Deep Optimal Sensor Placement for Black Box Stochastic Simulations

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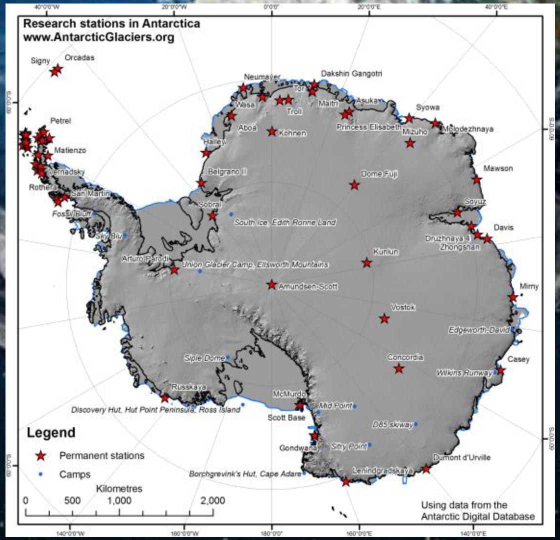

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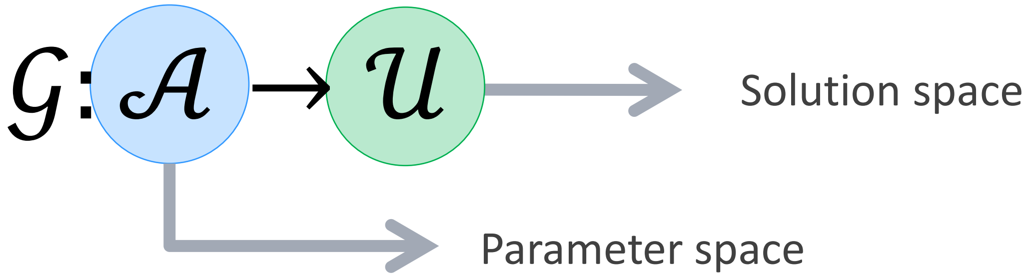
Lenindgradskaya
Legend
Permanent stations
Camps
Kilometres
0 500 1,000 2,000
Using data from the
Antarctic Digital Database

PROBLEM FORMULATION

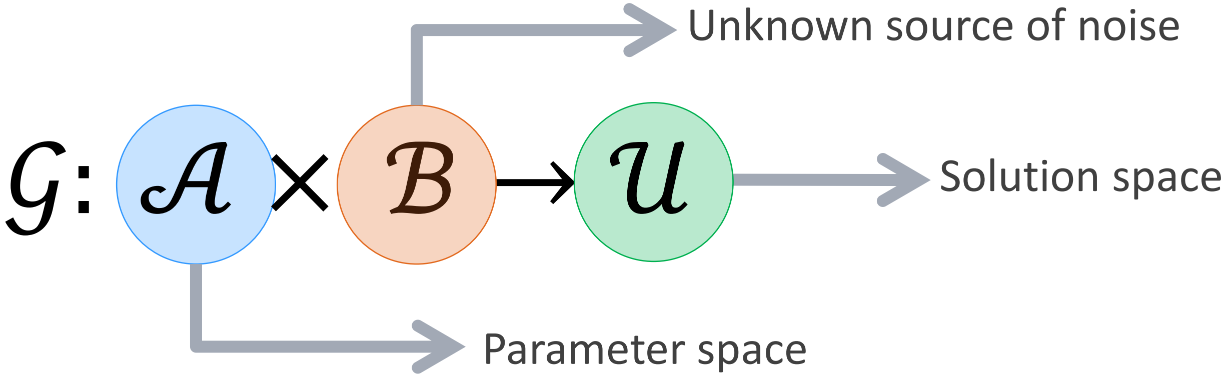
Consider a partial differential equation (PDE) model



Example: Poisson equation $\nabla u = a$. Given the functional parameter a, we compute the corresponding solution u.

PROBLEM FORMULATION

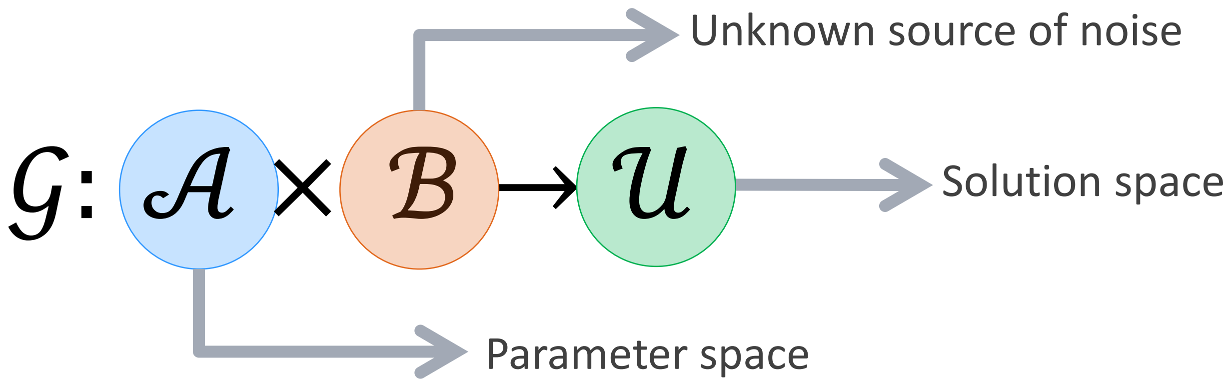
We go further and consider possibly stochastic PDEs



Example: Darcy flow $-\nabla \cdot (a(x)\nabla u(x)) = f(x) + \xi$, where ξ denotes space white noise. In this case, $u = \mathcal{G}_\xi(a)$.

PROBLEM FORMULATION

We will try to solve **inverse problems**



Given noisy observations of the sPDE solution $y_i = \mathcal{G}_\xi(a)(\boldsymbol{x}_i) + \eta_i$, **we want to infer $\boldsymbol{a}$**

In our scenario, η_i follows a standard Gaussian distribution. That is, $\eta_i \sim \mathcal{N}(0, \sigma^2)$.

PROBLEM FORMULATION

We will try to solve **inverse problems**

Unknown source of noise

$$\mathcal{G}: \mathcal{A} \times \mathcal{B} \rightarrow \mathcal{U}$$

Solution space

Parameter space

We take a Bayesian approach

Given noisy observations of the sPDE solution $y_i = \mathcal{G}_\xi(a)(\boldsymbol{x}_i) + \eta_i$, **we want to infer $\boldsymbol{a}$**

In our scenario, η_i follows a standard Gaussian distribution. That is, $\eta_i \sim \mathcal{N}(0, \sigma^2)$.

