Quantum-Enhanced Image Classification with Graph Neural Networks

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Resum– Aquest resum es centra en l'exploració de les Xarxes Neuronals Quàntiques de Grafs (QGNNs) i el seu potencial per a una revolució en l'aprenentatge automàtic quàntic, especialment a l'hora de resoldre problemes complexos basats en grafs. Les QGNNs aprofiten estats quàntics i operacions per a l'anàlisi de grafs, però l'òptim funcionament d'aquestes xarxes és un desafiament complex que implica tant aspectes algorísmics com de maquinari. Els avenços en el maquinari de computació quàntica, incloent-hi processadors quàntics més potents i estables, són crucials per a aconseguir les màximes capacitats de les QGNNs. L'òptim funcionament a nivell algorísmic inclou el disseny de circuits quàntics, l'optimització de portes quàntiques i l'ajustament de paràmetres per a millorar el rendiment de les QGNNs. Les aproximacions híbrides que combinen xarxes neuronals clàssiques amb components quàntics obren noves possibilitats per a l'optimització. Conforme les tecnologies de computació quàntica madurin i les tècniques d'optimització per a les QGNNs evolucionin, podem esperar avenços transformadors en la resolució de problemes reals que impliquin dades estructurades en forma de grafs.

Paraules clau– Xarxes Neuronals de Grafs, Algorismes Quàntics, Computació Quàntica, Aprenentatge Automàtic Quàntic, Visió per Computador

Abstract– The abstract discusses Quantum Graph Neural Networks (QGNNs) and their potential to revolutionize quantum machine learning by efficiently addressing complex graph-based problems. QGNNs leverage quantum states and operations for graph analysis. The optimization of QGNNs is a multifaceted challenge involving hardware and algorithmic aspects. Hardware advancements in quantum computing, including larger and more stable quantum processors, are crucial for maximizing QGNN capabilities. Algorithmic optimization entails designing quantum circuits, gate optimization, and parameter tuning to improve QGNN performance. Hybrid quantum-classical approaches, combining classical neural networks with quantum components, offer new avenues for optimization. As quantum computing technologies mature and optimization techniques for QGNNs evolve, we can expect transformative breakthroughs in solving real-world problems involving graph-structured data.

Keywords– Graph Neural Networks (GNNs), Quantum Algorithms, Quantum Computing, Quantum Machine Learning (QML), Computer Vision

1 INTRODUCTION

THE advent of quantum computing heralds a transformative era for various domains, with machine learning standing at the forefront of this revolution. Traditional image classification methods have achieved remarkable success, yet they are increasingly encountering limitations due to the growing complexity and volume of data. The intersection of quantum computing and machine learning, particularly Graph Neural Networks (GNNs), presents a promising frontier for overcoming these challenges. This research aims to harness the quantum mechanical phenomena of superposition and entanglement to enhance the capabilities of GNNs in image classification tasks.

The motivation for this study stems from the convergence

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of two cutting-edge technologies: quantum computing and GNNs. Quantum computers possess the unique capability to handle exponentially large computational spaces, which can be exploited to accelerate the learning process of GNNs. By translating image data into quantum states, we anticipate a significant enhancement in the speed and accuracy of classification tasks, surpassing what is achievable with classical computational resources alone.

2 STATE OF ART

The state of the art in quantum computing has been marked by significant advancements and challenges. As stated by Preskill [1], quantum computers with 50-100 qubits are expected to perform tasks that surpass the capabilities of today's classical digital computers. However, noise in quantum gates limits the size of quantum circuits that can be executed reliably. The exploration of the *entanglement frontier* is a promising avenue, where quantum computers might simulate natural processes that are intractable for classical computers, such as the properties of complex molecules, exotic materials, and fundamental physics phenomena [1].

