Discovering and forecasting extreme events via active learning in neural operators

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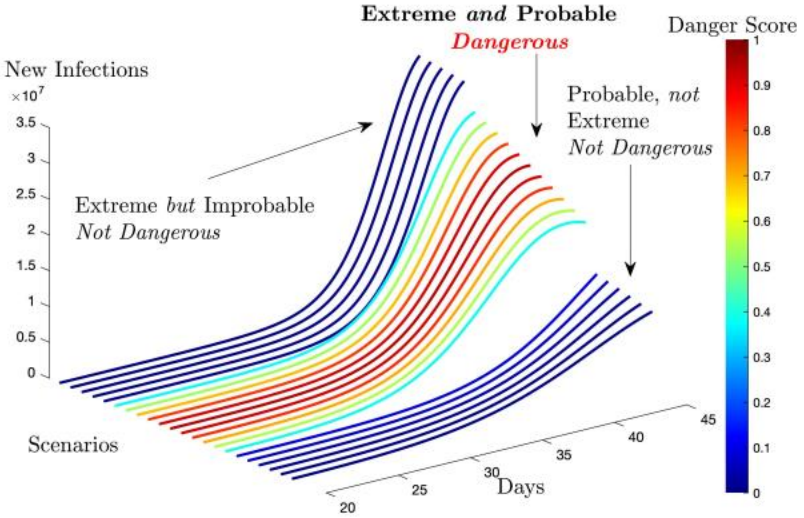
Extreme Phenomena

SIR

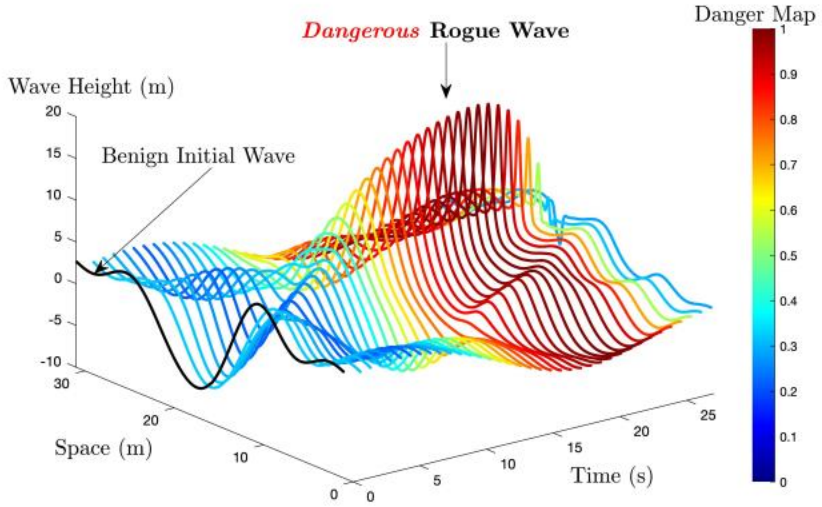
MMT

LAMP

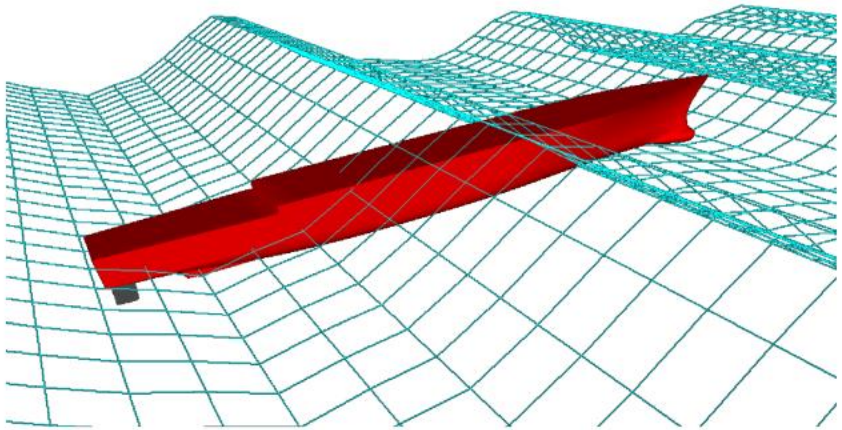
a) Pinpoint Dangerous Pandemic Spikes



b) Discover and Predict Rogue Ocean Waves



c) Estimate Peak Structural Ship Stress



$$\frac{\mathrm{d}S}{\mathrm{d}t} = -\beta IS + \delta R$$
$$\frac{\mathrm{d}I}{\mathrm{d}t} = \beta IS - \gamma I$$
$$\frac{\mathrm{d}R}{\mathrm{d}t} = \gamma I - \delta R,$$

$$iu_t = |\partial_x|^{\alpha} u + \lambda |\partial_x|^{-\beta/4} \left(\left| |\partial_x|^{-\beta/4} u \right|^2 |\partial_x|^{-\beta/4} u \right) + iDu,$$

