Physics-informed random fields. Application to Kriging

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Introduction and problem formulation

- Many functions of interest describe **physical quantities**. Often, they are partially known, e.g. through sensor measurements.
- Such quantities are constrained by **physical laws** which often take the form of **Partial Differential Equations (PDEs)**.

$\Longrightarrow$ Adopt a Bayesian approach, e.g. **Kriging** in the spirit of [1], which combines field data (sensors) and a **functional prior** that is constrained by such physical laws.

$\Longrightarrow$ Need to build a theory for PDE-constrained random fields compatible with the **standard tools of PDE theory**.

The tools : PDEs and random fields

- Consider an open set $\mathcal{D} \subset \mathbb{R}^d$ and a linear homogeneous PDE

$$L(u)(x) := \sum_{|\alpha|\leq n} a_\alpha(x)\partial^\alpha u(x) = 0, \quad x \in \mathcal{D} \tag{1}$$

For $\alpha = (\alpha_1, ..., \alpha_d)^T \in \mathbb{N}^d$, we used the notations $|\alpha| = \alpha_1 + ... + \alpha_d$ and $\partial^\alpha = (\partial_{x_1})^{\alpha_1}...(\partial_{x_d})^{\alpha_d}$.

- Let $U = (U(x))_{x\in\mathcal{D}}$ be a **random field (RF)**. A **sample path** of U is a deterministic function $U_\omega : x \mapsto U(x)(\omega)$.
- When a function u is unknown, it can be modelled as a sample path of U; U then defines a **prior over $\boldsymbol{u}$**.

Modelling consequence : if u is a solution to equation (1), the prior U should have all its sample paths verify $L(U_\omega) = 0$.

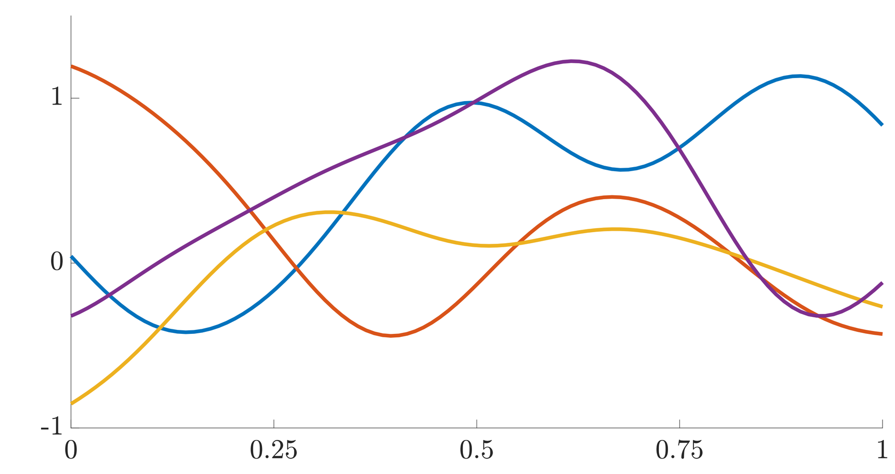

Fig. 1: Sample paths of a GP with $k(x,x') = s^2 \exp\left(-\frac{1}{2\ell^2}|x-x'|^2\right)$

What does $L(u) = 0$ really mean?

- Functions that verify equation (1) **pointwise**, i.e. for all $x \in \mathcal{D}$, are **strong solutions**.
- In some cases, this requirement is too strong. One relaxes (1) by requiring it to be verified only when **locally averaged**:

$$\forall\varphi \in C_c^\infty(\mathcal{D}),\ 0 = \int_{\mathcal{D}} \varphi(x)L(u)(x)dx = \sum_{|\alpha|\leq n}\int_{\mathcal{D}} \varphi(x)a_\alpha(x)\partial^\alpha u(x)dx \tag{2}$$

For each term, perform $|\alpha|$ successive integrations by parts :

$$\forall\varphi \in C_c^\infty(\mathcal{D}),\ \int_{\mathcal{D}} u(x)\sum_{|\alpha|\leq n}(-1)^{|\alpha|}\partial^\alpha(a_\alpha\varphi)(x)dx = 0 \tag{3}$$

One only needs u to be locally integrable ($\int_K |u| < +\infty$ if $K \subset \mathcal{D}$ is compact) to make sense of equation (3); if u verifies (3), it is a **distributional solution** of equation (1).