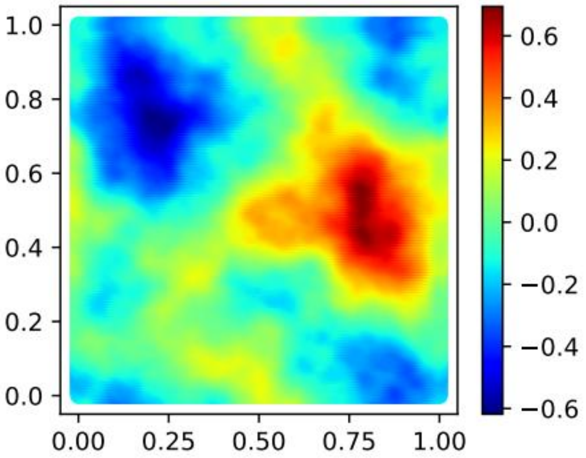
PROBLEM FORMULATION

An important challenge is sensor placement

What does this mean? Determine measurement positions $\boldsymbol{x}$ that yield the most information about the solution u and the functional parameter a.

Recall that we measure noisy observations of the sPDE solution $y_i = \mathcal{G}_\xi(a)(\boldsymbol{x}_i) + \eta_i$ at different points $\boldsymbol{x}_i$ to infer the solution and the parameter a. We want to choose the sensor locations $\boldsymbol{x}_i$ in an optimal way.

OUR OBJECTIVE: learn the initial parameter + optimise sensor locations



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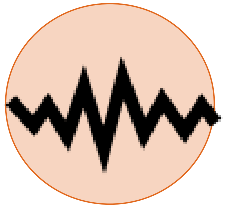
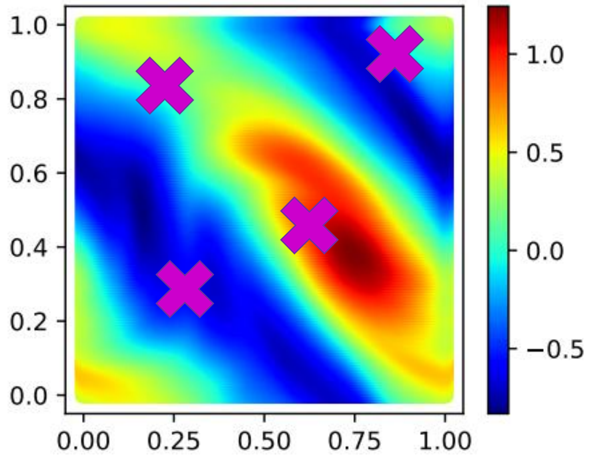




Based on measurements of the solution by different sensors

How do we choose to obtain the maximum amount of information?

Infer the initial parameter

CHALLENGES

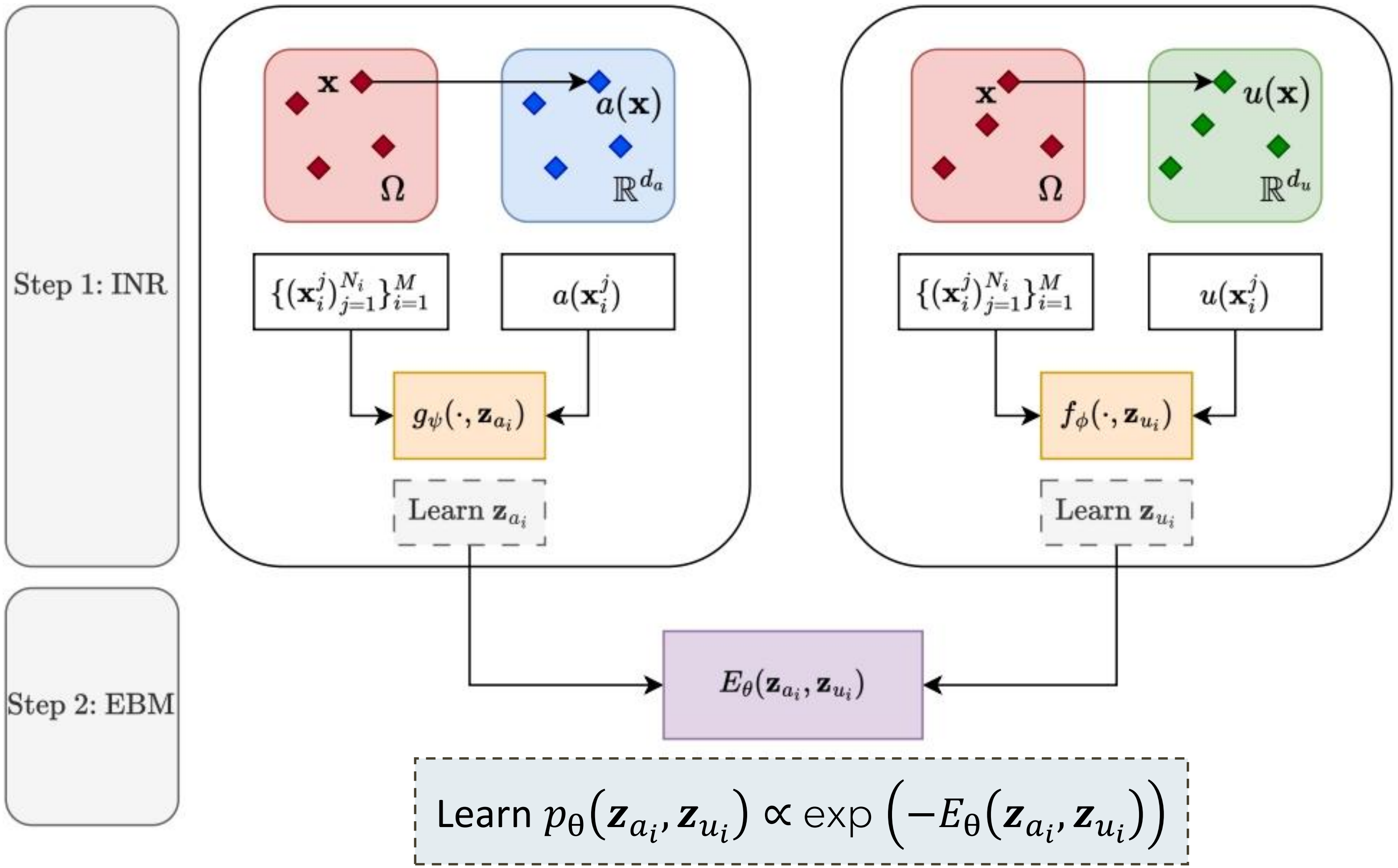
- Possibly stochastic operator $\mathcal{G}$
- Functional form parameter and solution
- Resolution invariant method
- Computationally efficient