Deep Neural Operator

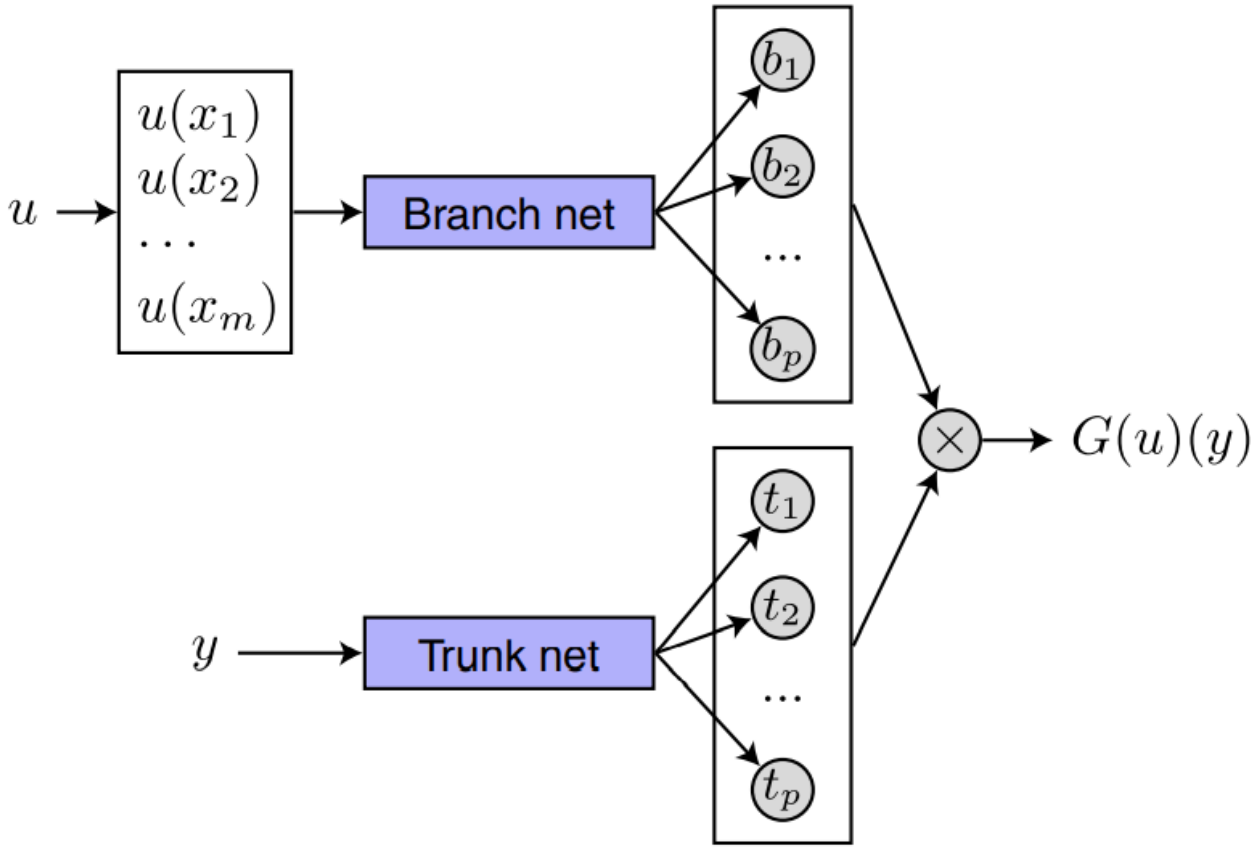
FNN: $x \rightarrow U(x)$

Neural Operator: $u(x) \rightarrow U(x)$

DeepONet

Universal Approximation Theorem for Operator

$$| G(u)(z) - \langle \underbrace{\mathbf{g}\left(u\left(x_1\right), u\left(x_2\right), \cdots, u\left(x_m\right)\right)}_{\text{branch}}, \underbrace{\mathbf{f}(z)}_{\text{trunk}} \rangle | < \epsilon.$$