Distributional PDE-constrained random fields

- Let U be a centered **measurable second order** RF whose covariance function $k(x,x') = \mathbb{E}[U(x)U(x')]$ is such that $\sigma : x \mapsto k(x,x)^{1/2}$ is locally integrable. We show that [2]

$$\mathbb{P}(\{\omega\in\Omega : L(U_\omega) = 0 \textbf{ in the distributional sense}\}) = 1 \\ \iff \forall x \in \mathcal{D}, L(k(x,\cdot)) = 0 \textbf{ in the distributional sense} \tag{7}$$

This extends a result from [3], where U is a Gaussian process (GP) and "distributional" is replaced by "strong". See also [4] for similar results in the stationary case.

- **Consequences for Kriging:** suppose that $U \sim GP(0,k)$ verifies the r.h.s. of (7) and define $V(x) = (U(x)|U(x_i) = u_i\ \forall i) \sim GP(\tilde{m},\tilde{k})$. Then $\tilde{m}$, $\tilde{k}(x,\cdot)$ and the sample paths of V also verify the PDE in the distributional sense.

A PDE with non-smooth solutions: the wave equation

Note $\Delta = \partial_{xx}^2 + \partial_{yy}^2 + \partial_{zz}^2$. Consider the following Cauchy problem in 3D:

$$\begin{cases} \square u = \left(\partial_{tt}^2 - c^2\Delta\right)u = 0 & x \in \mathbb{R}^3,\ t > 0 \\ u(x,0) = u_0(x) \ \text{ and } \ (\partial_t u)(x,0) = v_0(x) & x \in \mathbb{R}^3 \end{cases} \tag{4}$$

Its distributional solution u is

$$u(x,t) = (F_t * v_0)(x) + (\dot{F}_t * u_0)(x) \tag{5}$$

$$= \int_{S(0,1)} tv_0(x - c|t|\gamma) + u_0(x - c|t|\gamma) - c|t|\gamma\cdot\nabla u_0(x - c|t|\gamma)\frac{d\Omega}{4\pi} \tag{6}$$

Gaussian processes for the wave equation

- Suppose that u_0 and v_0 are sample paths of two independent GPs $U_0 \sim GP(0,k_u^0)$ and $V_0 \sim GP(0,k_v^0)$. Then we show that ([2]) u in equation (5) is a sample path of a centered GP whose covariance kernel is

$$k((x,t),(x',t')) = [(F_t \otimes F_{t'}) * k_v^0](x,x') + [(\dot{F}_t \otimes \dot{F}_{t'}) * k_u^0](x,x') \tag{8}$$

- This kernel verifies $\square k((x,t),\cdot) = 0$ for a fixed (x,t). It can then be used for physics-informed Kriging on partially observed solutions of (4).

Physics-informed Kriging for the wave equation

- **Aim:** consider u a solution of (4). Given a database $B = \{u(x_i,t_j)\}_{i,j}$ of values of u, **reconstruct its initial conditions $\boldsymbol{u_0}$ and $\boldsymbol{v_0}$**.
- **Physics-informed Kriging:** perform Kriging on B using kernel (8). Let $\tilde{m}(x,t)$ be the resulting Kriging mean, then **$\tilde{m}(\cdot,0)$ and $\partial_t\tilde{m}(\cdot,0)$ are approximations of u_0 and v_0**.

