Improving Article Classification with Edge-Heterogeneous Graph Neural Networks

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ABSTRACT

Classifying research output into context-specific label taxonomies is a challenging and relevant downstream task, given the volume of existing and newly published articles. We propose a method to enhance the performance of article classification by enriching simple Graph Neural Networks (GNN) pipelines with edge-heterogeneous graph representations. SciBERT is used for node feature generation to capture higher-order semantics within the articles’ textual metadata. Fully supervised transductive node classification experiments are conducted on the Open Graph Benchmark (OGB) ogbn-arxiv dataset and the PubMed diabetes dataset, augmented with additional metadata from Microsoft Academic Graph (MAG) and PubMed Central, respectively. The results demonstrate that edge-heterogeneous graphs consistently improve the performance of all GNN models compared to the edge-homogeneous graphs. The transformed data enable simple and shallow GNN pipelines to achieve results on par with more complex architectures. On ogbn-arxiv, we achieve a top-15 result in the OGB competition with a 2-layer GCN (accuracy 74.61%), being the highest-scoring solution with sub-1 million parameters. On PubMed, we closely trail SOTA GNN architectures using a 2-layer GraphSAGE by including additional co-authorship edges in the graph (accuracy 89.88%). The implementation is available at: https://github.com/lyvykhang/edgehetero-nodeproppred.

Keywords  Heterogeneous Graph Learning · Graph Neural Networks · Article Classification · Document Relatedness

1 Introduction

Article classification is a challenging downstream task within natural language processing (NLP) [Mirończuk and Protasiewicz 2018]. An important practical application is classifying existing or newly-published articles according to specific research taxonomies. The task can be approached as a graph node classification problem, where nodes represent articles with corresponding feature mappings, and edges are defined by a strong signal of article relatedness, e.g. citations/references. Conventionally, graph representation learning is handled in two phases: unsupervised node feature generation, followed by supervised learning on said features using the graph structure. Graph neural networks (GNNs) can be successfully employed for the second phase of such problems, being capable of preserving the rich structural information encoded by graphs. In recent years, prolific GNN architectures have achieved strong performance...
We focus on combining textual information from articles with various indicators of article relatedness (citation data, co-authorship, subject fields, and publication sources) to create a graph with multiple edge types; further referred to as an edge-heterogeneous graph, also known as multi-graphs or multipartite networks [Barabási and Pósfai, 2017]. We use two established node classification benchmarks - the citation graphs ogbn-arxiv and PubMed - and leverage their connection to large citation databases - Microsoft Academic Graph (MAG) and PubMed Central - to retrieve the metadata fields and enrich the graph structure with additional edge types [Hu et al., 2020, Sen et al., 2008]. For feature generation, SciBERT is used to infer embeddings based on articles’ titles and abstracts [Beltagy et al., 2019], with the intention of capturing higher-order semantics compared to the defaults, i.e. Skip-Gram or bag-of-words. We test our transformed graphs with a variety of GNN backbone models, converted to support heterogeneous input using the relational graph convolutional network (R-GCN) framework [Schlichtkrull et al., 2018]. In essence, we approach a typically homogeneous task using heterogeneous techniques. The method is intuitively simple and interpretable; we do not utilize complex model architectures and training frameworks, focusing primarily on data retrieval and preprocessing to boost the performance of simpler models, thus maintaining a reasonably low computational cost and small number of fitted parameters.

A considerable volume of research is devoted to article classification, graph representation learning with respect to citation networks, and the adaptation of these practices to heterogeneous graphs [Wu et al., 2019a, Bing et al., 2022]. However, the application of heterogeneous graph enrichment techniques to article classification is not well-studied and presents a research opportunity. Existing works on heterogeneous graphs often consider multiple node types, expanding

Figure 1: Illustration of the proposed edge heterogeneity, which enables the neighboring feature aggregation for a node $X_1$ to be performed across a variety of subgraphs, leveraging multiple signals of article relatedness (References, Authorship, and Journal depicted here).
from article to entity classification; we exclusively investigate the heterogeneity of paper-to-paper relationships to remain consistent with the single-node type problem setting. The emergence of rich metadata repositories for papers, e.g. OpenAlex, illustrates the relevance of our research [Priem et al., 2022].