DeepONet

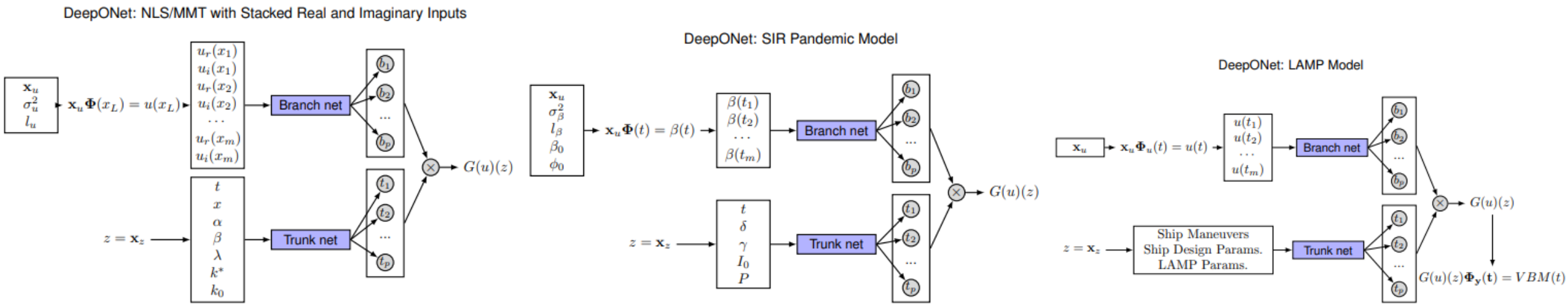
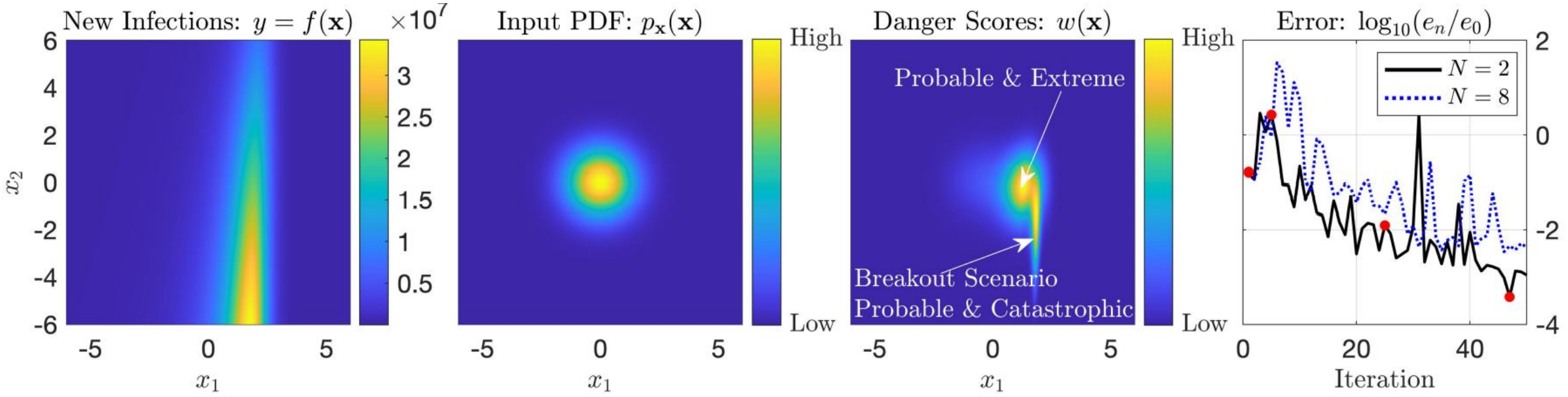


