Bayesian Graph Neural Networks for Interpretable Link Prediction

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***Abstract*—Link prediction is a fundamental problem in complex networks, with applications ranging from social media to bioinformatics. Existing methods often rely solely on either topological heuristics or latent variable models that neglect rich node attribute information. In this paper, we propose a Bayesian Graph Neural Network (BGNN) framework that simultaneously extracts deep node embeddings and leverages probabilistic graphical models to address these shortcomings. Specifically, our method first employs a multi-layer GNN to capture both local and global structural features. It then extracts non-topological features through attribute encoding. These complementary features are fused into a unified representation and fed into a Bayesian Network. The network computes the posterior probability of edge existence using Bayes' Theorem. This integration not only enhances prediction accuracy by leveraging both structural and attribute information, but also provides interpretable insights by quantifying the contribution of each feature to the final decision. Extensive experiments on standard datasets demonstrate that BGNN outperforms state-of-the-art methods both qualitatively and quantitatively. For instance, BGNN achieves an accuracy of 93% on the SCHOLAT dataset and 81% on the YST dataset, with significant improvements in precision, recall, and AUC.**

***Index Terms*—Link Prediction, Graph Neural Networks, Bayesian Inference, Interpretability**

I. Introduction

Link prediction has emerged as a cornerstone problem in the analysis of complex networks. It has drawn significant attention due to broad applications in various domains such as social networks [1], recommender systems [2], and bioinformatics networks [3]. In today's data-driven era, accurately forecasting potential connections not yet explicitly present in a graph is of paramount importance. This task not only relies on uncovering valuable patterns from the network topology but also leverages rich node attribute information to reveal hidden relationships. For instance, in social networks [4], the network topology captures explicit user interactions. Integrating additional node attributes, such as age, interests, and behavioral patterns, provides a more nuanced understanding of the underlying relational dynamics. The significance of link prediction extends beyond theoretical advancements. Its practical implications are substantial, contributing to enhanced accuracy in recommender systems and improved performance in critical applications like disease prediction.

Various approaches have been proposed to tackle the link prediction problem, which can be broadly classified into heuristic-based methods, latent factor or block models, and probabilistic graphical models. Heuristic-based approaches primarily utilize simple topological metrics, such as Common Neighbors [5], [6], Jaccard Similarity [7], and Resource Allocation [8]. However, these methods typically disregard valuable node attribute information. As a result, they potentially overlook critical nuances inherent in real-world networks. Latent factor methods, including Latent Variable Models [9] and Stochastic Block Models [10], [11], provide a more global view of network structure by modeling hidden relationships among nodes. Despite this advantage, they often struggle to accurately capture local structural details essential for pre-

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cise link prediction in complex and heterogeneous networks. Probabilistic Graphical Models (PGMs) [12] offer a clear, interpretable framework by explicitly modeling conditional dependencies among variables. Although PGMs are highly valuable for understanding and explaining underlying factors contributing to link formation, they frequently face scalability challenges. These challenges become particularly evident when integrating rich, deep embeddings generated by modern neural network techniques.

In recent years, deep learning models such as Convolutional Neural Networks (CNNs) [13] and Recurrent Neural Networks (RNNs) have demonstrated remarkable success in handling structured data like images and sequential data like text. CNNs excel at capturing spatial hierarchies through convolutional operations, while RNNs effectively process sequential dependencies via recurrent mechanisms. Building on these advances, Graph Neural Networks (GNNs) [14] have emerged as a powerful approach for modeling complex graph-structured data. By leveraging both topological information and node attributes, as demonstrated in multimodal fusion strategies [15], GNNs can learn high-quality node embeddings, substantially enhancing link prediction performance. Despite their predictive accuracy, GNNs face criticism for their "black-box" nature, lacking transparency in elucidating how specific structural or attribute features influence predictions. This limitation is particularly problematic in high-stakes applications such as disease prediction. Understanding the decision-making process is crucial in such cases. Consequently, this paper focuses on addressing two key issues: (1) effectively integrating topology and node attributes, and (2) improving interpretability.

