Adaptive Sampling to Reduce Epistemic Uncertainty Using Prediction Interval-Generation Neural Networks

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Abstract

Extensive experimentation required for model accuracy can be costly and time-consuming. This paper presents an **adaptive sampling (AS) approach to reduce epistemic uncertainty in predictive models**. Our specific contributions are:

1. We introduce a novel metric based on NN-generated prediction intervals (PIs) to quantify potential levels of epistemic uncertainty.
2. We present **ASPINN (Adaptive Sampling with Prediction-Interval Neural Networks)**. At each iteration, it builds a Gaussian Process (GP) from calculated potential epistemic uncertainty levels. The GP, a surrogate for the NN models, estimates potential epistemic uncertainty changes across the domain after sampling specific locations. An acquisition function then uses the GP to select sampling locations to minimize the epistemic uncertainty throughout the input domain.

We test ASPINN on three 1-D synthetic problems and a dataset based on an agricultural field for selecting experimental fertilizer rates. The results demonstrate that our method consistently converges faster to minimum epistemic uncertainty levels.

Problem Definition

Given $\mathcal{D}_t = (\mathbf{X}^{(t)}_{obs}, \mathbf{Y}^{(t)}_{obs})$ at iteration t, a model $\hat{f}_t : \mathcal{X} \to \mathcal{Y}$ is trained.

- *Epistemic uncertainty* (reducible): Due to the "lack of knowledge" of $\hat{f}_t$ about the underlying function.
- *Aleatoric uncertainty* (irreducible): Due to the random nature of the data.
- **Objective:** Identify $\mathbf{X}^{(t)}_{acq} = \{\mathbf{x}_{t,1}, \dots, \mathbf{x}_{t,B}\}$, a batch of B recommended sampling locations for iteration $t+1$.
- $\mathbf{X}^{(t)}_{acq}$ is chosen to minimize the epistemic uncertainty across $\mathcal{X}$ (Fig. 1).

