Neural Couplings for Optimal Bayesian Experimental Design of Inverse PDE Problems

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IMPERIAL

Problem Formulation

Consider a PDE model $\mathcal{G}: \mathcal{A} \to \mathcal{U}$ (Parameter space, Solution space)

We take a Bayesian approach

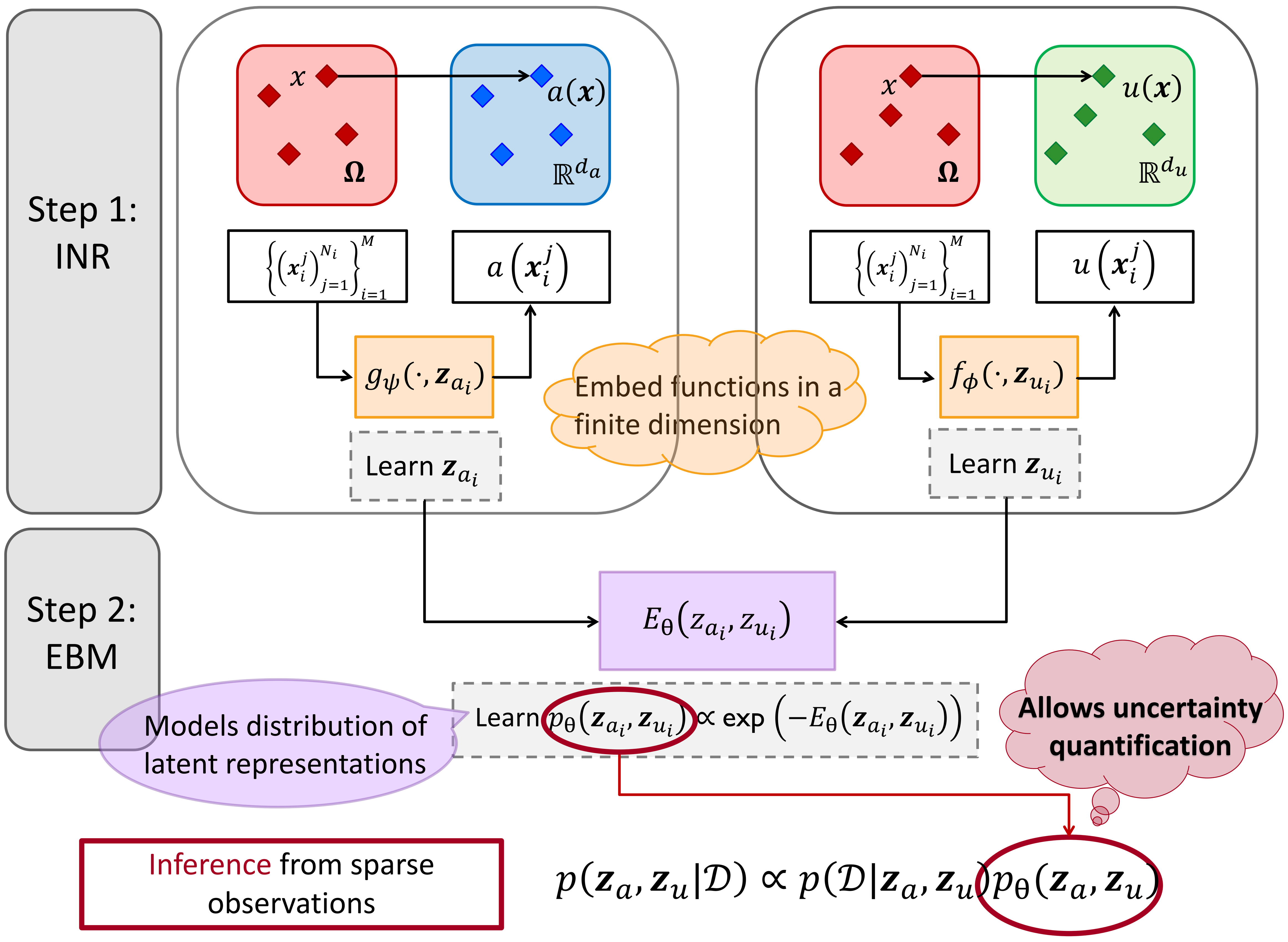
Inverse problem: Given noisy observations of PDE solution $y_i = \mathcal{G}(a)(\boldsymbol{x}_i) + \eta_i$, **infer** $\boldsymbol{a}$

Experimental design: Determine measurement positions $\boldsymbol{x}$ that yield the most information about solution

Challenges: Possibly stochastic operator $\mathcal{G}$
- Functional form parameter and solution
- Resolution invariant method
- Computationally efficient

Solution: Learn a **generative model** $\boldsymbol{p_\theta}$ for the joint distribution over parameters and PDE solutions $(a, u = \mathcal{G}(a))$.
Provides a **surrogate method** which allows for complex probabilistic relationship and that is **not dependent on a fixed discretisation** of the domain.