Scalability is often a concern with GNN architectures. For this reason, numerous approaches simplify typical GNN architectures with varying strategies, e.g. pre-computation or linearization, without sacrificing significant performance in most downstream tasks [Frasca et al., 2020; Wu et al., 2019b; Prieto et al., 2023]. Other solutions avoid GNNs altogether, opting for simpler approaches based on early graph-based techniques like label propagation, which outperform GNNs in several node classification benchmarks [Huang et al., 2021]. The success of these simple approaches raises questions about the potential impracticality of deep GNN architectures on large real-world networks with a strong notion of locality, and whether or not such architectures are actually necessary to achieve satisfactory performance.

Compared to simple homogeneous graphs, heterogeneous graphs encode rich structural and semantic information, and are more representative of real-world information networks and entity relationships [Bing et al., 2022]. For example, networks constructed from citation databases can feature relations between papers, their authors, and shared keywords, often expressed in an RDF triple, e.g. “paper $\xrightarrow{(co-authored by)}$ author,” “paper $\xrightarrow{includes}$ keyword,” “paper $\xrightarrow{cites}$ paper.” Heterogeneous GNN architectures share many similarities with their homogeneous counterparts; a common approach is to aggregate feature information from local neighborhoods, while using additional modules to account for varying node and/or edge types [Yang et al., 2022]. Notably, the relational graph convolutional network approach (R-GCN) by Schlichtkrull et al. [2018] shows that GCN-based frameworks can be effectively applied to modeling relational data, specifically for the task of node classification. The authors propose a modeling technique where the message passing functions are duplicated and applied individually to each relationship type. This transformation can be generalized to a variety of GNN convolutional operators in order to convert them into their relational (heterogeneous) counterparts.

2 Methodology

We propose an approach focusing on dataset provenance, leveraging their linkage to large citation and metadata repositories, e.g. MAG and PubMed Central, to retrieve additional features and enrich their graph representations. The proposed method is GNN-agnostic, compatible with a variety of model pipelines (provided they can function with heterogeneous input graphs) and node embedding techniques (results are presented with the provided features, plus the SciBERT embeddings). Figure 1 provides a high-level overview of the method.

The tested GNN backbones (see section 3) are converted to support heterogeneous input using the aforementioned R-GCN transformation defined by Schlichtkrull et al. [2018], involving the duplication of the message passing functions at each convolutional layer per relationship type; we employ the PyTorch Geometric (PyG) implementation of this technique, using the mean as the aggregation operator [Fey and Lenssen, 2019].

2.1 Datasets

Our experiments are conducted on two datasets: the Open Graph Benchmark (OGB) ogbn-arxiv dataset and the PubMed diabetes dataset.

The OGB ogbn-arxiv dataset consists of 169,343 Computer Science papers from arXiv, hand-labeled into 40 subject areas by paper authors and arXiv moderators, with 1,166,243 reference links [Hu et al., 2020]. Node features are constructed from textual information by averaging the embeddings of words (which are generated with the Skip-Gram model) in the articles’ titles and abstracts. The dataset provides the mapping used between papers’ node IDs and their original MAG IDs, which can be used to retrieve additional metadata.

The PubMed diabetes dataset consists of 19,717 papers from the National Library of Medicine’s (NLM) PubMed database labeled into one of three categories: “Diabetes Mellitus, Experimental,” “Diabetes Mellitus Type 1,” and “Diabetes Mellitus Type 2,” with 44,338 references links [Sen et al., 2008]. Bag-of-words vectors from a dictionary of 500 unique words are provided as node features. Similarly, the papers’ original PubMed IDs can be used to fetch relevant metadata.

2.2 Data Augmentation

We used a July-2020 snapshot of the complete Microsoft Academic Graph (MAG) index (240M papers) - since MAG (and the associated API) was discontinued later - to obtain additional metadata [Zhang et al., 2023]. Potential indicators

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1The data is hosted by AMiner’s Open Academic Graph project. All chunks were downloaded locally and metadata of IDs corresponding to papers in ogbn-arxiv were saved.
of paper relatedness include: authors, venue, and fields of study. Other metadata (DOI, volume, page numbers, etc.) are not useful for our purposes. Hence, we “heterogenize” the dataset with the following additional edge types (in addition to the References edges):

- (Co)-Authorship: Two papers are connected if they share an author, with a corresponding edge weight indicating the number of shared authors. This is based on the assumption that a given author tends to perform research on similar disciplines.
- Venue: Two papers are connected if they were published at the same venue (conference or journal), assuming that specific conferences contribute to relevant research areas.
- Fields of Study (FoS): Two papers are connected if they share at least one field, with an edge weight based on the number of shared fields. Fields of study, e.g. “computer science,” “neural networks,” etc. are automatically assigned with an associated confidence score (which we do not use), and each paper can have multiple fields of study, making them functionally similar to keywords.

