On the Bayesian formulation of fractional inverse problems and data-driven discretization of forward maps

> Nicolás García Trillos Brown University

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- Bayesian formulation of fractional inverse problems.
- ② Data driven discretization of forward maps.

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This presentation mostly based on:

- The Bayesian Formulation and Well-Posedness of Fractional Elliptic Inverse Problems (2017 Inverse Problems) with D. Sanz-Alonso.
- Data driven discretizations of forward maps in Bayesian inverse problems (In preparation) with D. Bigoni, Y. Marzouk and D. Sanz-Alonso.

# Part 1: Bayesian formulation of fractional inverse problems.

**Inverse problem**: learn a permeability field from partial and noisy observations of pressure field.

**PDE version**: Learn diffusion coefficient and **order** of a (FPDE) based on partial and noisy observations of its solution.

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**PDE version**: Learn diffusion coefficient and **order** of a (FPDE) based on partial and noisy observations of its solution.

$$u = (s, A) \longrightarrow \mathcal{F}(u) \longrightarrow \mathcal{O} \circ \mathcal{F}(u)$$
$$\mathcal{G} := \mathcal{O} \circ \mathcal{F}$$

$$y = \mathcal{G}(u) + Noise$$

**Inverse problem**: learn a permeability field from partial and noisy observations of pressure field.

**PDE version**: Learn diffusion coefficient and **order** of a (FPDE) based on partial and noisy observations of its solution.

$$u = (s, A) \longrightarrow \mathcal{F}(u) \longrightarrow \mathcal{O} \circ \mathcal{F}(u)$$
$$\mathcal{G} := \mathcal{O} \circ \mathcal{F}$$
$$\phi(y; \mathcal{G}(u))$$

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• Forward map:  $p = \mathcal{F}(u)$ .

$$\begin{cases} L_A^s p = f, & \text{in } D, \\ \partial_A p = 0, & \text{on } \partial D, \end{cases}$$
(1)

where  $\partial_A p := A(x) \nabla p \cdot \nu$ , and  $\nu$  is the exterior unit normal to  $\partial D$ .

- **Observation map:**  $\mathcal{O}(p) := (p(x_1), \dots, p(x_n))$  for some  $x_i \in D$ .
- Noise model:  $\phi(y, \mathcal{G}(u)) = \exp\left(-\frac{1}{2\gamma^2} \|y \mathcal{G}(u)\|^2\right)$ .

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• Forward map:  $p = \mathcal{F}(u)$ .

$$\begin{cases} L_A^s p = f, & \text{in } D, \\ \partial_A p = 0, & \text{on } \partial D, \end{cases}$$
(2)

where  $\partial_A p := A(x) \nabla p \cdot \nu$ , and  $\nu$  is the exterior unit normal to  $\partial D$ .

Here,

$$L_A^s p = \sum_{k=1}^\infty \lambda_{A,k}^s p_k \psi_{A,k}.$$

- **Observation map:**  $\mathcal{O}(p) := (p(z_1), \dots, p(z_m))$  for some  $z_i \in D$ .
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- A. M. Stuart. Inverse problems: a Bayesian perspective. (2010).
- J. Kaipio and E. Somersalo. Statistical and computational inverse problems (2006).

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- Prior:  $u \sim \pi_u$
- Likelihood model:  $\pi_{y|u}$
- Bayes rule (informally):

$$\nu^{y}(u) := \pi_{u|y} \propto \pi_{y|u} \cdot \pi_{u}$$

Posterior distribution.

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- $\nu^{\rm y}$  is the fundamental object in Bayesian inference.
  - Estimates:

$$\mathbb{E}_{u\sim \nu^{y}}\left(R(u)\right)$$

• Uncertainty quantification:

 $Var_{u\sim 
u^{y}}\left( R(u)
ight)$ 

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Well defined mathematical framework:

- Stability (Well-posedness).
- Posterior consistency (contraction rates, scalings for parameters, etc).
- Consistency of numerical methods.

