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THE HONG KONG UNIVERSITY OF SCIENCE & TECHNOLOGY

Department of Mathematics

PHD STUDENT SEMINAR

Stochastic Gradient Langevin Dynamic Based Uncertainty Quantification Framework for Neural Operators

By

Miss Yonglin LIU

Abstract

Uncertainty quantification (UQ) is critical for reliable predictions in complex systems, yet existing methods, such as Bayesian inference and ensemble-based approaches, face significant challenges in high-dimensional and computationally intensive scenarios, particularly in operator learning tasks. These methods often suffer from slow convergence, high computational costs, and limited scalability, which compromise their effectiveness and accuracy in capturing uncertainties.

To address these limitations, we propose a novel UQ framework based on stochastic gradient Langevin dynamics (SGLD) for operator learning. The framework is compatible with various neural operator architectures and leverages a perturbed gradient flow inspired by Langevin dynamics to simultaneously optimize model parameters and explore the parameter space. This dual mechanism enhances predictive accuracy while providing robust uncertainty estimates, especially for out-of-distribution (OOD) data, where conventional methods often fail. We validate our approach through experiments on learning nonlinear operators for partial differential equations (PDEs), demonstrating superior performance in both predictive accuracy and uncertainty quantification. Furthermore, we establish an approximation error bound for SGLD-based uncertainty estimates, providing theoretical guarantees for the reliability of our framework.

Date : 9 May 2025, Friday

Time : 5:00pm

Venue : Room 4472 (Lifts 25-26)

All are Welcome!