Link Prediction In Social Network with Graph Neural Network

A Report Submitted
in Partial Fulfillment of the Requirements
for the Degree of
Bachelor of Technology
in
Computer Science & Engineering

by
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to the
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ALLAHABAD PRAYAGRAJ
May, 2024

UNDERTAKING

I declare that the work presented in this report titled "*Link Prediction In Social Network with Graph Neural Network*", submitted to the Computer Science and Engineering Department, Motilal Nehru National Institute of Technology Allahabad, Prayagraj, for the award of the ***Bachelor of Technology*** degree in ***Computer Science & Engineering***, is my original work. I have not plagiarized or submitted the same work for the award of any other degree. In case this undertaking is found incorrect, I accept that my degree may be unconditionally withdrawn.

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CERTIFICATE

Certified that the work contained in the report titled "*Link Prediction In Social Network with Graph Neural Network*", by
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Tanya Dixit, 20214126, has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

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Preface

This project report delves into link prediction within social networks using graph neural networks (GNNs), aiming to forecast future connections. By merging social network analysis principles with GNN mechanics, we've devised a novel approach for this task. Our methodology emphasizes practicality and interpretability, ensuring applicability in real-world scenarios. Through extensive experimentation on diverse datasets, we've validated the effectiveness of our approach.

This project owes its success to the invaluable support of mentors and collaborators, whose guidance shaped its trajectory. We envision this report as a catalyst for further innovation in link prediction and GNN research, aiming to unlock actionable insights within social networks.

Abstract

This project report explores the application of Graph Neural Networks (GNNs) for link prediction in social networks. It discusses the significance of link prediction in facilitating information dissemination and understanding social dynamics. The report introduces the theoretical underpinnings of GNNs, highlighting their ability to capture complex structural patterns and semantic information in social graphs. The proposed approach involves a multi-layered architecture integrating Graph Convolutional Networks (GCNs), and GraphSAGE to leverage both local and global network features for enhanced prediction accuracy. Experimental evaluations on benchmark social network datasets demonstrate the superior performance of the proposed GNN-based approach compared to state-of-the-art baselines. The findings underscore the efficacy of GNNs in uncovering latent connections and adapting to evolving network structures over time. The insights gained from this research have implications for improving recommendation systems, personalized marketing strategies, and understanding social dynamics in the digital age. The algorithm achieved an impressive accuracy rate of 84.15% after running for 195 epochs.

Contents

Chapter 1

Introduction

Link prediction in social networks involves forecasting the likelihood of connections between nodes within a network, such as friendships or collaborations. Graph neural networks (GNNs) have become instrumental in this task due to their capacity to model complex relational structures found in social networks.GNNs work directly on graph-structured data, enabling them to capture both local and global patterns within the network. By learning representations of nodes that incorporate structural and feature information from their neighbors, GNNs can predict the existence of links between nodes effectively.

In link prediction, GNNs utilize techniques like message passing, graph convolution, and attention mechanisms to update node representations iteratively and predict link probabilities. These models leverage network topology and node attributes to make accurate predictions, even with incomplete or noisy data.

Overall, link prediction with graph neural networks offers a promising approach to uncovering hidden relationships and forecasting future connections in social networks, with applications ranging from recommendation systems to understanding social dynamics and community detection..