Specifically, most existing methods rely purely on topological information, making it difficult to capture heterogeneous relationships or incorporate valuable node attribute data when inferring potential links. Consequently, purely structural features alone often prove insufficient in complex real-world scenarios. On the other hand, although GNNs have achieved remarkable performance in link prediction, the underlying decision-making process remains largely opaque. This "black-box" nature hinders intuitive understanding and explanation of model outputs, which is particularly crucial in practical applications where reliable and interpretable predictions are required.

To address these challenges, this paper proposes a novel multi-stage link prediction framework. The framework leverages GNNs to extract deep node embeddings and uses probabilistic graphical models such as Bayesian Networks to infer topological structures and attribute features jointly. Specifically, we extract high-dimensional node embedding vectors via GNNs and combine node attribute similarity and local statistical features to perform joint inference through a Bayesian Network. Ultimately, we compute the posterior probability of edge existence.

The contributions of this paper are summarized as follows:

1) We propose a multi-stage framework that first extracts deep node embeddings via multi-layer GNNs. These embeddings effectively capture both local and global graph structures. Subsequently, embeddings are fused with statistical and node attribute features for joint inference through a Bayesian Network. This process enables comprehensive modeling of edge existence probability.
2) We introduce a unified strategy for integrating topology and node attributes into the prediction pipeline. Specifically, our framework seamlessly combines node attribute similarity and local statistical signals alongside topological information. This holistic integration enriches the feature representation and enhances predictive robustness, addressing the limitations of methods relying solely on structural information.
3) We conduct extensive experiments on two standard datasets using five evaluation metrics. The experimental results demonstrate that the proposed model consistently outperforms baseline methods, confirming its effectiveness and practical applicability.

The remainder of this paper is organized as follows. Section II reviews the existing research on link prediction, focusing on traditional methods, GNN-based approaches, and probabilistic graphical models. Section IV describes our proposed Bayesian Graph Neural Network (BGNN) framework, including topological feature extraction, non-topological feature extraction, and the fusion mechanism. Section V presents the experimental setup, results, and corresponding analyses. Finally, Section VI summarizes the main findings of this work and outlines possible future research directions.

II. Related Work

A. Traditional Link Prediction Methods

Early link prediction methods primarily relied on the topological structure of graphs for inference, such as heuristic methods like Common Neighbors [5], Jaccard Similarity [7], and Resource Allocation [8]. These methods mainly focused on the structural information of networks but ignored the attribute information of nodes. In addition, there are some statistical models, such as Latent Variable Models [9] and Block Models [10], which capture the latent relationships between nodes by modeling the network structure. However, these traditional methods often have certain limitations and cannot effectively handle complex real-world networks that contain rich non-structural information.

B. Graph Neural Networks

In the task of link prediction, GNN methods have made significant progress [16]. For link prediction in dynamic graphs, the GR model [17] effectively extracts spatio-temporal features and successfully addresses the issue of node count discrepancies across different time snapshots by stacking Graph Convolutional Networks (GCN) [18]. In addition, the Graph Isomorphism Network (GIN) [19] effectively preserves the structural information of the graph by modeling its isomorphism, while the Graph Attention Network (GAT) [20] utilizes attention mechanisms to learn relationships between nodes, which helps improve the accuracy of link prediction. In addition, recent approaches have leveraged hypergraph

neural networks [21], [22] to capture higher-order relationships among nodes. These methods play a crucial role in preserving the graph structure and capturing the complex relationships between nodes.

C. Probabilistic Graphical Models

The application of Probabilistic Graphical Models (PGMs) in link prediction is relatively rare [12], [23]. However, with the increasing demand for interpretability, more and more work is focusing on how to integrate PGMs into the link prediction framework [24], [25]. In particular, Bayesian Networks [26], as a typical PGM, can effectively describe the probabilistic dependencies between variables, providing interpretable analysis of the posterior probabilities of link existence. However, traditional PGM methods have often failed to fully integrate deep embeddings or local statistical features of nodes, limiting their performance in practical applications.

