Line Graph Quantum Embeddings for Learning on Edge-Centric Graphs

Luke J. Miller, PhD Student

Division of Computing, Analytics, and Mathematics, School of Science and Engineering, University of Missouri-Kansas City

Introduction

In many real-world systems, such as power grids and transportation networks, edges—not nodes—carry the most salient information. However, most graph learning models and quantum representations emphasize node-centric architectures. This misalignment limits the ability to capture edge-specific dynamics in learning tasks.

Graph line transformations, which map edges in the original graph to nodes in a derived graph, are a classical construct that has seen little exploration in quantum settings. This study addresses whether quantum encodings of line graphs can provide **a more expressive input space** for graph neural networks (**GNNs**), particularly in **edge-critical prediction tasks**.

Objectives: Goals and Hypotheses

This research has the following objectives:

- Evaluate whether **quantum state vector encodings** of **line graph node features** improve GNN performance on edge-focused tasks.
- **Benchmark line graph encodings** against direct edge-feature encodings on the original graph.
- Investigate the tradeoff between increased circuit width and potential gains in **structural expressivity** when using line graph-based embeddings.
- We hypothesize that **aligning qubits with edge representations** via line graphs, combined with quantum encodings, can enhance GNN accuracy on edge-importance classification tasks.

Methodology: Approach and Design

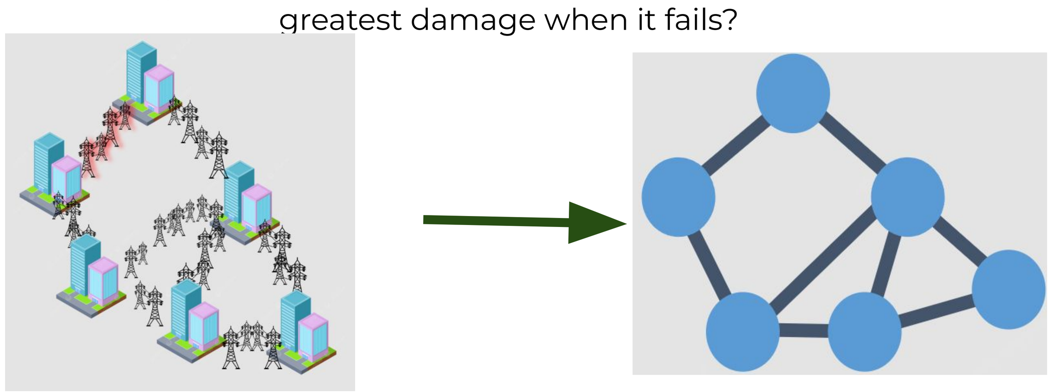
We construct synthetic power network topologies where edges represent critical infrastructure and are weighted by vulnerability. The task is to predict the edge whose removal would maximally disrupt the system.

- **Two** main **graph formats** are used:
  - **Original Graph**: Edges carry features; encoded directly via edgewise circuits.
  - **Line Graph:** Nodes represent edges in the original; node features encode edge weight.
- **Two quantum encoding strategies** are tested:
  - **Register-Based Binary Encoding**: Encodes features as binary strings across qubit registers.
  - **Amplitude-Based Rotation**: Uses scalar rotation gates proportional to edge weight, optionally with pairwise or full entanglement.
- Quantum circuits are simulated in **Qiskit**. Encoded graphs are input to a classical GCN implemented in **PyTorch Geometric**.

Methodology

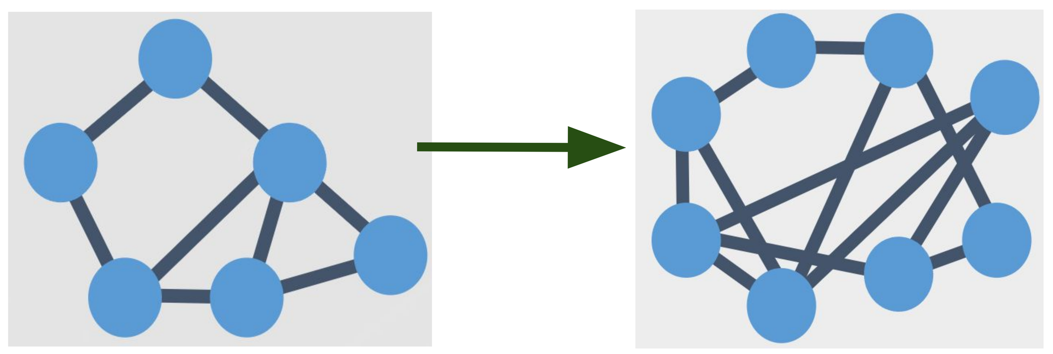
1. Synthetic Weighted Graph

Create a representation of a real problem. Which connection causes greatest damage when it fails?