SOLUTION

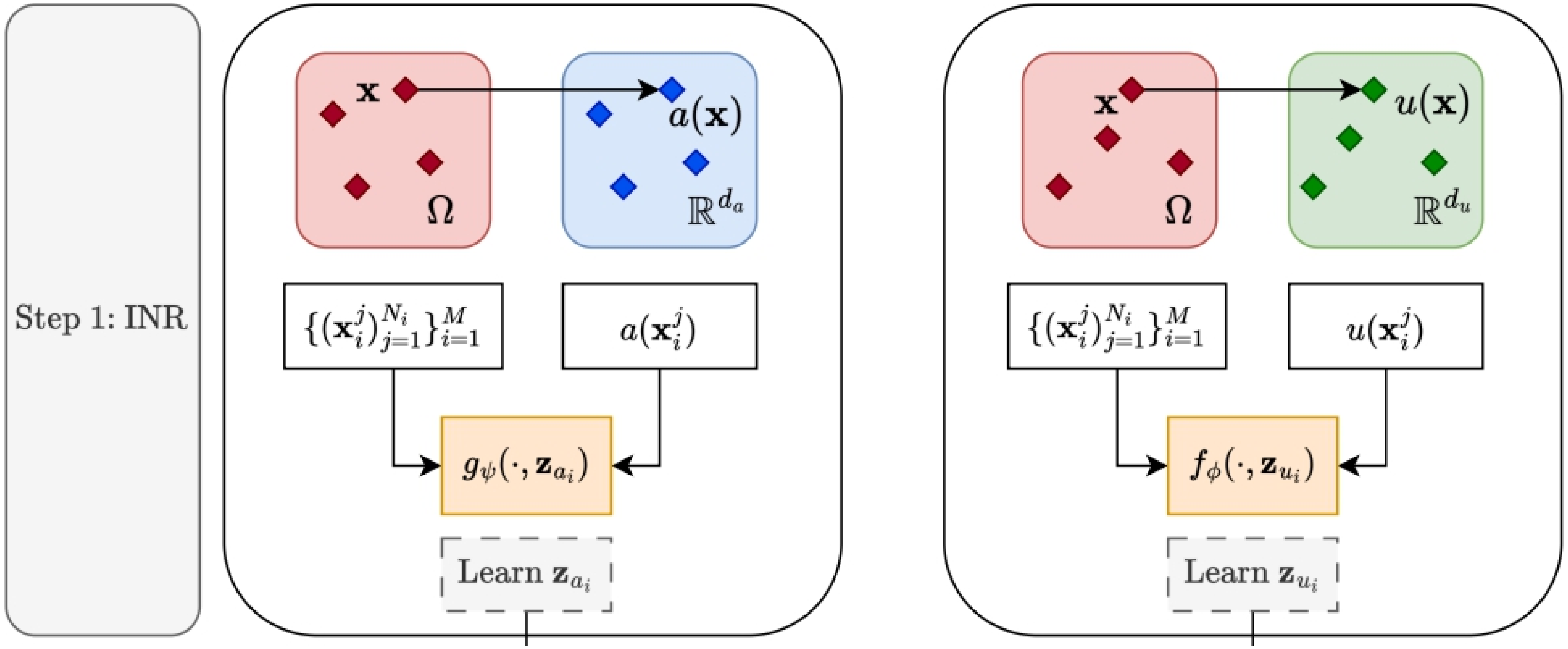
Learn a **generative model** $\boldsymbol{p_{\theta}}$ for the joint distribution over parameters and PDE solutions $(a\ , u = \mathcal{G}(a))$.

This provides a **surrogate method** which allows for complex probabilistic relationship and that is **not dependent on a fixed discretisation** of the domain.

TRAINING WORKFLOW



IMPLICIT NEURAL REPRESENTATIONS



- Shared weights among all functions in the dataset and particular weights for each function.
- Train them using an outer-inner optimisation loop to minimise the MSE.
- Very low reconstruction error.

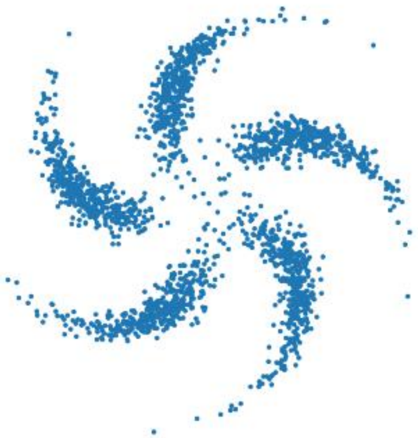
ENERGY-BASED MODELS

Learn $p_\theta(\boldsymbol{z}_{a_i}, \boldsymbol{z}_{u_i}) \propto \exp\left(-E_\theta(\boldsymbol{z}_{a_i}, \boldsymbol{z}_{u_i})\right)$

Energy Function (Neural Network)

Energy-Based Models (LeCun, 2006)

Data

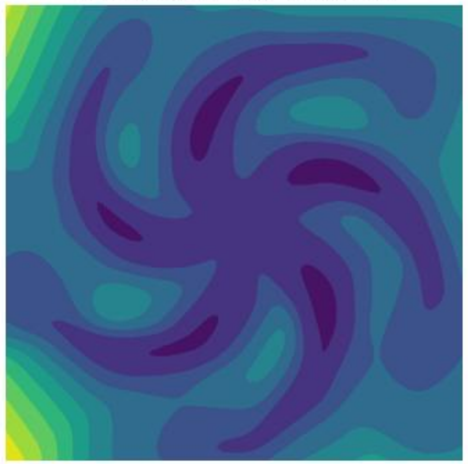


$\mathbf{x}^i \overset{i.i.d.}{\sim} p_{\text{data}}$

Model distribution

$$p_\theta(\mathbf{x}) = \frac{\exp(-U_\theta(\mathbf{x}))}{Z_\theta}$$

Learned Energy Function



$U_\theta(\mathbf{x})$

Intractable normalisation (partition function): $Z_\theta = \int \exp(-U_\theta(\mathbf{x}))\mathrm{d}\mathbf{x}$

ENERGY-BASED MODELS

Learn $p_\theta(\boldsymbol{z}_{a_i}, \boldsymbol{z}_{u_i}) \propto \exp\left(-E_\theta(\boldsymbol{z}_{a_i}, \boldsymbol{z}_{u_i})\right)$

- Training method:

