}{2\alpha(t,t')}\right), \quad (4)$$

where $\alpha(t,t') = 2D(t + t') + \ell^2$*, is symmetric, PSD and verifies*

$$\forall (t,x) \in \mathbb{R}_+^* \times \mathbb{R}, \quad Lk((t,x),\cdot) = 0, \quad L = \partial_t - D\partial_{xx}^2. \quad (5)$$

The kernel k is obtained by setting a GP prior $GP(0, k^0)$ over u_0 and propagating through the PDE solution map $u_0 \mapsto k_t * u_0$.

Example with 1D heat equation



A not-so-nice hyperbolic PDE : the 1D transport equation

Things were ok with the heat equation. Yet, other PDEs often have to be understood in a weakened sense.

Example 1 : transport equation

$$\begin{cases} \partial_t u(t,x) + c\partial_x u(t,x) = 0 & \forall t > 0, \forall x \in \mathbb{R} \\ u(t=0,x) = u_0(x) & \forall x \in \mathbb{R} \end{cases} \tag{6}$$

is solved as $u(t,x) = u_0(x-ct)$.

In hindsight, it makes no sense to assume that u is differentiable (e.g. if $u_0 \notin C^1(\mathbb{R})$! What is then the meaning of eq. (6)?

PDEs often reflect "balance laws" which can also be understood in an energetic/integrated sense $\rightarrow$ weak formulation.

Distributional formulation of the transport equation

Instead of the PDE being valid **pointwise**, we require that all the smooth and local averages of the PDE are zero : for all $\varphi \in C_c^\infty(\mathbb{R}_+^* \times \mathbb{R})$,

$$\begin{aligned} 0 &= \int_{\mathbb{R}\times\mathbb{R}_+^*} \varphi(t,x)\Big(\partial_t u(t,x) + c\partial_x u(t,x)\Big)dxdt \\ &= \int_{\mathbb{R}\times\mathbb{R}_+^*} \Big(-\partial_t\varphi(t,x) - c\partial_x\varphi(t,x)\Big)u(t,x)dxdt. \end{aligned} \tag{7}$$

$$(0 = \langle \varphi, Lu\rangle_{L^2} = \langle L^*\varphi, u\rangle_{L^2}...)$$

In equation (7), $u \in L^1_{loc}(\mathbb{R})$ is sufficient!

- To deal with non-smooth solutions of $Lu = 0$, we require instead that $\langle L^*\varphi, u\rangle = 0$ for all $\varphi \in C_c^\infty$: this is the distributional formulation of $Lu = 0$ (duality...).
- For applications (e.g. finite elements) we may require more, e.g. that u lies in the correct energy space $\to$ Sobolev spaces.

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PDE constrained random fields[3]

Given $U = (U(z))_{z\in\mathcal{D}}$ a RF, when does $\mathbb{P}(L(U) = 0) = 1$ hold?

Proposition 1

Let $\mathcal{D} \subset \mathbb{R}^d$ be an open set, and $L := \sum_{|\alpha|\leq n} a_\alpha \partial^\alpha$, $a_\alpha \in \mathcal{C}^{|\alpha|}(\mathcal{D})$. Let $U = \left(U(z)\right)_{z\in\mathcal{D}}$ be a second order centred measurable random field, with covariance function k; assume that $\sigma : z \longmapsto k(z,z)^{1/2} \in L^1_{loc}(\mathcal{D})$. Then the following statements are equivalent.

- $\mathbb{P}(\{\omega \in \Omega : L(U_\omega) = 0$ *in the distributional sense*$\}) = 1$
- $\forall z \in \mathcal{D}, L(k(z,\cdot)) = 0$ *in the distributional sense.*

Distributional sense $\rightarrow$ also takes into account non-smooth solutions !
Generalisation of a result from[2]; inherited to conditioned GPs.

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Sketch of proof 1/2

Assume that $\forall z \in \mathcal{D}, L(k(z,\cdot)) = 0$ in the distrib. sense. Show that

$$\text{a.s.},\ \forall \varphi \in C_c^\infty(\mathcal{D}),\ \langle L^*\varphi, U\rangle = 0.$$

Let $\varphi \in C_c^\infty(\mathcal{D})$. Then

$$\begin{aligned}
\mathbb{E}[\langle L^*\varphi, U\rangle^2] &= \mathbb{E}\left[\left(\int_{\mathcal{D}} L^*\varphi(z)U(z)dz\right)^2\right] \\
&= \int_{\mathcal{D}}\int_{\mathcal{D}} L^*\varphi(z)L^*\varphi(z')\mathbb{E}[U(z)U(z')]dz'dz \\
&= \int_{\mathcal{D}} L^*\varphi(z)\int_{\mathcal{D}} L^*\varphi(z')k(z,z')dz'dz = 0.
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Hence $\langle L^*\varphi, U\rangle^2 = 0$ a.s., and

