Comparing Graph Neural Network task choices on their stability in face of perturbations

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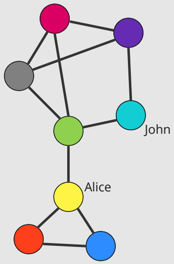
1. Background

Graph Neural Network (GNN) - solution to Machine Learning problems on graph data (i.e. a graph of connected friends) [1].
Perturbations - A modification done to a graph, i.e. an attack could remove a node [2].
Stability - A GNN's ability to keep its accuracy high in spite of perturbations [2].



Various tasks:

- Node Classification: Is John an accountant [1]?
- Link Prediction: Could John and Alice be friends [1]?
- Graph Classification: Is this structure a protein [1]?

2. Problem Definition

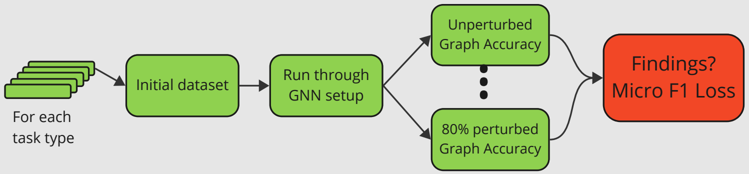
Main Research Question:

How does choice of task types, namely node classification, link prediction, graph classification, impact the stability of a GNN in the face of perturbations?

Why?

Identify weak points in GNNs to fend off potential attacks.

3. Methodology



Task	Dataset	Backbone	Graphs	Nodes	Edges	Features	Classes
Node Classification	Planetoid	Pubmed	1	19717	88648	500	3
Graph Classification	TUDatasetEnzymes	MUTAG	188	17.9	39.6	7	2
Link Prediction	Planetoid	Cora	1	2708	10556	1433	7

Table 1: Datasets used during the experiments per task

GNN setups:

- Graph Convolutional Network, makes use of global structure (spectral method) through normalized graph Laplacians and Fourier transforms [3].
- Graph Attention Network, only makes use of local structure (non-spectral). uses attention heads to use as edge weights [4].

Perturbation methods:

- Random Edge Removal
- Random Node Removal
- Edge Rewiring: Moving edges around to new locations

4. Results

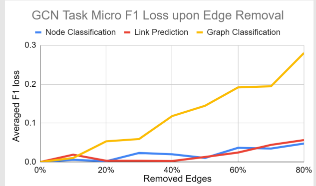


Figure 1: GCN (3 layers, 64 hidden channels each) results on Edge Removal. 25 trials per data point.

Experiment 1:
Initial Performance Comparison on GCN Edge Removal

- Graph Classification performs the worst.
- Link Prediction and Node Classification relatively stable.

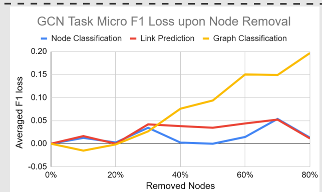


Figure 2: GCN (3 layers, 64 hidden channels each) results on Node Removal. 25 trials per data point.

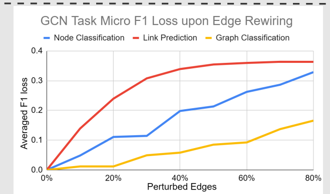


Figure 3: GCN (3 layers, 64 hidden channels each) results on Edge Rewiring. 10 trials per data point.

Experiment 2:
Performance Comparison on different perturbation methods

- Figure 2 has roughly the same results, but more inconsistent.
- Figure 3 has new results: Graph Classification now has the best stability, and Link Prediction the worst.

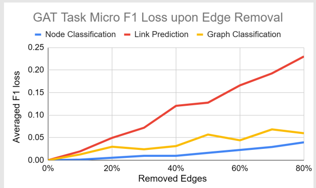


Figure 4: GAT (3 layers, 64 hidden channels each, 5 attention heads) Results on Edge Removal. 25 trials per data point.

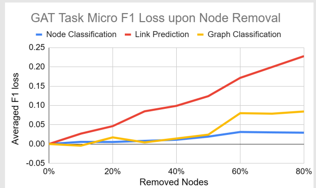


Figure 5: GAT (3 layers, 64 hidden channels each, 5 attention heads) Results on Node Removal. 25 trials per data point.

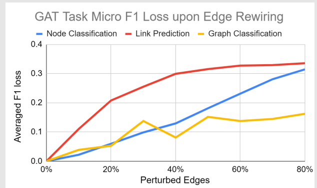


Figure 6: GAT (3 layers, 64 hidden channels each, 5 attention heads) Results on Edge Rewiring. 10 trials per data point.

Experiment 3:
Performance Comparison on different architectures (GAT)

- Under the GAT, Link Prediction performs the worst.
- In Figures 4 and 5 Node Classification performs the best.
- GAT Edge Rewiring (Figure 6) approaches similar results to GCN Edge Rewiring (Figure 3).

5. Conclusion

The GNN task seems to matter!
But there is no definitive ranking...

- Different architectures have different results. Graph Classification usually more stable under non-spectral GAT, Link Prediction always more stable under spectral method GCN.
- Different perturbation methods have different results.
- Link Prediction performed the worst in 4 out of 6 Figures.
- Graph Classification struggled the most under the GCN when removing items.
- Node Classification was never the least stable, though also not always the best.

6. Limitations + Future Work

Limitations:

- Limited computer hardware resulted in fewer trials, Figure 2 most affected.
- Link Prediction has more than one implementation: What if a different method was utilized?

Future Work:

- Compare more Link Prediction implementations: Which one is more stable?
- Explore architectures which are more resilient to Edge Rewiring.

Sources

[1] Aman, "A Comprehensive Introduction to Graph Neural Networks (GNNs)," *DataCamp*, 2024. https://www.datacamp.com/tutorial/comprehensive-introduction-graph-neural-networks-gnns-tutorial
[2] H. Kenlay, D. Thano, and X. Dong, "On the stability of graph convolutional neural networks under edge rewiring," in ICASSP 2021 - 2021 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), IEEE, June 2021
[3] T. N. Kipf and M. Welling, "Semi-supervised classification with graph convolutional networks," 2017.
[4] P. Velickovic, G. Cucurull, A. Casanova, A. Romero, P. Lio, and Y. Bengio, "Graph attention networks," 2018.