Energy Discrepancy

Energy-Based distribution: $p(\mathbf{x}) \propto \exp(-U(\mathbf{x}))$

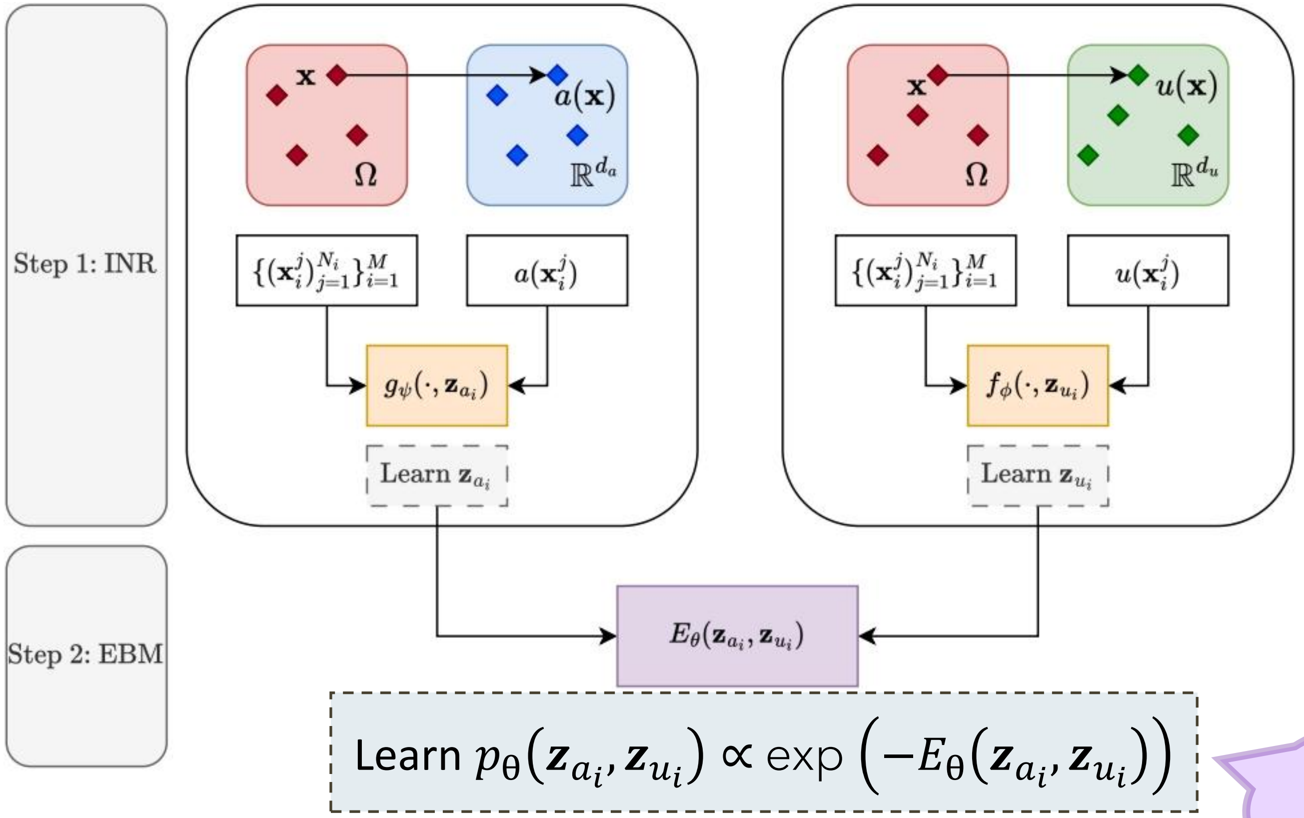
Conditional (noising) distribution: $q(\mathbf{y} \mid \mathbf{x})$

Contrastive potential: $U_q(\mathbf{y}) = -\log \int \exp(-U(\mathbf{x}))q(\mathbf{y} \mid \mathbf{x})\mathrm{d}\mathbf{x}$

$$\boxed{\mathrm{ED}_q(p_{\mathrm{data}}, p) := \mathbb{E}_{p_{\mathrm{data}}(\mathbf{x})}[U(\mathbf{x})] - \mathbb{E}_{p_{\mathrm{data}}(\mathbf{x})}\mathbb{E}_{q(\mathbf{y}|\mathbf{x})}[U(\mathbf{y})]}$$

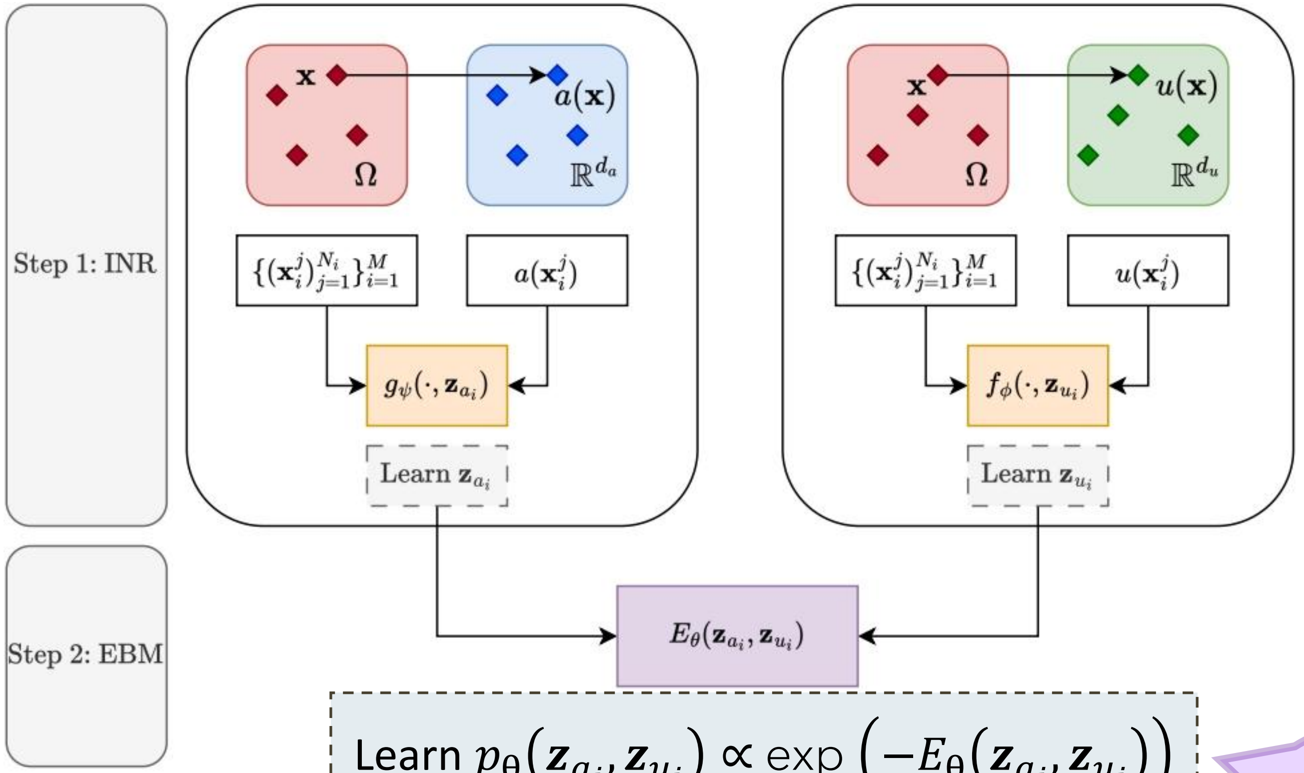
- Data processing inequality implies that $\mathrm{ED}_q(p_{data}, p) \geq 0$.
- Energy Discrepancy is functionally convex in U.
- For nice q, ED has a unique global minimiser at $\exp(-U^*) \propto p_{\mathrm{data}}$