Figure 8: **The application of the MMT, SIR, and LAMP operators to DeepONet.**

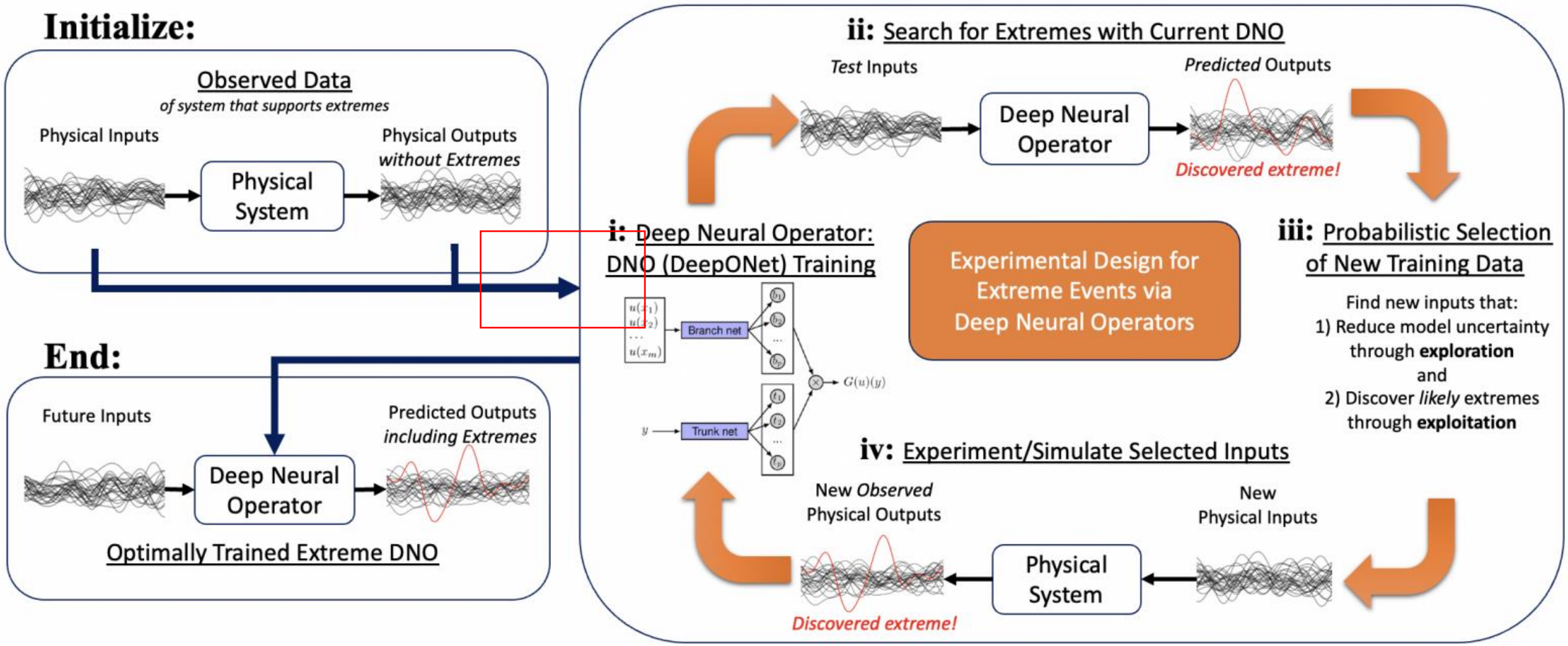
Method

Goal: accurately quantify the probability distribution function (PDF) of a stochastic quantity of interest (QoI), y

The variable y results from an observed random variable input, x, that is transformed by the underlying system or map, y = G(x).



DNO+BED Framework



DNO+BED Framework

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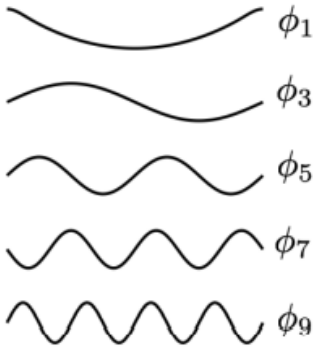
I. Stochastic Process

u

II. Parameterize

$$u = \sum_{i=1}^{D} x_i \phi_i = \mathbf{x}\mathbf{\Phi}$$



III. Map

GP Approach

Parameter Mapping to QoI

$$\mathbf{x} \rightarrow \tilde{G}_{\mathrm{GP}}(\mathbf{x}) \approx y$$

DNO Approach

Functional Mapping to QoI

$$u = \mathbf{x}\mathbf{\Phi} \rightarrow \tilde{G}_{\mathrm{DNO}}(u = \mathbf{x}\mathbf{\Phi}) \approx y$$

1. Different Mapping

$$\tilde{G}_{\mathrm{GP}} \neq \tilde{G}_{\mathrm{DNO}}$$

2. Both Learn via $\mathbf{x}$

3. DNO Leverages Basis Information: $\mathbf{\Phi}$

Active Learning

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Algorithm 1 Sequential search for active learning/training of DNOs and GPs .

Input: Number of iterations: n_{iter}

Initialize: Train GP/DNO on initial dataset of input-output pairs

GP: $\mathcal{D}_0 = \{\mathbf{x}_i, y_i = G(\mathbf{x}_i)\}_{i=1}^{n_{\text{init}}}$ DNO: $\mathcal{D}_0 = \{\mathbf{x}_i, y_i = G(\mathbf{x}_{u,i}\mathbf{\Phi}(x_1, ...x_m), \mathbf{x}_{z,i})\}_{i=1}^{n_{\text{init}}}$

for $n = 1$ **to** n_{iter} **do**

Select next sample $\mathbf{x}_n$ by maximizing* acquisition function $a(\mathbf{x})$:

*Maximization using Monte Carlo, See Section 4.4 and Appendix G

$$\mathbf{x}_n = \arg\max_{\mathbf{x}\in\mathcal{X}} \ (a(\mathbf{x}; y), \mathcal{D}_{n-1})$$

Evaluate objective function at $\boldsymbol{x}_n$ and record y_n

Augment dataset: $\mathcal{D}_n = \mathcal{D}_{n-1} \cup \mathbf{x}_n, y_n$

Retrain GP/DNO.

end for

return Final GP/DNO Model

Ensemble of Neural Networks and Uncertainty Quantification

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train N randomly weight-initialized DNO models, each denoted as G˜ n

$$\sigma^2(u,z) = \frac{1}{(N-1)} \sum_{n=1}^{N} (\tilde{G}_n(u)(z) - \overline{\tilde{G}(u)(z)})^2$$

Acquisiton functions

1. $$a_{US}(\mathbf{x}) = \sigma^2(\mathbf{x}).$$

2. both highly uncertain and high magnitude

likelihood ratio $$w(\mathbf{x}) = \frac{p_{\mathbf{x}}(\mathbf{x})}{p_{\mu}(\mu(\mathbf{x}))}.$$ $$a_{US-LW}(\mathbf{x}) = w(\mathbf{x})\sigma^2(\mathbf{x})$$