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Sketch of proof 2/2

But "a.s." and "$\forall\varphi$" do not commute ! Expect if the "$\forall\varphi$" statement is countable... For this we use that

1. $C_c^\infty(\mathcal{D})$ is (sequentially) separable endowed with its standard topology (i.e. there exists a countable dense subset $F \subset C_c^\infty(\mathcal{D})$).
2. The assumptions that $x \mapsto \sigma(x) \in L^1_{loc}(\mathcal{D})$ and $a_\alpha \in C^{|\alpha|}(\mathcal{D})$ imply that for almost every $\omega \in \Omega$,

$$\varphi \mapsto \langle L^*\varphi, U_\omega \rangle \quad (U_\omega = \text{sample path at } \omega \in \Omega)$$

is a continuous linear form over $C_c^\infty(\mathcal{D})$ for its topology!

Thus (...), one can commute "a.s." and "$\forall\varphi$" so that

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Plan

Some examples of kernels such that $L(k(z,\cdot)) = 0 \ \forall z$

- **Heat equation** in $\mathbb{R}$: $Lu = \partial_t u - D\partial^2_{xx} u = 0$. Let $k_t(x)$ = density of $\mathcal{N}(0, 2Dt)$ and k_0 a kernel over $\mathbb{R}$.

$$k((t,x),(t',x')) = [(k_t \otimes k_{t'}) * k_0](x,x') \quad \text{(general form.)}$$

If $k_0(x,x') = \sigma^2 e^{-\|x-x'\|^2/2\ell^2}$, and $\alpha_D(t,t') = 2D(t+t') + \ell^2$:

$$k((t,x),(t',x')) = \frac{\ell\sigma^2}{\sqrt{\alpha_D(t,t')}} \exp\left(-\frac{\|x-x\|)^2}{2\alpha_D(t,t')}\right).$$

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They both verify $L(k(t,x),\cdot)) = 0$ for all (t,x) and for their respective differential operators, and depend on their physical parameters.

Some examples of kernels such that $L(k(z,\cdot)) = 0 \ \forall z$

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More examples of kernels verifying $L(k(z,\cdot)) = 0 \;\; \forall z$

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

- Laplace: $\Delta u = 0$ (Mendes and da Costa Júnior, 2012), (Ginsbourger et al., 2016) : use harmonic basis functions.
- Heat: $\partial_t - D\Delta u = 0$ (Albert and Rath, 2020)
- Div/Curl free: $\nabla \cdot u = 0$, $\nabla \times u = 0$ (Scheuerer and Schlather, 2012),(Owhadi, 2023)
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1. Introduction
   - Generalities on GP modelling
   - Two simple examples of PDEs
2. PDE constrained random fields
   - Theorem
   - Examples
3. Sobolev regularity of the samples of a GP
   - Motivation : Sobolev spaces and PDEs
   - Gaussian measures and processes on L^2
   - Sobolev regularity of the samples of a GP
4. Application to the 3D wave equation
   - Covariance kernels for the wave equation
   - Estimation of initial data and physical parameters
5. Conclusion and perspectives

Sobolev spaces and PDEs

Let us construct some relevant energy functionals for given PDEs :

- Heat : $T(x,t), (x,t) \in \mathbb{R}^d \times \mathbb{R}_+$, $\partial_t T - \Delta T = 0$.

$$\frac{1}{2}\partial_t \|T(\cdot,t)\|_{L^2}^2 = -\|\nabla T(\cdot,t)\|_{L^2}^2 < 0 \quad \text{(diffusion)}. \tag{8}$$

- Wave : $\partial_{tt}^2 u - \Delta u = 0$.

$$\partial_t \Big(\|\partial_t u(\cdot,t)\|_{L^2}^2 + \|\nabla u(\cdot,t)\|_{L^2}^2 \Big) = 0 \quad \text{(conservation)}. \tag{9}$$

Transport : if $\partial_t u + \partial_x u = 0$, then $\partial_t \|u(\cdot,t)\|_{L^p} = 0$.

→ "natural" Euclidean structure associated to some PDEs : L^2 norm of the solution and of its derivatives.