The power of quantum computing rests on principles such as quantum complexity and quantum error correction, with quantum entanglement as a core concept differentiating it from classical information processing. Quantum algorithms can solve classically intractable problems, and complexity theory suggests that quantum states prepared by quantum computers have superclassical properties [1]. However, there is a recognition that quantum computing's power is not unlimited, particularly when it comes to NP-hard problems which remain challenging for both classical and quantum computers.

These developments and investments signal a period of consolidation and scaling in quantum computing, suggesting that while the most significant hardware milestones may yet be on the horizon, the groundwork laid by researchers and industry is paving the way for a future where quantum computing could fulfill its transformative promise.

2.1 Quantum Machine Learning (QML)

Quantum Machine Learning (QML) represents a burgeoning field that merges quantum computing's strengths with machine learning's versatility, aiming to enhance computational efficiency and problem-solving capabilities. The state of the art in QML is highlighted by the potential of quantum algorithms to expedite solutions for problems that are computationally intensive on classical systems, as discussed by Preskill [1].

Recent advances explore Quantum Approximate Optimization Algorithms (QAOA) applied to optimization problems like the *MaxCut* for specific models such as the *2-D Antiferromagnetic Ising Model*, showcasing the innovative use of reinforcement learning to optimize quantum algorithms [2].

The exploration of these quantum-classical hybrids, particularly in QAOA, reveals a nuanced understanding of quantum states and entanglement's role in problem-solving, which could lead to quantum advantages in complex systems analysis [1]. Moreover, the development of QML algorithms considers not only the potential speed-ups but also the practical constraints of current and near-term quantum hardware, which shapes the realistic deployment of QML models.

As quantum technology advances into the Noisy Intermediate-Scale Quantum (NISQ) era, the focus on error correction and noise-resilient algorithms becomes crucial for the practical implementation of QML. While the theoretical foundations suggest substantial advantages over classical counterparts, the empirical applications remain in nascent stages, with much research directed towards scalability and error mitigation [1].

In summary, QML is poised at a pivotal intersection of theory and application, with significant research directed towards leveraging quantum phenomena for learning and optimization, which is expected to evolve alongside quantum hardware advancements.

2.2 QNNs: Quantum Neural Networks

Quantum Neural Networks (QNNs) have shown significant promise in improving machine learning through speed-ups in computation or improved model scalability. As demonstrated by Abbas et al. [3], well-designed QNNs offer an advantage over classical neural networks through a higher effective dimension and faster training ability.

In terms of expressibility, QNNs are able to achieve a significantly better effective dimension than comparable classical neural networks. To assess the trainability of quantum models, the Fisher information spectrum is connected to barren plateaus, the problem of vanishing gradients. Certain QNNs can show resilience to this phenomenon and train faster than classical models due to their favourable optimisation landscapes, captured by a more evenly spread Fisher information spectrum [3].

2.2.1 Circuit Ansatz

An ansatz quantum circuit is a heuristic quantum circuit used in quantum computing, particularly in variational algorithms, where the form of the circuit is guessed or conjectured based on intuition, physical insight, or numerical experiments. An ansatz circuit is typically parameterized with a set of variables that can be tuned algorithmically to minimize a certain objective function, making it suitable for optimization problems [4].

The state of the art in quantum ansatzes, particularly for Variational Quantum Eigensolvers (VQEs), has been advanced through the development of size-extensive ansatzes. These ansatzes are designed to compactly represent ground state quantum correlations without the need for *Trotterization*[1], which often introduces errors and additional computational costs. Researchers have worked on designing VQE ansatzes that span the entire Hilbert space with the minimum number of parameters, focusing on symmetry constraints of target systems to create increasingly accurate sub-ansatzes. This approach has shown good convergence to the ground state in models like the transverse-field Ising model [5].

[1] As a real time evolution technique, the *Trotterization* or *Trotterized Real Time Evolution (RTE)* consists in the successive application of a quantum gate, assumed to approximate the time evolution of a system for a time slice.