- $\pi_u$  is a distribution on  $(0,1) \times \mathcal{H}$ .
- For example,

$$\pi_u = \pi_s \otimes \pi_A$$
  
 $A = e^{v} I_d, \quad ext{where } v \sim N(0, K)$ 

• Karhunen-Loeve expansion:

$$\mathbf{v} = \sum_{i=1}^{\infty} \lambda_{K,i} \zeta_i \Psi_i, \quad \zeta_i \sim \mathcal{N}(0,1).$$

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#### Theorem (NGT and D. Sanz-Alonso 17')

Suppose that  $\mathcal{G}$  is continuous in supp $(\pi_u)$ . Then, posterior distribution  $\nu^y$  is absolutely continuous with respect to prior:

 $d\nu^{y}(u) \propto \phi(y; \mathcal{G}(u)) d\pi_{u}(u),$ 

*Recall:*  $\mathcal{G}$  :  $(s, A) \rightarrow \mathbb{R}^m$ .

Theorem (NGT and D. Sanz-Alonso 17')

Suppose that  $\mathcal{G} \in L^2_{\pi_u}$ . Then the map

 $y \mapsto \nu^y$ 

is Locally Lipschitz in the Hellinger distance. That is, For  $|y_1|, |y_2| \leq r$  we have

$$d_{hell}(\nu^{y_1}, \nu^{y_2}) \leq C_r \|y_1 - y_2\|.$$

The analysis reduces to studying stability through regularity of FPDEs.

• L. A. Caffarelli and P. R. Stinga. Fractional elliptic equations, Caccioppoli estimates and regularity. (2016)

- M. Dashti and A. M. Stuart. Uncertainty quantification and weak approximation of an elliptic inverse problem. (2011).
- S. Agapiou, S. Larsson, and A.M. Stuart. Posterior contraction rates for the Bayesian approach to linear ill-posed inverse problems. (2013).
- S. Volmer. Posterior consistency for Bayesian inverse problems through stability and regression results. (2013).

## Numerical methods: MCMC

- Need a way to approximate expectations with respect to  $\nu^{y}$ .
- Standard procedure: MCMC.
   Generate a path of a Markov chain with invariant distribution
   ν<sup>y</sup>: u<sub>1</sub>,..., u<sub>k</sub>,... and then use

$$\frac{1}{k}\sum_{i=1}^{k}R(u_i)$$

- However, careful with:
  - Discretization of u.
  - ② Discretization of forward map.

For the sake of simplicity assume  $A = e^{v} \cdot I_d$  and known  $s \in (0, 1)$ . **Metropolis Hastings with pCN proposal:** Having defined  $v_k$ ,  $v_{k+1}$  is generated according to:

• Proposal:  $\tilde{v} = \sqrt{1 - \beta^2} v_k + \beta \xi$ , where  $\xi \sim \pi_v$ .

2 Acceptance probability:

(3)

$$\alpha(\tilde{u}, u_k) := \min\left\{1, \frac{\phi(y; \mathcal{G}(\tilde{u}))}{\phi(y; \mathcal{G}(u_k))}\right\}$$
$$v_{k+1} := \begin{cases} \tilde{v} & \text{with prob } \alpha(\tilde{u}, u_k) \\ v_k & \text{with prob } 1 - \alpha(\tilde{u}, u_k) \end{cases}$$

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• Proposal: 
$$\tilde{v} = \sqrt{1 - \beta^2} v_k + \beta \xi$$
, where  $\xi \sim \pi_v$ .  
Compare to:  $\tilde{v} = v_k + \beta \xi$ 

S. L. Cotter, G. O. Roberts, A. M. Stuart, and D. White. MCMC methods for functions: modifying old algorithms to make them faster. Statistical Science.

2 Acceptance probability:

$$\alpha(\tilde{u}, u_k) := \min\left\{1, \frac{\phi(y; \mathcal{G}(\tilde{u}))}{\phi(y; \mathcal{G}(u_k))}\right\}$$

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## Idealized MCMC algorithm

For the sake of simplicity assume  $A = e^{v} \cdot I_d$  and known  $s \in (0, 1)$ . **Metropolis Hastings with pCN proposal:** Having defined  $v_k$ ,  $v_{k+1}$  is generated according to:

• Proposal:  $\tilde{v} = \sqrt{1 - \beta^2} v_k + \beta \xi$ , where  $\xi \sim \pi_v$ . Compare to:  $\tilde{v} = v_k + \beta \xi$ 

S. L. Cotter, G. O. Roberts, A. M. Stuart, and D. White. MCMC methods for functions: modifying old algorithms to make them faster. Statistical Science. Robustness to truncation:

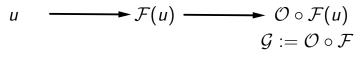
$$\xi = \sum_{i=1}^{L} \lambda_{\mathcal{K},i} \zeta_i \Psi_i, \quad \zeta_i \sim \mathcal{N}(0,1)$$