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Finite energy derivatives and Sobolev spaces

Some functions are "almost" differentiable: $h(x) = \max(0, 1 - |x|)$.

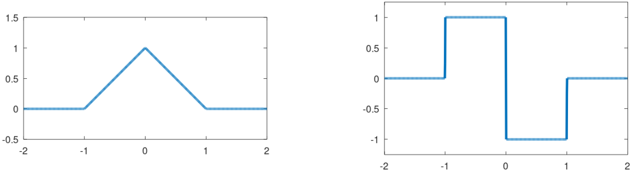

Figure 4: Left: $h(x)$. Right: $h'(x)$ (hopefully).

Unfortunately, $h' \notin C^0$... but $h' \in L^2$ (finite energy)!

A function g is the weak derivative of h if for all $\varphi \in C_c^\infty(\mathbb{R})$,

$$\int_{\mathbb{R}} h(x)\varphi'(x)dx = -\int_{\mathbb{R}} g(x)\varphi(x)dx.$$

$$H^1(\mathbb{R}) := \{u \in L^2(\mathbb{R}) : u' \text{ exists in the weak sense and } u' \in L^2(\mathbb{R})\},$$

$$H^m(\mathcal{D}) := \{u \in L^2(\mathcal{D}) : \forall\ |\alpha| \leq m, \partial^\alpha u \text{ exists ITWS and } \partial^\alpha u \in L^2(\mathcal{D})\}.$$

Caveat : $H^m(\mathbb{R}^d) \subset C^0(\mathbb{R}^d) \iff m > d/2\ !$ $\rightarrow$ *not* a RKHS if $m \leq d/2$.

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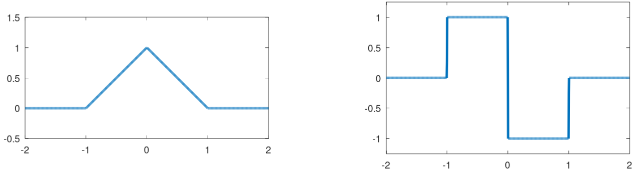

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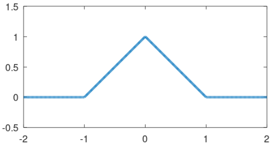

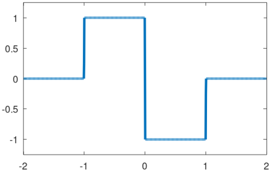

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Sobolev regularity of GPs

Modelling question :

Under what conditions can we ensure that

$$\mathbb{P}(U \in H^m(\mathcal{D})) = 1 \quad ???$$

- We assume that $\mathcal{D}$ is *any* open set of $\mathbb{R}^d$ $\rightarrow$ no smoothness assumptions on $\partial\mathcal{D}$, hence no extension operators, no Fourier analysis, no series representations for weak derivatives...
- We also wish to replace $H^m(\mathcal{D})$ with $W^{m,p}(\mathcal{D})$ where $p \in (1, +\infty) \rightarrow$ even less Fourier analysis.

Plan

Gaussian measures 1/3

Change the point of view : Gaussian process/vector $\leftrightarrow$ Gaussian measure.

- A Gaussian measure μ over $\mathbb{R}^d$ is the distribution of some Gaussian random vector U with values in $\mathbb{R}^d$ ($\mu = \mathcal{N}(m, \Sigma)$).
- If μ is abs. continuous, density $\propto \exp(-(x-m)^\top \Sigma^{-1}(x-m))$.
- Defining property for U : for any $(a_1, \ldots, a_d) \in \mathbb{R}^d$, $\sum_{i=1}^d a_i U_i$ is a 1D Gaussian random variable.
- Equivalent in terms of μ : the pushforward of μ through the map

$$\ell_a : \begin{cases} (\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d), \mu) & \to (\mathbb{R}, \mathcal{B}(\mathbb{R})) \\ u & \mapsto \langle a, u \rangle = \sum_{i=1}^d a_i u_i \end{cases}$$

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Gaussian measures 2/3

Let $(H, \|\cdot\|)$ be a Hilbert space and $\mathcal{B}(H)$ be its Borel σ-algebra.

Definition 2 (Gaussian measures)

A measure μ over $(H, \mathcal{B}(H))$ is Gaussian if for all $h \in H$, the pushforward of μ via the continuous linear form ℓ_x

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is s a 1D Gaussian distribution (i.e. $\ell_{x\#}\mu =$ some $\mathcal{N}(m_x, \sigma_x^2)$).

