H-UniMP: A Heterogeneity-Aware Unified Message Passing Model for Citation Networks

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***Abstract*—Citation networks have long served as canonical benchmarks for semi-supervised node classification, where the goal is to predict publication venues or categories based on graph structure and limited labeled nodes. Traditional Graph Neural Networks (GNNs) such as GCN and GAT improved over classical methods by propagating node features through graph neighborhoods, but they often treated citation graphs as homogeneous and underutilized available label information. Recent advances such as UniMP introduced masked label prediction, unifying feature and label propagation and achieving state-of-the-art results on Open Graph Benchmark (OGB) datasets. Extensions like R-UniMP incorporated heterogeneous relations (e.g., paper-to-paper, author-to-paper), relation-wise normalization, and metapath embeddings, leading to a winning solution in the KDD Cup 2021 MAG240M-LSC challenge.**

Despite these advances, UniMP and R-UniMP remain sensitive to hyperparameter choices–particularly the masking rate for label injection–and require substantial GPU resources for training at scale. This paper proposes H-UniMP, an enhanced framework designed to address these limitations. The model integrates (i) relation-aware propagation to handle multiple edge types, (ii) relation-aware attention to weight heterogeneous relations differently during message passing, and (iii) systematic optimization of masked label prediction hyperparameters to improve robustness and stability.

Experiments on the Citation-Network V1 dataset demonstrate that H-UniMP achieves 0.20-0.22% improvements in accuracy over R-UniMP under comparable settings. Importantly, all experiments were conducted under CPU-only training conditions, highlighting the practicality of the approach in resource-constrained environments. These results indicate that relation-aware mechanisms combined with careful hyperparameter tuning can significantly improve the effectiveness of GNNs for heterogeneous citation networks while reducing dependence on large-scale compute.

***Index Terms*—Graph Neural Networks, Citation Networks, Semi-Supervised Classification, UniMP, R-UniMP, Heterogeneous Graphs**

I. Introduction

Graph Neural Networks (GNNs) have become the suitable paradigm for learning from citation networks, where nodes represent papers and edges represent citations or authorship relations. Early models such as Graph Convolutional Networks (GCN) [1] and Graph Attention Networks (GAT) [2] demonstrated the effectiveness of message passing in homogeneous citation graphs. However, these approaches largely ignored heterogeneity (different node and edge types) and underutilized supervision from labels.

The UniMP framework [5] introduced masked label prediction, treating labels as learnable embeddings injected into the feature space. This unified message passing of features and labels significantly boosted performance. Building upon this, R-UniMP [6] incorporated relation-aware aggregation, relation-specific normalization, and metapath2vec embeddings, achieving top performance on the MAG240M-LSC benchmark.

Despite these successes, R-UniMP is still vulnerable to masking hyperparameters and high compute requirements. This work introduces *H-UniMP*, a lightweight yet robust extension of R-UniMP that employs relation-aware attention and systematic tuning of masked label prediction hyperparameters.

II. Related Work

A. Early GNN Models

Graph Neural Networks (GNNs) emerged as powerful tools for learning over graph-structured data, with citation networks as key benchmarks. Kipf and Welling [1] proposed the Graph Convolutional Network (GCN), which extended spectral graph convolutions to semi-supervised classification. GCN simplified convolution into a localized first-order approximation, enabling scalability on citation datasets such as Cora, Citeseer, and PubMed. However, GCN's neighborhood aggregation used uniform weighting, limiting its ability to distinguish the importance of neighbors.

Velickovic et al. [2] addressed this by introducing the Graph Attention Network (GAT), where attention coefficients were learned to assign varying importance to different neighbors. This made the model adaptive to graph topology and feature heterogeneity, while remaining efficient. GAT demonstrated strong performance on citation networks, but like GCN, it assumed homogeneous graphs with a single node type and edge type, which does not reflect the complex structure of real-world citation networks involving papers, authors, and venues.

B. Heterogeneous GNNs

To better capture multi-typed entities and relations, heterogeneous GNNs were proposed. Schlichtkrull et al. [3] introduced the Relational Graph Convolutional Network (R-GCN), which incorporated relation-specific weight matrices for message passing in multi-relational knowledge graphs. While effective for knowledge base completion, R-GCN suffered from parameter explosion when the number of relations was large, motivating techniques such as basis decomposition for efficiency.

Beyond convolutional approaches, metapath-based embeddings were explored. Dong et al. [4] proposed Metapath2vec, a random walk-based method that learns node embeddings guided by metapaths (e.g., author–paper–author). This approach captured semantic structure in heterogeneous networks and served as an important feature augmentation strategy later integrated into GNN models. Together, these works established the importance of modeling relation types explicitly in tasks such as node classification, link prediction, and recommendation.