The optimization of VQEs is critical for outperforming classical supercomputers, especially in the Noisy Intermediate-Scale Quantum (NISQ) era and beyond. The variational ansatz is central to this process, as it must be carefully designed to cover a sufficient portion of the Hilbert space and avoid local minima or barren plateaus that hinder optimization. In practical terms, a VQE is executed on a quantum register to approximate the minimum eigenvalue of a system, and the variational ansatz is a parameterized circuit that can be tuned to minimize the energy of the resulting state. The efficiency and success of these algorithms depend on the careful design of the ansatz and its adaptability to the hardware constraints of quantum computers [5]. The efficiency and success of these algorithms depend on the careful design of the ansatz and its adaptability to the hardware constraints of quantum computers [5].

The state of the art on ansatzes for QGNNs centers around the development of ansatzes that respect graph symmetries, specifically equivariance under node permutations. These ansatzes are designed to address complex learning tasks on weighted graphs such as neural combinatorial optimization. The study demonstrates that symmetry-preserving ansatzes are vital for success in Quantum Machine Learning (QML). The Equivariant Quantum Circuit (EQC) ansatz introduced by Skolik et al. [6] provide trainability advantages by avoiding issues like barren plateaus, which hamper the scaling of quantum circuits. This novel approach to ansatz design is motivated by geometric deep learning principles, which focus on the mathematical properties of data to create more efficient learning architectures.

2.2.2 QGNNs: Quantum Graph Neural Networks

Classical Graph Neural Networks (GNNs), by leveraging the rich relational information inherent in graph data, have demonstrated exceptional performance on a variety of deep learning tasks, such as modeling physical systems, learning molecular fingerprints, predicting protein interfaces, and classifying diseases [7]. Their design considerations, and the computational modules that constitute them, offer insights into both the current state of the art and potential future directions for research.

Quantum Graph Neural Networks (QGNNs) are a novel quantum neural network ansatz specifically designed to represent quantum processes with graph structures, making them particularly well-suited for distributed quantum systems operating over a quantum network. They are an emerging subset within the broader domain of variational quantum algorithms, which are gaining prominence in quantum computing. QGNNs are inspired by the successes of classical Graph Neural Networks (GNNs), which have achieved notable breakthroughs by adapting convolutional operations to graph-structured data [8].

The QGNN framework encompasses a parameterized quantum circuit that evolves through sequences of Hamiltonian evolutions, each associated with graph structures. Specialized versions of QGNNs include Quantum Graph Recurrent Neural Networks (QGRNNs), which are designed to learn effective quantum Hamiltonian dynamics of systems organized in graph structures, and Quantum Graph Convolutional Neural Networks (QGCNNs), which exploit permutation invariance to perform convolutional operations on quantum graphs, as discussed by Verdon et al. [8].

The QGCN leverages quantum parametric circuits to perform graph classification tasks, a common challenge in traditional machine learning. The model architecture parallels classical graph convolutional neural networks, allowing it to efficiently represent graph topology and learn hidden node feature representations. Numerical simulations have shown that this model can be effectively trained, displaying promising performance in graph-level classification tasks [9]. It was noted by Zheng et al. [9] that increasing the model's complexity did not substantially improve accuracy for simple test data, suggesting that the model's effectiveness may scale with the complexity of the graph's structure.

The Quantum Spectral Graph Convolutional Neural Network (QSGCNN) is a variant that aligns with Laplacian-based graph convolutional networks, utilizing alternating layers of quantum operations to pass messages and update node information in a manner that mimics classical spectral-based graph convolutions [8].