Unlike previous models that focus solely on either deep GNN embeddings or traditional statistical features, our approach uniquely integrates both. By combining node attribute similarity and local statistics with multi-layer GNN representations through a Bayesian Network, our model not only enhances prediction accuracy but also offers clear interpretability, revealing how each feature contributes to the final prediction.

III. Problem Formulation

Link prediction aims to predict the existence of an edge between two nodes in a graph $G = (V, E)$, where V is the set of nodes and E is the set of edges. Given the graph G, each node $v \in V$ has an associated feature vector $\mathbf{x}_v$, which may include both topological and non-topological attributes. The task is to predict whether an edge exists between a pair of nodes $(u, v) \in V \times V$, where $u \neq v$.

Formally, for a node pair (u, v), the goal is to predict the probability that an edge exists between these nodes, i.e., to estimate $\Pr(y_{uv} = 1 \mid \mathbf{x}_u, \mathbf{x}_v)$, where y_{uv} is a binary random variable that indicates the presence of an edge between u and v:

$$y_{uv} = \begin{cases} 1, & \text{if there is an edge between } u \text{ and } v, \\ 0, & \text{otherwise.} \end{cases} \tag{1}$$

Here, $\mathbf{x}_u$ and $\mathbf{x}_v$ are the feature vectors of nodes u and v, respectively. These feature vectors are derived from both topological information (graph structure) and non-topological information (node attributes). The challenge lies in efficiently combining these two types of information and leveraging them for accurate link prediction.

IV. Proposed BGNN

In this section, we describe the proposed approach for link prediction, which combines multi-layer GNN embeddings with Bayesian Network inference.

A. Overview

The method consists of two main stages: first, the extraction of topological and non-topological features of the nodes, and then the fusion of these two types of features followed by link prediction.

The input data are a graph $G = (V, E)$, where each node $v \in V$ has an associated attribute vector $\mathbf{x}_v$. The topological features are extracted using a multi-layer GNN, resulting in the node embedding vector $\mathbf{h}_v^{(L)}$. The non-topological features are processed by transforming node attributes into feature vectors $\mathbf{x}_v$.

In the fusion module, the topological and non-topological feature vectors are concatenated into a single vector, which is then used by the link-prediction module. This module employs a Bayesian Network to compute the posterior probability of an edge between two nodes. Specifically, the fused feature vector $\mathbf{f}_{uv}$ is used to evaluate $\Pr\big(y_{uv} = 1 \mid \mathbf{f}_{uv}\big)$, thus performing link prediction via Bayes' theorem. This probabilistic approach not only enhances interpretability by helping to understand which features influence the link prediction outcome, but also provides the potential for risk assessment and decision-making support through the quantification of uncertainty.

B. Topological Features Extraction Module

We use a multi-layer GNN to capture the topological features of the graph. The embedding of a node v is updated in two steps. First, we aggregate information from its neighbors:

$$\mathbf{m}_v^{(l)} = \text{AGGREGATE}\big\{\mathbf{h}_u^{(l-1)} : u \in \mathcal{N}(v)\big\}. \tag{2}$$

Next, the aggregated message is transformed:

$$\mathbf{h}_v^{(l)} = \sigma\big(\mathbf{W}^{(l)}\mathbf{m}_v^{(l)} + \mathbf{b}^{(l)}\big), \tag{3}$$

where $\mathbf{W}^{(l)}$ and $\mathbf{b}^{(l)}$ are learnable parameters and $\sigma(\cdot)$ denotes the ReLU activation. After L layers, the final embeddings $\mathbf{h}_v^{(L)}$ capture information from both local neighborhoods and broader graph structure.

C. Non-Topological Features Extraction Module

Non-topological features are encoded from node attributes (e.g., labels or categorical data):

$$\mathbf{x}_v = \text{ENCODE}(\text{Attributes of node } v). \tag{4}$$

These vectors provide complementary information and are normalized before fusion.