An unprocessed version of the PubMed dataset preserving the original paper IDs was used [Namata et al., 2012]. A January-2023 snapshot of the complete PubMed citation database (35M papers) was accessed for additional metadata. Relevant features include: title, abstract, authors, published journal (indicated by unique NLM journal IDs), and Medical Subject Headings (MeSH®). The latter is an NLM-controlled hierarchical vocabulary used to characterize biomedical article content. As with the Fields of Study, they are functionally similar to curated keywords. As before, we use three additional edge types:

- (Co)-Authorship: Two papers are connected if they share an author, with a corresponding edge weight indicating the number of shared authors. Unlike MAG, PubMed Central does not provide unique identifiers for authors, so exact author names are used, which can lead to some ambiguity in a minority of cases, e.g. two distinct authors with the same name.
- Journal: Two papers are connected if they were published in the same journal. The intuition is that journals publish papers on similar topics.
- MeSH: Two papers are connected if they share at least one MeSH subject heading, with an edge weight based on the number of shared subjects.

Since the ogbn-arxiv venue and fields and PubMed MeSH relationships result in massive edge lists, posing out-of-memory issues on the utilized hardware, we only create edges between up to \( k \) nodes per unique venue/field/heading, where \( k \) is the mean number of papers per venue/field/heading, in order to reduce the subgraphs’ sizes. All edge weights are normalized using logistic sigmoid.

In a traditional citation network, the links are typically directed, but in our experiments, they are undirected to strengthen the connections of communities in the graph. The graph includes only one node type, “paper.” Other approaches, notably in the citation recommendation domain, leverage node types to represent authors and journals [Guo et al., 2017]. However, this work strictly concerns relationships between papers and not between papers and other entities, in order to apply the homogeneous problem settings. Practically, the resultant graph would contain too many nodes, while there the number of features and metadata is insufficient to generate informative representations of other node types, limiting their usefulness in the feature aggregation step.

For textual node feature representation, embeddings of the concatenated paper titles and abstracts are inferred using SciBERT [Beltagy et al., 2019]; this is inspired by the work of Cohan et al. [2020], in which SciBERT was pretrained on a citation graph and used to generate high-quality document-level embeddings for node classification purposes. Here, we utilize the base model (scibert-scivocab-uncased) without additional fine-tuning.

2.3 Subgraph Properties

Some insights on the characteristics of the defined subgraphs can be derived from Table 1, which lists the following: number of nodes and edges (post-conversion to undirected) in the largest connected component (LCC), total number of edges, average degree, network average clustering coefficient [Schank and Wagner, 2005], and edge homophily ratio (fraction of edges connecting nodes with the same label) [Ma et al., 2022]. While the References graphs do not exhibit the tight clustering typical of real-world information networks, the strong signal of relatedness in the edges has

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2This version of the dataset is hosted by the [LINQS Statistical Relational Learning Group](https://linqs.cs.cornell.edu/). The 2023 annual baseline on the NLM FTP server is accessed to retrieve metadata. All files were downloaded locally and metadata of matching IDs were extracted (19,716 records matched, 1 missing).
nonetheless ensured their compatibility with message passing GNN paradigms [Wu et al., 2019a]. This relatedness is also evident in the Authorship graphs, and the high level of clustering confirms the initial hypothesis that researchers co-author papers within similar topics. The topic-based relationships (FoS and MeSH), include many edges formed between shared generic keywords, e.g. “computer science,” leading to rather average homophily. The publication source subgraphs (Venue and Journal) consist of isolated fully-connected clusters per unique source, with no inter-cluster connections, as each paper belongs to only one journal or venue. As with the topic-based relationships, the research area covered by a given publication conference or journal can be quite broad with respect to the paper labels.

Table 1: Properties of constructed subgraphs. Note that the References subgraphs are the only ones without isolated nodes. Note that the network average clustering coefficient computation accounts for isolated nodes (which are treated as having “zero” local clustering), hence the value for sparser subgraphs, e.g. ogbn-arxiv Venue, is notably lower than intuitively expected (1, in the absence of isolated nodes).

