Benchmarking GNN and Graph Transformer Models for Dynamic Link Prediction

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Abstract. Dynamic Link Prediction (DLP) aims to forecast the formation or disappearance of links in evolving networks. Traditional GNN-based models (e.g., GCN-GRU, GAT-GRU) effectively capture localized spatial-temporal dependencies but often fall short in modeling long-range structural and temporal patterns. Recent advancements in Graph Transformers introduce global attention mechanisms that better capture such dependencies. This paper presents a benchmarking study of six representative models—RoleGRU, GCN-GRU, GAT-GRU, Transformer, GraphTransformer-GRU, and a hybrid GCN+Transformer evaluated on two real-world datasets: MOOC and Enron. Results show that GraphTransformer-GRU consistently achieves the highest AUC and Average Precision, outperforming both recurrent and hybrid designs. These findings offer key insights into architectural trade-offs and reinforce the importance of integrating spatial structure and temporal dynamics in DLP, addressing gaps noted in recent studies.

Keywords: Dynamic Link Prediction, Temporal Graphs, Graph Neural Networks, Graph Transformers.

1 Introduction

Networks in real-world systems evolve continuously, with new connections forming and existing ones disappearing over time. Dynamic Link Prediction (DLP) addresses the challenge of forecasting future links in such temporal graphs, with applications in social recommendation systems [1], transaction networks [2], and social networks [3].

Traditional methods rely on static graph snapshots and fail to capture temporal dynamics. Dynamic GNNs like GCN-GRU and GAT-GRU integrate spatial and temporal information using graph convolutions and recurrent units [29, 4], but their locality limits long-range dependency modeling. Transformer architectures, originally from NLP, have shown promise for graph learning due to their global attention mechanisms [28, 14]. When combined with GRUs, Graph Transformers can model both structure and temporal evolution effectively [28].

This paper benchmarks six representative models—RoleGRU, GCN-GRU, GAT-GRU, Transformer, Hybrid GCN+Transformer, and GraphTransformer-GRU—on two dynamic datasets: Enron and MOOC. We evaluate each model's performance using AUC, Average Precision (AP), and loss.

The objectives of this paper are threefold:

- How do recurrent GNNs compare to Transformer-based models in capturing temporal and structural dependencies in DLP tasks?
- Can hybrid models combining local structural encoding and global attention outperform purely recurrent or purely attention-based models?
- How does graph density or structure affect model performance across different architectural designs?

Although we do not propose a new model, our systematic benchmarking provides a unified and practical comparison of state-of-the-art GNN and Transformer approaches under consistent training conditions. Our findings show that Transformer-based models—particularly GraphTransformer-GRU—consistently outperform others across both sparse and dense networks.

We also discuss limitations in scalability, dataset diversity, and CPU-only training, offering insights for real-world deployment and future research in dynamic link prediction.

2 Related Work on Dynamic Link Prediction

Link prediction has long been a core problem in graph mining. Traditional methods like Common Neighbors (CN), Jaccard Coefficient (JC), and Adamic-Adar (AA) [14, 15] estimate link likelihood based on static neighborhood overlap. While efficient, these heuristics fail to capture temporal evolution.

To address dynamics, early approaches incorporated probabilistic modeling and supervised learning over temporal snapshots [7, 8]. Techniques like Hawkes processes and dynamic matrix factorization [9, 10] introduced time-awareness, but often struggled with scalability and irregular updates.

Graph Neural Networks (GNNs) advanced the field by learning evolving node embeddings through spatial-temporal architectures. Models like GCN-GRU and GAT-GRU [11, 6] leverage recurrent units and local aggregation but are limited in capturing long-range dependencies.

To overcome this, Transformer-based models were introduced to dynamic graphs. Self-attention enables global context modeling across time and structure. Works such as FreeDyG and Temporal Graph Transformer [7, 10] show notable gains in capturing complex dynamics and outperform local models in various DLP settings.

Despite these developments, comparative studies are fragmented and often lack a unified evaluation framework. To fill this gap, we benchmark six representative models—RoleGRU, GCN-GRU, GAT-GRU, Transformer, GCN +Transformer, and GraphTransformer-GRU—on two diverse real-world datasets. This unified analysis provides deeper insights into how architectural choices influence DLP performance under different structural and temporal conditions, addressing the lack of interpretability and generalizability noted in recent reviews.