INFERENCE FROM SPARSE OBSERVATIONS



Models distribution of latent representations

INFERENCE FROM SPARSE OBSERVATIONS

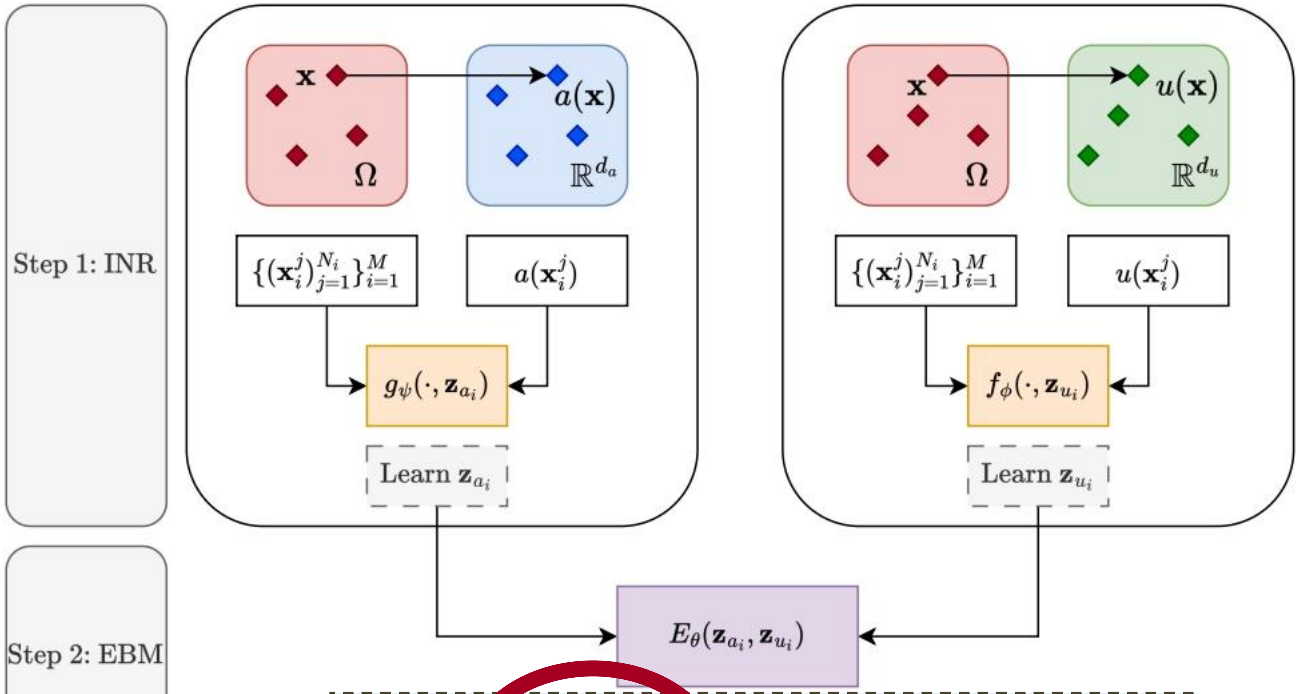


Learn $p_\theta(\mathbf{z}_{a_i}, \mathbf{z}_{u_i}) \propto \exp\left(-E_\theta(\mathbf{z}_{a_i}, \mathbf{z}_{u_i})\right)$

Models distribution of latent representations

It also provides a "prior" distribution for our problem

INFERENCE FROM SPARSE OBSERVATIONS



Learn $p_\theta(\boldsymbol{z}_{a_i}, \boldsymbol{z}_{u_i}) \propto \exp\left(-E_\theta(\boldsymbol{z}_{a_i}, \boldsymbol{z}_{u_i})\right)$

Allows uncertainty quantification

$$p(\boldsymbol{z}_a, \boldsymbol{z}_u | \mathcal{D}) \propto p(\mathcal{D} | \boldsymbol{z}_a, \boldsymbol{z}_u) p_\theta(\boldsymbol{z}_a, \boldsymbol{z}_u)$$

Bayes rule

OPTIMAL SENSOR PLACEMENT

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?

We need to define what is a good placement position, that is, an utility function.

OPTIMAL SENSOR PLACEMENT

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

HOW?

Maximise utility of sensor placement positions

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

OPTIMAL SENSOR PLACEMENT

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

HOW?

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

In practice, we maximise the PCE bound

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

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.

OPTIMAL SENSOR PLACEMENT

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

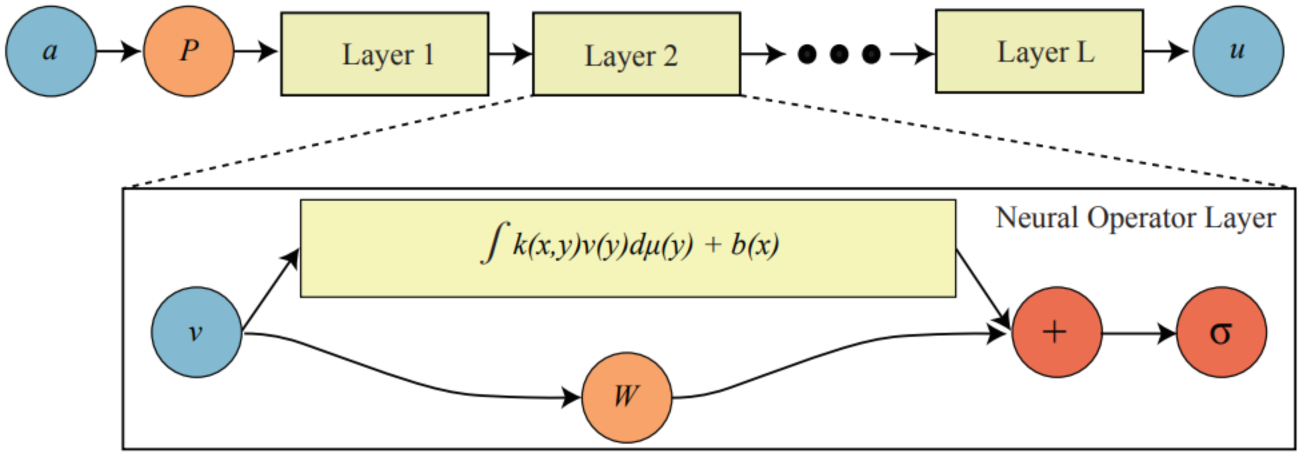
HOW TO DO THE SELECTION SEQUENTIALLY?