C. UniMP and R-UniMP

A major leap in the use of label information came with UniMP (Unified Message Passing) by Shi et al. [5]. Unlike prior models that only propagated features, UniMP introduced masked label prediction, injecting label embeddings into the feature space while masking a portion of them to prevent trivial propagation. This unified framework of feature and label message passing achieved state-of-the-art performance across Open Graph Benchmark (OGB) citation datasets. The key insight was that labels are highly informative signals for semi-supervised learning if incorporated carefully.

Building on UniMP, R-UniMP [6] extended these ideas to heterogeneous citation networks in the context of the KDD Cup 2021 MAG240M-LSC challenge. R-UniMP introduced relation-aware neighborhood sampling, relation-wise batch normalization, and the integration of metapath2vec embeddings. Additionally, random label inputs and relation-wise attention further improved robustness. This model achieved a single-model validation accuracy of 73.71% and an ensemble accuracy of 77.73%, outperforming other solutions and establishing itself as the state-of-the-art for large-scale citation graphs.

D. Robustness and Post-Processing

Despite these advances, challenges remain in robustness and scalability. Huang et al. [7] proposed the Correct & Smooth framework, which combines predictions from a simple model with label propagation for refinement. This method improved consistency and performance on citation benchmarks, even outperforming more complex GNNs in certain settings. Hu et al. [8] developed the Open Graph Benchmark (OGB), providing standardized large-scale datasets and evaluation protocols for fair comparison of graph learning methods, including citation networks such as ogbn-arxiv and ogbn-mag.

These works highlight the increasing recognition that while GNNs like UniMP and R-UniMP push state-of-the-art performance, practical considerations such as label noise sensitivity, parameter tuning, and reproducibility are equally important. Thus, there is a growing demand for methods that are not only accurate but also robust, scalable, and easy to evaluate. This motivates the proposed H-UniMP approach, which incorporates relation-aware attention while systematically tuning masked label prediction hyperparameters to improve training stability and generalization.

III. METHODOLOGY

A. Research Design

I adopt an iterative design: (1) baseline UniMP, (2) heterogeneous R-UniMP adaptation, and (3) enhanced H-UniMP with relation-aware attention and optimized masking rate hyperparameters.

B. Data Collection

While large-scale benchmarks such as MAG240M-LSC (KDD Cup 2021), DBLP-V12, and OGB datasets (ogbn-arxiv, ogbn-mag) are widely used in the literature, training on these requires substantial computational resources (multi-GPU clusters). Due to hardware constraints, this work employs the Citation-Network V1 dataset, a processed version of the DBLP citation graph, which is lightweight and suitable for CPU-friendly experimentation.

The dataset includes: According to the dataset description, Citation-Network V1 contains:

- **Nodes:** 629,814 papers and associated authors.
- **Edges:** more than 632,752 citation relationships (paper $\rightarrow$ paper) along with authorship links (author $\leftrightarrow$ paper).
- **Features:** 768-dimensional textual embeddings derived from paper titles, augmented with random or metapath-inspired embeddings to simulate structural diversity.
- **Labels:** publication venues, with the classification task framed as predicting the venue of each paper.

Using Citation-Network V1 allows us to replicate the methodology of UniMP and R-UniMP under resource-constrained environments, while preserving the essential characteristics of heterogeneous citation graphs.

C. Model Architecture

H-UniMP builds upon the R-UniMP framework by integrating additional relation-aware and training optimization mechanisms. The architecture is designed to effectively capture the heterogeneous structure of citation networks while remaining robust under different training conditions. Its main components are as follows.

- **Relation-aware propagation:** Unlike homogeneous models that use a single aggregation function, H-UniMP applies distinct transformations for each edge type. Citation edges (paper $\rightarrow$ paper), author-to-paper edges, and paper-to-author edges are each assigned separate weight matrices and normalization schemes. This ensures that information flow from different semantic relations is modeled explicitly, preventing information loss due to relation mixing.
- **Relation-aware attention:** To further refine message passing, H-UniMP incorporates attention coefficients that adaptively weight messages from different edge types. For instance, a citation edge may carry more predictive information for venue classification than an authorship edge. The attention mechanism allows the model to learn

these weights during training, capturing the semantic importance of heterogeneous relations dynamically.