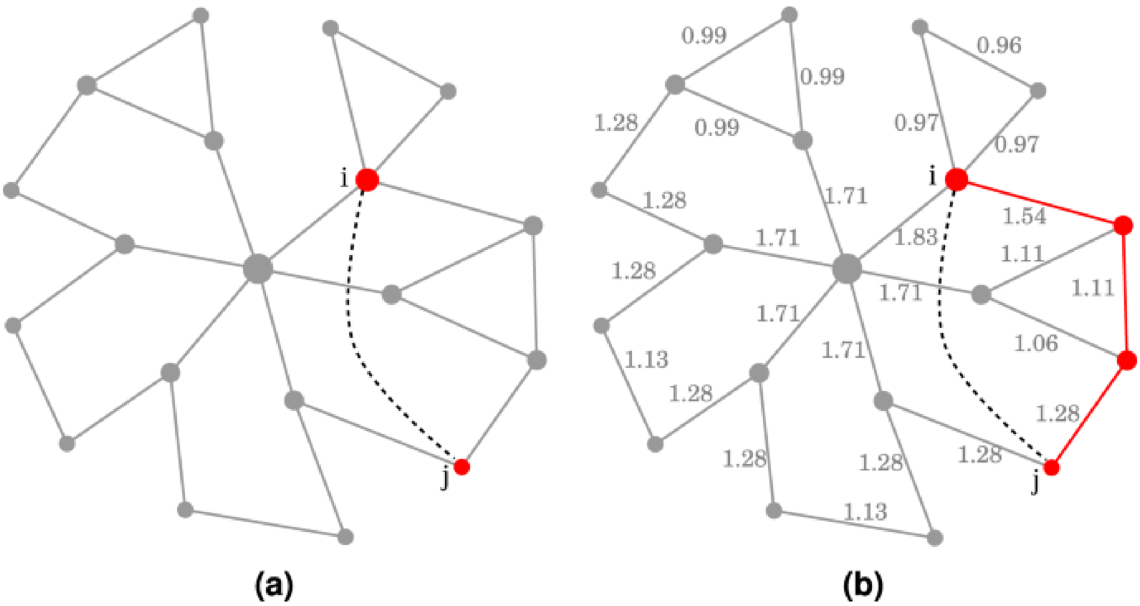

Fig.1: Example of link prediction

Dataset	#Nodes	#Edges	Avg. node deg.	Density	Attr. Dimension
Cora	2708	10556	3.90	0.2880%	1433
Citeseer	3327	9104	2.74	0.1645%	3703
Pubmed	19717	88648	4.50	0.0456%	500
USAir	332	4252	12.81	7.7385%	-
NS	1589	5484	3.45	0.4347%	-
PB	1222	33428	27.36	4.4808%	-
Yeast	2375	23386	9.85	0.8295%	-
C.ele	297	4296	14.46	9.7734%	-
Power	4941	13188	2.67	0.1081%	-
Router	5022	12516	2.49	0.0993%	-
E.coli	1805	29320	16.24	1.8009%	-

Fig. 2: Example of datasets used in link prediction

1.1 Motivation

Link prediction in social networks is still a relatively new problem as of this writing, with the seminal study on the subject, published only in 2003. As a result, there is much room for improvement in the methods used to solve the issue. Temporal methods have been entirely disregarded by

Researchers have used a network at one point in time for the majority of their study . Additionally, these networks have typically been tiny, with fewer nodes than what would fit in a memory-based adjacency matrix. This results in irrational analytical methods because most real-world analysis would be carried out on enormous criminal intelligence databases, which would include extensive Internet email logs. Additionally, researchers have not made a distinction between link detection and link forecast and it appears that the issues are taken for granted that they are the same. Almost 80% of the papers that are taken into consideration do not differentiate between the issues. Link detection isn't even discussed in many articles. It describes how metrics can be modified to calculate more quickly and the differences between link identification and prediction. A mathematical and statistical method called link prediction has numerous applications in the economic, social, and software domains. There are numerous uses for link prediction.

- Identifying the composition of a criminal network, for instance, involves forecasting inadequate data to identify gaps in a criminal network).
- Using collaborative filtering to solve the data-sparsity issue in recommender systems.
- Quickening the formation of a mutually beneficial academic or professional relationship that would have taken longer to occur by accident.
- Enhancing hypertext analysis for search engines and information retrieval.
- Keeping an eye out for and managing computer infections that spread via email .
- Making predictions about the pages visitors will visit next to enhance the effectiveness and efficiency of a website's navigation.
- Assisting in the forecasting of an entity's network-wide spread. Examples include an illness like HIV or information like rumors or a certain style of clothes.

1.2 Problem and Idea

Link prediction in social networks is challenging due to the inherent sparsity and noise in the data, as well as the evolving nature of social interactions. Traditional methods for link prediction often rely on handcrafted features or simplistic graph-based algorithms, which may not capture the complex patterns present in real-world social networks. Hence, there is a need for more advanced techniques that can effectively model the underlying structure and dynamics of social networks.

The objective of this project is to explore the use of Graph Neural Networks (GNNs) for link prediction in social networks. GNNs have shown promising results in various graph-related tasks by leveraging the graph structure and node attributes to learn powerful node representations. By applying GNNs to the task of link prediction, we aim to capture the latent features of nodes and their relationships, thus improving the accuracy and robustness of predictions in social networks.