<table>
<thead>
<tr>
<th>Subgraph</th>
<th>Nodes in LCC</th>
<th>Edges in LCC</th>
<th>Edges total</th>
<th>Avg. degree</th>
<th>Avg. clustering coeff.</th>
<th>Homophily</th>
</tr>
</thead>
<tbody>
<tr>
<td>ogbn-arxiv</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>References</td>
<td>169,343</td>
<td>2,315,598</td>
<td>2,315,598</td>
<td>13.7</td>
<td>0.247</td>
<td>0.654</td>
</tr>
<tr>
<td>Authorship</td>
<td>145,973</td>
<td>6,697,998</td>
<td>6,749,335</td>
<td>39.9</td>
<td>0.702</td>
<td>0.580</td>
</tr>
<tr>
<td>Venue</td>
<td>63</td>
<td>3,906</td>
<td>600,930</td>
<td>3.5</td>
<td>0.112</td>
<td>0.077</td>
</tr>
<tr>
<td>FoS</td>
<td>144,529</td>
<td>8,279,492</td>
<td>8,279,687</td>
<td>48.9</td>
<td>0.505</td>
<td>0.319</td>
</tr>
<tr>
<td>PubMed</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>References</td>
<td>19,716</td>
<td>88,649</td>
<td>88,649</td>
<td>4.5</td>
<td>0.057</td>
<td>0.802</td>
</tr>
<tr>
<td>Authorship</td>
<td>17,683</td>
<td>729,468</td>
<td>731,376</td>
<td>37.1</td>
<td>0.623</td>
<td>0.721</td>
</tr>
<tr>
<td>Journal</td>
<td>2,213</td>
<td>4,895,156</td>
<td>11,426,930</td>
<td>579.6</td>
<td>0.940</td>
<td>0.414</td>
</tr>
<tr>
<td>MeSH</td>
<td>18,345</td>
<td>1,578,526</td>
<td>1,578,530</td>
<td>80.1</td>
<td>0.456</td>
<td>0.550</td>
</tr>
</tbody>
</table>

Figure 2: Degree distribution, i.e. frequency of each degree value, of all subgraphs for ogbn-arxiv (left) and PubMed (right), plotted on a log-log scale. Points indicate the unique degree values.

Figure 3 shows the degree distribution of all edge type subgraphs in both datasets, which gives a clear view of the subgraphs’ structures when interpreted with the above metrics. The high frequency of large node degrees in the PubMed Journal subgraph corresponds to large journals; the size of the LCC (2,213) is the number of papers in the largest journal. While not visible for the ogbn-arxiv Venue subgraph due to the aforementioned sampling, a similar distribution would occur for large venues if all possible edges had been included. In contrast, the lower occurrence of high degree nodes and low clustering in the References subgraphs of both datasets indicates greater average distance across the LCC compared to the other subgraphs; such a structure stands to benefit the most from the multi-hop neighborhood
We evaluate model performance on the task of fully supervised transductive node classification. The metric is multi-class accuracy on the test set. The proposed data preparation scheme is tested with several GNN architectures commonly deployed in benchmarks. We consider two GCN setups (base one and with a jumping knowledge module using concatenation as the aggregation scheme), as well as GraphSAGE [Kipf and Welling, 2017, Xu et al., 2018, Hamilton et al., 2017]. We also run experiments with the simplified graph convolutional operator (SGC) [Wu et al., 2019b]. The increased graph footprint can lead to scalability concerns, hence the performance of such lightweight and parameter-efficient methods is of interest.

For ogbn-arxiv, the provided time-based split is used: train on papers published until 2017, test on those published in 2018, test on those published since 2019. For PubMed diabetes, nodes of each class are randomly split into 60% - 20% - 20% for training - validation - and testing for each run (as performed by Pei et al., 2020 and Chen et al., 2020). Ablation experiments are also performed to examine the impact of the different edge types (averaged across 3 runs) and to identify the optimal configuration for both datasets, on which we then report final results (averaged across 10 runs). Experiments were conducted on a g4dn.2xlarge EC2 instance (32 GB RAM, 1 NVIDIA Tesla T4 16 GB VRAM). Models are trained with negative log-likelihood loss and early stopping based on validation accuracy (patience of 50 epochs, with an upper limit of 500 epochs). We also scale down the learning rate as the validation loss plateaus. The ScIBERT embeddings are pre-computed using multi-GPU distributed inference.