Applications of QGNNs have been explored in several areas by Verdon et al. [8]:

- **Learning Quantum Hamiltonian Dynamics:** QGRNNs have been utilized to learn the dynamics of quantum systems, such as Ising spin systems, by evolving a known quantum state over time and adjusting the network to minimize the deviation from the expected evolution.
- **Quantum Sensor Networks:** QGCNNs have been employed to optimize quantum sensor networks, including the preparation of multipartite entangled states that can improve the sensitivity of quantum sensors beyond classical limits.
- **Unsupervised Graph Clustering:** QSGCNNs have been applied to spectral clustering tasks, demonstrating the potential of quantum neural networks to find clusters within graph-structured data, even with low-qubit precision suitable for near-term quantum computers.
- **Graph Isomorphism Classification:** QSGCNNs have also been benchmarked for their ability to determine graph isomorphism, a key problem in graph theory, by comparing the distributions of Hamiltonian ”energies” corresponding to different graph structures.

These initial explorations into QGNN applications are promising and suggest a variety of future research directions, including the development of hybrid methods for quantum chemistry, generalization of QGNN architectures to include more quantum features, and the use of quantum optimization techniques for training

2.2.3 Quantum Graph Encoding

The state of the art in quantum graph encoding circuits, particularly in the context of solving the combinatorial optimization problems using quantum algorithms, can be discussed in terms of three main approaches: Equivariant Quantum Circuits (EQCs), Quantum Approximate Optimization Algorithm (QAOA), and Quantum Graph Neural Networks (QGNNs).

The EQC approach is a specialization of a QAOA-type ansatz. Instead of encoding a problem Hamiltonian, EQCs encode the graph instance directly and include mixing terms for a problem-dependent subset of qubits. This encoding enables the derivation of exact formulations of expectation values at depth one from those of the QAOA. EQCs consider the one-step neighborhood of each candidate node at depth one, which is essential for quantum models because, for QAOA to find optimal solutions, it must "see the whole graph." A recursive version of QAOA, known as RQAOA, was introduced to overcome depth limitations by iteratively eliminating variables based on their correlation, reducing the problem to a smaller instance that can be solved efficiently by classical algorithms [6].

In Neural Combinatorial Optimization (NCO) with reinforcement learning, a machine learning model learns a heuristic for a given optimization problem based on data. In Q-learning, a popular method within NCO, a Neural Network (NN) or a Parameterized Quantum Circuit (PQC) approximates the optimal Q-function, which is used to predict the expected return of actions taken in states. This is particularly relevant for problems like the Travelling Salesperson Problem (TSP), where the goal is to find the shortest route connecting all locations without revisiting any [6].

The QAOA for solving TSP employs a Trotterization of Adiabatic Quantum Computation (AQC), alternating between a starting Hamiltonian and a problem Hamiltonian, parameterized by values that are optimized to approximate the solution to the combinatorial optimization problem. However, this method requires a large number of qubits, and finding good parameters for QAOA to solve the TSP is challenging. Moreover, the performance of QAOA is still not on par with EQC, even for instances as small as five cities, despite considerable computational efforts and optimization techniques like COBYLA [6].

In addition to EQCs, Sopena et al. [10] introduced a novel method to exactly prepare eigenstates of quantum integrable vertex models on programmable digital quantum computers. This method relies on the QR decomposition to convert the Algebraic Bethe Ansatz (ABA) to a unitary form, functioning effectively for both real and complex roots of the Bethe equations. The approach scales linearly with the number of qubits regarding circuit depth and gate complexity, though an exponential scaling is expected with the number of magnons, potentially affecting preprocessing, compilation, and circuit depth. The process can create a unitary circuit representation for interesting states with modest classical computational resources. It's especially efficient for the quantum *XX model*[2], leading to quantum circuits that match the state-of-the-art $O(N)$ depth.

Moreover, this method could be used for a variety of applications, such as studying Hamiltonian quenches that may be challenging for classical methods or as inputs for other quantum algorithms, potentially aiding in the initialization of variational quantum algorithms, thus addressing trainability issues. It also offers a new way to benchmark quantum hardware using strongly-correlated states, when analytical solutions for some expectation values are known, which could serve as a type of application-oriented benchmark [10].

In summary, while EQCs and QAOA both encode graph instances to solve optimization problems like the TSP, EQCs seem to be more promising due to their ability to handle problem-specific features and their performance over classical approaches. However, the full potential for quantum advantage in these settings is still an open area of research.