Acceptance probability:

$$\alpha(\tilde{u}, u_k) := \min\left\{1, \frac{\phi(y; \mathcal{G}(\tilde{u}))}{\phi(y; \mathcal{G}(u_k))}\right\}$$

# Part 2: Data driven discretization of forward maps

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 $\phi(y;\mathcal{G}(u))$ 

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#### MCMC: Metropolis with pCN proposal

To produce  $u_{k+1}$ :

**9** Proposal: 
$$ilde{u} = \sqrt{1-eta^2}u_k + eta\xi$$
 ,  $\xi \sim \pi_u$ .

Ompute acceptance probability:

$$\alpha(\tilde{u}, u_k) := \min\left\{1, \frac{\phi(y; \mathcal{G}(\tilde{u}))}{\phi(y; \mathcal{G}(u_k))}\right\}$$

$$u_{k+1} := \begin{cases} \tilde{u} & \text{with prob } \alpha(\tilde{u}, u_k) \\ u_k & \text{with prob } 1 - \alpha(\tilde{u}, u_k) \end{cases}$$

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 ,  $\xi \sim \pi_u$ .

Ompute acceptance probability:

$$\alpha(\tilde{u}, u_k) := \min\left\{1, \frac{\phi(y; \mathcal{G}_X(\tilde{u}))}{\phi(y; \mathcal{G}_X(u_k))}\right\}$$

$$\mathbf{0} \ v_{k+1} := \begin{cases} \tilde{v} & \text{with prob } \alpha(\tilde{u}, u_k) \\ v_k & \text{with prob } 1 - \alpha(\tilde{u}, u_k) \end{cases}$$

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#### MCMC:Metropolis with pCN proposal

To produce  $u_{k+1}$ :

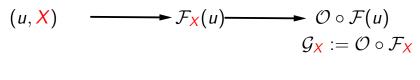
**9** Proposal: 
$$\tilde{u} = \sqrt{1 - \beta^2} u_k + \beta \xi$$
,  $\xi \sim \pi_u$ .

Ompute acceptance probability:

$$\alpha(\tilde{u}, u_k) := \min\left\{1, \frac{\phi(y; \mathcal{G}_{\mathcal{X}}(\tilde{u})}{\phi(y; \mathcal{G}_{\mathcal{X}}(u_k))}\right\}$$

How do we choose the discretization? How fine? Inhomogeneous in space?

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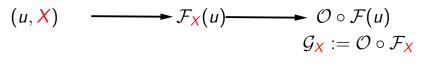


 $\phi(y; \mathcal{G}_{\mathbf{X}}(u))$ 

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 $\phi(y; \mathcal{G}_{\mathbf{X}}(u))$ 

More specifically:  $X = (N, \{x_1, \ldots, x_N\}).$ 

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Prior:  $u \sim \pi_u$ . Likelihood:  $\phi(y; \mathcal{G}(u))$ Posterior: Prior:  $(u, X) \sim \pi_{u,X}$ . Likelihood:  $\phi(y; \mathcal{G}_X(u))$ Posterior:

 $d\nu^{y}(u) \propto \phi(y; \mathcal{G}(u)) d\pi_{u}(u)$ 

 $d\nu^{y}(u,X) \propto \phi(y;\mathcal{G}_{X}(u))d\pi_{u,X}(u,X)$ 

For simplicity our prior takes the form:

$$\pi_{u,X} = \pi_{x_1,\dots,x_N|N} \cdot \pi_N \cdot \pi_u.$$

- $\pi_u$  is as for the true problem.
- $\pi_{u,X}$  treats X and u independently.
- $\pi_{x_1,...,x_N|N} = dx_1...dx_N$  on  $D^N$ .
- $\pi_N$  takes into account cost of discretization of  $\mathcal{F}$  using N elements:

$$\pi_N \propto \exp(-C(N))$$

### $\phi(y;\mathcal{G}_X(u))$

Recall  $\mathcal{G}_X = \mathcal{O} \circ \mathcal{F}_X$ .

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#### $\phi(y;\mathcal{G}_X(u))$

Recall  $\mathcal{G}_X = \mathcal{O} \circ \mathcal{F}_X$ . However, we don't triangulate directly using X. First, we regularize the points  $x_1, \ldots, x_n$ .