Energy-Based Coupling on Function Space



Bayesian experimental design

Find optimal sparse sensor placement positions $\xi = \{\xi_1, \ldots, \xi_D\}$ to improve posterior inference based on new measurements $y_i = u(\xi_i) + \eta_i$.

HOW?

Maximise utility of sensor placement positions

$$U(\xi) := \mathbb{E}_{p(y|\xi)} D_{KL}(p(\boldsymbol{z}_a, \boldsymbol{z}_u | y, \xi) || p_\theta(\boldsymbol{z}_a, \boldsymbol{z}_u))$$

In practice, we maximise the PCE bound

$$\hat{U}_{PCE}(\xi) := \mathbb{E}\left[\log \frac{p(y|\boldsymbol{z}_{a,0}, \boldsymbol{z}_{u,0}, \xi)}{\frac{1}{L+1}\sum_{l=0}^{L} p(y|\boldsymbol{z}_{a,l}, \boldsymbol{z}_{u,l}, \xi)}\right] \le U(\xi)$$

where the expectation is over $\prod p_\theta(\boldsymbol{z}_{a,i}, \boldsymbol{z}_{u,i})\, p(y|\boldsymbol{z}_{a,0}, \boldsymbol{z}_{u,0})$.
The selection of ξ_i is conducted sequentially.

Conclusion and future work

Our combination of implicit neural representation (INR) and generative model captures the often intractable stochasticity that is propagated through the PDE and provides a **novel method for BED of inverse PDE problems avoiding costly MCMC methods** with runtimes of days vs minutes for our approach.

Future work: explore improved sample efficient methods for the modelling and training of EBMs for functional data.

Numerical experiments

Boundary value problem in 1D: $u''(x) - u^2(x)u'(x) = f(x)$

- Boundary conditions $u(x_{min}) = X_a \sim N(a, 0.3^2), u(x_{max}) = X_b \sim Unif(b - 0.3, b + 0.4)$
  Training data: a, b and observations of solution for a realisation of X_a, X_b
- Perform inference on a, b based on 2 sparse observations of solution ✖

Design points	$\|\|\hat{u} - u_{tr}\|\|^2/\|\|u_{tr}\|\|^2$	$\|\|\hat{a} - a_{tr}\|\|^2/\|\|a_{tr}\|\|^2$	$\|\|\hat{b} - b_{tr}\|\|^2/\|\|b_{tr}\|\|^2$
BED	0.064 ± 0.009	0.073 ± 0.085	0.130 ± 0.062
Sobol points	0.433	0.291	1.326

Steady-state difussion in 2D: $-\nabla \cdot (\kappa(x)\nabla u(x)) = f(x)$

- Learn functional difussion coefficient κ
- Based on initial observations ✖, find optimal locations ✖ of u maximising PCE

Design points	$\|\|\log\hat{\kappa} - \log\kappa_{tr}\|\|^2/\|\|\log\kappa_{tr}\|\|^2$	$\|\|\hat{u} - u_{tr}\|\|^2/\|\|u_{tr}\|\|^2$
BED w/ Neural Coupling (Ours)	0.016 ± 0.007	0.020 ± 0.005
Sobol points	0.054	0.098

Navier Stokes equation: $\partial_t \omega(x,t) + u(x,t) \cdot \nabla\omega(x,t) = \nu\Delta\omega(x,t) + f(x)$

- Learn initial vorticity $\omega_0(x) = \omega(x, 0)$ generated according to a Gaussian random field
- Find 15 optimal locations ✖ of the vorticity at t=5 maximising PCE bound

Design points	$\|\|\hat{\omega}_0 - \omega_0\|\|^2/\|\|\omega_0\|\|^2$	$\|\|\hat{\omega}_{t=5} - \omega_{t=5}\|\|^2/\|\|\omega_{t=5}\|\|^2$
BED w/ Neural Coupling (Ours)	0.226 ± 0.042	0.046 ± 0.003
Sobol points	0.311	0.108