Experiment Batching

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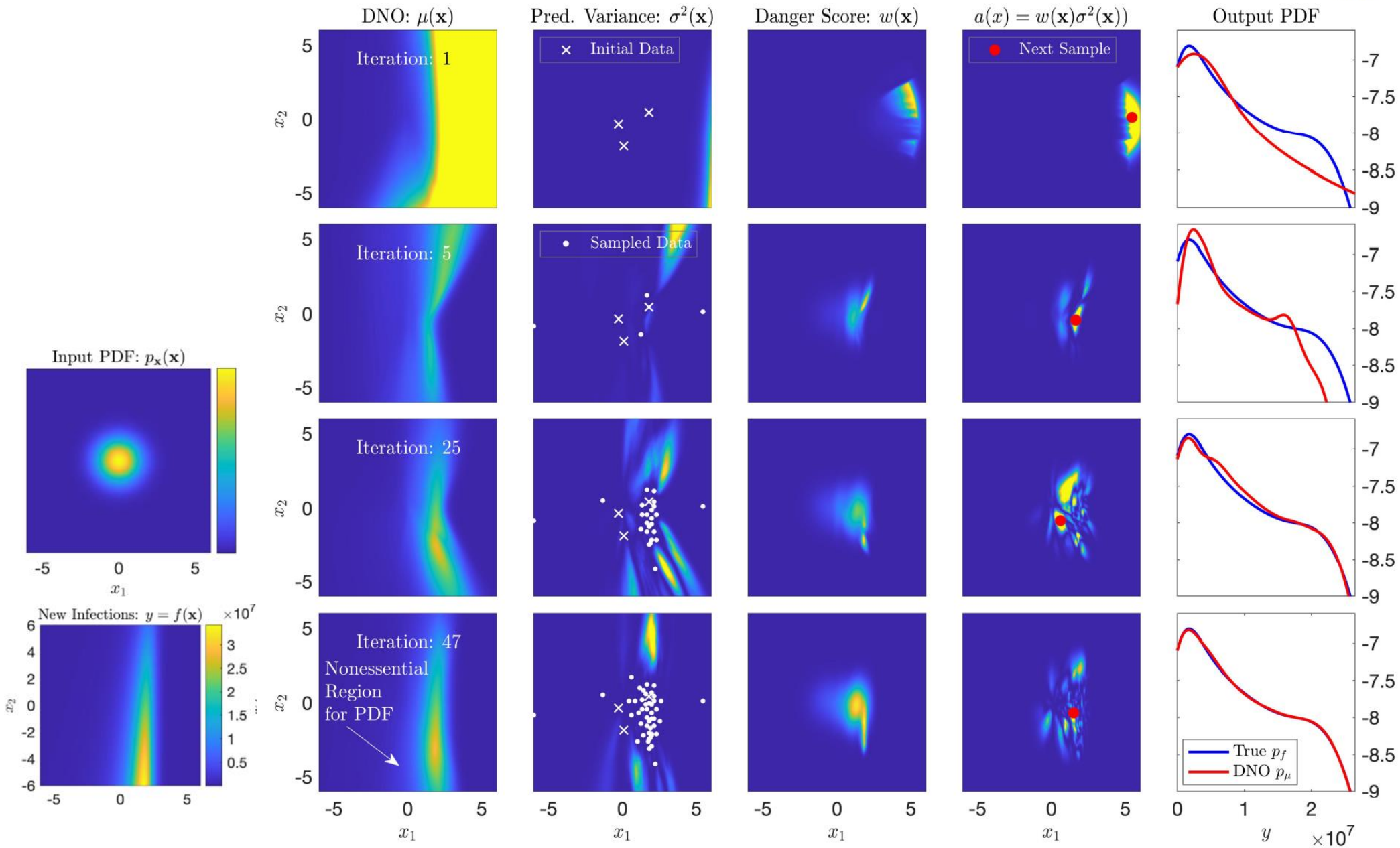
The purpose of batching is to find multiple regions of local optima of the acquisition function, rather than finding several optima in the same region.

Algorithm 2 Sequential selection of samples for batch sampling.

1: **Evaluate** acquisition function for n_q query points.
2: **for** Acquisition samples smaller than batch size $n_a < n_b$
3: **Choose** the maximum score, $\max(a) = a(\mathbf{x}_c)$, from n_q points.
4: **Augment** $\mathbf{x}_a$ with chosen point, $\mathbf{x}_c$.
5: **Compute** the distances, r, between the chosen point and the remaining query points.
6: **Eliminate** all samples from n_q where $r < r_{\min}$.
7: **end for**
8: **return** samples for the next experiment: $\mathbf{x}_a$