D. Fusion Module

Topological and non-topological features are concatenated:

$$\mathbf{f}_{uv} = \mathbf{h}_u^{(L)} \| \mathbf{h}_v^{(L)} \| \mathbf{x}_u \| \mathbf{x}_v. \tag{5}$$

E. Link Prediction Module

The Bayesian Network models

$$\Pr\big(y_{uv} = 1 \mid \mathbf{f}_{uv}\big) = \frac{\Pr\big(\mathbf{f}_{uv} \mid y_{uv} = 1\big)\Pr\big(y_{uv} = 1\big)}{\Pr\big(\mathbf{f}_{uv}\big)}. \tag{6}$$

This yields interpretable posterior probabilities and feature contributions.

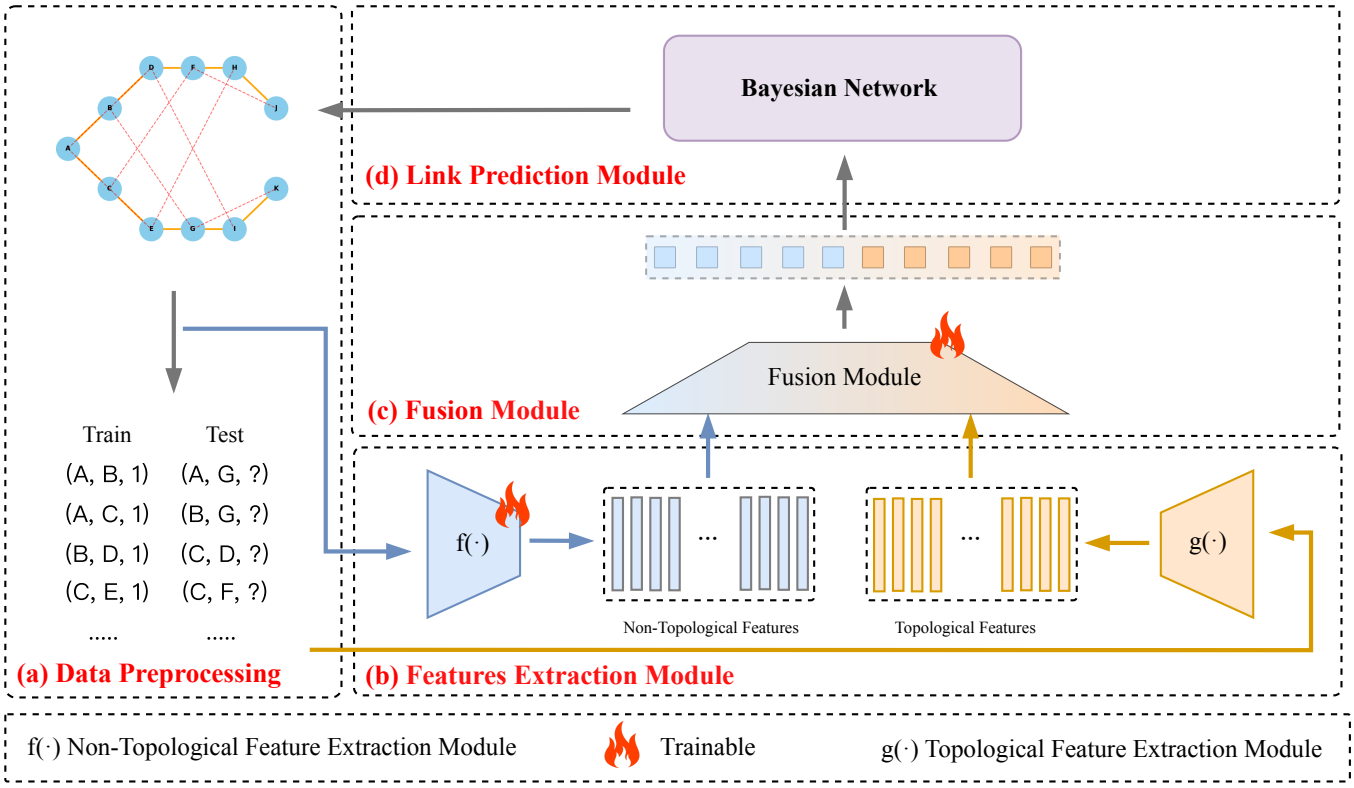

Fig. 1. Block diagram of the proposed network

TABLE I
COMPARISON RESULTS: PERFORMANCE OF DIFFERENT METHODS ON TWO DATASETS.

Category	Model	SCHOLAT				YST			
		AUC	Prec.	Rec.	F1	AUC	Prec.	Rec.	F1
G	GIN	0.96	0.91	0.91	0.91	0.49	0.55	0.26	0.36
	GAT	0.96	**0.93**	0.94	0.94	0.52	0.59	0.31	0.40
	GAT v2	0.96	0.92	0.94	0.93	0.50	0.57	0.34	0.43
	LAGCN	0.93	0.83	0.91	0.87	0.52	0.60	0.41	0.49
HG	SELAR	0.94	0.87	0.90	0.89	0.59	0.58	0.68	0.35
	MAGNN	0.94	0.88	0.89	0.89	0.57	0.65	0.35	0.46
	MAHGA	0.92	0.85	0.86	0.85	0.62	0.66	0.44	0.53
Ours	**BGNN***	**0.96**	0.89	**0.97**	**0.93**	**0.85**	**0.81**	**0.82**	**0.82**

[1] G: Graph Neural Network Methods; HG: Heterogeneous Graph Methods
[2] *: Our proposed method; Prec.: Precision; Rec.: Recall

F. Pseudocode Flowchart

V. EXPERIMENTS

A. Experimental Setups

1) Datasets: **SCHOLAT Link Prediction Dataset** [27] originates from the SCHOLAT open data platform and mainly focuses on the link prediction problem in academic social networks. This dataset comprises 10,755 user nodes and provides 168,540, 16,854, and 16,854 undirected edges for the training, development, and test sets, respectively, while integrating both the users' social topology and attribute information.

