Machine Learning-Based Ground State Estimation: A Comparison of Neural Network Architectures

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***Abstract*—We employ the Neural Network Quantum State (NQS) approach to approximate the ground state of a quantum many-body system. Different architectures are compared, and their respective advantages and limitations are discussed. Owing to recent advances in machine learning and computing hardware, NQS has gained increasing attention as it can describe complex many-body systems with significantly fewer parameters than traditional methods.**

***Index Terms*—Machine Learning, Quantum Many-Body, NQS, Ground State Estimation**

I. Introduction

A better theoretical understanding of quantum many-body physics is likely to be directly linked to improvements in the field of quantum computing. Traditional approaches suffer from exponential scaling of the many-body wave function, rendering them inefficient on classical hardware. Employing artificial neural networks to represent the many-body wavefunction provides a more efficient and scalable alternative. However, the landscape of neural network architectures is vast, and determining the optimal design and architecture for a given problem remains a major challenge, particularly in the study of quantum many-body systems.

We employ multiple neural network architectures to approximate the ground state of a quantum many-body system, resulting in a significant reduction in the parameters required to describe the system compared to non-machine-learning approaches. The approach is called *Neural Network Quantum States* (NQS) and relies on the ansatz of *variational wavefunctions*. We then compare the different architectures and evaluate their advantages and potential limitations.

II. Background

As we will later compare the capabilities of different NQS architectures, which are designed to accurately find the ground state of a quantum many-body system, we will briefly review the underlying concepts first.

A. Physical Background

Determining the ground state of a quantum many-body system is a pronouncedly non-trivial task. As recent developments have shown, machine learning (ML) algorithms can be successfully employed to provide accurate estimates for the ground state function $|\psi_0\rangle$ of the underlying Hamiltonian $\hat{\mathcal{H}}$. NQS is an ML-based approach using *variational wavefunctions* $|\psi_\theta\rangle$, which are described by the learnable parameter θ. The estimate of the ground state is found by minimizing the system's energy, as seen in Eqn. (1) [1]

$$E_\theta = \frac{\langle \psi_\theta | \hat{\mathcal{H}} | \psi_\theta \rangle}{\langle \psi_\theta \mid \psi_\theta \rangle} \geq E_0 \equiv E_{\text{Ground-State}}. \tag{1}$$

B. Computational Background

Computational complexity theory provides a framework for classifying problems according to the computational resources required for their solution. While problems in class P can be solved efficiently on classical computers, those in NP or its quantum counterpart QMA can only be verified efficiently. Determining the ground-state energy of a general local Hamiltonian is QMA-hard [2], placing it among the most computationally intractable problems known.

In quantum many-body problems, the complexity arises from the exponential growth of the Hilbert space with system size N, requiring $\mathcal{O}(d^N)$ parameters to describe a wavefunction, rendering exact diagonalization infeasible. Classical approaches, such as Quantum Monte Carlo [3] and tensor network [4] methods, offer approximate solutions but are limited by issues like the sign problem [5] and restricted entanglement scaling. NQS addresses these limitations by parametrizing the wavefunction $|\psi_\theta\rangle$ through a neural network.

C. Neural Networks' Architectures

Neural Networks and Deep Learning [6] have undergone significant advancements in recent years. A wide range of neural network architectures has emerged, each designed with unique properties suited to different application domains. Selecting an appropriate architecture is therefore highly task-dependent. [7] For instance, convolutional neural networks [8] are predominantly used for image recognition tasks due to their ability to capture spatial correlations. Recurrent neural networks [9] are particularly suited for sequential data, such as speech recognition, while transformer architectures [10] have become the standard in large-scale language modeling for learning long-range dependencies. Neural Quantum States can be realized using various neural network architectures. [1] The field initially began with restricted Boltzmann machines (RBMs) [11] and has since evolved to include many other architectures.

III. Implementation

First, we will present the implementations of various NQS architectures to find the ground state of a given physical system. These implementations are compared employing the J_1-J_2 model [12], a commonly used model to evaluate NQS architectures [1].

IV. Discussion

We discuss the results obtained by the different architectures used for our NQS approach and compare them in terms of performance, efficiency, and accuracy here. Furthermore, we point out the potential and limitations of the architectures, respectively.

V. Conclusion

Finally, we can conclude the following....

VI. Outlook

Regarding the presented work, some next steps could be .... Further, the concept of ... seems promising. Moreover, it seems worth considering .... Furthermore, NQS can be used for quantum state tomography (QST) and the analysis of dynamical systems (at finite temperatures) as well [1], [13].

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