Danger Score Convergence in 50 Samples



Convergence

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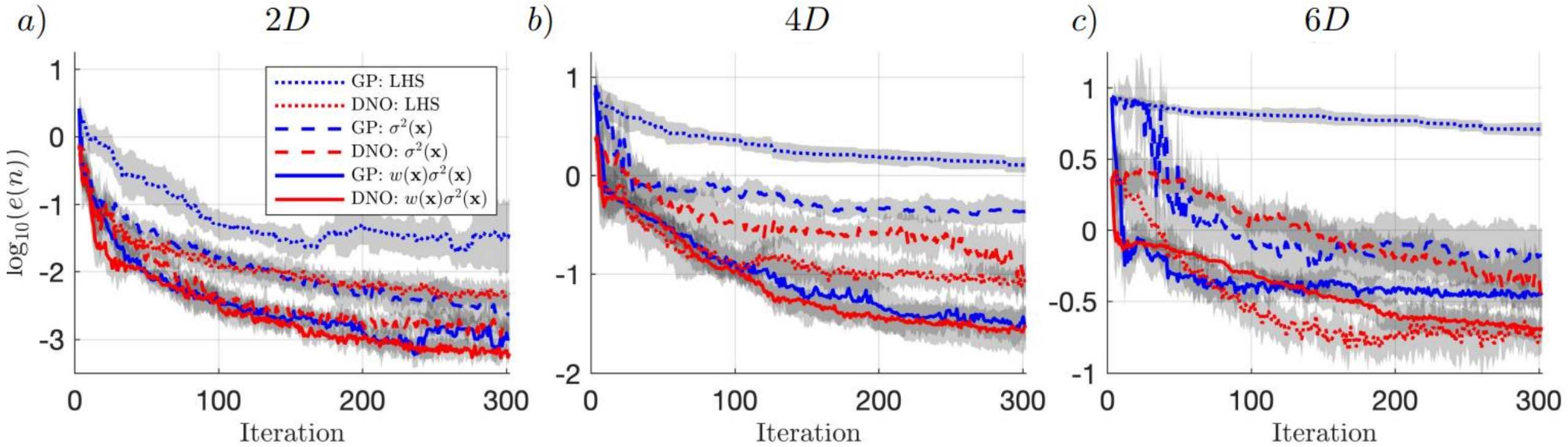
Accelerated convergence with DNOs plus extreme acquisition functions regardless of dimensionality

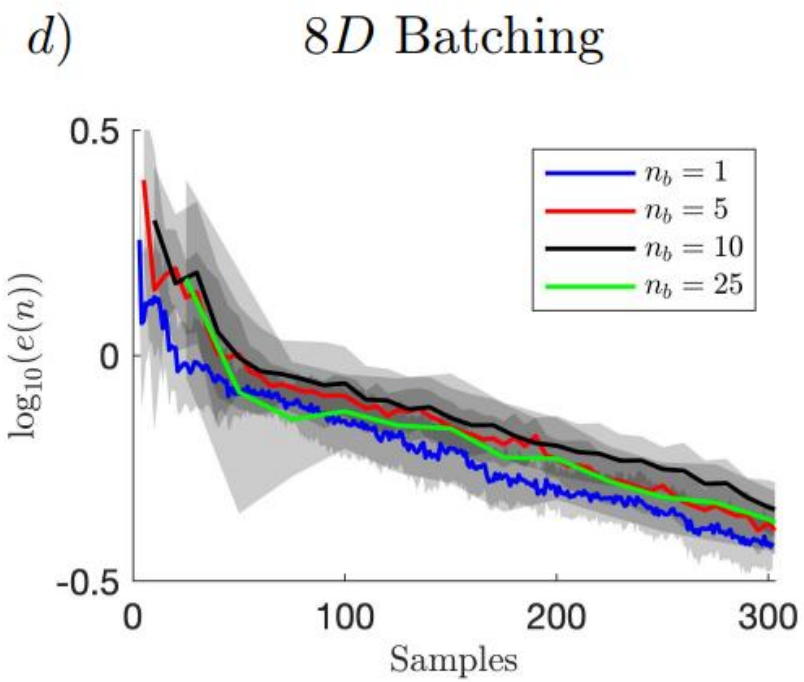
$$e(n) = \int |\log_{10} p_{\mu_n}(y) - \log_{10} p_G(y)| \mathrm{d}y.$$