YST Dataset [28] is based on the work by von Mering et al. This study compared different large-scale protein–protein interaction (PPI) datasets, with a particular focus on the interaction network in yeast, and revealed the tremendous potential of using integrated protein interaction maps to decipher complex cellular regulatory networks.

2) Baselines: To comprehensively evaluate our proposed model, we compare it with several benchmark methods, which can be categorized into two types: GNN-based methods, and methods for heterogeneous graphs and meta-paths.

GNN-based Methods. These methods learn node represen-

Algorithm 1 Simplified BGNN Framework

Input: Graph $G = (V, E)$, node attributes $\mathbf{X}$
Output: Probabilities $\hat{y}_{uv}$ for each node pair (u, v)
▷ Step 1: Feature extraction
Extract topological features $\mathbf{h}_v^{(L)}$ via GNN
Extract non-topological features $\mathbf{x}_v$ from attributes
▷ Step 2: Feature fusion
$\mathbf{f}_{uv} \leftarrow \mathbf{h}_u^{(L)} \| \mathbf{h}_v^{(L)} \| \mathbf{x}_u \| \mathbf{x}_v$
▷ Step 3: Bayesian inference
$\hat{y}_{uv} \leftarrow \Pr\big(y_{uv} = 1 \mid \mathbf{f}_{uv}\big)$

tations to capture complex graph structure information for link prediction. We compare *Graph Isomorphism Network* (GIN), *Graph Attention Network* (GAT), *Graph Attention Network v2* (GAT v2), and *Local Attention Graph Convolution Network* (LAGCN), which all leverage different mechanisms, such as isomorphism, attention, and local enhancements.

Heterogeneous Graph and Meta-Path-based Methods. We compare *SELAR*, which uses meta-paths for heterogeneous graph representation learning with attention residuals; *MAGNN*, which aggregates information from different meta-paths using attention; and *MAHGA*, a multi-faceted framework combining structural and meta-path-level enhancements for robust link prediction.