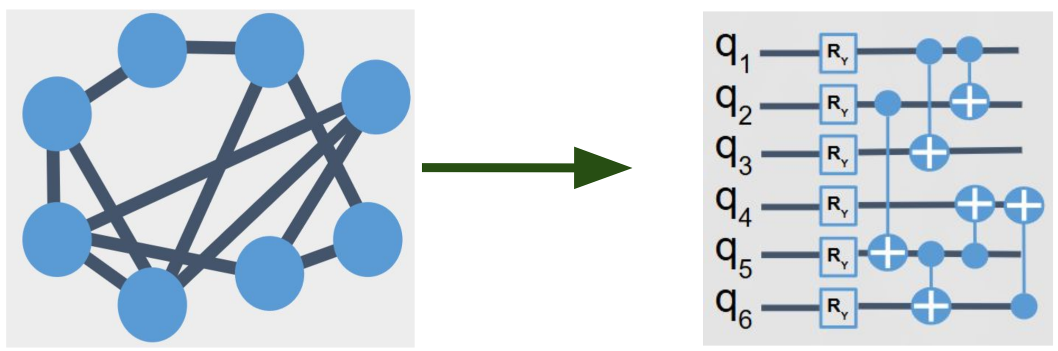
2. Convert to Line Graph

Turn adjacent edges into adjacent nodes. The representation works with existing architectures. Exposes most critical edges.



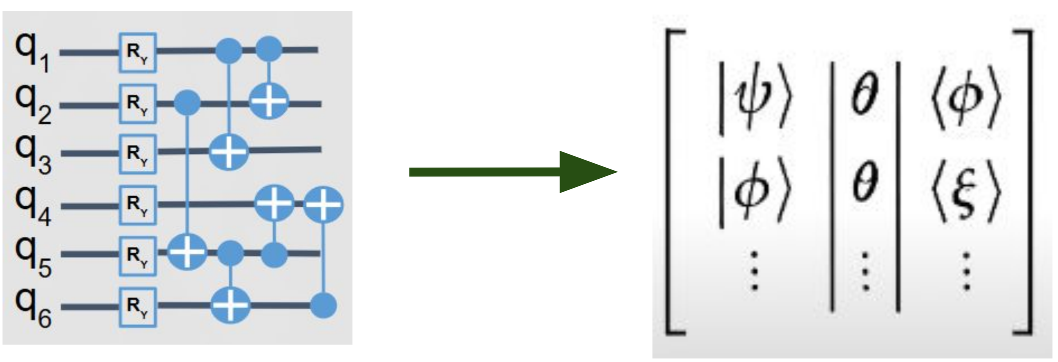
2. Encode Line Graph in Quantum Circuit

Manipulate qubits to encode weights and graph structure.4



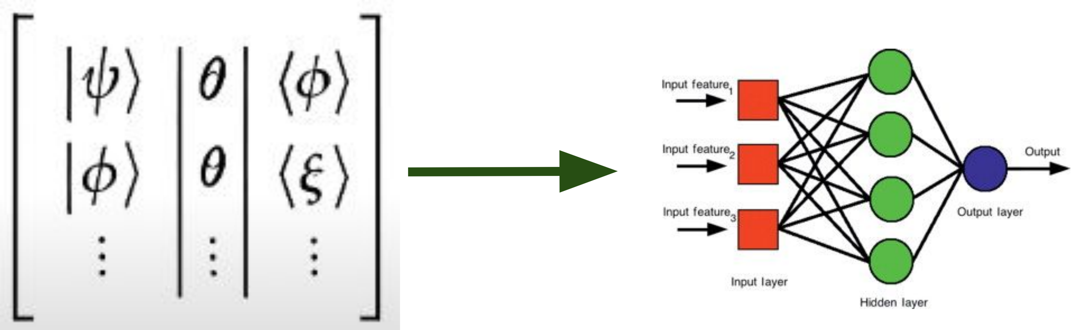
3. Extract State Vector from Quantum Circuit

Represent the entangled structure of the quantum circuit.