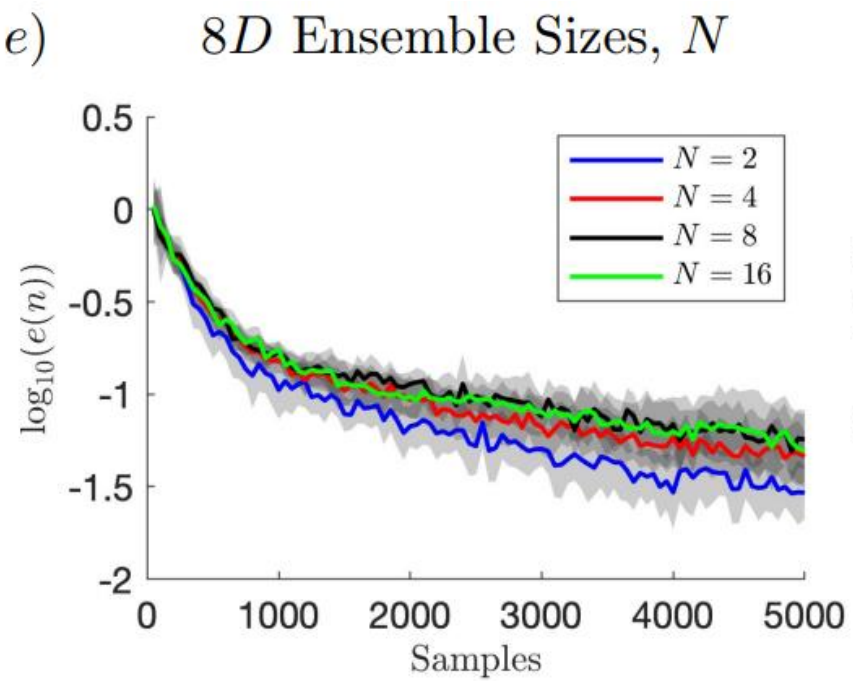
DNO ✓ w(x)σ2(x) ✓

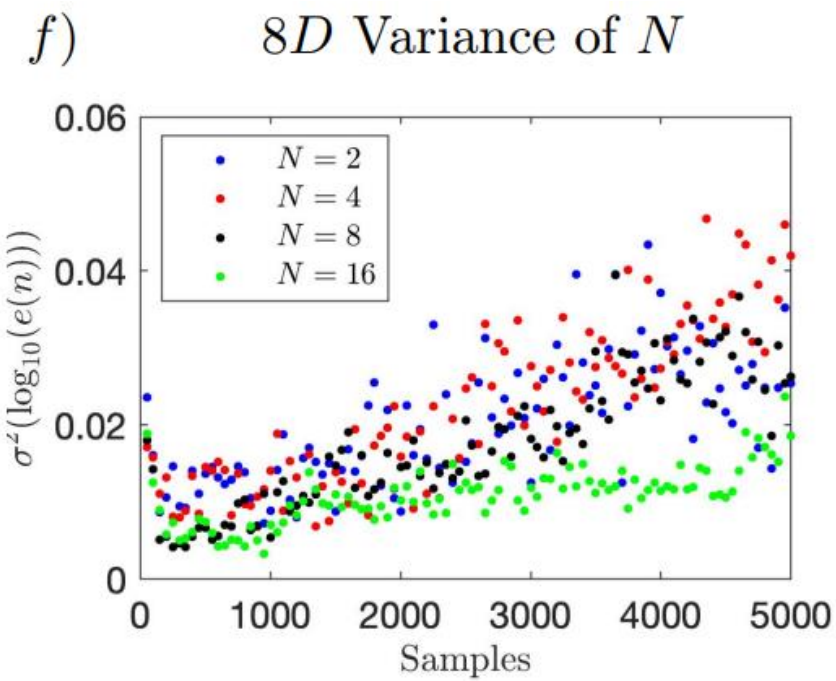


Convergence

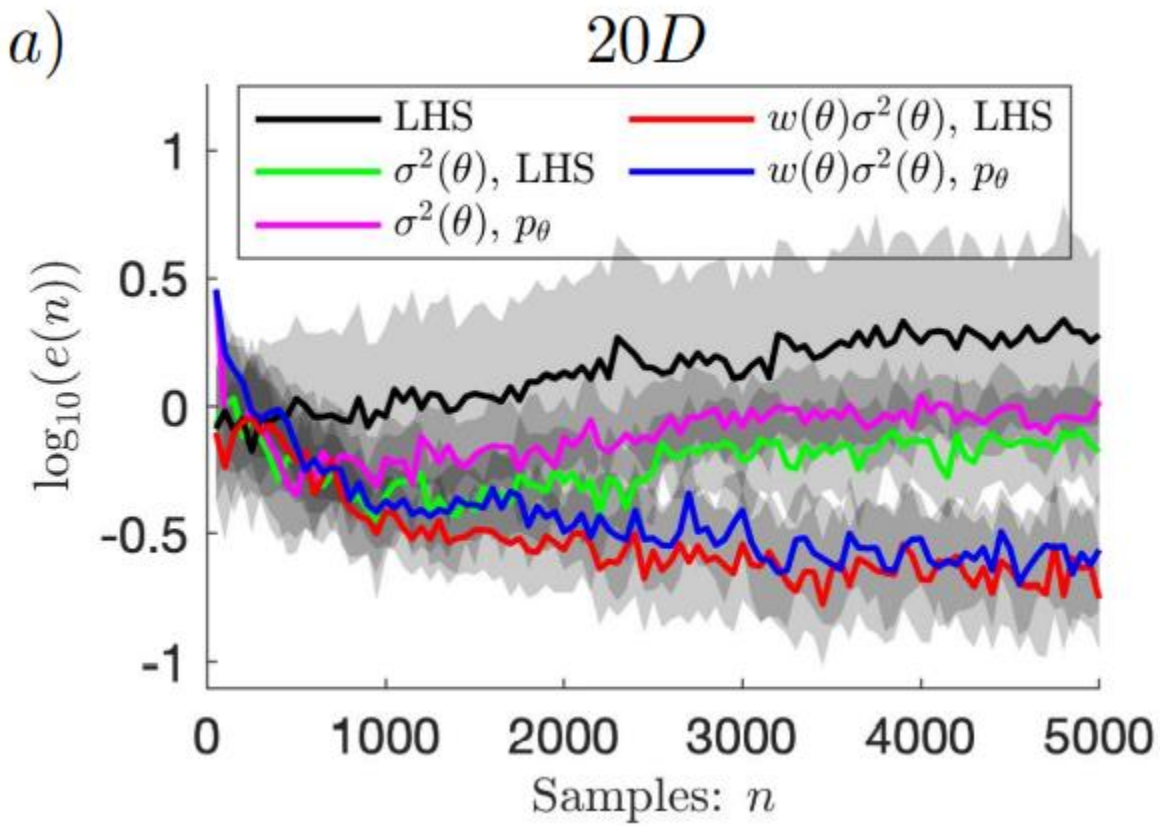
1. reducing computational cost in high dimensions
2. N=2 seems performs better, appears to disagree with the natural hypothesis (maybe use small N imposes a greedy search)
3. larger ensembles lead to a higher fidelity predictive variance

