Dissertation Defense

Improving Sampling and Function Approximation in Machine Learning Methods for Solving Partial Differential Equations

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Abstract: Numerical solutions to partial differential equations (PDEs) remain one of the main focus in the field of scientific computing. Deep learning and neural network based methods for solving PDEs have gained much attention and popularity in recent years. The universal approximation property of neural networks allows for a cheaper approximation of functions in high dimensions compared to many traditional numerical methods. Reformulating PDE problems as optimization tasks also enables straightforward implementation and can sometimes circumvent stability concerns common for classic numerical methods that rely on explicit or semi-explicit time discretization. However low accuracy and convergence difficulty stand as challenges to deep learning based schemes, fine-tuning neural networks can also be time-consuming at times.

In our work, we present some of our findings using machine learning methods for solving certain PDEs. We divide our work into two sections, in the first half we focus on the popular Physics Informed Neural Networks (PINNs) framework, specifically in problems with dimensions less than or equal to three. We present an alternative optimization based algorithm using a B-spline polynomial function approximator and accurate numerical integration with a grid based sampling scheme. With implementation using popular machine learning libraries, our approach serves as a direct substitute for PINNs, and through performance comparison between the two methods over a wide selection of examples, we find that for low dimensional problems, our proposed method can improve both accuracy and reliability when compared to PINNs. In the second half, we focus on a general class of stochastic optimal control (SOC) problems. By leveraging the underlying theory we propose a neural network solver that solves the SOC problem and the corresponding Hamilton–Jacobi–Bellman (HJB) equation simultaneously. Our method utilizes the stochastic Pontryagin maximum principle and is thus unique in the sampling strategy, this combined with modifying the loss function enables us to tackle high-dimensional problems efficiently.

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