Graph Neural Networks on Quantum Computers

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Graph Neural Networks (GNNs) are powerful machine learning models for analyzing structured data represented as graphs, demonstrating remarkable success in applications like social network analysis and recommendation systems [1]. However, classical GNNs face scalability challenges when dealing with large-scale graphs [2]. This paper proposes frameworks for implementing GNNs on quantum computers to potentially address the scalability challenges. We devise Quantum GNN architectures mirroring the the structure and functionality of three fundamental types of classical GNNs [3]: Graph Convolutional Networks (GCNs), Graph Attention Networks (GATs), and Message-Passing GNNs. Figure 1 and 2 present the overall circuit constructions for the three Quantum GNN architectures.

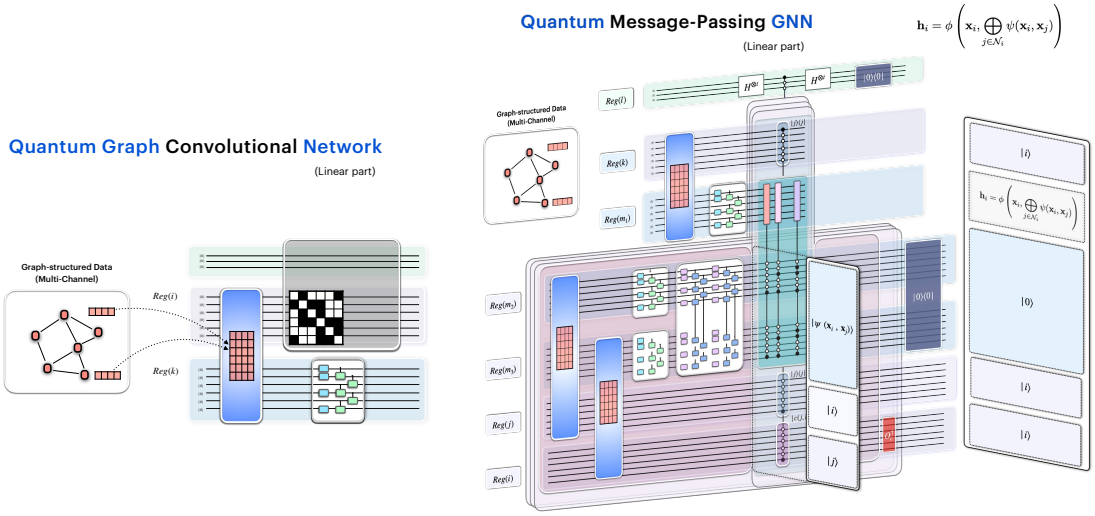

FIG. 1. *Overall circuit constructions for our Quantum Graph Convolutional Networks and Quantum Message-Passing GNNs.*

For GCNs, we develop quantum algorithms corresponding to the vanilla Graph Convolutional Networks (GCNs) [4] and two of its variants - the Simplified Graph Convolution (SGC) [5] and Linear Graph Convolution (LGC) [6]. A complexity analysis of the quantum SGC demonstrates potential quantum advantages (Table 1).

Algorithm	**Time Complexity**	**Space Complexity**[a]
Quantum SGC (Min. Depth)	$\tilde{O}(\log(1/\delta)\cdot(\log(NC)+\log(Ns)))$	$O(NC+N\log N\cdot s\log s)$
Quantum SGC (Min. Qubits)	$\tilde{O}(\log(1/\delta)\cdot(NC/\log(NC)+Ns\log s))$	$O(\log(NC))$
Classical SGC	$O(\lvert E\rvert C+NC^2))=O(NdC+NC^2)$	$O(\lvert E\rvert+NC+C^2)=O(Nd+NC+C^2)$

[a] space complexity in the quantum case refers to the number of qubits, including the ancilla qubits used by the circuit [7].

TABLE 1. Complexity comparison between quantum and classical SGC [5] for a single forward pass and cost function evaluation, with $K=2$ (where K is the number of layers in the original GCN formulation, though this concept becomes irrelevant in the context of SGC) and fixed precision parameters. N is the number of nodes, C is the number of features per node. $|E|$ is the number of edges. d is the average degree of the nodes in the graph. s is the maximum number of non-zero elements in each row/column of the normalized adjacency matrix. The quantum SGC provides a probabilistic result with a success probability of $1-\delta$.

When optimizing for minimal circuit depth, the quantum SGC achieves logarithmic time complexity in the input sizes (albeit at the cost of linear space complexity), providing a substantial speedup over classical SGCs. When optimizing for minimal qubit usage, the quantum SGC exhibits space complexity logarithmic in the input sizes, offering an exponential reduction compared to classical SGCs, while still maintaining better time complexity. The space-time trade-off provides flexibility to adapt to specific quantum hardware constraints and problem instances. Similar complexity improvements are shown for quantum LGC.