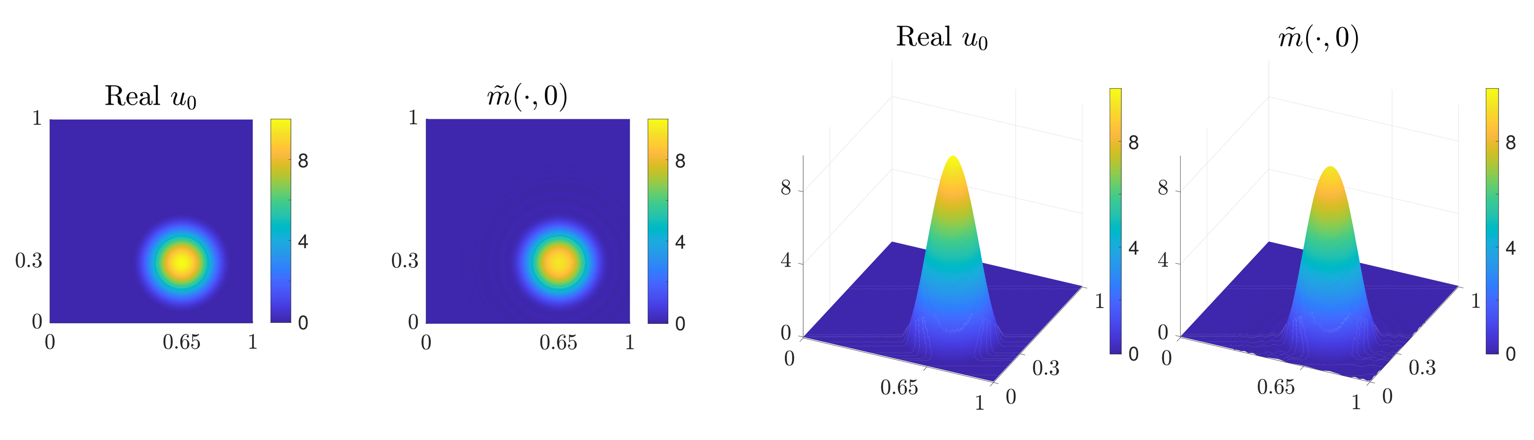

Fig. 2: Comparison of u_0 and $\tilde{m}(\cdot,0)$ on a slice $z = Cst$

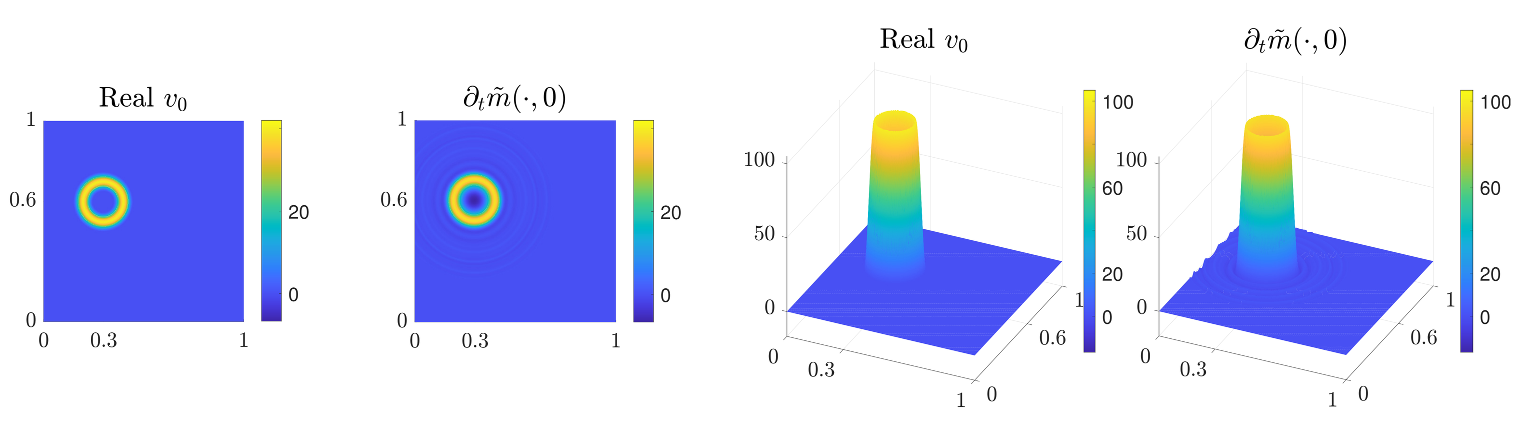

Fig. 3: Comparison of v_0 and $\partial_t\tilde{m}(\cdot,0)$ on a slice $z = Cst$

- **DOE and Kriging model :** for B, we use 30 sensors scattered in $[0,1]^3$ acquiring values of u at a frequency of $50Hz$ during 1.5 s. We impose radial symmetry and compact support around unknown points x_0^u and x_0^v in the covariance structures of U_0 and V_0. The physical parameters (c, x_0^u, x_0^v, source sizes) are estimated through **log-marginal likelihood maximization**.

Conclusion and acknowledgements

- We provided a characterization of distributional PDE constrained RFs.
- Kriging for the wave equation: we performed initial condition reconstruction and physical parameter estimation.

Perspectives:

- Replace "distributional" by "weak" in equation (7).
- Tackle nonlinear PDEs.

We gratefully thank the SHOM and Rémy Baraille in particular for funding this work.

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