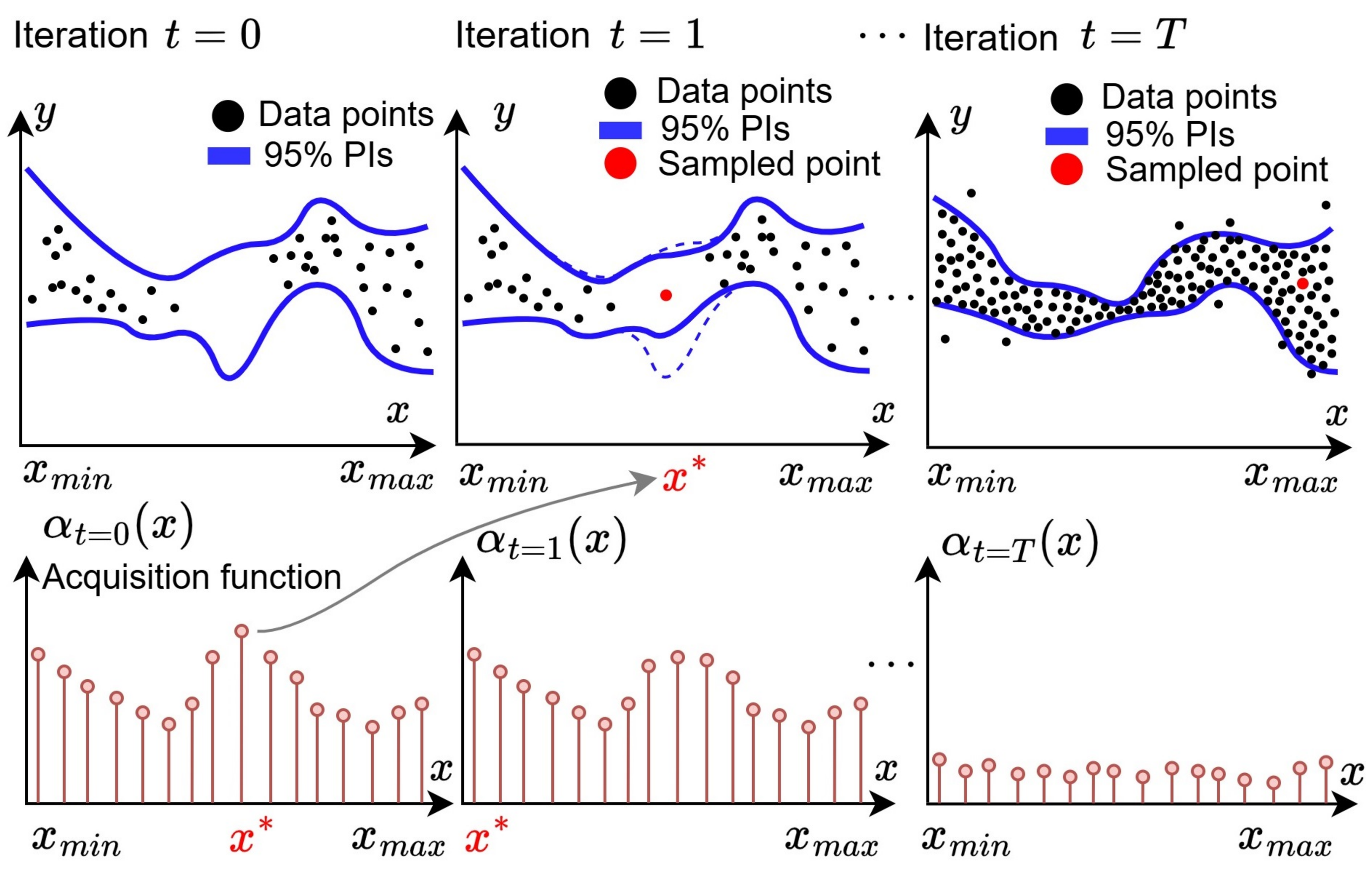

Figure 1. Epistemic uncertainty minimization through AS.