3 Problem Definition

Dynamic Link Prediction (DLP) involves forecasting the formation or disappearance of links in a temporal graph, where the structure evolves over discrete time steps [12–14]. Formally, a dynamic graph is denoted by $\mathcal{G} = \{G_1, G_2, \ldots, G_T\}$, where each snapshot $G_t = (V_t, E_t)$ contains nodes V_t and edges E_t observed at time t.

Given snapshots up to time T, the goal is to predict future edges $\hat{E}_{T+1}$ in G_{T+1} [15, 16]. This is commonly formulated as a supervised task, where a model learns a scoring function:

$$s(i,j) = \text{likelihood that } (i,j) \in E_{T+1} \tag{1}$$

Candidate node pairs are ranked by $s(i,j)$, and top-k scores indicate predicted links. Model effectiveness depends on how well it captures both structural context and temporal evolution.

In this study, we benchmark six DLP models—spanning recurrent, attention-based, and hybrid architectures—on the Enron and MOOC datasets. Each dataset is divided into T snapshots, and models are evaluated using AUC and Average Precision (AP), enabling consistent comparison of dynamic modeling capabilities.

4 Benchmarking Methods

4.1 RoleGRU

Structural roles have long been used to identify node equivalence based on graph topology [23]. While traditional role-based methods often neglect temporal evolution, RoleGRU addresses this by applying Gated Recurrent Units (GRUs) over learned role representations [22]. This design enables tracking of structural role transitions over time, allowing the model to effectively capture dynamic behavior for link prediction without relying on direct neighborhood aggregation.

4.2 Graph Convolutional Network with GRU (GCN-GRU)

GCN-GRU integrates spatial and temporal modeling by combining Graph Convolutional Networks (GCNs) with Gated Recurrent Units (GRUs). At each time step t, a GCN processes the snapshot $G_t = (A_t, X_t)$ to produce node embeddings H_t, which are then fed into a GRU to capture temporal dynamics: $Z_t = \text{GRU}(H_t, Z_{t-1})$. Link scores are computed via inner product: $s_{ij} = \sigma(\mathbf{z}_i^T \mathbf{z}_j)$ [17]. This model is widely used in DLP for its ability to learn evolving node interactions [18, 19].

4.3 Graph Attention Network with GRU (GAT-GRU)

GAT-GRU combines Graph Attention Networks (GATs) with Gated Recurrent Units (GRUs) to capture dynamic graph patterns. GAT layers assign attention weights to neighbors, enabling context-aware spatial encoding, while GRUs model temporal evolution across snapshots [20]. This architecture maintains memory of past states and adapts to topological shifts, enhancing DLP performance on evolving graphs [21].

4.4 Transformer

Transformer models have gained traction in DLP for their ability to capture global temporal dependencies through self-attention. Unlike GCN or GAT, which aggregate local neighborhoods, Transformers attend over all nodes, modeling non-local structural shifts.

Their success spans multiple domains—including traffic [24], heterogeneous networks [25], and trajectory forecasting [26, 27]—highlighting their utility in temporal graphs.

We employ a standard Transformer encoder over evolving node embeddings without structural priors. While effective in learning temporal trends, this approach may struggle on sparse graphs due to the absence of graph topology. These limitations motivate the hybrid models introduced in Section 4.5.

4.5 Hybrid Models: GCN + Transformer

To address the limitations of Transformers in sparse graphs, we benchmark a hybrid model that combines GCNs for local structure encoding with Transformer encoders for global temporal reasoning [16, 24]. GCNs process each snapshot to embed topological context, which is then passed to the Transformer to capture long-range dynamics [25, 26].

This architecture improves generalization in irregular or sparse temporal graphs by integrating spatial priors into attention-based models. Our results show that this hybrid approach offers more consistent DLP performance across diverse datasets, demonstrating a valuable trade-off between structural bias and temporal flexibility.