- Data Preprocessing: We start by preprocessing the raw social network data, including cleaning, normalization, and feature extraction. We represent the social network as a graph where nodes correspond to individuals and edges represent their connections.

- Graph Neural Network Architecture: We design a GNN architecture tailored for link prediction tasks in social networks. The GNN will consist of multiple layers of graph convolutional operations, which aggregate information from neighboring nodes to update the node representations.

- Training and Evaluation: We train the GNN model using a subset of the social network data with known links. We employ techniques such as mini-batch training and early stopping to prevent overfitting. The model performance is evaluated using standard evaluation metrics such as precision, recall, and F1-score on a held-out validation set.

In this project, we propose to tackle the problem of link prediction in social networks using Graph Neural Networks. By leveraging the power of GNNs to capture complex dependencies in graph-structured data, we aim to improve the accuracy and robustness of link predictions in social networks. This research has the potential to advance our understanding of social network dynamics and facilitate the development of more effective social network analysis techniques

Given a social network $G(V, E)$ in which an edge represents interactions between its vertices on nodes at a given time t, the Link Prediction Problem aims to forecast modifications to the network. Liben-Nowell and Kleinberg describe it as predicting the edges that will be added to the network during the interval from time t to a given future time t'. The problem involves a training interval $[t_0, t_{00}]$ and a test interval $[t_1, t_{01}]$.

1.2.1 Node Neighborhood Algorithms

Node neighborhood algorithms, such as Common Neighbors, Jaccard Coefficient, Adamic/Adar, and Preferential Attachment, focus on local features of the network, considering the number of common friends between two nodes to predict future linkage.

- *Common Neighbors*

The Common Neighbors method provides a measure for similarity by calculating the intersection of the sets of neighbors of the nodes to predict future linkage:

$$CN(x, y) = |N(x) \cap N(y)|$$

- *Jaccard Coefficient*

Jaccard's coefficient measures the number of shared neighbors between two nodes relative to all the neighbors of both nodes:

$$J(x, y) = \frac{|N(x) \cap N(y)|}{|N(x) \cup N(y)|}$$

■ *Adamic/Adar*

Adamic/Adar measures the similarity between nodes based on shared neighbors, emphasizing nodes with few common neighbors:

$$AA(x, y) = \sum_{z \in N(x) \cap N(y)} \frac{1}{\log(|N(z)|)}$$

1.2.2 Path Based Algorithms

Path based algorithms, such as Katz, SimRank, Hitting Time, and Commute Time, consider all paths between two nodes.

1.2.3 Meta-Approaches

Meta-approaches, like low-rank approximation and clustering, alter the data before applying algorithms.

1.2.4 Bayesian Probabilistic Model

Probabilistic relational models capture interactions between attributes and link structures, aiding in predicting links based on attributes of related entities.

1.2.5 Linear Algebraic Method

Linear algebraic methods directly operate on the graph adjacency or Laplacian matrix, reducing the link prediction problem to a one-dimensional regression problem.

Chapter 2

Overview and Related Work

A sociogram's nodes are connected by an intricate web of relationships that evolve over time. Individuals' positions within the network, their actions, and the environment's influence all play a role in the emergence, strengthening, and degradation of these ties. The Link Prediction Problem is the task of forecasting modifications to a social network. As explained by Liben-Nowell and Kleinberg, it is:

Given a snapshot of a social network at time t, we seek to accurately predict the edges that will be added to the network during the interval from time t to a given future time t'.

The problem is illustrated in the graphs below, where a link is forming between the orange nodes. This scenario represents a common task in social network analysis known as "link prediction." In social networks, nodes often represent entities such as users, and edges represent relationships or interactions between these entities.

This predictive task holds significant implications for various applications, including recommendation systems, community detection, and anomaly detection, contributing to a deeper understanding of social dynamics and network evolution.