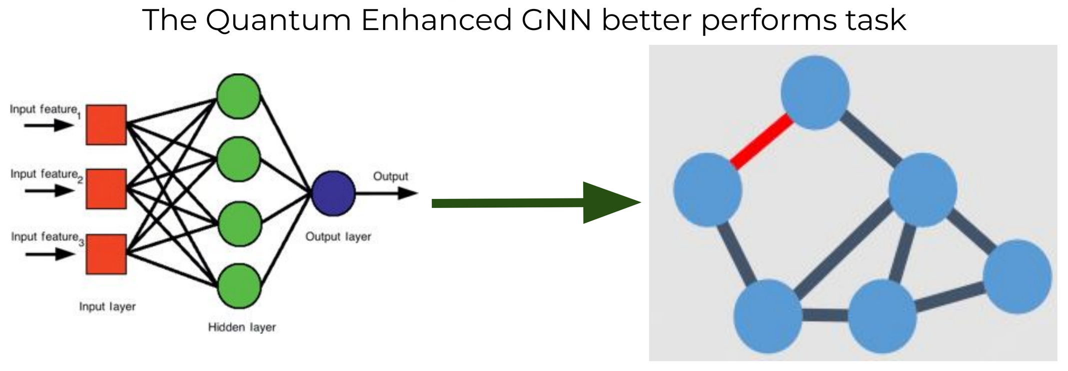
4. Pass State Vectors to GNN as Features

Use the learned representation to enable GNN training



5. Identify Vulnerabilities

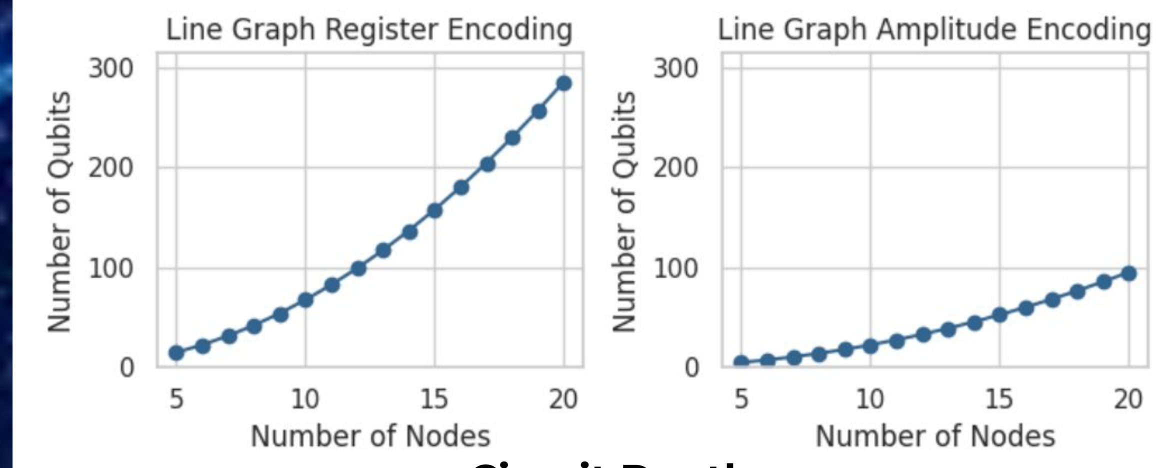
The Quantum Enhanced GNN better performs task