Potential Epistemic Uncertainty

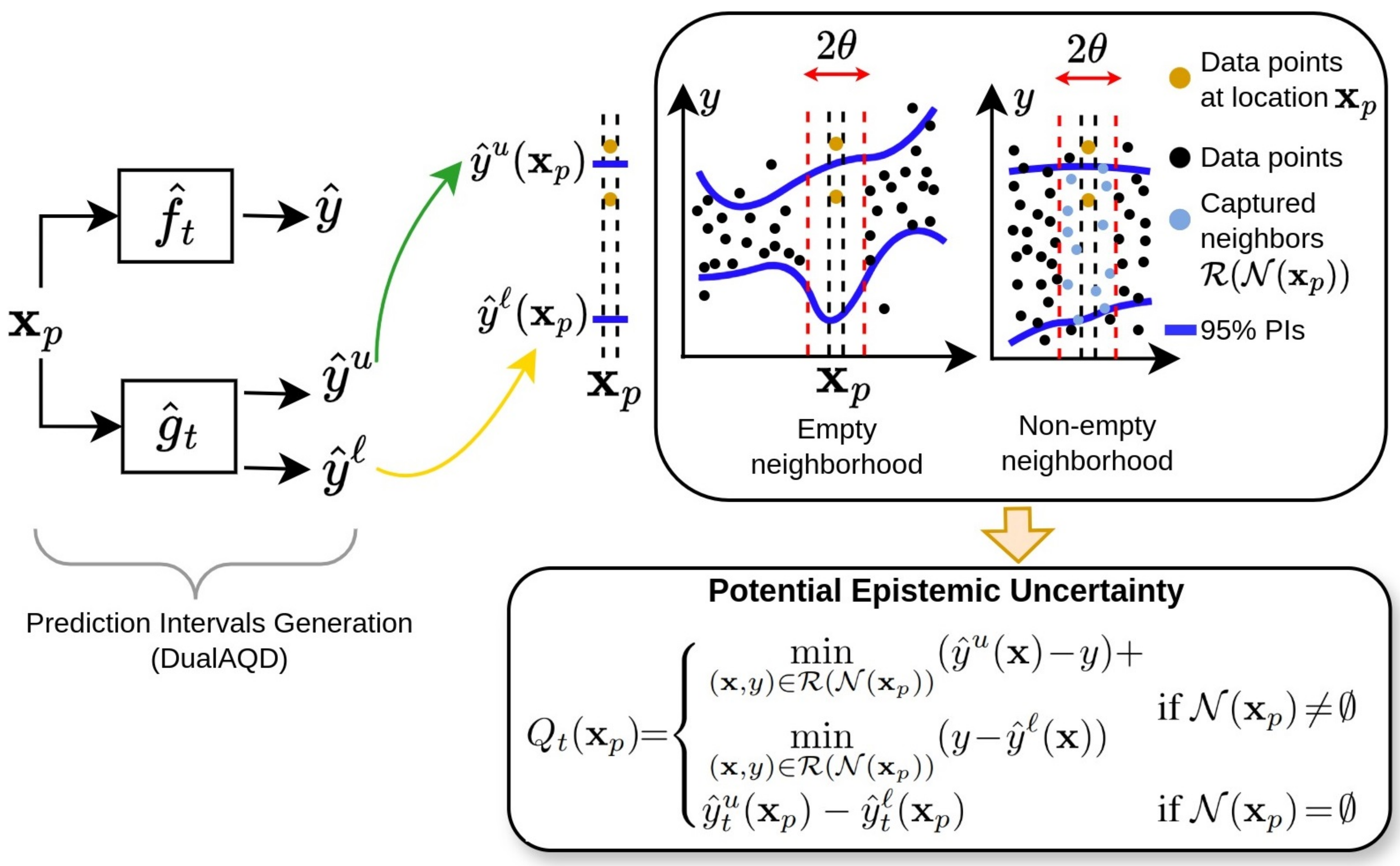

Figure 2. Potential epistemic uncertainty $Q_t(\mathbf{x}_p)$.

Batch Sampling

Selection of the k-th element of the t-th batch, $\mathbf{x}_{t,k}$:

$$\mathbf{x}_{t,k} = \underset{\mathbf{x}_p \in \mathcal{X}}{\text{argmax}}\ \alpha_t(\mathbf{x}_p \,|\, \mathbf{x}_{t,1:k-1}).$$

The acquisition function α_t estimates the **reduction in the total potential epistemic uncertainty across** $\mathcal{X}$ when making an observation at $\mathbf{x}_p$.

Batch Sampling (Cont.)

$\mathcal{D}_{t,0} = \mathcal{D}_t \leftarrow$ Dataset $\mathcal{D}_t$ augmented with the first $k-1$ samples of the batch

$$\alpha_t(\mathbf{x}_p|\mathbf{x}_{t,1:k-1}) = \underbrace{J(\mathcal{D}_{t,k-1})}_{\text{Total potential epistemic uncertainty for a model trained on } \mathcal{D}_{t,k-1}} - J\left(\mathcal{D}_{t,k-1} \cup (\overset{\text{Candidate sampling location}}{\mathbf{x}_p}, \underbrace{\hat{f}(\mathbf{x}_p)}_{\text{Estimated response at } \mathbf{x}_p})\right)$$

$J(\mathcal{D}_{t,k-1}) = \sum_{\mathbf{x}\in\mathcal{X}} Q_{t,k-1}(\mathbf{x})$

Figure 3. Acquisition function $\alpha_t(\mathbf{x}_p)$.