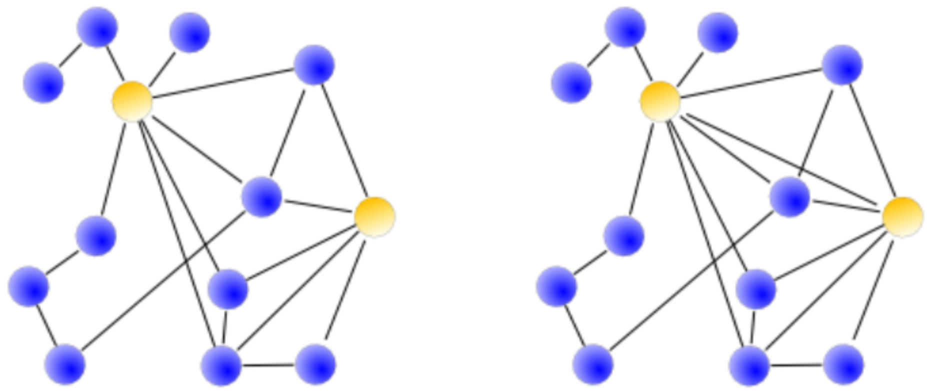

Fig. 3-4: A graph where a link is forming at time step t and where a link has been formed at time step t+1

Given below is an overview of the work studying link prediction:

2.0.1 Popescul and Ungar (2003)

- Paper: Citation prediction systems using statistical learning techniques
- Year: 2003
- Developed citation prediction systems using statistical learning techniques that extended inductive logic programming.
- Learnt link prediction patterns from queries to a relational database, incorporating joins, selections, and aggregations.

2.0.2 Taskar, Abbeel, and Koller

- Paper: Relational Markov models for learning patterns of cliques and transitivity in web pages and hyperlinks
- Year: Unknown
- Utilized relational Markov models to learn patterns of cliques and transitivity in web pages and hyperlinks.
- Incorporated node attributes (e.g., web page text) alongside relational features, enhancing prediction accuracy.

2.0.3 Popescul and Ungar (2004)

- Paper: Enhanced link prediction of author-document bipartite networks
- Year: 2004
- Enhanced link prediction of author-document bipartite networks by employing clustering.
- Clustered documents and authors by topic and research community, generating new entities used in logistic regression of features and relations.

2.0.4 Zhou and Scholkopf

- Paper: Discrete calculus for graphs: classification, ranking, and link prediction
- Year: Unknown
- Approached classification, ranking, and link prediction in graph problems using discrete calculus for graphs.
- Shifted classical regularization from the continuous case to graph data, though empirical testing was not included.

2.0.5 Liben-Nowell and Kleinberg

- Paper: Proximity metrics for link prediction in social networks
- Year: Unknown
- Tested the predictive power of proximity metrics, including common neighbors, Katz measure, and variants of PageRank.
- Found that some measures had predictive accuracy of up to 16%.
- Hypothesized that link prediction could be performed from topology alone, which was validated through empirical testing, but with limitations due to network size constraints.

2.0.6 Getoor and Diehl (2005)

- Paper: Survey of link analysis in social networks
- Year: 2005
- Summarized various link prediction papers in their survey of link analysis.

2.0.7 Additional Papers

- *Huang, Li, and Chen*
  - Paper: Enhancing collaborative filtering with link prediction in recommender systems
  - Year: Unknown
  - Explored link prediction's utility in enhancing collaborative filtering for recommender systems.
  - Found the Katz measure to be the most effective, followed by preferential attachment, common neighbors, and the Adamic-Adar measure.
  - Path-based and neighbor-based measures outperformed simpler metrics, with distance between nodes proving less useful due to short path connections in their dataset.

- *Farrell, Campbell, and Myagmar*
  - Paper: Academic networking: link prediction for new connections
  - Year: Unknown
  - Implemented link prediction to develop a system recommending new academic connections at a computer science conference.
  - Received feedback through a survey, revealing that established researchers found the system less useful compared to newer researchers.
  - Advocated for relation-oriented computing, emphasizing the potential of social network systems in managing professional contacts.

- *Zhu*
  - Paper: Predicting users' next web page visits with link prediction
  - Year: Unknown
  - Utilized link prediction to predict users' next web page visits, aiming to enhance site navigation and efficiency.
  - Employed Markov chain modeling to store lists of visited web pages, deviating from the assumption of independent link formation typical in social networks.
  - This approach assumes a sequential link formation process, unlike the sporadic link formation observed in social networks.