Gaussian measures have a mean vector $a_\mu \in H$ and cov. op. $K_\mu : H \to H$,

$$a_\mu = \int_H x\mu(dx) \in H \quad \text{(Bochner integral)}$$

$$\langle u, K_\mu v \rangle = \int_H \langle u, x - a_\mu \rangle \langle v, x - a_\mu \rangle \mu(dx) = \int_H \langle u, x \rangle \langle v, x \rangle \mu(dx) \text{ if } a_\mu = 0.$$

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Proposition 2 (Gaussian covariance operators)

$K : H \to H$ is the covariance operator of a centred Gaussian measure μ over $(H, \|\cdot\|)$ $\iff$ $K = K^*$, $K \geq 0$ and K is trace class, i.e. for any orthonormal basis (ONB) $(e_n)_{n\in\mathbb{N}}$ of H,

$$Tr(K) := \sum_{n=0}^{+\infty} \langle e_n, Ke_n \rangle < +\infty.$$

- Trace class operators are compact : there exists an ONB of H of eigenvectors, eigenvalues $\lambda_n \geq 0$ leading to

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Gaussian processes and Gaussian measures 1/2

What is the link between Gaussian measures and Gaussian processes ?

Let $U = (U(x))_{x \in \mathcal{D}} \sim GP(0, k)$ be measurable, i.e. the map below is measurable :

$$\begin{cases} (\mathcal{D} \times \Omega, \mathcal{B}(\mathcal{D}) \otimes \mathcal{F}) & \to (\mathbb{R}, \mathcal{B}(\mathbb{R})) \\ (x, \omega) & \mapsto U(x)(\omega) \end{cases}.$$

Assume also that $\mathbb{P}(\|U\|_{L^2(\mathcal{D})} < +\infty) = 1$. Then the random function map

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where $U_\omega : x \mapsto U(x)(\omega)$, is well-defined and measurable.

Moreover, $\mathbb{P}_{\widetilde{U}}$, the pushforward of $\mathbb{P}$ through $\widetilde{U}$ is a Gaussian measure!

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$$(\mathcal{E}_k f)(x) := \int_{\mathcal{D}} k(x,y) f(y) dy.$$

Hence $\mathcal{E}_k$ is necessarily trace class, with

$$Tr(\mathcal{E}_k) = \int_{\mathcal{D}} k(x,x)dx \overset{Fubini}{=} \mathbb{E}\left[\int_{\mathcal{D}} U(x)^2 dx\right] = \mathbb{E}[\|U\|_2^2] < +\infty.$$

In fact, in $L^2(\mathcal{D})$ we have the following equivalence.

Proposition 3 (GPs vs GMs over $L^2(\mathcal{D})$)

Let μ be a Gaussian measure over $(L^2(\mathcal{D}), \mathcal{B}(L^2(\mathcal{D}))$.

- *Then there exists a measurable Gaussian process $U \sim GP(0,k)$ such that $\mathbb{P}(\widetilde{U} \in L^2(\mathcal{D})) = 1$ and $\mu = \mathbb{P}_{\widetilde{U}}$.*
- *Its covariance operator K_μ is of the form $K_\mu = \mathcal{E}_k$ and k can be chosen as the cov. function of the GP U, with $\int_{\mathcal{D}} k(x,x)dx < +\infty$.*

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In fact, in $L^2(\mathcal{D})$ we have the following equivalence.

Proposition 3 (GPs vs GMs over $L^2(\mathcal{D})$)

Let μ be a Gaussian measure over $(L^2(\mathcal{D}), \mathcal{B}(L^2(\mathcal{D}))$.

- *Then there exists a measurable Gaussian process $U \sim GP(0,k)$ such that $\mathbb{P}(\widetilde{U} \in L^2(\mathcal{D})) = 1$ and $\mu = \mathbb{P}_{\widetilde{U}}$.*
- *Its covariance operator K_μ is of the form $K_\mu = \mathcal{E}_k$ and k can be chosen as the cov. function of the GP U, with $\int_{\mathcal{D}} k(x,x) dx < +\infty$.*

L^2 regularity of a Gaussian process[4]

To summarise again, let $(U(x))_{x\in\mathcal{D}} \sim GP(0,k)$ be a measurable GP, then

→ Integral criterion:

$$\mathbb{P}\big(U \in L^2(\mathcal{D})\big) = 1 \iff \int_{\mathcal{D}} k(x,x)dx < +\infty. \quad (10)$$