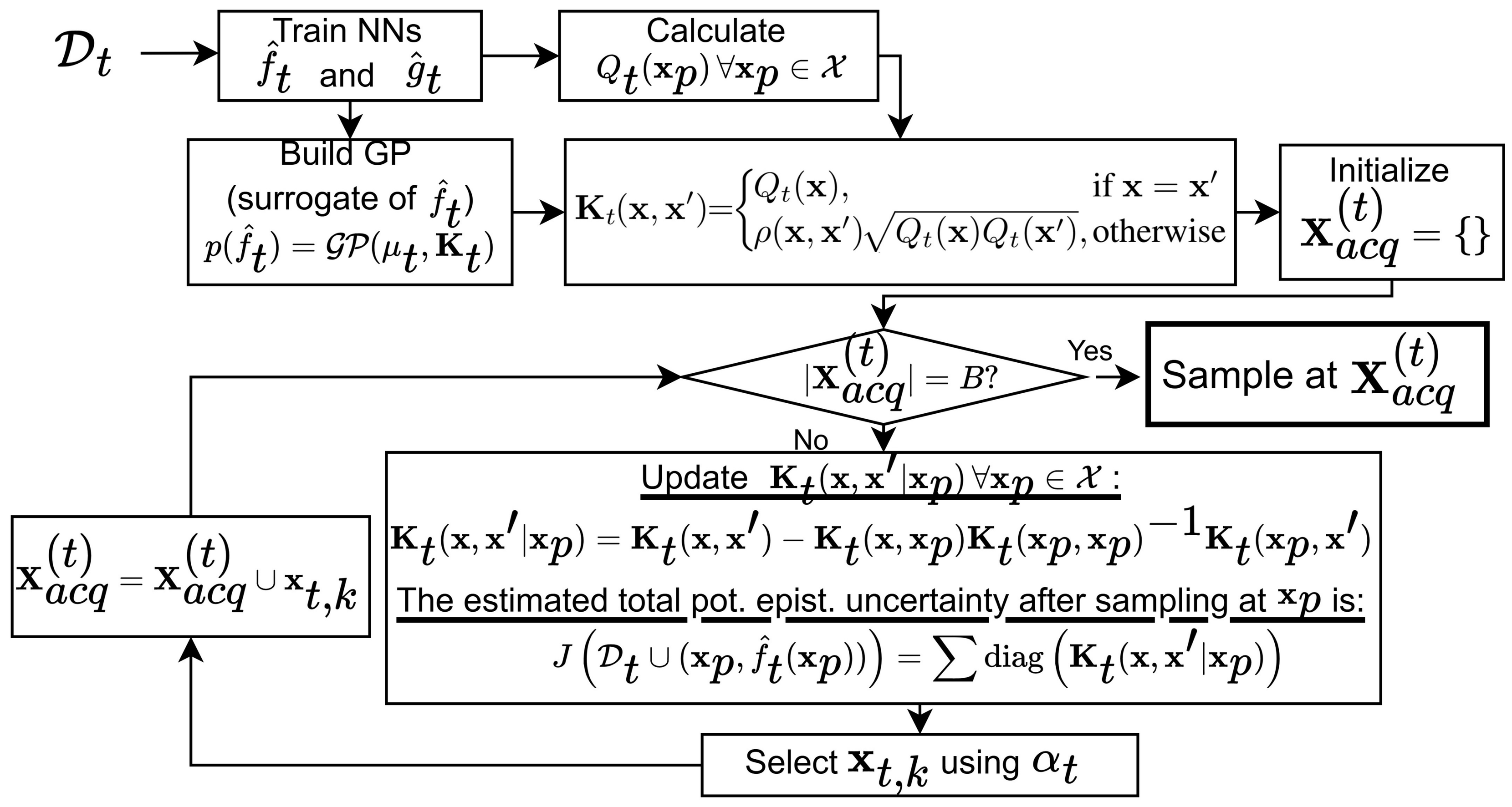

Figure 4. Acquisition function $\alpha_t(\mathbf{x}_p)$.

Experimental Results

Table 1. Functions, noise terms, and area under the uncertainty curve (AUCC) comparison.

Name	Function $f(\mathbf{x})$	Noise $\varepsilon_a(\mathbf{x})$	MCDropout	GP	NF-Ensemble	ASPINN
cos	$10 + 5\cos(\mathbf{x}+2)$	$\mathcal{N}(0, 2 + 2\cos(1.2\mathbf{x}))$	112.6 ± 24.2	123.9 ± 26.2	113.4 ± 19.5	$\mathbf{97.3 \pm 7.9}$
hetero	$7\sin(\mathbf{x})$	$\mathcal{N}(0, 3\cos(\mathbf{x}/2))$	113.8 ± 13.4	110.2 ± 13.6	106.4 ± 16.3	$\mathbf{85.9 \pm 9.1}$
cosqr	$10 + 5\cos(\frac{\mathbf{x}^2}{5})$	$\mathcal{N}(0, \frac{1}{2}(1 - \frac{\mathbf{x}^2}{100}))$	30.4 ± 3.6	23.1 ± 5.6	25.6 ± 2.7	$\mathbf{17.1 \pm 1.42}$
Simul. Field	$\frac{\mathbf{x}^P}{15} + \left(\frac{\mathbf{x}^A}{\pi} + 1\right) \times \tanh\left(\frac{0.1\mathbf{x}^{Nr}}{3\mathbf{x}^{VH}+2}\right)$	$\mathcal{N}(0, (\mathbf{x}^P + \mathbf{x}^{Nr})/150)$	614.68 ± 112.48	593.54 ± 107.42	730.80 ± 74.63	$\mathbf{496.85 \pm 71.65}$