3) Implementation Details: In our implementation, we employed a three-layer GAT network as the node feature extractor. The first GAT layer utilizes 8 attention heads, each with an output dimension of 128, to fully capture local neighborhood information. Subsequently, the second and third layers further aggregate and map the features, resulting in a final node embedding dimension of 64, which ensures both compactness and expressive power. Meanwhile, the initial node attributes are generated using Node2Vec with a dimension of 32, reflecting the latent relationships among nodes in the entire graph. The model is trained using the Adam optimizer with an initial learning rate of 0.001 and a weight decay of 0.0005 to mitigate overfitting. Dropout (rate 0.2) is applied in each layer to enhance generalization. A learning-rate scheduler automatically reduces the learning rate if validation metrics fail to improve for 100 consecutive epochs. The model is trained for 1000 epochs, evaluating on the validation set every 100 epochs, and the checkpoint with the best validation performance is selected for testing.

4) Evaluation Metrics: We assess link prediction performance using five metrics:

Accuracy (Acc)

$$\text{Acc} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}}. \tag{7}$$

Area Under Curve (AUC) quantifies discrimination ability by measuring the area under the ROC curve.

Precision

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}. \tag{8}$$

Recall

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}. \tag{9}$$

F1-score

$$\text{F1-score} = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}. \tag{10}$$

TABLE II
ACCURACY COMPARISON OF DIFFERENT METHODS ON TWO DATASETS

Category	Model	SCHOLAT	YST
G	GIN	0.91	0.52
	GAT	0.93	0.55
	GAT v2	0.93	0.54
	LAGCN	0.87	0.57
HG	SELAR	0.88	0.59
	MAGNN	0.89	0.58
	MAHGA	0.85	0.60
Ours	**BGNN***	**0.93**	**0.81**

[1] G: Graph Neural Network Methods; HG: Heterogeneous Graph Methods
[2] *: Our proposed method

B. Comparison Results and Analyses

Our proposed BGNN model was evaluated against several baseline models on two datasets, SCHOLAT and YST, with results summarized in Table II. As shown in the table, BGNN achieves the highest Accuracy scores among all baseline methods, demonstrating its strong overall performance in the task of link prediction. Specifically, BGNN achieved an Accuracy of 93% on the SCHOLAT dataset and 81% on the YST dataset. This performance significantly outperforms other models, such as GIN, GAT, and LAGCN, which achieved accuracy values ranging from 0.87 to 0.93 on SCHOLAT and from 0.52 to 0.60 on YST. These results indicate that our proposed method excels in correctly identifying both positive and negative links. The higher accuracy achieved on SCHOLAT can be attributed to the more structured nature of the graph, where BGNN is able to leverage both node embeddings and topological information effectively. On YST, the slightly lower accuracy suggests that the graph may have more complex, heterogeneous relationships, but BGNN still manages to achieve a strong performance compared to other models, proving its robustness across different types of data.

In addition to Accuracy, we further evaluated BGNN's performance using four other important metrics: AUC, Precision, Recall, and F1-score. The results, summarized in Table I, reinforce the advantages of the BGNN model. Specifically, BGNN achieved an AUC of 0.96 on SCHOLAT, which is comparable to the top-performing GNN models such as GIN and GAT. The AUC score is crucial as it evaluates the model's ability to distinguish between positive and negative link predictions, and BGNN's high AUC indicates its superior capability in this aspect. This shows that BGNN not only

TABLE III
PERFORMANCE COMPARISON OF DIFFERENT GNN ENCODERS ON TWO DATASETS.