→ Spectral/Mercer-type criterion: let $\mathcal{E}_k : L^2(\mathcal{D}) \to L^2(\mathcal{D})$ be

$$(\mathcal{E}_k f)(x) := \int k(x,y)f(y)dy. \quad (11)$$

If $\int k(x,x)dx < +\infty$, then we have an ONB (ψ_n) of eigenvectors of $\mathcal{E}_k$, with eigenvalue $\lambda_n \geq 0$. This yields the Mercer decomposition

$$k(x,y) = \sum_{n=0}^{+\infty} \lambda_n \psi_n(x)\psi_n(y) \quad \text{in} \quad L^2(\mathcal{D}\times\mathcal{D}). \quad (12)$$

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Moreover, this Mercer decomposition verifies

$$\int_{\mathcal{D}} k(x,x)dx = \int_{\mathcal{D}} \sum_{n=0}^{+\infty} \lambda_n \psi_n(x)^2 dx = \sum_{n=0}^{+\infty} \lambda_n \int_{\mathcal{D}} \psi_n(x)^2 dx \tag{13}$$

$$= \sum_{n=0}^{+\infty} \lambda_n = \text{Tr}(\mathcal{E}_k) < +\infty \quad \text{(trace class)}. \tag{14}$$

→ Imbedding of the RKHS (other criterion) : if $\int k(x,x)dx < +\infty$, then $RKHS(k) \subset L^2(\mathcal{D})$, and denoting $\mathcal{I}$ the associated imbedding, $\mathcal{I}\mathcal{I}^*(= \mathcal{E}_k)$ is trace class ("∼Driscoll's theorem but for L^2" [5]).

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Plan

Tool : Sobolev norm as a countable supremum

- Recall that, from the Cauchy-Schwarz inequality,

$$\|f\|_2 = \sup_{g \in B_{L^2}(0,1)} |\langle f, g \rangle_{L^2}|.$$

- Likewise, $f \in L^1_{loc}(\mathcal{D})$ admits a weak derivative f' s.t. $f' \in L^2(\mathcal{D})$ iff

$$S := \sup_{\substack{\varphi \in C_c^\infty(\mathcal{D}) \\ \|\varphi\|_2 = 1}} |\langle f, \varphi' \rangle_{L^2}| < +\infty, \quad \text{with} \quad \|f'\|_2 = S.$$

Proof : extension of C^0 linear forms via the density of $C_c^\infty(\mathcal{D})$ in $L^2(\mathcal{D})$ + Riesz lemma (see e.g. Brézis book).
Utility : $\langle f, \varphi' \rangle_{L^2}$ is well-defined if $f \in L^1_{loc}(\mathcal{D})$.

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H^m regularity of a Gaussian process, $m \in \mathbb{N}$[7]

Proposition 4

Let $(U(z))_{z\in\mathcal{D}} \sim GP(0,k)$ be a measurable GP, there is an equiv. between

(i) (Sobolev) $\mathbb{P}(U \in H^m(\mathcal{D})) = 1$

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Sketch of proof 1/3

Prove the case $m = 1$ (one weak derivative), $d = 1$ ($\mathcal{D} \subset \mathbb{R}$). We only prove $(i) \iff (ii)$.

(i) : *Sobolev* $\implies$ (ii) : *Spectral* : assume (i) that $\mathbb{P}(U \in H^1(\mathcal{D})) = 1$.

- Then (...) the map $\omega \mapsto U'_\omega$ induces a Gaussian measure μ_D over $L^2(\mathcal{D})$. Let k_D be the covariance function of a GP s.t. $K_{\mu_D} = \mathcal{E}_{k_D}$.
- Direct computation of its covariance operator (...) : we show that $\partial_x \partial_y k \in L^2(\mathcal{D} \times \mathcal{D})$ (weak partial derivatives) and that

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Thus

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Hence, ω-a.s., $U_\omega \in H^1(\mathcal{D})$, i.e. (i) !

Other equivalences $(ii) \iff (iii) \iff (iv)$: analysis (... Spectral theory, Sobolev space theory.)

Sketch of proof 3/3

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$$= \mathbb{P}(\sup_{\varphi\in F_2} |\langle\varphi', U\rangle_{L^2}| < +\infty).$$

Hence, ω-a.s., $U_\omega \in H^1(\mathcal{D})$, i.e. (i) !

Other equivalences $(ii) \iff (iii) \iff (iv)$: analysis (... Spectral theory, Sobolev space theory.)