Considering the sequence of locations $\{\xi_1, \dots, \xi_{t-1}\}$ and outcomes $\{y_1, \dots, y_{t-1}\}$ up to step t, we maximise the utility given the history h_{t-1}

$$U(\xi_t | h_{t-1}) := \mathbb{E}\left[\log \frac{p(y | \mathbf{z}_a, \mathbf{z}_u, \xi_t, h_{t-1})}{p(y | \xi_t, h_{t-1})}\right]$$

BENCHMARK ALGORITHMS

- **Neural Operator Surrogate:** It can only learn deterministic maps. Therefore, it fails to incorporate the effect that a spatio-temporal external random signal has on the system described.



- **Neural Operator Surrogate With Noise Oracle** (Ideal setting not realistic): Takes as the driving noise of the stochastic model

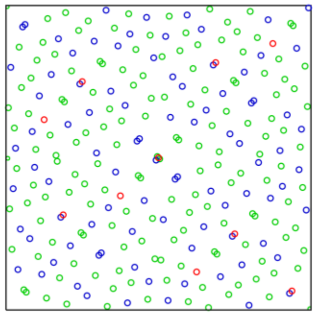
ALTERNATIVE METHODS

Methods	Direct PDE solves	Neural Operator surrogate	Neural Operator surrogate with oracle noise	Functional Neural Coupling (ours)
Low-cost evaluation	✗	✓	✓	✓
Low-cost inversion	✗	✓	✓	✓
Supports sensor placement pipeline	✓	✓	✓	✓
Supports stochastic PDEs	✓	✗	✓	✓
Tractable likelihood	✗	✗	✗	✓

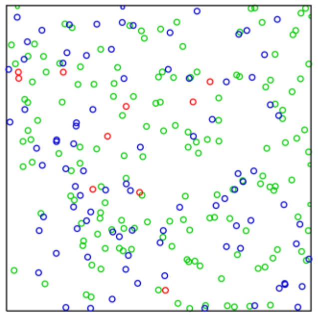
NUMERICAL EXAMPLES

- Our training data consists of M pairs of parameters and their corresponding solutions, $\{a_i,\ u_i\}_{i=1,\dots,M}$. We assume access to only N_i point observations for each of them, where the set of N_i locations varies across the M function realisations and need not be the same for a and u.
- PDE solutions are only required to train the INR and EBM models. Once trained, these models are reused for inference leading to high savings in terms of computational cost.
- For each method (ours and benchmarks) we compare optimal sensor placement against a quasi-Monte Carlo sequence

QMC



Uniform



NUMERICAL EXPERIMENTS

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

Boundary conditions $u(-1) = X_a \sim N(a, 0.3^2), u(1) = X_b \sim Unif(b - 0.3, b + 0.4)$
Training data: a, b and observations of solution for a realisation of X_a, X_b

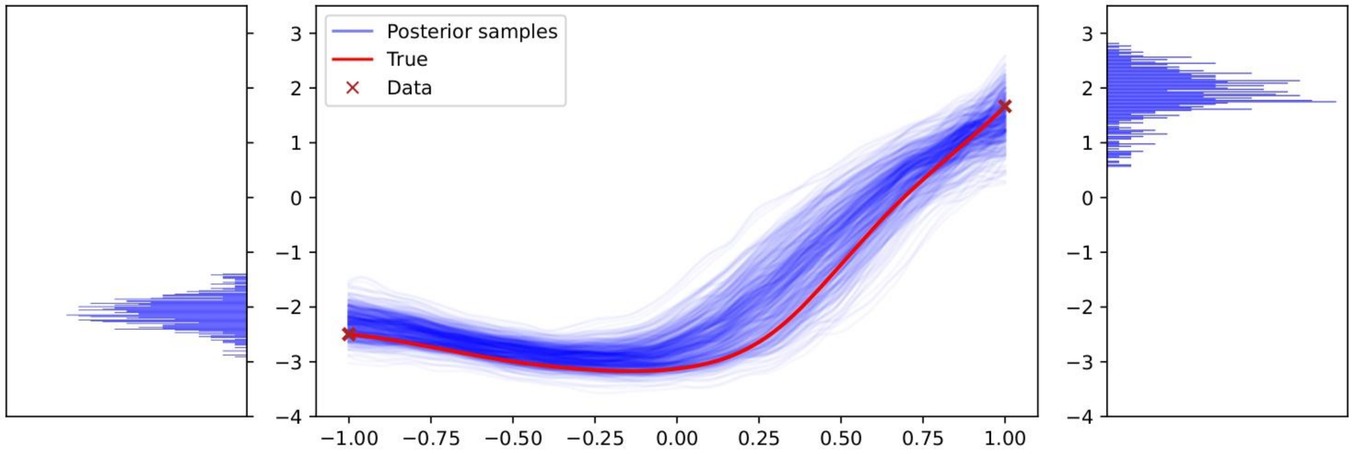
TO-DO

Perform inference on a, b based on 2 sparse observations of solution

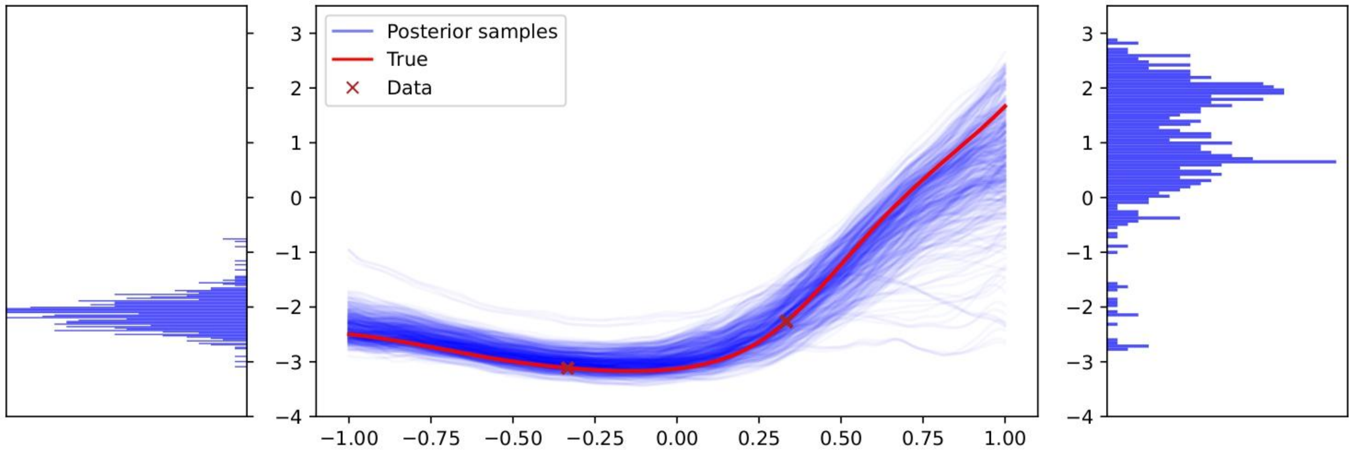
Method	Design points	$\|\widehat{u} - u_{\text{tr}}\|^2/\|u_{\text{tr}}\|^2$	MSE($\hat{a}$)	MSE($\hat{b}$)
Functional Neural Coupling (Ours)	Adaptive BED	0.124 ± 0.101	0.135 ± 0.099	1.441 ± 1.003
	Batch non-adaptive BED	$\mathbf{0.097 \pm 0.081}$	$\mathbf{0.103 \pm 0.193}$	$\mathbf{1.074 \pm 0.906}$
	Random sequence	0.331 ± 0.259	0.476 ± 0.888	4.162 ± 3.885
FNO surrogate (Li et al., 2021)	Adaptive BED	0.137 ± 0.308	0.441 ± 1.337	1.224 ± 2.084
	Batch non-adaptive BED	0.125 ± 0.255	0.428 ± 1.239	1.111 ± 1.785
	Random sequence	0.251 ± 0.507	0.484 ± 0.947	3.839 ± 7.457
FNO w/ oracle noise surrogate (Salvi et al., 2022)	Adaptive BED	0.116 ± 0.250	$\underline{0.021 \pm 0.058}$	1.580 ± 2.888
	Batch non-adaptive BED	$\underline{0.090 \pm 0.131}$	0.041 ± 0.105	$\underline{1.046 \pm 1.620}$
	Random sequence	0.356 ± 0.613	0.494 ± 1.412	8.372 ± 11.856