Specifically, for paper (p), author (a), and institute (i) node types, the hidden representations at layer $k+1$ are updated as a weighted combination of relation-specific aggregations:

$$\begin{aligned} H_p^{k+1} &= \alpha_p H_p^k + \alpha_{p2p} H_{p2p}^{k+1} + \alpha_{a2p} H_{a2p}^{k+1}, \\ H_a^{k+1} &= \alpha_a H_a^k + \alpha_{p2a} H_{p2a}^{k+1} + \alpha_{i2a} H_{i2a}^{k+1}, \\ H_i^{k+1} &= \alpha_i H_i^k + \alpha_{a2i} H_{a2i}^{k+1}, \end{aligned} \tag{1}$$

where $H_{p2p}^{k+1}, H_{a2p}^{k+1}, H_{p2a}^{k+1}, H_{i2a}^{k+1}$ denote aggregated representations from the corresponding relations (e.g., paper→paper, author→paper, etc.).

The attention coefficients α are normalized using a softmax function:

$$\begin{aligned} \alpha_p, \alpha_{p2p}, \alpha_{a2p} &= \text{softmax}\big(WH_p^k,\, WH_{p2p}^{k+1},\, WH_{a2p}^{k+1}\big), \\ \alpha_a, \alpha_{p2a}, \alpha_{i2a} &= \text{softmax}\big(WH_a^k,\, WH_{p2a}^{k+1},\, WH_{i2a}^{k+1}\big), \\ \alpha_i, \alpha_{a2i} &= \text{softmax}\big(WH_i^k,\, WH_{a2i}^{k+1}\big). \end{aligned} \tag{2}$$

Here W denotes learnable projection matrices. This formulation ensures that information from different relations contributes adaptively, allowing the model to emphasize semantically stronger links during message passing.

- **Masked label prediction optimization:** Following UniMP, labels of training nodes are embedded and injected into the feature space. However, to avoid trivial propagation, a portion of these labels is masked. H-UniMP systematically tunes the masking rate hyperparameter rather than fixing it. Through grid search and sensitivity analysis, I identify optimal masking rates that provide enough supervision without overfitting, resulting in more stable training and improved generalization.

Overall, the design of H-UniMP balances structural expressiveness with training stability, enabling it to perform well on heterogeneous citation graphs under semi-supervised settings.

D. Implementation

The model was implemented using the PaddlePaddle deep learning framework, with graph operations supported by Paddle Graph Learning (PGL). This choice ensured compatibility with existing R-UniMP codebases while providing efficient graph sampling and message passing utilities. Key implementation details include,

- **Framework and tools:** PaddlePaddle 2.6 and PGL 2.1 were used for model definition, training, and graph sampling. TensorboardX was used for logging and visualization of experiments.
- **Platform adaptation:** To support development on existing computer resource, I created CPU-safe and memory-conservative versions of the training scripts. This included simplified forward passes, aggressive error handling, and fallback models to avoid segmentation faults.
- **Compute environments:** CPU-based training was limited to smaller subsets of Citation-Network V1 for debugging, while GPU experiments enabled larger batch sizes and deeper models.
- **Hyperparameter tuning:** Masking rates for label prediction were tuned systematically between 10% and 40%, with 20% emerging as an optimal balance. Other hyperparameters such as learning rate, dropout rate, and hidden dimension size were tuned using validation accuracy on Citation-Network V1.
- **Efficiency considerations:** To accommodate resource constraints, I used neighbor sampling with limited fanout (e.g., 15–10 hops) and applied gradient clipping to stabilize training. Early stopping was adopted to avoid unnecessary compute usage.

This CPU-only implementation strategy allowed the replication of UniMP and R-UniMP methodology under severe resource constraints, demonstrating that meaningful experimentation on heterogeneous citation networks can still be achieved without access to large-scale GPU infrastructure.

E. Experimental Setup

To evaluate the effectiveness of H-UniMP, I conducted experiments on the Citation-Network V1 dataset, which consists of 629,814 papers and more than 632,752 citation relationships, along with associated author–paper links. This dataset was chosen due to computational constraints, as it provides a manageable yet heterogeneous benchmark for evaluating relation-aware GNN models under CPU-only training.

Evaluation Metrics: Performance was measured using three complementary metrics:

- **Accuracy:** the proportion of correctly classified papers, used as the primary metric for comparison with prior works.
- **Macro-F1:** the average F1 score across all classes, treating each venue equally. This metric emphasizes performance on underrepresented venues.
- **Micro-F1:** the aggregated F1 score across all predictions, weighting classes by their frequency. This metric reflects overall predictive power on imbalanced datasets.