Sketch of proof 3/3

Hence the GPs $(V_\varphi)_{\varphi\in C_c^\infty(\mathcal{D})}$ and $(U'_\varphi)_{\varphi\in C_c^\infty(\mathcal{D})}$ have the same finite dimension marginals. In particular, because F_2 is countable,

$$(\|V\|_2 =) \quad \sup_{\varphi\in F_2} |V_\varphi| \overset{distribution}{=} \sup_{\varphi\in F_2} |U'_\varphi|.$$

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Sobolev spaces of non Hilbert type

The spaces $W^{m,p}(\mathcal{D})$ are also useful for the analysis of PDEs :

$$W^{1,p}(\mathbb{R}) := \{u \in L^p(\mathbb{R}) : u' \text{ exists in the weak sense and } u' \in L^p(\mathbb{R})\},$$
$$W^{m,p}(\mathcal{D}) := \{u \in L^p(\mathcal{D}) : \forall\ |\alpha| \leq m, \partial^\alpha u \text{ exists ITWS and } \partial^\alpha u \in L^p(\mathcal{D})\}.$$

L^p regularity of GPs : if $X \sim \mathcal{N}(0, \sigma^2)$, then $\mathbb{E}[|X|^p] = C_p \sigma^p$ for some C_p.

$$\mathbb{E}[\int |U(x)|^p dx] = \int \mathbb{E}\Big[|U(x)|^p\Big] dx = C_p \int k(x,x)^{p/2} dx = C_p \|\sigma\|_p^p.$$

Moreover if $\sigma \in L^p$ then there exists $(\psi_n) \subset L^p(\mathcal{D})$ s.t. $\sum_n \|\psi_n\|_p^2 < +\infty$,

$$k(x,y) = \sum_{n=0}^{+\infty} \psi_n(x)\psi_n(y) \quad \text{in} \quad L^p(\mathcal{D} \times \mathcal{D}) \quad \text{(nuclear operator).}$$

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$W^{m,p}$ regularity of a GP, $m \in \mathbb{N}, p \in (1, +\infty)$[8]

Proposition 5

Let $(U(z))_{z\in\mathcal{D}} \sim GP(0, k)$ be a measurable GP, there is an equiv. between
(i) $\mathbb{P}(U \in W^{m,p}(\mathcal{D})) = 1$
(ii) For all $|\alpha| \leq m$, $\partial^{\alpha,\alpha} k \in L^p(\mathcal{D} \times \mathcal{D})$ and the operator $\mathcal{E}_k^\alpha$

$$\mathcal{E}_k^\alpha : L^q(\mathcal{D}) \to L^p(\mathcal{D}), \quad \mathcal{E}_k^\alpha f(x) = \int_{\mathcal{D}} \partial^{\alpha,\alpha} k(x,y) f(y) dy$$

is symmetric, nonnegative and nuclear: there exists $(\phi_n^\alpha) \subset L^p(\mathcal{D})$ s.t.
$\partial^{\alpha,\alpha} k(x,y) = \sum_n \psi_n^\alpha(x)\psi_n^\alpha(y)$ *in $L^p(\mathcal{D} \times \mathcal{D})$ with*

$$\sum_{n=0}^{+\infty} \|\psi_n^\alpha\|_p^2 < +\infty \quad (+\textit{refinement if } 1 \leq p \leq 2)$$

(iii) For all $|\alpha| \leq m$, $\partial^{\alpha,\alpha} k \in L^p(\mathcal{D} \times \mathcal{D})$, $\int_{\mathcal{D}} [\partial^{\alpha,\alpha} k(x,x)]^{p/2} dx < +\infty$.

[8]H., I. (2024).Sobolev regularity of Gaussian random fields. *J. Func. Anal., 286(3)*, Paper No. 110241.

Some comments

- Matérn of order ν,$RKHS(k_\nu) = H^{\nu+d/2}$, target Sobolev space H^m : $\mathcal{I}\mathcal{I}^*$ is trace class $\iff \nu > m \iff \mathbb{P}(U_\nu \in H^m(\mathcal{D})) = 1$.
- Integral criterion for stationary kernels becomes trivial! For $L^2(\mathcal{D})$,

$$\int_{\mathcal{D}} k(x,x)dx < +\infty \iff \lambda(\mathcal{D}) < +\infty...$$

For $H^m(\mathcal{D})$,

$$\int_{\mathcal{D}} \partial^{\alpha,\alpha} k(x,x)dx < +\infty \iff \partial^{2\alpha} k_s(0) \text{ exists and } \lambda(\mathcal{D}) < +\infty...$$

Conclusion : do not use stationary GPs for modelling Sobolev functions ! E.g. choose k of the form

$$k(x,x') = \sigma(x)\sigma(x')k_S(x-x')...$$

- More interesting for Mercer decompositions.