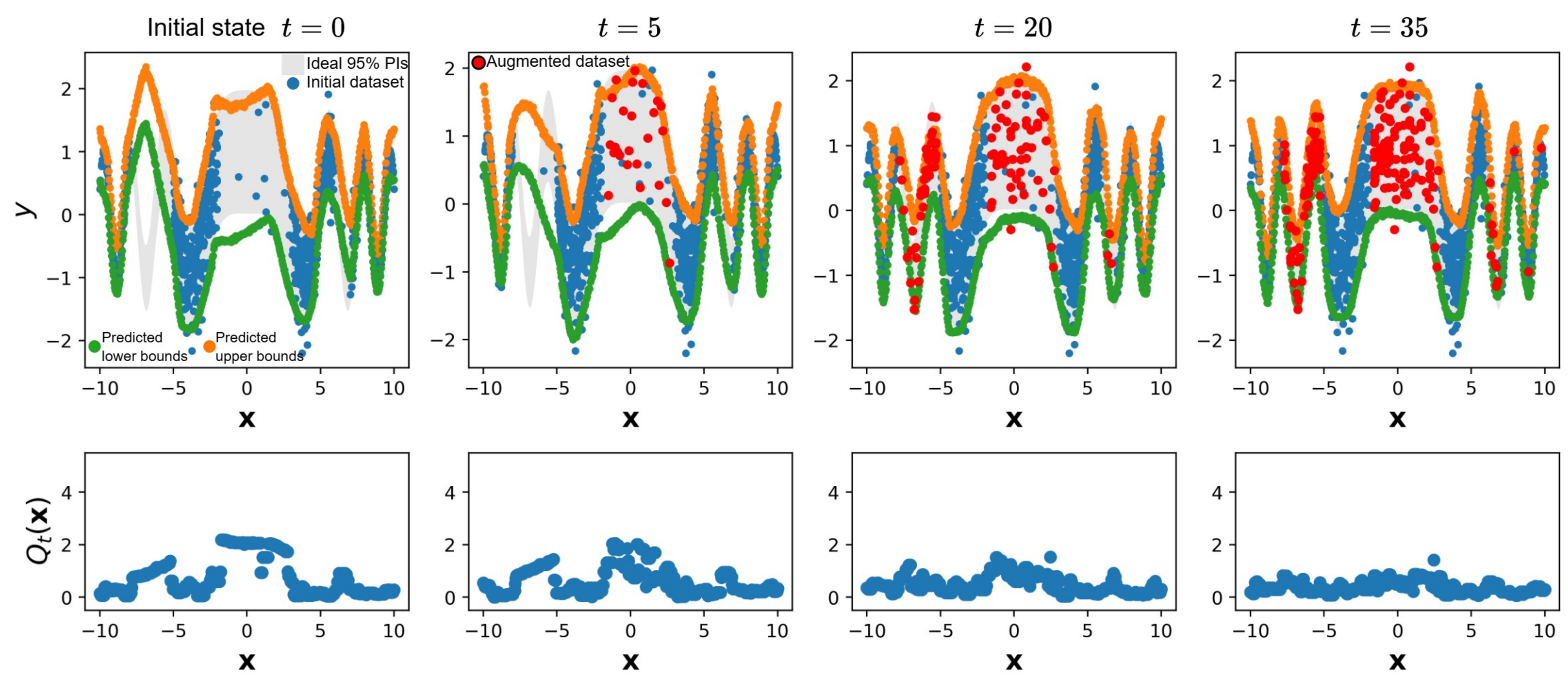

Figure 5. AS process using ASPINN on the `cosqr` problem.