Chapter 3

Proposed Work

3.1 Dataset

The dataset utilized for link prediction in this study originates from snap.stanford.edu, a repository of large-scale network datasets. Specifically, the dataset contains a collection of graph instances representing various social networks. These networks encompass diverse domains such as academic collaborations, online social platforms, and communication networks. Each graph instance consists of nodes representing individuals or entities and edges denoting relationships or interactions between them. While the exact composition of the dataset may vary, it typically includes attributes associated with nodes and edges, facilitating the exploration of both topological and attribute-based link prediction techniques. Detailed statistics regarding the size, structure, and characteristics of the dataset are typically provided, enabling researchers to effectively analyze and evaluate their link prediction algorithms.

3.2 Technologies Used

In developing our project, we utilized a range of technologies such as:

- **Python and Python Standard Library**: Python is widely used in machine learning because of its ease of use, flexibility, and large ecosystem of libraries and tools.It provides a wide range of machine learning algorithms that can be used for tasks such as regression, classification, clustering, and dimensionality reduction. The code also makes use of standard Python libraries for general-purpose programming tasks and functionalities, such as itertools for generating combinations and permutations, scikit-learn is used for computing the AUC score (roc-auc-score) for evaluating the performance of the trained model on the test set and NumPy and SciPy are fundamental libraries for numerical computing and scientific computing in Python.

- **PyTorch**: PyTorch is a popular deep learning framework primarily used for building and training neural networks. The code uses PyTorch for defining and training the GraphSAGE model (GraphSAGE), implementing the predictor (DotPredictor), computing loss functions, performing backpropagation, and updating model parameters using optimizers.

- **Deep Graph Library(DGL)**: DGL is a Python library built for deep learning on graphs. It provides a wide range of functionalities for creating, manipulating, and training graph neural networks (GNNs). In the code, DGL is used for loading and preprocessing the Cora dataset, creating and manipulating graphs, implementing GraphSAGE layers (SAGEConv), and performing operations on nodes and edges.

- **Google Colab**: Google Colab offers a platform for data exploration and analysis through Jupyter notebooks, empowering users to manipulate and visualize data using Python. Within the notebook environment, users can seamlessly write and execute code, facilitating the creation and testing of machine learning models directly within the Colab interface.

3.3 Project Implementation

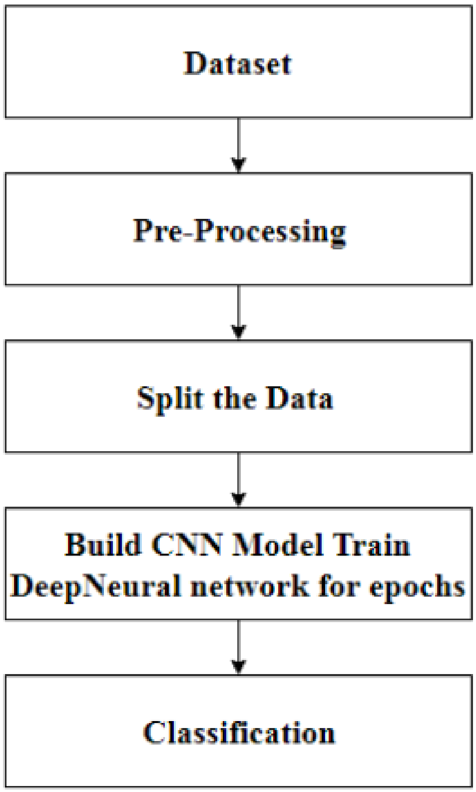

Fig. 5: Proposed work flow of Link Prediction

3.3.1 Program Flow

- **Imports and Setup:** This section includes importing necessary libraries and setting up the environment, including checking for GPU availability and updating data visualization settings.

- **Data Loading and Preprocessing:** Loading the Cora dataset using 'dgl.data.CoraGraphDatase Obtaining the graph (g) and spliting the edge set into training and testing sets as to prepare positive and negative edges for training and testing.

- **Model Description:** Implementing a two-layer GraphSAGE model ('GraphSAGE') using 'dgl.nn.SAGEConv' and Define a predictor (DotPredictor) to compute edge scores based on dot product of node features.