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Plan

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GPR and the wave equation[9]

3D homogeneous wave equation : $\Delta := \partial^2_{xx} + \partial^2_{yy} + \partial^2_{zz}$

$$\begin{cases} Lu & = \partial^2_{tt} u - c^2 \Delta u = \Box u = 0, \quad (x,t) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ u(x,0) & = u_0(x), \quad \partial_t u(x,0) = v_0(x). \end{cases} \tag{15}$$

Representation of u (Krichhoff) : $F_t = \sigma_{ct}/4\pi c^2 t$ et $\dot{F}_t = \partial_t F_t$

$$u(x,t) = (F_t * v_0)(x) + (\dot{F}_t * u_0)(x). \tag{16}$$

Assume that u_0, v_0 are unknown $\rightarrow u_0 \sim GP(0, k_u)$ and $v_0 \sim GP(0, k_v)$, independant. u given by (16) is a centered GP, its kernel is

$$k((x,t),(x',t')) = [(F_t \otimes F_{t'}) * k_v](x,x') + [(\dot{F}_t \otimes \dot{F}_{t'}) * k_u](x,x'). \tag{17}$$

The kernel k verifies $\Box k((x,t),\cdot) = 0$ for all $(x,t) \in \mathbb{R}^3 \times \mathbb{R}_+$.

[9]H., I., Noble, P., & Roustant, O. (2023a).Covariance models and gaussian process regression for the wave equation. application to related inverse problems. *Journal of Computational Physics*, *494*, Paper No. 112519.

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Plan

1. Introduction
   - Generalities on GP modelling
   - Two simple examples of PDEs
2. PDE constrained random fields
   - Theorem
   - Examples
3. Sobolev regularity of the samples of a GP
   - Motivation : Sobolev spaces and PDEs
   - Gaussian measures and processes on L^2
   - Sobolev regularity of the samples of a GP
4. Application to the 3D wave equation
   - Covariance kernels for the wave equation
   - **Estimation of initial data and physical parameters**
5. Conclusion and perspectives

Estimation of physical parameters and initial conditions

- Initial condition reconstruction: the GPR mean verifies $\Box\tilde{m} = 0$. Hence

$$\tilde{m}(\cdot, t = 0) \simeq u_0, \quad \partial_t \tilde{m}(\cdot, t = 0) \simeq v_0$$

Recover u_0: photoacoustic tomography.

- Parameters of the PDE may also be estimated with GPR : celerity c, source position, source size...

  $\rightarrow$ can be estimated using marginal likelihood (standard in GPR).

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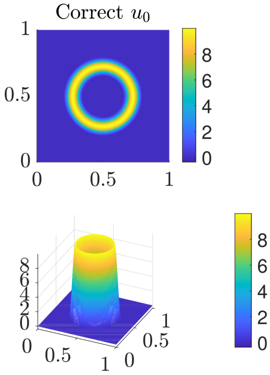
Numerical application

Restrictive framework

Expensive convolutions (4D) → radial symmetry framework (explicit convolutions).

- Numerical solution of the wave equation in $[0,1]^3$, $v_0 = 0$ and



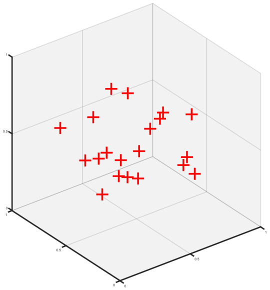


Figure 5: Sensor positions

Data visulatization

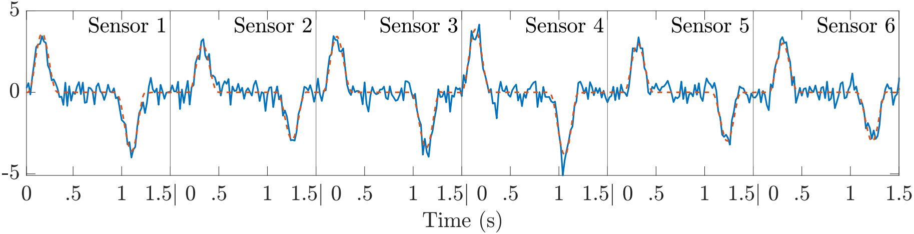


Figure 6: Examples of captured signals. Red: noiseless signal. Blue: noisy signal.