Resource Requirements and Accuracy

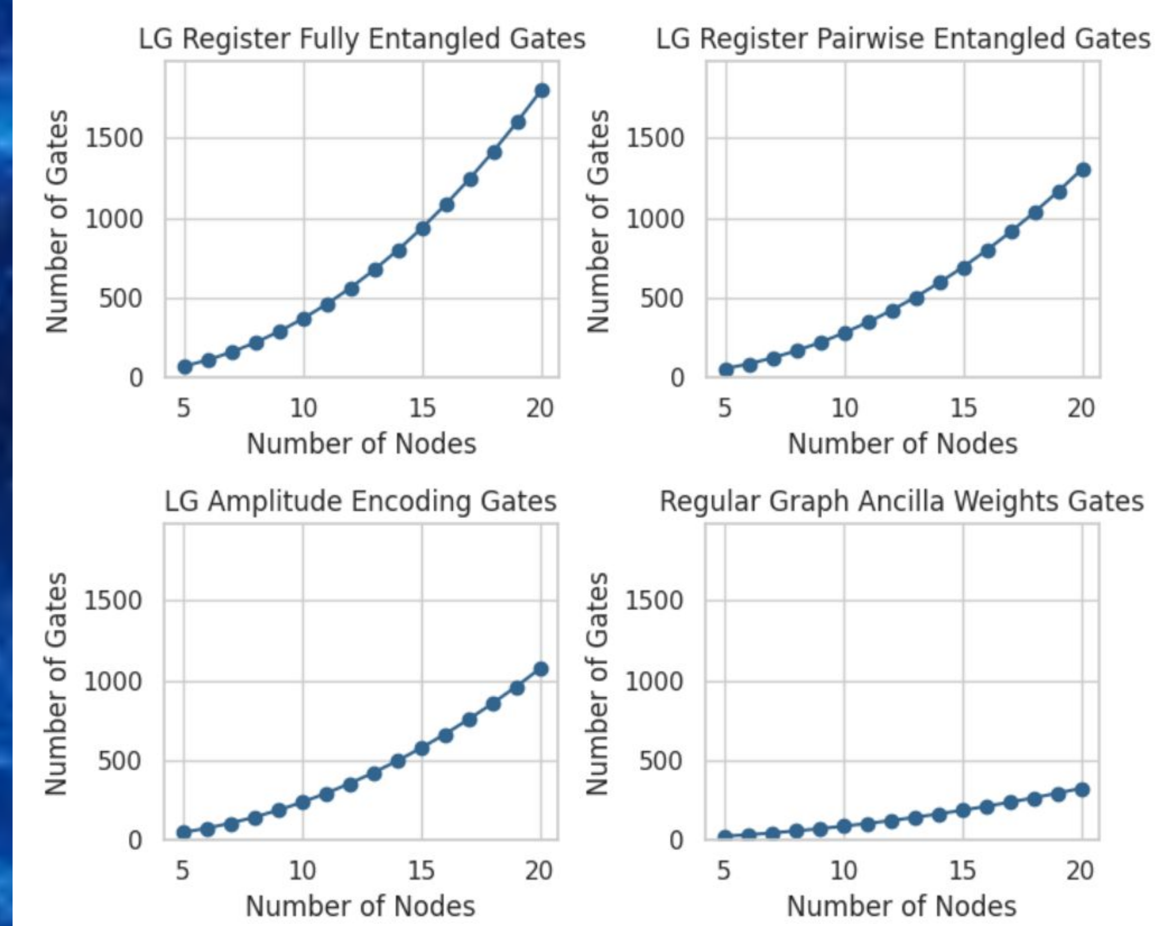
Circuit Width

Top Left: Line Graph Register Encoding **-** Qubit count increases quadratically with node count. Register-based encoding is the most resource-intensive method tested.
Top Right Line Graph Amplitude Encoding - Requires fewer qubits than register-based encoding, but still scales with the square of the number of nodes.