[2]The quantum Heisenberg model (XX-model), developed by Werner Heisenberg, is a statistical mechanical model used in the study of critical points and phase transitions of magnetic systems, in which the spins of the magnetic systems are treated quantum mechanically.

3 METHODOLOGY

The aim of this research is to enhance the efficacy of document classification through the integration of Quantum Graph Neural Networks (QGNN) and reinforcement learning techniques. The methodology entails a series of interconnected steps to harness the potential of quantum computing paradigms and reinforcement learning for document classification tasks, as discussed in the following subsections.

3.1 Development of Quantum Graph Encoding

The foundational step involves designing a quantum circuit capable of encoding classical document data into a quantum state, thereby representing the inter-document relationships in a graph format amenable to quantum computation. Leveraging Qiskit, IBM's open-source quantum computing framework, the encoding circuit is meticulously structured to preserve the semantic and relational dynamics between document elements, ensuring that the contextual and structural integrity of the documents is upheld within the quantum graph. This quantum graph serves as the input for subsequent quantum-enhanced graph neural network processing.

This encoding process draws upon the methodologies proposed by Skolik et al. [6], Sopena et al. [10], Yan et al. [11], Shah et al. [12], offering a blueprint for transposing classical document data into a quantum representation. The circuit architecture ensures the preservation of the semantic and relational information among document elements, thereby retaining the global structural significance within the quantum domain.

3.2 Integration of Quantum Graph Neural Networks

Following quantum graph preparation, quantum algorithms are integrated within the Graph Neural Network (GNN) architecture, as observed in the work by Verdon et al. [8], to exploit the computational capabilities of quantum processing. This fusion gives rise to a hybrid framework where quantum states representing document data undergo manipulations via quantum gates. Measurements derived from these states are pivotal for feature extraction, essential for document classification.

3.3 Parameter Optimization using Reinforcement Learning

Optimization of the quantum circuit and the QGNN involves the application of reinforcement learning strategies based on the work by Jerbi et al. [13]. The primary objective is to formulate an optimal policy that refines the quantum circuit parameters, thereby enhancing the efficacy of document classification. The algorithm's performance, in terms of navigating the quantum state space and ascertaining optimal parameter adjustments, is predicated on feedback from the QGNN's classification outcomes.

3.4 Benchmarking and Performance Evaluation

A critical phase involves evaluating the quantum-augmented QGNN against conventional techniques by employing standard document classification datasets. This analysis encompasses accuracy, computational efficiency, and scalability assessments. Quantitative metrics including classification accuracy, processing duration, and resource allocation will be meticulously recorded to illustrate the comparative advantage of the quantum approach.

In summary, the methodology amalgamates Qiskit's robust quantum circuit construction capabilities, the profound learning potential from graph-structured data via Quantum Graph Neural Networks, and the dynamic optimization faculties of reinforcement learning, all aimed at setting a new precedent in document classification efficiency facilitated by quantum computing innovations.

4 DEVELOPMENT

The development phase of the project is characterized by the execution of the planned methodology, leading to the construction of a foundational framework for a Quantum-Enhanced Graph Neural Network (QGNN). This section outlines the sequential progress made and the steps planned for the near future.

4.1 Design of Graph Encoding Circuit

The initial phase of development focused on designing the graph encoding circuit that is pivotal for translating classical graph data into a quantum-compatible format. Utilizing the theoretical groundwork laid out in Skolik et al. [6] and subsection 2.2.3, a quantum circuit, as the one you can see on Fig. 1, was constructed using Qiskit that encodes classical graphs as quantum graphs.

As of the latest development cycle, the project has successfully completed the graph encoding circuit design. The circuit has been verified to correctly encode sample nodes and edges into quantum states that reflect the graph structure, thus preparing the ground for the subsequent integration with a GNN model.