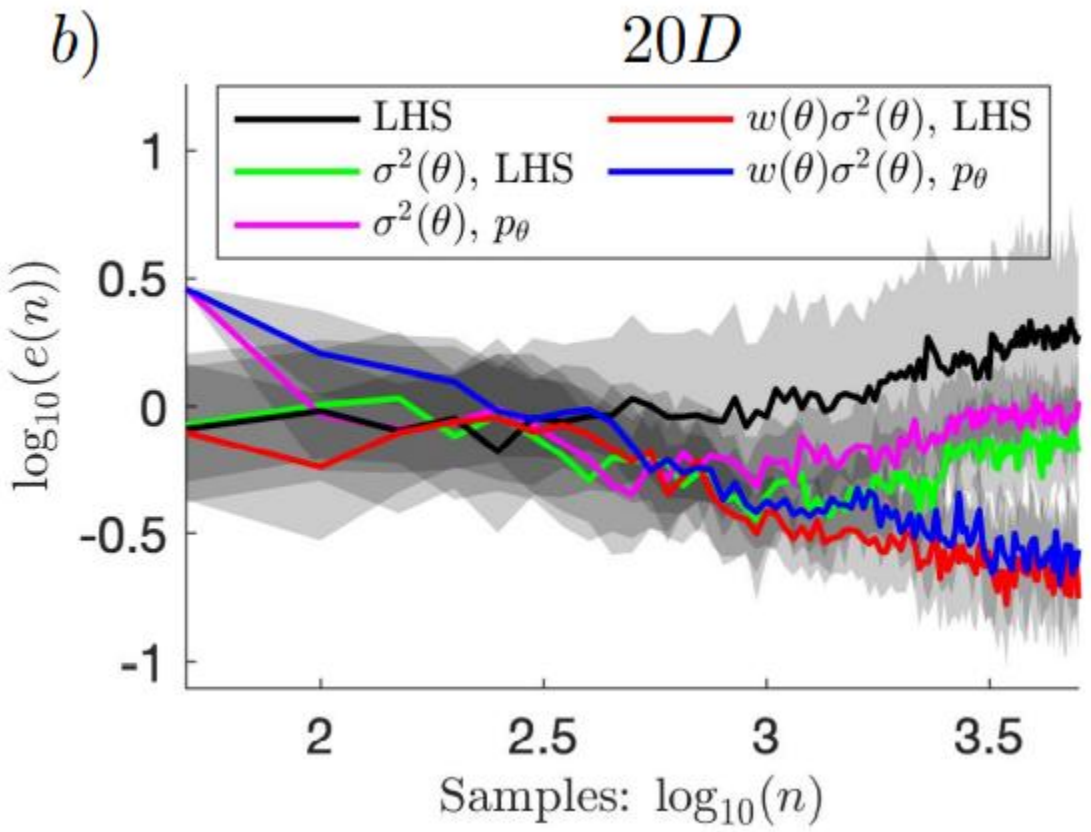






Robustness


a)
20D
LHS
$\sigma^2(\theta)$, LHS
$\sigma^2(\theta)$, p_θ
$w(\theta)\sigma^2(\theta)$, LHS
$w(\theta)\sigma^2(\theta)$, p_θ
$\log_{10}(e(n))$
1
0.5
0
-0.5
-1
0
1000
2000
3000
4000
5000
Samples: n


b)
20D
LHS
$\sigma^2(\theta)$, LHS
$\sigma^2(\theta)$, p_θ
$w(\theta)\sigma^2(\theta)$, LHS
$w(\theta)\sigma^2(\theta)$, p_θ
$\log_{10}(e(n))$
1
0.5
0
-0.5
-1
2
2.5
3
3.5
Samples: $\log_{10}(n)$

Thanks