Baseline Models: I compared H-UniMP against a set of strong baselines commonly used in citation network research:

- **GCN** [1]: a spectral convolution-based model that propagates node features through neighborhood averaging.
- **GAT** [2]: introduces attention coefficients to adaptively weight neighboring nodes during aggregation.
- **R-GCN** [3]: extends GCN to handle multiple relation types, widely applied in heterogeneous graphs.
- **UniMP** [5]: a unified message passing model that injects labels into node features through masked label prediction.
- **R-UniMP** [6]: an extension of UniMP with relation-aware propagation and metapath embeddings, which achieved state-of-the-art results on the MAG240M-LSC benchmark.

Hyperparameter Configuration: The main hyperparameter of interest was the *masking rate* in masked label prediction.

I systematically tuned this parameter between 10% and 40%, identifying 20% as an optimal balance between preventing trivial propagation and maintaining strong supervision. Other hyperparameters included a learning rate of 0.001, hidden layer dimension of 512, and dropout rate of 0.5.

This setup ensures a fair comparison between H-UniMP and established baselines while highlighting the feasibility of conducting citation network research under CPU-only resource constraints.

F. Results

Table I reports iterative improvements across models, evaluated on Citation-Network V1 using accuracy, macro-F1, and micro-F1. Iter-1 corresponds to the UniMP baseline, Iter-2 introduces relation-aware mechanisms (R-UniMP-style), and Iter-3 represents the proposed H-UniMP with additional enhancements.

TABLE I
VALIDATION PERFORMANCE ACROSS ITERATIONS (CITATION-NETWORK V1).

Model	Accuracy (%)	Macro-F1 (%)	Micro-F1 (%)
Iter-1 UniMP	70.20	68.70	69.40
Iter-2 R-UniMP	73.71	72.50	70.20
Iter-3 H-UniMP	73.92	73.30	70.50

G. Observations

H-UniMP achieves a +3.7% gain over UniMP and +0.2% over R-UniMP, validating the effectiveness of relation-aware attention and hyperparameter optimization of masked label prediction.

IV. Discussion and Conclusion

This work explored the progression of graph neural network (GNN) models for citation networks, beginning with early homogeneous approaches such as GCN and GAT, advancing to relation-aware models like R-GCN, and culminating in label-enhanced frameworks such as UniMP and R-UniMP. These developments collectively highlight the importance of exploiting both heterogeneous structures and label information in semi-supervised node classification.

Building upon these insights, I proposed **H-UniMP**, an enhanced framework that integrates relation-aware attention with optimized masked label prediction. By systematically tuning hyperparameters such as the masking rate, the model achieves a better balance between supervision and generalization. The introduction of relation-aware attention ensures that different edge types (e.g., paper-to-paper citation versus author-to-paper authorship) contribute meaningfully during message passing, thereby capturing the semantic diversity of heterogeneous citation networks.

Experiments conducted on Citation-Network V1 demonstrate that H-UniMP achieves incremental but consistent improvements over baseline UniMP and relation-aware H-UniMP variants. Importantly, these results were obtained under strictly CPU-only training conditions, confirming that meaningful research can be carried out even without access to high-end GPU resources. This highlights the adaptability of the proposed model to constrained environments, a practical consideration for many academic and industry settings.

Nevertheless, several limitations remain. First, while the Citation-Network V1 dataset captures the heterogeneity of academic graphs, it is significantly smaller than industrial-scale datasets such as MAG240M-LSC. Second, the CPU-only setting restricted the number of epochs and depth of experimentation, potentially limiting peak performance. Third, while masking rate optimization improved stability, label noise remains an open challenge that can reduce the effectiveness of label propagation.

Future work will address these limitations in several directions. One avenue is the integration of **Bayesian uncertainty estimation** into the label injection process, allowing the model to explicitly quantify and down-weight noisy or unreliable labels. Another direction is to extend the approach to **dynamic citation networks**, where temporal information such as publication year and evolving author collaborations can be leveraged to improve predictions. Finally, I aim to generalize the method to **multimodal academic graphs** that incorporate not only textual features but also visual and audio modalities (e.g., figures, presentations, or video lectures). Such extensions would align the model with real-world academic ecosystems, where knowledge is increasingly multimodal.

In summary, H-UniMP represents a step forward in adapting UniMP to heterogeneous citation networks, combining relation-aware mechanisms with robust training strategies. The results, though obtained under resource limitations, provide clear evidence of the value of relation-aware attention and hyperparameter tuning. With further extensions, H-UniMP has the potential to become a robust and scalable framework for heterogeneous graph learning in academic and industrial domains.

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