RADemics

Variational Quantum Eigensolver Applications in Quantum Machine Learning

M. Amshavalli, Shambhu Sharan Srivastava
ERODE SENGUNTHAR ENGINEERING COLLEGE, SCHOOL OF MANAGEMENT SCIENCES

Variational Quantum Eigensolver Applications in Quantum Machine Learning

M. Amshavalli, Assistant Professor, Department of Computer Science and Engineering, Erode Sengunthar Engineering College, Erode, Taminadu, India, amshavalli1494@gmail.com

Shambhu Sharan Srivastava, Associate Professor, School of Management Sciences, Varanasi, shambhuss@yahoo.com

Abstract

The Variational Quantum Eigensolver (VQE) has emerged as a transformative approach in quantum computing, providing a practical means to tackle complex quantum systems. This chapter delves into the essential components and strategies for enhancing VQE performance, focusing on key areas such as hybrid optimization techniques, quantum circuit design, and measurement efficiency. By integrating classical and quantum resources, hybrid optimization methods significantly improve convergence rates while reducing the computational burden on quantum devices. The chapter explores the design of quantum circuits, emphasizing the importance of selecting appropriate variational ansätze to achieve optimal results. Challenges related to Hamiltonian simulation and measurement are critically examined, alongside innovative solutions to mitigate noise and enhance measurement fidelity. Through these comprehensive insights, this chapter aims to illuminate the potential of VQE in advancing quantum machine learning applications across diverse scientific domains.

Keywords:

Variational Quantum Eigensolver, quantum computing, hybrid optimization, measurement efficiency, quantum circuit design, Hamiltonian simulation.

Introduction

The Variational Quantum Eigensolver (VQE) has emerged as a pivotal algorithm in the realm of quantum computing, particularly for addressing the complexities inherent in quantum chemistry and many-body physics [1,2]. As a hybrid algorithm, VQE leverages both quantum and classical computing resources to efficiently estimate the ground state energies of quantum systems [3]. This methodology capitalizes on the strengths of current noisy intermediate-scale quantum (NISQ) devices, which are characterized by their limited qubit count and error rates [4,5]. By combining variational techniques with quantum measurements, VQE provides a promising avenue for exploring the quantum landscape, ultimately aiming to unlock new insights into chemical reactions, materials properties, and more[6,7,8,9].

One of the core strengths of VQE lies in its adaptability to various quantum systems [10]. The algorithm can be tailored to accommodate a wide range of Hamiltonians, allowing researchers to investigate diverse physical phenomena [11,12]. For instance, the ability to incorporate different ansätze, or parameterized quantum circuits, enhances the flexibility of VQE, enabling it to represent complex quantum states more accurately [13]. This adaptability was crucial in the quest for reliable quantum simulations, as it allows researchers to fine-tune their approaches based on the specific characteristics of the system under study [14]. Consequently, VQE stands out as a versatile tool for both theoretical investigations and practical applications in quantum chemistry and beyond [15].

The convergence of VQE was significantly influenced by the optimization strategies employed throughout the process. Classical optimization methods play a vital role in refining the parameters of the variational ansatz, guiding the algorithm toward an optimal solution [16,17]. Various techniques, such as gradient-based optimization and derivative-free methods, have been explored to enhance convergence rates [18]. Additionally, the choice of initial parameters can substantially impact the efficiency of the optimization process [19,20,21]. By intelligently selecting starting points based on prior knowledge or computational heuristics, researchers can improve the likelihood of reaching the global minimum and thus achieve more accurate results [22].

Measurement efficiency was another critical aspect that influences the overall performance of VQE. The quantum nature of the VQE process necessitates multiple measurements to extract meaningful expectation values from the quantum states generated by the algorithm. The inherent noise and errors present in quantum devices complicate this task, potentially leading to inaccurate results [23]. Therefore, advanced techniques for error mitigation and measurement optimization are essential for maximizing the reliability of VQE outcomes [24]. Implementing strategies such as measurement error correction, variance reduction, and adaptive sampling can help improve measurement fidelity and enhance the algorithm's overall efficiency [25].