- **Loss Function and Optimizer:** Using binary cross-entropy loss (compute-loss) for training and Adam optimizer for updating model parameters.
- **Training:** Iterate over epochs, compute loss, perform backpropagation, and update model parameters. Monitor loss during training.
- **Training:** Iterate over epochs, compute loss, perform backpropagation, and update model parameters. Monitor loss during training.
- **Testing and Evaluation:** Lastly, the model is tested on test dataset, and predictions are made and displayed alongside. Computing AUC score using the trained model on the test set.

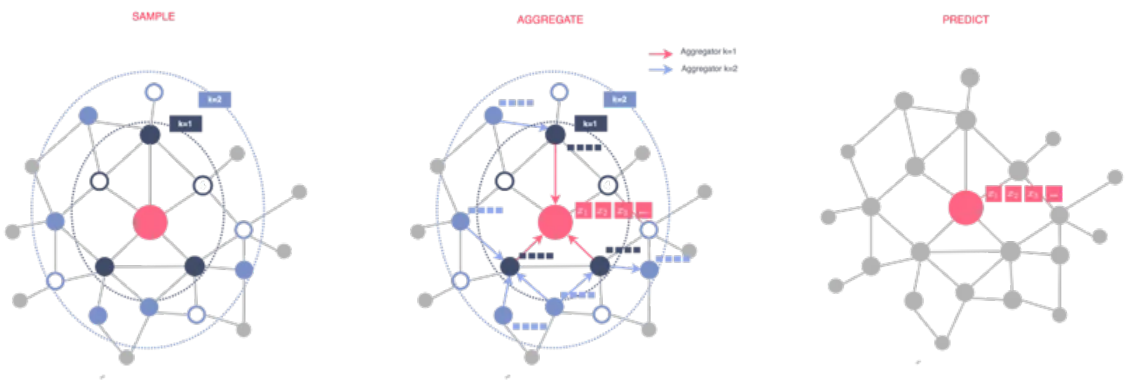

Fig. 6: Workflow

Chapter 4

Experimental Setup & Result Analysis

After training the model the maximum frequency in 195 epochs turned out to be 84.15%. Following are the detailed results out of each epoch.

4.0.1 Result Analysis

- *Accuracy:*

Accuracy measures how well a machine learning model can correctly predict or classify a given set of data. It is calculated as the ratio of the number of correct predictions to the total number of predictions made by the model.

$$Accuracy = \frac{Correctlypredictedsamples}{Totalsamples}$$

- *Precision:*

Precision is the percentage of true positive predictions.

$$Precision = \frac{TP}{TP + FP}$$

▮ *Recall:*

Recall calculates the percentage of true positive predictions out of all actual positive cases in the data.

$$Recall = \frac{TP}{TP + FN}$$

▮ *Receiver Operating Characteristic (ROC) Curve:*

The Area Under the Receiver Operating Characteristic (ROC) Curve (AUC) is used as a performance metric. The ROC curve and AUC provide valuable insights into the classification performance of the model, especially in binary classification tasks like link prediction.

- **Prediction and Scoring:** After training, the model makes predictions for both positive and negative edges in the test set. For each edge, the dot product predictor computes a score representing the likelihood of the edge being positive.

- **ROC Curve:** The ROC curve is a graphical plot that illustrates the performance of a binary classification model across various threshold settings. The true positive rate (Sensitivity) is plotted on the y-axis, and the false positive rate (1 - Specificity) is plotted on the x-axis. For each possible threshold value, the true positive rate and false positive rate are computed based on the predicted scores and corresponding ground truth labels. By varying the threshold, different points are plotted on the ROC curve, representing the trade-off between sensitivity and specificity.

- **AUC Calculation:** The AUC is calculated by computing the area under the ROC curve. A perfect classifier would have an AUC of 1.0, indicating that it achieves a true positive rate of 1 and a false positive rate of 0 across all threshold settings. A random classifier would have an AUC of 0.5, indicating that its performance is no better than random guessing. The AUC provides a single scalar value that summarizes the model's ability to distinguish between positive and negative examples. Higher AUC values indicate better performance.

- **Interpretation:** A higher AUC indicates better discrimination ability of the model: it can effectively distinguish between positive and negative examples. An AUC of 0.5 suggests that the model's performance is no better than random guessing. The ROC curve and AUC are useful for evaluating and comparing different models, especially in scenarios where class imbalance or different misclassification costs are present.