NUMERICAL EXPERIMENTS

Boundary value problem in 1D:



Batch non-adaptive



Sobol points

NUMERICAL EXPERIMENTS

Steady-state diffusion in 2D: $-\nabla \cdot \left(\kappa(x)\nabla u(x)\right) = f(x) + \alpha\omega$

Learn functional diffusion coefficient κ generated as the push-forward of a Gaussian random field. $f(x) = 0.5$ and ω is space white noise

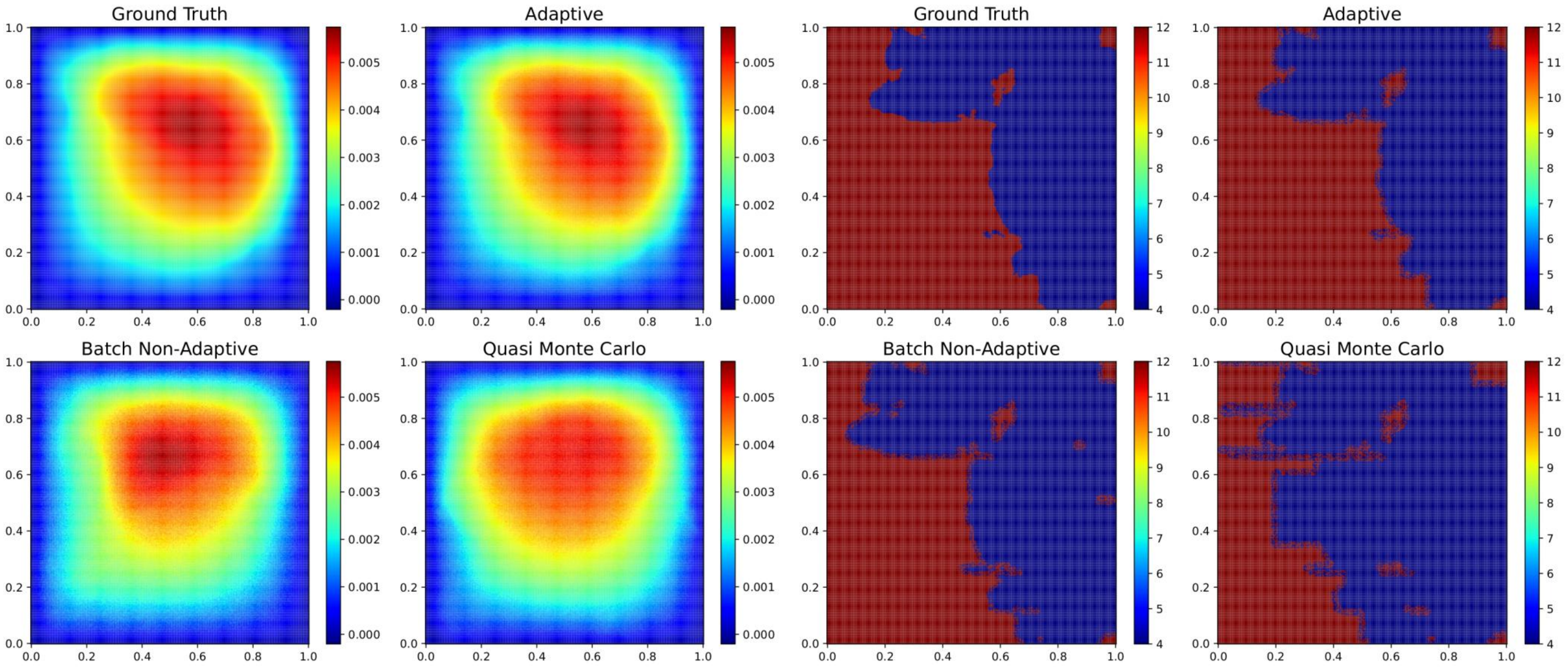
TO-DO

Based on 5 initial observations ✖ , find optimal locations ✖ for 15 additional measurement sites

Method	Design points	$\\|\log\widehat{\kappa} - \log\kappa_{\mathrm{tr}}\\|^2/\\|\log\kappa_{\mathrm{tr}}\\|^2$	$\\|\widehat{u} - u_{\mathrm{tr}}\\|^2/\\|u_{\mathrm{tr}}\\|^2$
Functional Neural Coupling (Ours)	Adaptive BED	$\mathbf{0.234 \pm 0.078}$	$\mathbf{0.102 \pm 0.083}$
	Batch non-adaptive BED	0.337 ± 0.091	0.192 ± 0.087
	Quasi-Monte Carlo sequence	0.711	0.328
FNO surrogate (Li et al., 2021)	Adaptive BED	0.306 ± 0.130	0.117 ± 0.106
	Batch non-adaptive BED	0.551 ± 0.172	0.220 ± 0.118
	Quasi-Monte Carlo sequence	1.182	0.379
FNO w/ oracle noise surrogate (Salvi et al., 2022)	Adaptive BED	$\underline{0.155 \pm 0.101}$	$\underline{0.093 \pm 0.089}$
	Batch non-adaptive BED	$\underline{0.291 \pm 0.089}$	$\underline{0.124 \pm 0.110}$
	Quasi-Monte Carlo sequence	0.459	0.255

NUMERICAL EXPERIMENTS

Steady-state diffusion in 2D:



Solutions

Diffusion coefficient

NUMERICAL EXPERIMENTS

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

Learn initial vorticity $\omega_0(x) = \omega(x,0)$ generated according to a Gaussian random field with periodic boundary conditions. $f(x)$ is the deterministic forcing function and ε is the stochastic forcing function

TO-DO

We learn a Functional Neural Coupling between the initial vorticity ω_0 and the vorticity at times $t = 1, 2, 3$.
Find optimal locations for 15 measurements sites of the vorticity based on 5 initial observations.