For GATs, we design quantum circuits to evaluate and store the attention scores between each pair of nodes, allowing the incorporation of self-attention mechanisms [8]. Our quantum GAT performs quantum linear algebraic operations to achieve the graph attention operation, updating each node's feature from the attention-scores-weighted features of its neighbors.

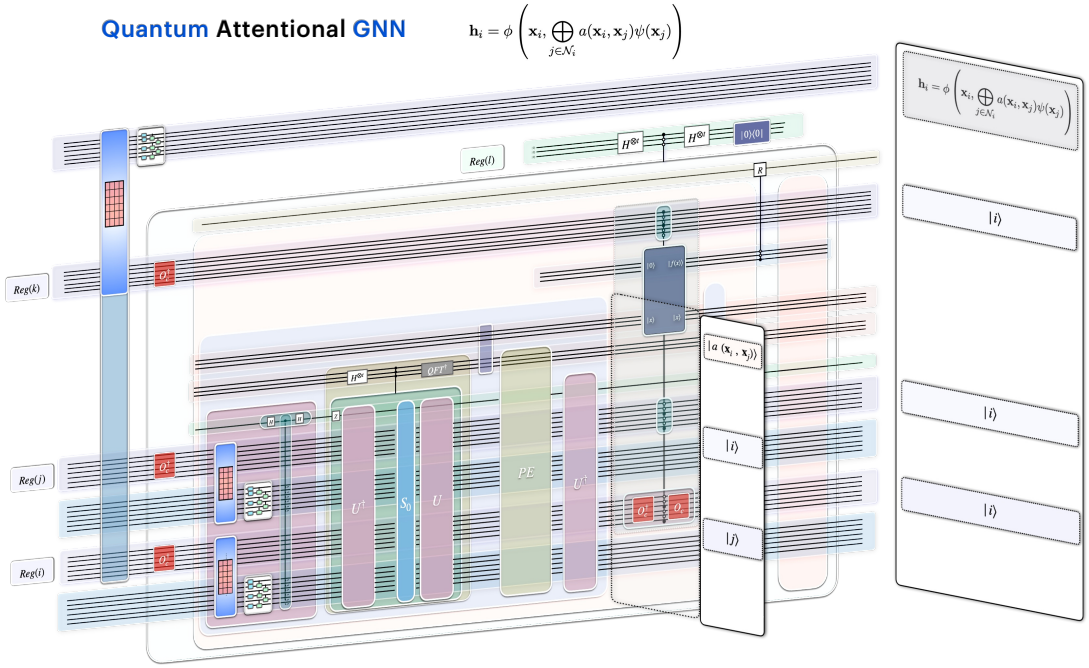

FIG. 2. *Overall circuit construction for our Quantum Graph Attention Networks.*

For Message-Passing GNNs, we propose a quantum algorithm to load and transform the node features according to the message-passing operation [9]. The training of our quantum GNNs can be performed using either classical or quantum optimization techniques [10].

The proposed quantum GNN architectures offer several advantages:

1. Improved Scalability: The logarithmic space and time complexities of the quantum SGC suggest that our quantum GNN frameworks can efficiently process large-scale graphs that are intractable for classical GNNs. This capability is particularly valuable in domains such as social network analysis, where graphs can reach billions of nodes, making it infeasible to store and process such graphs using classical computing hardware.

2. Inductive Bias Incorporation: By designing quantum circuits that respect the structure of graph-structured data, our quantum GNNs align with the principles of Geometric Quantum Machine Learning (GQML) [11], potentially leading to improvements over problem-agnostic quantum machine learning models.

3. Quantum-Classical Alignment: Our quantum GNN architectures are designed to closely mirror the functionality of classical GNNs, allowing the leverage of classical GNNs' proven effectiveness while harnessing quantum computing's power. This alignment facilitates the translation of insights and techniques from the well-established field of classical GNNs to the emerging area of quantum GNNs, paving the way for the development of more advanced architectures.

In conclusion, this work makes significant contributions to the emerging area of Quantum Graph Neural Networks by introducing quantum GNN architectures that go beyond generic parameterized quantum circuits, providing rigorous complexity analysis that demonstrates potential quantum advantages, and laying the foundation for harnessing the power of quantum computing in graph representation learning. These advances not only expand the theoretical understanding of quantum GNNs but also pave the way for their practical applications in real-world scenarios where classical GNNs face scalability challenges. As quantum hardware continues to advance, our quantum GNN frameworks provide promising avenues for developing scalable and efficient quantum-enhanced graph learning algorithms, opening up new possibilities for analyzing graph-structured data and tackling previously intractable problems in various domains.

A preprint of this work is available on ArXiv: https://arxiv.org/pdf/2405.17060.

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