Reconstruction of initial conditions and position parameters

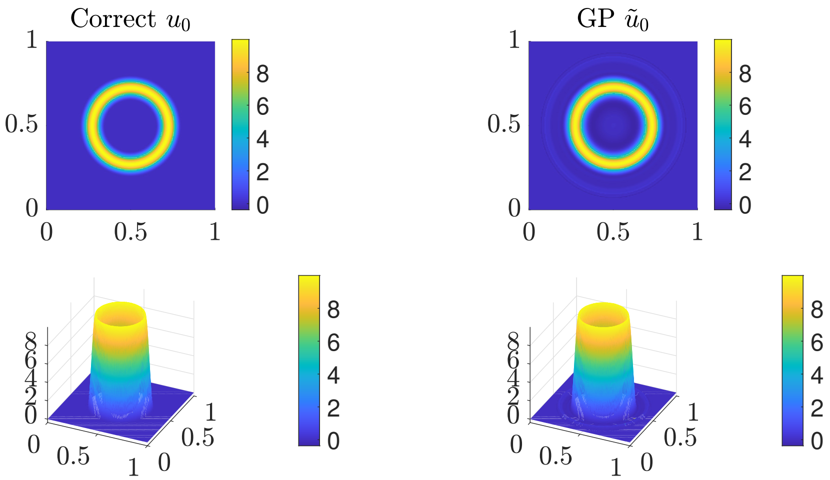


Figure 7: True u_0 (left column) vs GPR u_0 (right column). 15 sensors are used. Images correspond to 3D slices at $z = 0.5$.

Plan

Retrospective

GPR, GPs constrained by physical laws :

- Linear distributional PDE constraints[10]
- Energy constraints: $H^m, W^{m,p}$[11]

$\rightarrow$ Theorems with necessary and sufficient conditions without continuity assumptions.

Practical application : Wave equation and related inverse problems[12]

[10]H., I., Noble, P., & Roustant, O. (2023b).Characterization of the second order random fields subject to linear distributional pde constraints. *Bernoulli*, *29*(4), 3396–3422.

[11]H., I. (2024).Sobolev regularity of Gaussian random fields. *J. Func. Anal.*, *286(3)*, Paper No. 110241.

[12]H., I., Noble, P., & Roustant, O. (2023a).Covariance models and gaussian process regression for the wave equation. application to related inverse problems. *Journal of Computational Physics*, *494*, Paper No. 112519.

Perspectives

Short term :

- PDE kernels for bathymetry inversion in data assimilation, with INSA Toulouse.
- ANR SHORECAST lead by Déborah Idier (BRGM), : large scale surrogate models with functional inputs-outputs to emulate complex physical models for the evolution of sandy shores,

PhD position available for Autumn 2026 !

- Student processes : like GPs, but more general !

Less short term :

- Error analysis of GPR using Sobolev norms[13].
- 3D wave equation : computational issues (convolutions)[14].

[13]Batlle, P., Chen, Y., Hosseini, B., Owhadi, H., & Stuart, A. M. (2023). Error analysis of kernel/gp methods for nonlinear and parametric pdes.

[14]Tick, J., Pulkkinen, A., Lucka, F., Ellwood, R., Cox, B. T., Kaipio, J. P., Arridge, S. R., & Tarvainen, T. (2018).Three dimensional photoacoustic tomography in bayesian framework. *The Journal of the Acoustical Society of America*, *144*(4), 2061–2071.

Thank you for your attention!

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GPR : Bayesian inference of functions

Bayesian inference : to estimate $\eta \in H$ given partial data $\mathcal{B}$,

1. introduce a **prior** probability distribution π over H,
2. **condition it on** $\mathcal{B}$ to obtain the **posterior** distribution $\pi_{\mathcal{B}}$
3. construct $\widehat{\theta}$ and perform UQ on it with

$$\widehat{\eta} = \int_H s \ \pi_{\mathcal{B}}(ds) = \mathbb{E}_{S \sim \pi_{\mathcal{B}}}[S] = \text{posterior expectation} \tag{18}$$

$$v(\widehat{\eta}) = \int_H (s - \widehat{\eta})^2 \pi_{\mathcal{B}}(ds) = \text{Var}_{S \sim \pi_{\mathcal{B}}}(S) = \text{posterior variance} \tag{19}$$

For us,

- $\eta = u$ (function), $H =$ space of functions , $\mathcal{B} = \{u(z_1), \dots, u(z_n)\}$.
- prior $\pi = GP(m, k)$, posterior $\pi_{\mathcal{B}} = GP(\widetilde{m}, \widetilde{k})$.