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A Symplectic Based Neural Network Algorithm for Quantum Controls under Uncertainty

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Abstract. Robust quantum control with uncertainty plays a crucial role in practical quantum technologies. This paper presents a method for solving a quantum control problem by combining neural network and symplectic finite difference methods. The neural network approach provides a framework that is easy to establish and train. At the same time, the symplectic methods possess the norm-preserving property for the quantum system to produce a realistic solution in physics. We construct a general high dimensional quantum optimal control problem to evaluate the proposed method and an approach that combines a neural network with forward Euler's method. Our analysis and numerical experiments confirm that the neural network-based symplectic method achieves significantly better accuracy and robustness against noises.

AMS subject classifications: 81Q93, 81Q05, 65P10, 49M25

Key words: Quantum (noise) control, neural network, symplectic methods, norm-preservation.

1 Introduction

Developing quantum technologies [11, 17, 34] in practice requires the robust control of quantum systems. The main goal of quantum control is to drive a quantum system to the desired state with high fidelity [5]. The theory of deterministic quantum control has

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been well established in various applications [5, 10]. Still, in practice, the presence of uncertainty in the process is inevitable, which is commonly due to imperfect knowledge of the system or the fluctuations in the experiment parameters [25, 31]. As a result, robustness becomes a critical bottleneck in designing control strategies for practical quantum systems. A theoretical study of quantum noise control can be found in [21] and we refer to a list of robust quantum control methods in references [8, 12, 13, 16, 19, 24, 32, 37].

In this paper, we aim to construct an efficient numerical algorithm for quantum control problems under uncertainty which incorporates a symplectic method for the Schrödinger equation and a deep learning method for the optimization process. In the past decades, many efforts have been made to explore the applications of machine learning techniques, particularly neural network, in solving differential equation [6, 14, 43], partial differential equation [4, 20, 22, 35, 39], stochastic differential equations [3, 18, 42], which naturally extends to the classical control problems [1, 28]. In addition, a number of recent literature have successfully demonstrated the close connection between several state-of-the-art deep network architectures and the traditional discrete dynamical systems such as forward Euler's method [15, 27]. The neural network-based method has attained promising success in alleviating challenges facing classical approaches such as high dimensionality in a system. For quantum control problems, one branch of ideas takes the data-driven approach, where networks, such as deep reinforcement learning, are built to learn the control of quantum systems [30, 33] from the data collected under an experimental setting. On the other hand, a model-driven approach avoids the necessity of data collection. It focuses on solving the quantum system with the neural network as a substitution of traditional numerical methods [36, 40]. Following the approach, In our previous work [26], we followed the second approach by combining neural networks with a sampling-based learning method to solve a quantum control problem with uncertainty. The technique exploited the auto-differentiation function provided by standard machine learning algorithms to bypass the necessity of the manual computation of the gradient of the loss function, as required in conventional methods such as the gradient flow method or Hamilton Jacobi equations. The algorithms are easy to implement and the networks can be efficiently trained thanks to the sophisticated software and hardware available for training deep neural networks. Two approaches, neural network-based learning control (NNLC) and finite difference integrated neural network-based learning control (FDI-NNLC) were considered.

Recently, there has been growing interest in symplectic neural networks in learning Hamiltonian systems and applications to normalizing flows [7, 23, 38]. In this paper, we use the symplectic finite difference schemes to discretize the Schrödinger equation, which are known to have better accuracy than simple schemes such as Euler's method for solving the Hamiltonian system and have the additional property of norm-preservation, which is essential to produce realistic physical solution of the quantum systems. The two symplectic schemes under consideration are the symplectic Euler method and the midpoint symplectic method. Both methods are compared to the NNLC and FDI-NNLC methods. In practice, the size of a realistic quantum system grows fast as more interac-