4.6 Graph Transformer + GRU Hybrid Model

This model combines Graph Transformers for snapshot-wise global structural encoding with GRUs for capturing temporal dependencies. Inspired by prior works such as AuxGT [28] and FreeDyG [29], this modular architecture separates spatial and temporal modeling, enabling effective handling of irregular graph topologies and non-uniform evolution over time.

Empirically, this hybrid outperforms both GCN-GRU and Transformer-only models, particularly on datasets with complex structural and temporal dynamics. These results highlight the benefits of fusing self-attention and recurrent modeling for robust dynamic link prediction.

5 Experimental Setup

We evaluate six models—RoleGRU, GCN-GRU, GAT-GRU, Transformer, Hybrid GCN+Transformer, and GraphTransformer-GRU—on two dynamic graph datasets: Enron (email communications) and MOOC (student-platform interactions), each split into 100 snapshots.

These models vary in how they model spatial-temporal dependencies (see Section 4). RoleGRU encodes evolving roles; GCN-GRU and GAT-GRU integrate structural and temporal signals using convolution and attention, respectively; Transformer models temporal patterns without graph priors; the Hybrid and GraphTransformer-GRU models combine structural encoding with global attention and temporal modeling.

All models are trained for 100 epochs on CPU using Adam (learning rate 0.001) and binary cross-entropy loss. Metrics include AUC, Average Precision

(AP), and loss, evaluated on test snapshots and logged for reproducibility and comparison.

6 Results and Analysis

We evaluate six models—RoleGRU, GCN-GRU, GAT-GRU, Transformer, Hybrid GCN+Transformer, and GraphTransformer-GRU—on the Enron and MOOC datasets, each split into 100 temporal snapshots.

Model performance is measured using AUC, Average Precision (AP), and Binary Cross-Entropy Loss, capturing link prediction accuracy and convergence stability. All models were trained and tested under consistent preprocessing and evaluation protocols for fair comparison. Table 1 summarizes the dataset characteristics used in this benchmarking.

Table 1: Description of the dynamic graph datasets used in the experiments.

Dataset	**Type**	**Nodes**	**Edges**	**Time Steps**	**Task**	**Source**
MOOC	Interaction Network	6,319	411,749	100	LP	[SNAP]
Enron	Email Communication	143	20,217	100	LP	[SNAP]

These datasets differ significantly in scale and structure: MOOC is dense and regular, while Enron is sparse and irregular. This contrast enables an analysis of model robustness under varied temporal and structural dynamics.

6.1 Enron Results

Table 2 shows that GraphTransformer-GRU achieves the best results on Enron (AUC: 0.6326, AP: 0.6110, Loss: 0.6642), capturing both structural complexity and temporal patterns. Among GNNs, GAT-GRU outperforms GCN-GRU and RoleGRU, benefiting from attention-based aggregation.

The pure Transformer and Hybrid models perform worse, likely due to Enron's sparse, role-based structure requiring strong structural priors. Figure 1 highlights faster convergence and better generalization by GraphTransformer-GRU.

6.2 MOOC Results

All models perform better on MOOC due to its regular structure. GraphTransformer -GRU again leads (AUC: 0.9996, AP: 0.9997, Loss: 0.0459), followed by GCN-GRU and the Hybrid model. RoleGRU remains competitive, while GAT-GRU shows signs of overfitting.

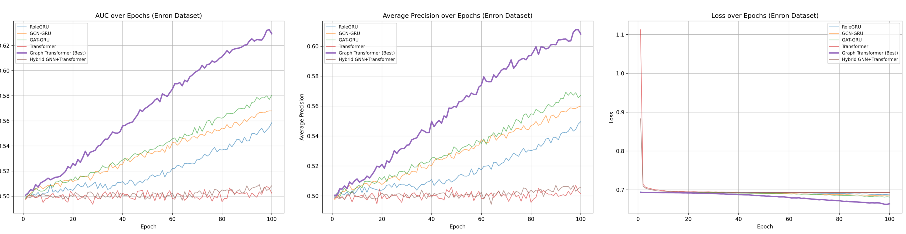
As shown in Figure 1, GraphTransformer-GRU maintains stable training and superior generalization, confirming its robustness across both datasets.