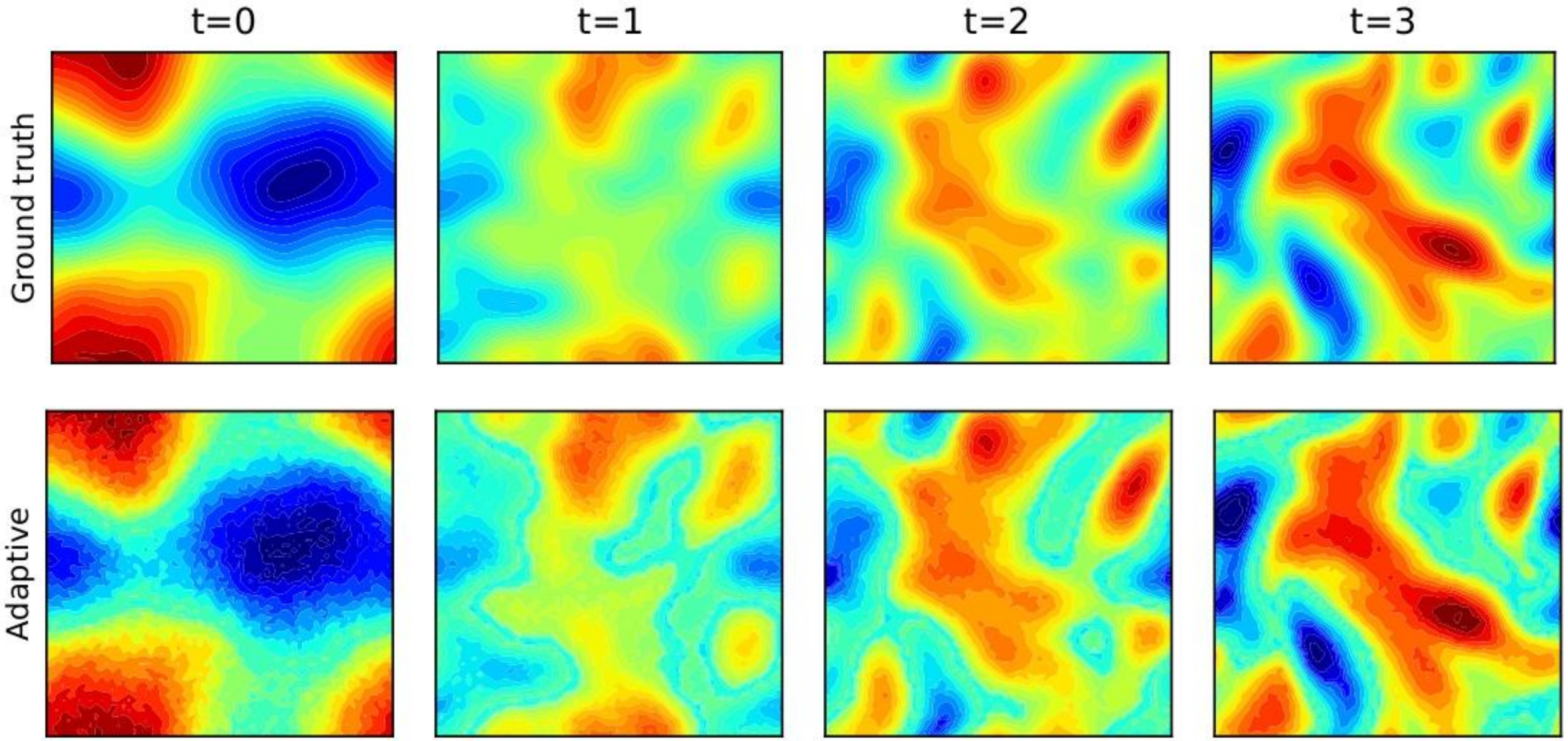
NUMERICAL EXPERIMENTS

Navier Stokes equation:

Method	Design points	$\|\widehat{w}_0 - w_{\mathrm{tr},0}\|^2 / \|w_{\mathrm{tr},0}\|^2$	$\|\underline{\widehat{w}}_t - \underline{w}_{\mathrm{tr},t}\|^2 / \|\underline{w}_{\mathrm{tr},t}\|^2$
	Adaptive BED	$\mathbf{0.293 \pm 0.077}$	$\mathbf{0.175 \pm 0.091}$
Functional Neural Coupling (Ours)	Batch non-adaptive BED	0.321 ± 0.083	0.239 ± 0.090
	Quasi-Monte Carlo sequence	0.578	0.422
FNO surrogate	Adaptive BED	0.382 ± 0.067	0.242 ± 0.095
(Li et al., 2021)	Batch non-adaptive BED	0.454 ± 0.092	0.288 ± 0.089
	Quasi-Monte Carlo sequence	0.652	0.576
FNO w/ oracle noise surrogate	Adaptive BED	$\underline{0.221 \pm 0.065}$	$\underline{0.103 \pm 0.079}$
(Salvi et al., 2022)	Batch non-adaptive BED	$\underline{0.301 \pm 0.080}$	$\underline{0.169 \pm 0.083}$
	Quasi-Monte Carlo sequence	0.454	0.332

NUMERICAL EXPERIMENTS

Navier Stokes equation:



LIMITATIONS

Limitations:

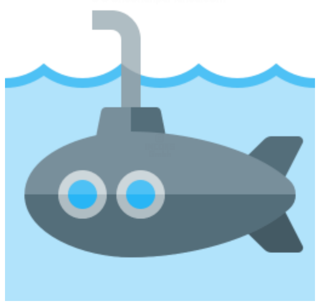
- Assumption that the density of the parameter-solution pairs is positive everywhere might be restrictive. For example, only a few parameter choices lead to stable behaviour of the system.
- EBM will not necessarily generalise to parts of the space not covered by the prior from which a was sampled. Therefore, we need to carefully choose training data.

Future work:

- Study sequential strategies that use the observation data more effectively for fine-tuning the base EBM. Generating more data as needed.

MORE FUTURE WORK

❓ If we have different sensors and some of them provide better measurements than others, how do we place them?



What if we have to select not a set of sensor points ✖️ but the route that a submarine follows to take measurements?

CONCLUSIONS

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 sensor placement in inverse PDE problems avoiding costly MCMC methods** with runtimes of days vs minutes for our approach.