Method	SCHOLAT					YST				
	AUC	**Prec.**	**Rec.**	**F1**	**Acc.**	**AUC**	**Prec.**	**Rec.**	**F1**	**Acc.**
SAG	0.90	0.89	0.85	0.87	0.87	0.68	0.75	0.53	0.62	0.68
GIN	0.87	0.89	0.80	0.84	0.85	0.64	0.72	0.43	0.54	0.63
Ours	**0.96**	**0.89**	**0.97**	**0.93**	**0.93**	**0.85**	**0.81**	**0.82**	**0.82**	**0.81**

[1] Prec.: Precision; Rec.: Recall; Acc.: Accuracy.
[2] All results use identical hyperparameters, data processing, and training pipelines.

excels in making correct predictions but also in its ability to rank links correctly in terms of likelihood.

Moreover, BGNN outperforms the other models in both Precision and Recall, achieving 0.89 and 0.97, respectively, on the SCHOLAT dataset, and 0.85 and 0.81 on the YST dataset. The Precision score indicates that among the predicted positive links, a high proportion are indeed correct, and BGNN's high Precision on both datasets suggests that it is highly effective in minimizing false positives. In contrast, the Recall score indicates that BGNN is able to correctly identify a large portion of the actual positive links, particularly excelling in SCHOLAT with a Recall of 0.97, which demonstrates its effectiveness in capturing true links.

The F1-score, which balances Precision and Recall, further confirms BGNN's ability to provide high-quality predictions, achieving 0.93 for SCHOLAT and 0.82 for YST. The F1-score is particularly important in imbalanced datasets, as it considers both false positives and false negatives, and BGNN's high F1-score across both datasets demonstrates its robustness in providing a balanced prediction without overfitting to either false positives or false negatives.

In summary, BGNN not only excels in overall accuracy but also provides high-quality predictions across all performance metrics. These results demonstrate that BGNN is highly reliable and effective in link prediction tasks, providing a strong foundation for its application in various domains that require high prediction quality and interpretability.

C. Influence Investigation of GNN

To examine the effectiveness of the GNN encoder used in our proposed framework, we conduct an ablation study by replacing the GNN component while keeping all other modules identical Specifically, we compare two widely used graph convolutional variants: SAG [29] and GIN [19], against our proposed architecture that employs GAT [20], [30].

SAG efficiently aggregates neighborhood features via mean pooling but may miss detailed node interactions, while GIN employs MLP-based aggregation capable of distinguishing structural variations yet struggles with flexible attribute integration. Our multi-layer GAT encoder, using attention mechanisms, selectively captures nuanced structural and attribute-level interactions effectively.

Table III presents the comparative performance. On the SCHOLAT dataset, while SAG and GIN achieve reasonable AUC scores of 0.90 and 0.87 respectively, our model surpasses them significantly, reaching an AUC of 0.96 and notably higher Recall (0.97) and F1-score (0.93). Similar trends are observed on the more challenging YST dataset, where SAG and GIN exhibit substantial performance degradation, particularly in Recall and F1 metrics. Our GAT-based Bayesian model maintains robust performance, achieving an F1-score of 0.82 and AUC of 0.85. These improvements underscore the superiority of the attention mechanism in effectively capturing node interactions, especially in heterogeneous or noisy environments, and validate the value of the Bayesian integration in handling feature uncertainty comprehensively.

VI. CONCLUSION AND FUTURE WORK

In this paper, we introduced BGNN, a novel framework that integrates deep node embeddings from multi-layer GNNs with non-topological features through Bayesian inference. This fusion not only enhances prediction accuracy—demonstrated by superior performance across multiple metrics on benchmark datasets—but also significantly improves interpretability by quantifying the contribution of each feature in predicting link existence. Our comprehensive experiments validate BGNN's robustness and effectiveness in addressing the challenges of link prediction by capturing both local and global structural information along with rich attribute data.

Looking ahead, future work will extend BGNN to more complex scenarios, such as dynamic and heterogeneous graphs, where evolving network structures and diverse data sources further complicate link prediction tasks. Additionally, we aim to incorporate domain-specific features and refine the interpretability of our probabilistic framework, thereby enhancing decision-making support in critical real-world applications and expanding the utility of our approach across various domains.

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