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$$\phi(y;\mathcal{G}_X(u))$$

Recall  $\mathcal{G}_X = \mathcal{O} \circ \mathcal{F}_X$ .

However, we don't triangulate directly using X. We regularize the points  $x_1, \ldots, x_n$ .  $X = (\{x_1, \ldots, x_n\}, N)$  induces a density estimator  $\rho_X$ .

•  $\rho_X$  is used to choose points in a master grid.

#### or

Using \(\rho\_X\) we start a flow of the points \(x\_1, \ldots, x\_n\) attempting to minimize an energy of the form:

$$E(x_1,\ldots,x_n)\sim \sum_{i,j}\exp(-|x_i-x_j|^2/(h_N\cdot\rho_X(x_i))^2)$$

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#### Metropolis within Gibbs:

Alternate:

- **1** Update the unknown; discretization is fixed. u|X, y|
- **2** Change distribution of elements.  $x_1, \ldots, x_N | N, u, y$
- **③** Coarsen or refine discretization.  $x_1, \ldots, x_N, N|u, y$

Given  $(u_k, X_k)$  produce  $u_{k+1}$  by:

 $\ \, {\rm Proposal:} \ \, \widetilde{u}=\sqrt{1-\beta^2}u_k+\beta\xi \ \, , \ \xi\sim\pi_u. \ \ \,$ 

Ompute acceptance probability:

$$\alpha(\tilde{u}, u_k) := \min\left\{1, \frac{\phi(y; \mathcal{G}_{X_k}(\tilde{u}))}{\phi(y; \mathcal{G}_{X_k}(u_k))}\right\}$$

$$\mathbf{3} \ u_{k+1} := \begin{cases} \tilde{u} & \text{with prob } \alpha(\tilde{u}, u_k) \\ u_k & \text{with prob } 1 - \alpha(\tilde{u}, u_k) \end{cases}$$

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#### Change distribution of elements

Given 
$$(u_k, X_k)$$
 produce  $x_1^{k+1}, \ldots, x_N^{k+1}$  by:  
Proposal:  $\tilde{x}_i = x_i + F(x_i)$ , for all  $i = 1, \ldots, N$ .  
 $F := (\Psi_1, \Psi_2) \sim N(0, K_1 \otimes K_2)$ 

Ompute acceptance probability:

$$\alpha(\tilde{X}, X_k) := \min\left\{1, \frac{\phi(y; \mathcal{G}_{\tilde{X}}(u_k)}{\phi(y; \mathcal{G}_{X_k}(u_k))} \cdot \frac{p(X_k | \tilde{X})}{p(\tilde{X} | X_k)}\right\}$$
  

$$X_{k+1} := \begin{cases} \tilde{X} & \text{with prob } \alpha(\tilde{X}, X_k) \\ X_k & \text{with prob } 1 - \alpha(\tilde{X}, X_k) \end{cases}$$

## Coarsen or refine discretization

Given  $(u_k, X_k)$  we produce  $N_{k+1}$  and  $x_1^{k+1}, \ldots, x_{N_{k+1}}^{k+1}$  by:

**9** Proposal: First construct  $\rho_X$  and generate  $\tilde{N} \sim p(\cdot|N_k)$ .

• If 
$$\tilde{N} < N$$
 let  $\tilde{x}_i = x_i$  for  $i = 1, \dots, \tilde{N}$ .

- If  $\tilde{N} \ge N$  let  $\tilde{x}_i = x_i$  for i = 1, ..., N and generate  $\tilde{x}_{N+j} \sim \rho_X$  for  $j = 1, ..., \tilde{N} N$ .
- Ompute acceptance probability:

$$\alpha(\tilde{X}, X_{k}) := \min \left\{ 1, \frac{\phi(y; \mathcal{G}_{\tilde{X}}(u_{k}))}{\phi(y; \mathcal{G}_{X_{k}}(u_{k}))} \cdot p(X, \tilde{X}) \\ \cdot \frac{p(\tilde{N}|N_{k})}{p(N_{k}|\tilde{N})} \cdot \frac{\exp(-C(\tilde{N}))}{\exp(-C(N))} \right\}$$

$$(3)$$

$$\mathbf{S} \quad X_{k+1} := \begin{cases} \tilde{X} & \text{with prob } \alpha(\tilde{X}, X_{k}) \\ X_{k} & \text{with prob } 1 - \alpha(\tilde{X}, X_{k}) \end{cases}$$

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#### Thank you for your attention!

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