Unsupervised Link Prediction in Sparse Biomedical Knowledge Graphs for Clinical Insight Enhancement

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DATA 7300 Final Project Report | Fall 2024

December 10, 2024

1. Background
2. Dataset
3. Methodology
4. Model Architecture
5. Experiment and Results
6. Conclusion, Recommendations

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Main Focus

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Main Focus

- Biomedical knowledge graphs: Tools to analyze relationships between diseases, drugs, symptoms, and genes, [1].
- Challenge: Graph sparsity limits clinical applications.
- Example: Hetionet (47,031 nodes, 2,250,197 edges; density: 0.10%).
- **Objective:** Predict unknown links using unsupervised techniques to enhance clinical insights.

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- Leverage GraphSAGE and PubBERT for structural and semantic feature learning.
- Validate the models effectiveness for clinical applications like drug repurposing and disease diagnosis.

Related Work

- **Hetionet:** Aggregates diverse biomedical data for applications like drug discovery and precision medicine.
- **Traditional Approaches:** Heuristic methods like common neighbors, supervised embeddings (Node2Vec, DeepWalk).
- Graph Neural Networks (GNNs) like GCNs, GATs, and GraphSAGE.
- Addressing sparsity in biomedical graphs with unsupervised methods.

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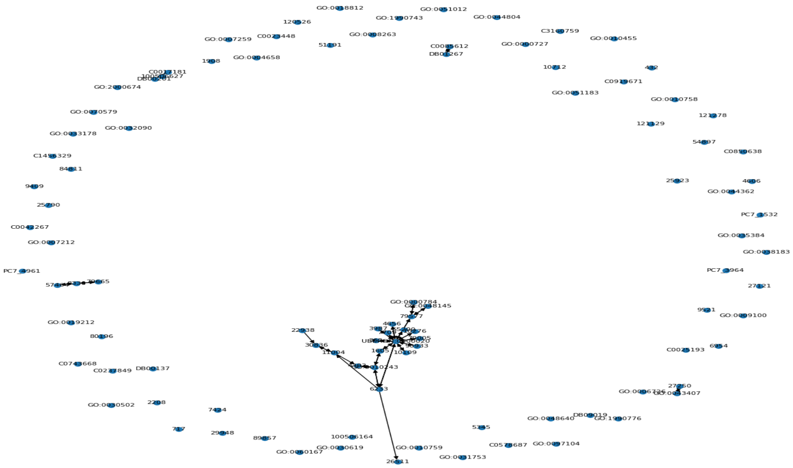
- **Edges: Relationships like treats, interacts, associates.**

Dataset Overview



Dataset Stats

Nodes: 47,031, Edges: 2,250,197, Density: 0.10%.

Preprocessing: Extracted **k-core subgraph** to reduce sparsity.

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Methodology

Data Preprocessing:

- Sampled 60% connected, 40% unconnected nodes.

Graph Representation Learning:

Link Prediction:

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Link Prediction:

- Similarity scoring, thresholding, *validation.*

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Model Architecture

Components:

- PubMedBERT: Captures semantic features.

Layers:

Training:

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- Three SAGEConv Layers with ReLU activation.

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Training:

- Positive and negative sampling.
- Loss function: Binary cross-entropy.

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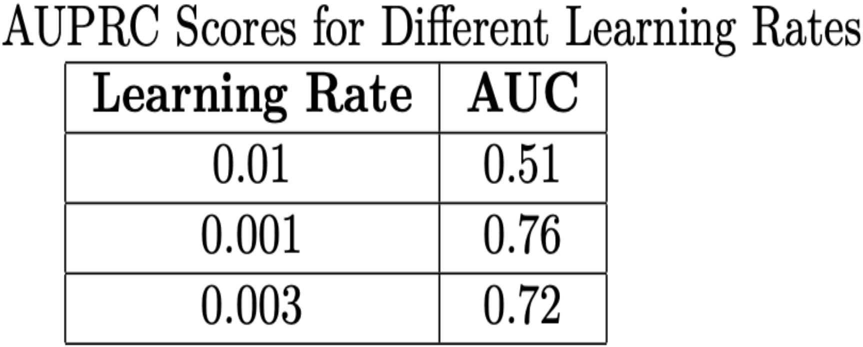
Experiment & Results



AUPRC Scores for Different Learning Rates

Learning Rate	AUC
0.01	0.51
0.001	0.76
0.003	0.72

Figure 2:

Limitations and Challenges

- Sparsity: Limits link prediction.
- Data Imbalance: Affects negative sampling.
- Performance Limitations: Modest AUPRC (0.508).
- Threshold Sensitivity: High threshold excludes plausible links.

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Conclusion

- Demonstrated utility of GraphSAGE and PubBERT for sparse graphs.
- Challenges highlight areas for future improvement in graph-based machine learning.

Recommendations

- Graph augmentation methods to address sparsity.
- Experiment with sparsity reduction methods.

Future Directions

- Validate predicted links with biomedical experts.
- Experiment with advanced architectures (e.g., GATs).
- Consider other embedding methods for text features of node.

References

1. Himmelstein DS, Lizee A, Hessler C, et al. Systematic integration of biomedical knowledge prioritizes drugs for repurposing. Elife 2017;6:e26726.

Thank you!