6.3 Comparative Insights

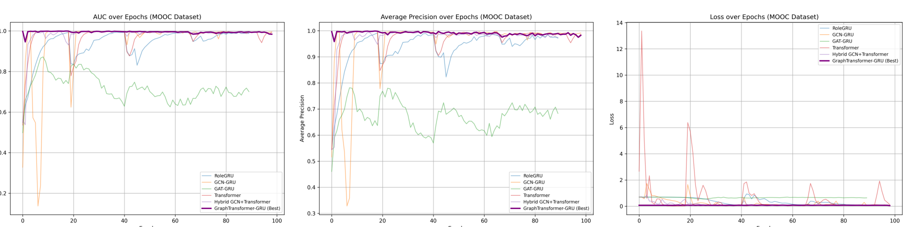
GraphTransformer-GRU outperforms other models by effectively integrating spatial and temporal dynamics, highlighting the value of hybrid attention-based architectures for DLP. GCN+Transformer and GraphTransformer-GRU show strong generalization across both dense (MOOC) and sparse (Enron) graphs, while pure Transformer models underperform on irregular structures. RoleGRU remains competitive in stable environments but lacks adaptability. These results affirm that modular, hybrid models with global attention and structural awareness are better suited for scalable and robust dynamic link prediction.

Table 2: Performance comparison of models on Enron and MOOC datasets.

Model	**Enron**			**MOOC**		
	AUC	**AP**	**Loss**	**AUC**	**AP**	**Loss**
RoleGRU	0.5585	0.5496	0.6870	0.9938	0.9918	0.0863
GCN-GRU	0.5679	0.5600	0.6845	0.9985	0.9983	0.0466
GAT-GRU	0.5804	0.5693	0.6815	0.8719	0.7817	0.6363
Transformer	0.5077	0.5071	0.6933	0.9994	0.9990	0.1195
Hybrid GCN+Transformer	0.5092	0.5071	0.6931	0.9974	0.9950	0.0670
GraphTransformer-GRU	**0.6326**	**0.6110**	**0.6642**	**0.9996**	**0.9997**	**0.0459**



(a) Performance of models on the Enron dataset.



(b) Performance of models on the MOOC dataset.

Fig. 1: Performance plots for Enron and MOOC datasets across AUC, AP, and Loss.

7 Discussion

Our experiments across the Enron and MOOC datasets reveal clear trends in model performance for DLP. The GraphTransformer-GRU consistently outperforms all other models, achieving near-perfect AUC and AP on MOOC and maintaining strong results on the noisier Enron dataset. These results highlight the advantage of integrating global attention with temporal modeling in a unified architecture.

The model's robustness across both sparse and dense networks demonstrates its flexibility in capturing complex temporal-structural patterns. In contrast, GAT-GRU underperforms, particularly on MOOC, indicating that local attention alone is insufficient without dedicated temporal reasoning. Hybrid models (e.g., GCN+Transformer) offer improvements over traditional baselines but still fall short of the fully integrated GraphTransformer-GRU.

8 Conclusion and Future Work

We benchmarked six dynamic link prediction models on the Enron and MOOC datasets under a unified experimental setup. Among them, the Graph-Transformer -GRU consistently outperformed others, demonstrating the value of combining global attention with temporal and structural modeling. Our results reveal that hybrid architectures, which integrate spatial priors with temporal reasoning, offer clear advantages over purely local or sequential models.

This work fills a critical gap in the DLP literature by systematically comparing traditional GNN-based approaches with emerging Transformer-based models, offering a structured perspective on when and why certain architectures succeed. While this study does not propose a new model, it offers actionable insights for designing future dynamic graph models that balance interpretability, scalability, and performance.

Future research should explore generalization across more diverse and challenging datasets—including heterogeneous, multi-relational, and irregularly timed graphs—to validate robustness in real-world scenarios. Incorporating GPU-based training can enable deeper architectures and large-scale experiments. Additionally, self-supervised learning (SSL) techniques tailored to temporal graphs hold promise for improving performance in low-label conditions. Designing SSL objectives that align with evolving graph structures and temporal dependencies is a particularly promising direction for scalable and transferable DLP models.

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