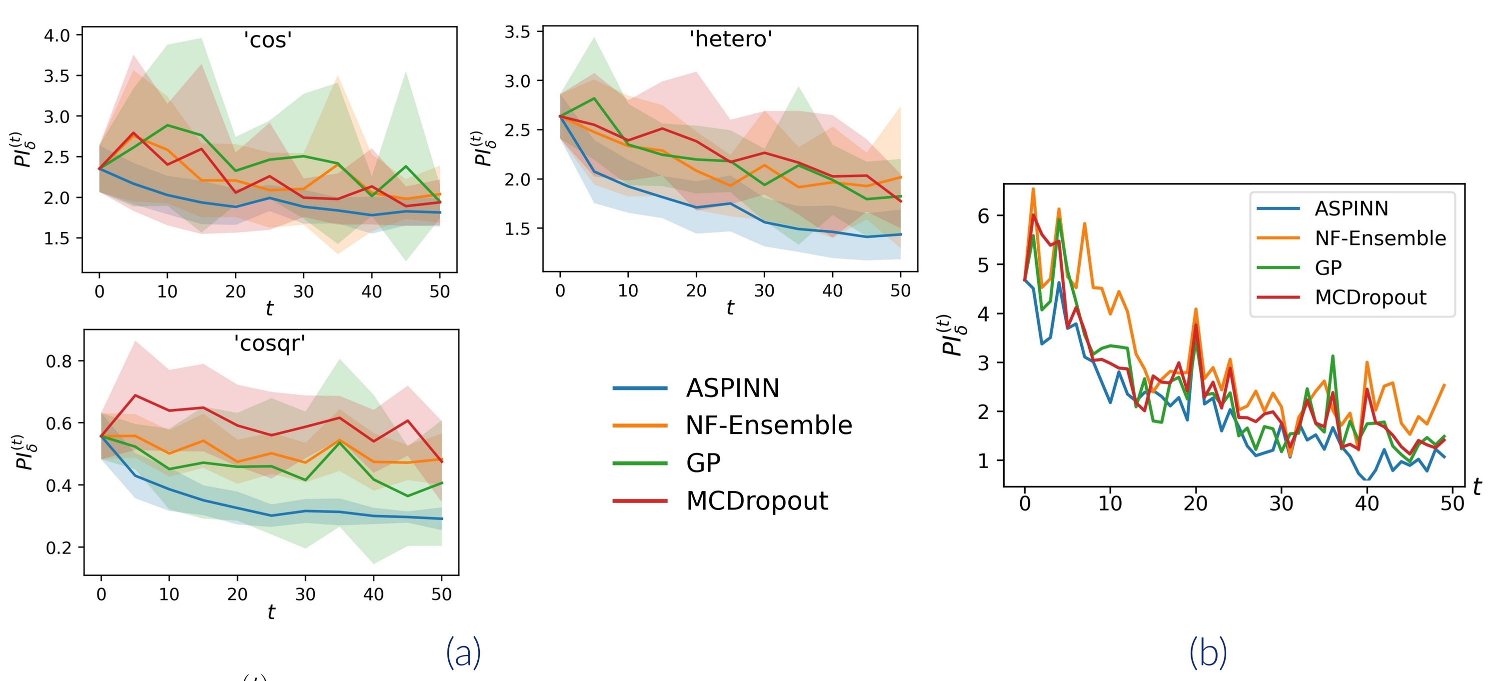

Figure 6. $PI^{(t)}_\delta$ value evolution for the **(a)** 1-D problems and the **(b)** Simulated field data.

Conclusions

1. We introduced ASPINN, an AS technique designed to reduce epistemic uncertainty across an input domain using PIs generated by NNs.
2. The novel potential epistemic uncertainty metric, central to ASPINN, provided a robust basis for guiding the sampling process.
3. The effectiveness of our approach was demonstrated through its consistent ability to achieve faster convergence rates with lower and more stable learning curves compared to other methods.