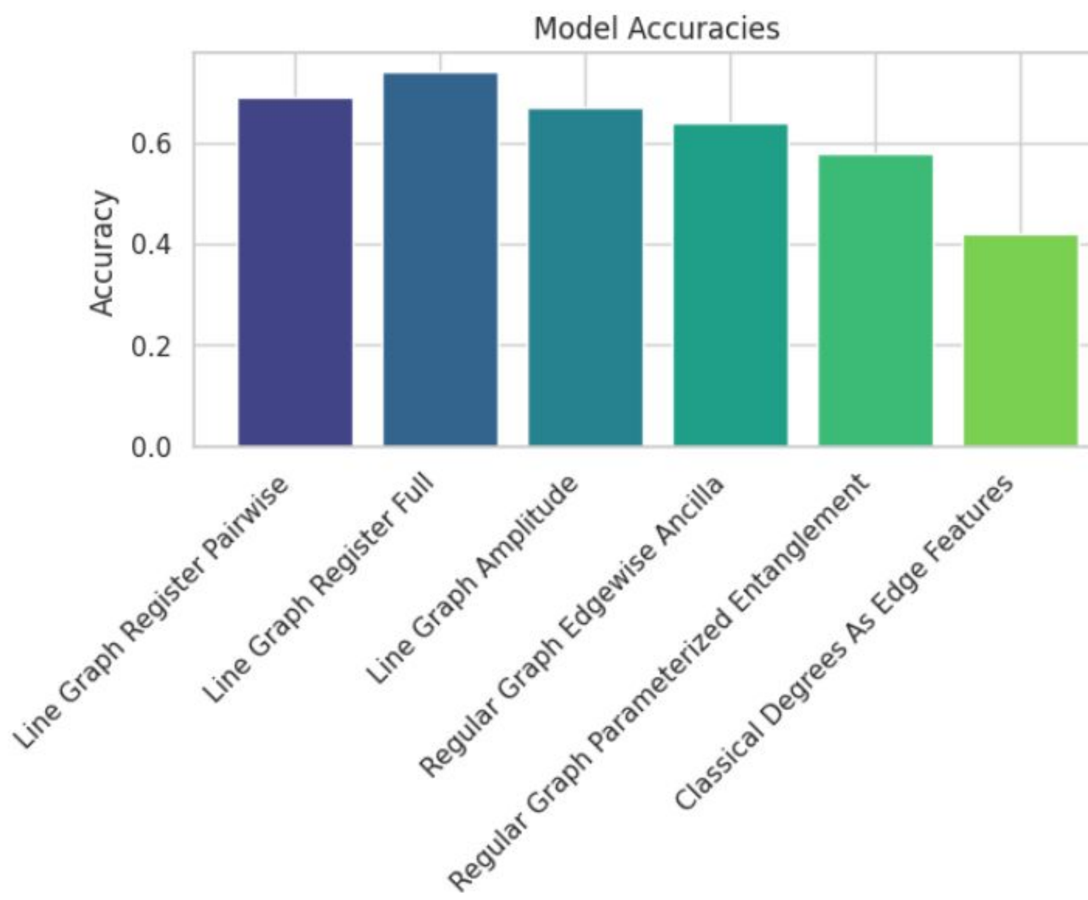
Circuit Depth

Top Left LG Register Fully Entangled Gates: Gate count grows fastest under full entanglement. This strategy achieved the highest accuracy.
Top Right LG Register Pairwise Entangled Gates**:** Pairwise entanglement reduces gate count compared to fully entangled circuits. Small accuracy drop.
Bottom Left LG Amplitude Encoding Gates - Amplitude encoding offers a middle ground—lower gate count with modest performance.
Bottom Right Plot Regular Graph Ancilla Gates - Classical edge-feature encoding on the original graph requires fewer gates, but also produced the lowest model accuracy.



Accuracy Across Encoding Strategies

Quantum line graph methods outperformed classical edge-feature baselines in this synthetic setting. Full entanglement with register encoding achieved the highest accuracy at 74%.



Discussion: Significance and Innovation

- Introduces classical line graph transformations into **quantum machine learning pipelines**.
- Mapping edges to nodes **enables direct alignment of qubits with edge features,** unlike node-centric methods.
- While circuit width increases, **line graphs capture connectivity, path adjacency, and neighborhoods.**
- Synthetic datasets support line graph quantum embeddings **improve learning on edge-focused tasks**.

Conclusion: Summary and Impact

- Demonstrates feasibility of **line graph quantum embeddings** for **edge-based predictions** using GNNs.
- Quantum encoding of edge features via line graphs **enhances structural representation** in input features.
- The proposed method offers a controlled testbed for evaluating **hybrid quantum-classical pipelines.**
- Especially effective for small or structurally sparse graphs, where **richer feature encoding** is valuable.

Future Work: Next Steps

- Extend benchmarks to **real-world infrastructure** datasets with known edge criticality.
- Explore integration with **fully quantum** graph learning architectures, quantum convolutional networks and quantum support vector machines.
- Analyze **circuit efficiency and decoherence tolerance** of line graph circuits on noisy intermediate-scale quantum (NISQ) devices.

Acknowledgments

- Advisor: Dr. Yugyung Lee
- Support: Division of Computing, Analytics, and Mathematics, School of Science and Engineering, UMKC
- Tools and simulation support: Qiskit

References

1. Langerer A. et al., Graph Neural Networks in Power Systems: State-of-the-Art and Future Directions, arXiv:2202.10859
2. Schuld M., Petruccione F., Machine Learning with Quantum Computers, Springer, 2021
3. Kipf T., Welling M., Semi-Supervised Classification with Graph Convolutional Networks, ICLR 2017
4. Koehler J., Quantum Machine Learning of Graph-Structured Data, Master's Thesis, Leibniz Universität Hannover, 2021
5. Kamalzadeh M. et al., Quantum Feature Embeddings for Graph Neural Networks, University of Hawai'i at Mānoa, 2023
6. Choudhary S. et al., Quantum Machine Learning Algorithm for Knowledge Graphs, KDD 2021, DOI: 10.1145/3467982
7. Xu Y. et al., A Quantum-based Transformer for Graph Representation Learning, arXiv:2412.02285
8. Torlay L. et al., Bond-Centric Shapley Value-Based Explanation Method for GNNs, Patterns, 3(3), 100519, 2022
9. Budhathoki K. et al., Edge-Centric Embeddings of Digraphs: Properties and Stability, Entropy, 27(3), 304, 2023
10. Wang Z. et al., Theoretical Insights into Line Graph Transformation on GNNs, arXiv:2410.16138