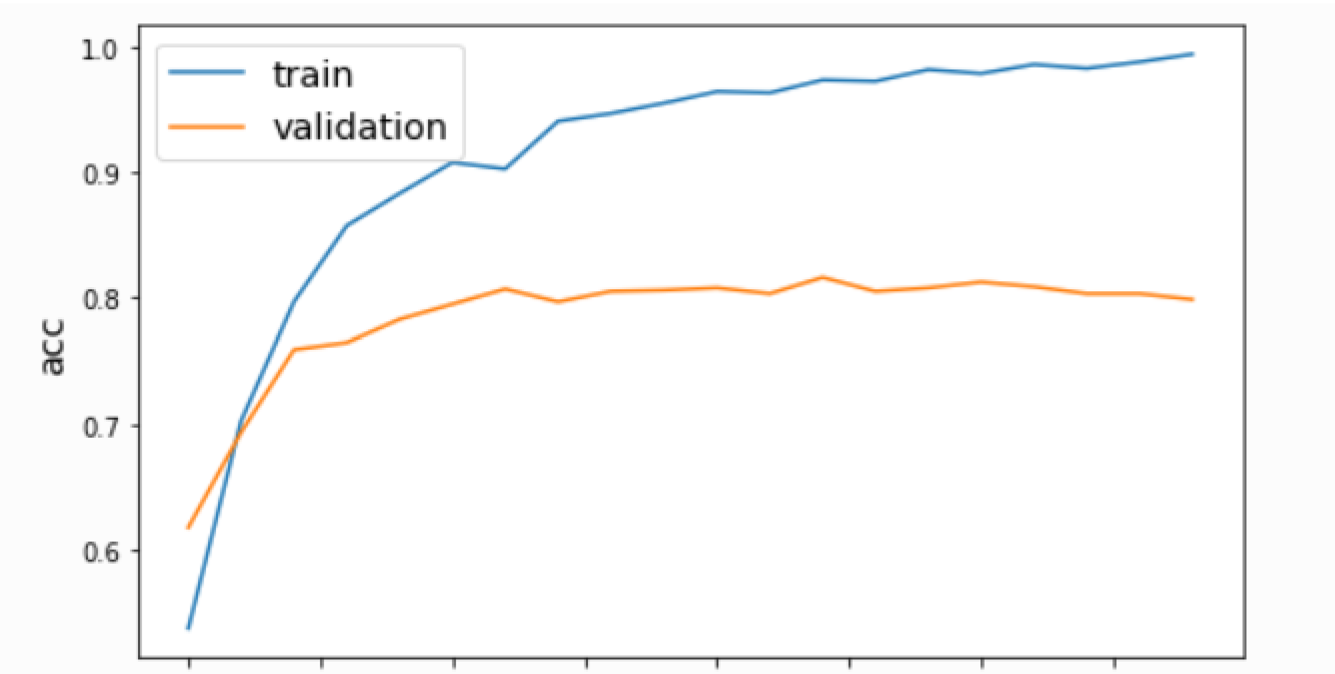

Fig. 7: Accuracy Curve

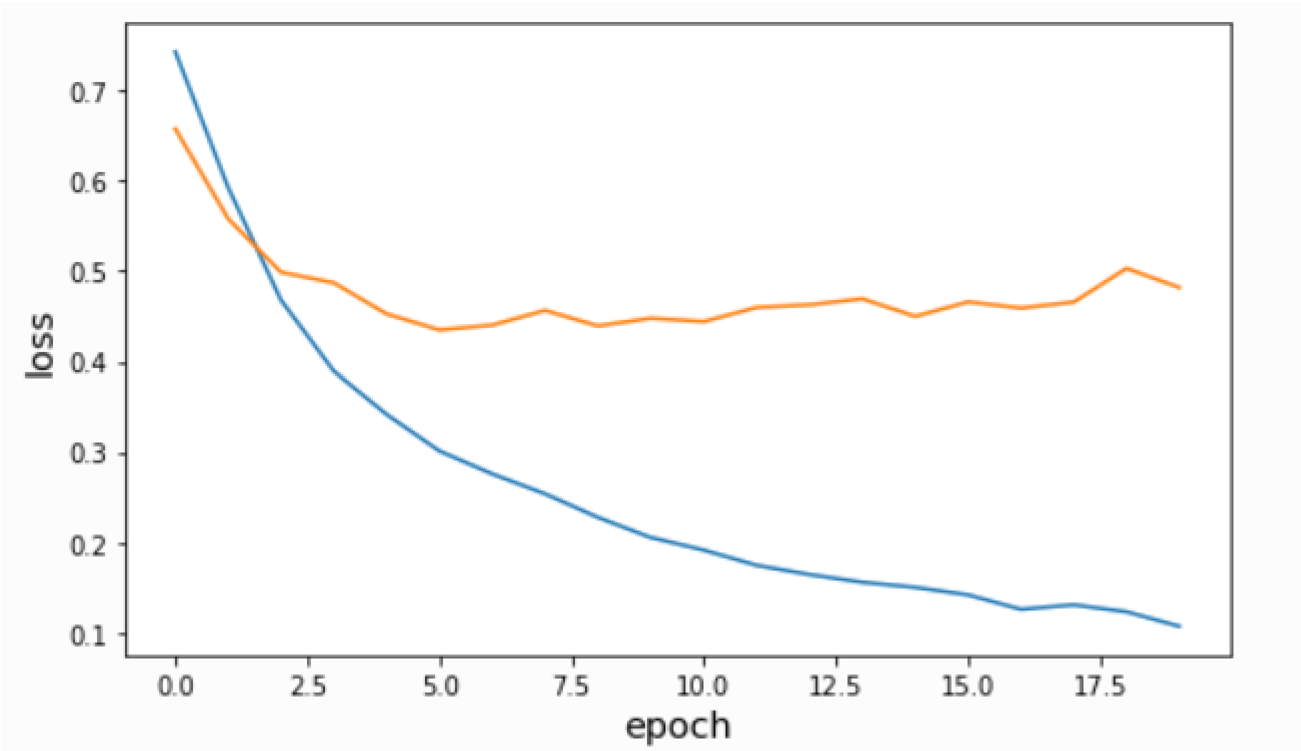

Fig.8 Loss Curve

Chapter 5

Conclusion & Future Work

5.1 Conclusion

The progression of loss values across epochs indicates a consistent improvement in our link prediction model's performance. Starting with a loss of 0.705 at epoch 0, we observe a steady decline, reaching 0.0088 by epoch 195, showcasing effective learning and parameter optimization. Additionally, achieving an AUC value of 0.8415 underscores the strong predictive capability of our GraphSAGE-based model in discerning future connections within social networks. This performance surpasses random chance, reaffirming its efficacy in link prediction tasks. In conclusion, our approach demonstrates the effectiveness of leveraging GraphSAGE and machine learning techniques, offering accurate identification of potential connections with implications for recommendation systems, community detection, and anomaly detection in social network analysis.

5.2 Future Work

In the realm of social network analysis, the future of link prediction presents numerous opportunities for advancement, catering to a wide array of applications crucial in understanding and enhancing social interactions.

- **Recommendation Systems:** Enhancing recommendation algorithms by predicting potential friendships, collaborations, or interactions between users, thus providing more personalized and relevant suggestions.
- **Community Detection:** Identifying latent communities within social networks by predicting links that bridge different groups or clusters, aiding in the understanding of network structure and dynamics.
- **Anomaly Detection:** Utilizing link prediction to detect anomalous behavior or potential threats, such as fake accounts or malicious activities, thereby bolstering cybersecurity measures.
- **Influence Maximization:** Predicting future influential connections or information diffusion paths to optimize strategies for maximizing influence spread or marketing campaigns.
- **Social Network Growth Prediction:** Forecasting the evolution of social networks by predicting future connections, helping in resource allocation and infrastructure planning.

Moving forward, research endeavors could focus on leveraging advanced machine learning techniques, such as graph neural networks and reinforcement learning, to capture intricate patterns and temporal dynamics inherent in social networks. Additionally, integrating multi-modal data sources, including text, images, and user behavior, could enrich link prediction models and provide a more comprehensive understanding of social interactions. Furthermore, addressing ethical considerations, such as privacy preservation and algorithmic fairness, will be essential to ensure responsible and equitable deployment of link prediction techniques in social network applications.

Chapter 6

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