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Convergence Analysis of a Quasi-Monte Carlo-Based Deep Learning Algorithm for Solving Partial Differential Equations

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Abstract. Deep learning has achieved great success in solving partial differential equations (PDEs), where the loss is often defined as an integral. The accuracy and efficiency of these algorithms depend greatly on the quadrature method. We propose to apply quasi-Monte Carlo (QMC) methods to the Deep Ritz Method (DRM) for solving the Neumann problems for the Poisson equation and the static Schrödinger equation. For error estimation, we decompose the error of using the deep learning algorithm to solve PDEs into the generalization error, the approximation error and the training error. We establish the upper bounds and prove that QMC-based DRM achieves an asymptotically smaller error bound than DRM. Numerical experiments show that the proposed method converges faster in all cases and the variances of the gradient estimators of randomized QMC-based DRM are much smaller than those of DRM, which illustrates the superiority of QMC in deep learning over MC.

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Key words: Deep Ritz method, quasi-Monte Carlo, Poisson equation, static Schrödinger equation, error bound.

1. Introduction

Partial differential equations (PDEs) are classical models for describing problems arising in physics, finance and engineering. Solving PDEs by deep learning has attracted considerable attention, see [9, 14, 19]. Recently, a variety of well-designed deep learning algorithms for solving PDEs have been proposed, such as the physics-informed neural networks (PINNs) [29], the Deep Ritz Method (DRM) [10] and the Deep Galerkin Method (DGM) [30]. The basic idea of these algorithms is to minimize the loss by training the deep neural network. These deep learning algorithms have

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shown satisfactory efficiency and a wide range of application scenarios. However, researchers are not satisfied with treating a deep learning algorithm as a black box. It is desirable to identify the factors that drive the algorithm in mathematics and improve the algorithm by modifying these factors.

In this paper, we study the effect of the different sampling strategies on DRM. There have been some papers about the error analysis of DRM, see [8, 16, 22]. Briefly, the essence of DRM is to solve

$$\min_{u\in H^1(\Omega)} I(u),$$

where $I(u)$ is in the form of an integral and $H^1(\Omega)$ is a Sobolev space. Obviously, the quadrature method plays an important role in DRM. For high-dimensional PDEs, the algorithm may suffer from the curse of dimensionality. We aim to enhance the accuracy and efficiency of DRM by combining it with a new sampling strategy. To be specific, the accuracy is expressed in terms of the total error, namely the difference between the limit of the algorithm output and the exact solution of the PDE, and the efficiency is measured by the convergence rate and stability of the algorithm.

Quasi-Monte Carlo (QMC) methods are efficient quadrature methods, which choose deterministic points, rather than random points, as sample points. QMC methods are widely used in finance [20], statistics [11], etc. The Koksma-Hlawka inequality [26] yields that QMC integration has an error bound in the order of $\mathcal{O}(n^{-1}(\log n)^d)$ for the integrands with suitable smoothness, where n is the sample size and d is the dimension of the domain of the integrand. It is easy to see that the order of QMC is asymptotically better than that of Monte Carlo (MC). Although the error bound of QMC depends on the dimension, there have been many results that indicate the superiority of QMC over MC in high dimension [32]. Furthermore, Caflisch *et al.* [3] and Wang *et al.* [35] attribute the superiority of QMC to the effective dimension of the integrand, which is usually much lower than the nominal dimension. We believe that the integrands arising in deep learning outlined in this paper have similar characteristics.

Recently, the application of QMC methods combined with finite element methods to solve some classes of PDEs with random coefficients has achieved good performance [18] and some researchers have applied QMC methods to machine learning successfully [6, 21, 23, 24]. We propose to combine QMC methods with DRM (abbreviated as DRM-QMC) for solving the Poisson equation and the static Schrödinger equation equipped with the Neumann boundary condition. DRM-QMC can achieve asymptotically smaller error bound than DRM. The proposed algorithm converges faster and is more stable than DRM. To prove these results, we will

- formalize DRM-QMC through training the deep neural network by low discrepancy sequences,
- decompose the total error into three parts, which correspond to the generalization error, the approximation error and the training error, and then establish their upper bounds to demonstrate their relationship with the mini-batch size,