4.2 Next Steps

The forthcoming development efforts are slated to focus on the integration of the graph encoding circuit with a GNN. This step will involve the translation of quantum state measurements into features that can be processed by the GNN to perform document classification tasks.

Following the circuit-GNN integration, the project will embark on implementing reinforcement learning techniques. These techniques will be adapted from the strategies outlined in the referenced paper, with the objective of optimizing the QGNN's performance. The reinforcement learning algorithm will be trained to fine-tune the parameters of the quantum circuit based on the classification results obtained from the GNN, thereby establishing a feedback loop for continuous improvement.

The key milestones for the upcoming weeks include:

- Completion of the quantum circuit-GNN integration.
- Implementation and training of the reinforcement learning algorithm.
- Initial benchmarking of the QGNN against classical GNN models using small-scale document datasets.

In conclusion, the development phase has achieved a significant breakthrough with the design of the graph encoding circuit. The project is now well-positioned to proceed to the integration of quantum computing techniques with GNNs, a step that promises to push the boundaries of quantum document classification technology. With the reinforcement learning optimization and benchmarking phases on the horizon, the project is on track to fulfill its objectives and contribute a novel approach to the domain of quantum-enhanced machine learning.

5 PRELIMINARY RESULTS

The preliminary results highlight the foundational achievements and ongoing insights in the development of a quantum graph neural network (QGNN) for image classification. The successful design and simulation of the graph encoding quantum circuit represent a significant milestone, demonstrating the feasibility of representing graph data in a quantum state for processing by a GNN.

The technical exploration has provided valuable insights into quantum state preparation and simulating quantum circuits using Qiskit, revealing challenges in integrating quantum computing with classical neural network architectures, particularly in data interfacing and algorithmic efficiency. The immediate focus is on integrating reinforcement learning techniques to optimize the QGNN's performance, aiming to dynamically tune the model based on empirical results to enhance document classification accuracy.

Although promising, the true efficacy and practicality of quantum-enhanced machine learning models will become clear through further development. If successful, the QGNN could advance document classification methodology and inspire future quantum computing applications in machine learning, potentially leading to the creation of new quantum algorithms optimized for graph-structured data.

In conclusion, while the project is still in development, the outcomes of upcoming phases will be crucial in determining the practical applications of the proposed QGNN model. The work to date lays a solid foundation, reflecting the innovative spirit of quantum machine learning research.

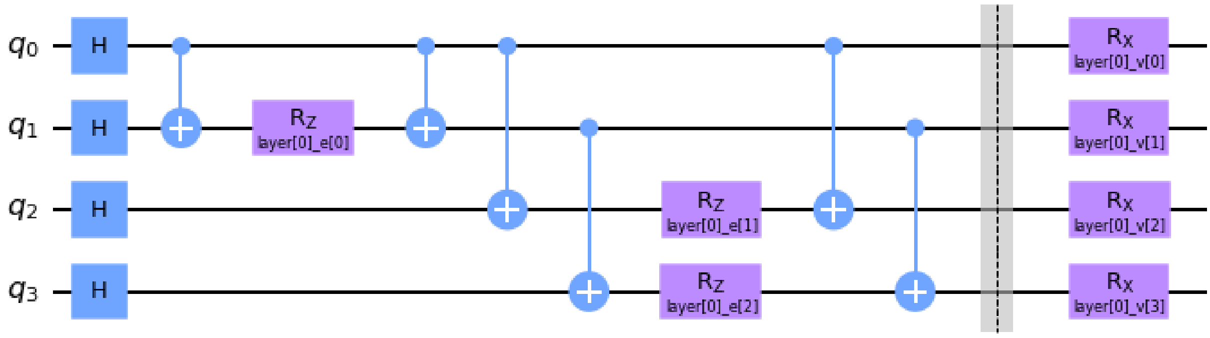

Fig. 1: Quantum Graph Encoding Circuit

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Code Availability

The full code used during all these first steps of the project can be found on our Github public repository[3].

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