### 3 Experiments and Results

We evaluate model performance on the task of fully supervised transductive node classification. The metric is multi-class accuracy on the test set. The proposed data preparation scheme is tested with several GNN architectures commonly deployed in benchmarks. We consider two GCN setups (base one and with a jumping knowledge module using concatenation as the aggregation scheme), as well as GraphSAGE [Kipf and Welling, 2017, Xu et al., 2018, Hamilton et al., 2017]. We also run experiments with the simplified graph convolutional operator (SGC) [Wu et al., 2019b]. The increased graph footprint can lead to scalability concerns, hence the performance of such lightweight and parameter-efficient methods is of interest.

For ogbn-arxiv, the provided time-based split is used: train on papers published until 2017, test on those published in 2018, test on those published since 2019. For PubMed diabetes, nodes of each class are randomly split into 60% - 20% - 20% for training - validation - and testing for each run (as performed by Pei et al., 2020 and Chen et al., 2020). Ablation experiments are also performed to examine the impact of the different edge types (averaged across 3 runs) and to identify the optimal configuration for both datasets, on which we then report final results (averaged across 10 runs). Experiments were conducted on a g4dn.2xlarge EC2 instance (32 GB RAM, 1 NVIDIA Tesla T4 16 GB VRAM). Models are trained with negative log-likelihood loss and early stopping based on validation accuracy (patience of 50 epochs, with an upper limit of 500 epochs). We also scale down the learning rate as the validation loss plateaus. The ScIBERT embeddings are pre-computed using multi-GPU distributed inference.

#### 3.1 Ablation Study

Ablation results for both datasets are presented in Table 2, separated by node embedding type. First, all possible homogeneous subgraphs are inspected, as this is the conventional input data for this task (see the first 4 rows). The best performance is achieved on the References graphs, followed by the Authorship graphs. Then we build upon the References graph by adding different combinations of other subgraphs. The results demonstrate that transitioning to edge-heterogeneous graphs can yield up to 2.87% performance improvement on ogbn-arxiv and 2.05% on PubMed (see the difference between the yellow- and green-highlighted cells). These results were obtained with a 2-layer GCN base, using the following fixed hyperparameter values: optimizer weight decay of 0.001 and initial learning rate of 0.01, hidden layer dropout probability of 0.5, and hidden feature dimensionality of 128 (ogbn-arxiv) or 64 (PubMed).

Cross-checking with the metrics in Table 1 implies improvements from edge-heterogeneity roughly correspond to the edge homophily ratio of the utilized subgraphs, as strong homophily is implicitly assumed by the neighborhood aggregation mechanism of GCN-based models. Subsequently, their performance can be erratic and unpredictable in graphs with comparatively low homophily [Kipf and Welling, 2017, Ma et al., 2022]. Since the R-GCN transformation collects neighborhoods from input subgraphs with equal weighting, including a comparatively noisy subgraphs (like ogbn-arxiv Venue) can worsen predictive performance. Changing the R-GCN aggregation operator, e.g. from mean to concatenation, does not alleviate this. This study suggests publication sources do not yield beneficial subgraphs with their current definition; while the aforementioned tight clustering could provide a strong signal for classification with sufficient homophily, any potential benefit is absent because these clusters are noisy. The topic-based subgraphs are more structurally preferable, but noisy edges (from keywords tied to concepts that are higher-level than the paper labels) reduce their usefulness in classification. In all experimental settings, the largest gain from heterogeneity comes from the co-authorship graph, often outperforming configurations that use more subgraphs. These trends are expected, given the characteristics discussed in section 2.3.

Replacing the PubMed bag-of-words vectors with ScIBERT embeddings does not improve raw accuracy in most cases. Though, the increased feature dimensionality of ScIBERT embeddings do stabilize convergence behavior in configurations using multiple subgraphs. A paper might possess only a few non-zero feature dimensions when using bag-of-words; combined with the additional feature averaging step from the R-GCN transformation, the risk of oversmoothing is increased even on shallow 2-layer networks in edge-heterogeneous configurations (however, note that tested single-layer models underfit and thus do not improve performance). In accordance with the findings of Chen et al., 2020, these hypothesized oversmoothing effects are more pronounced when using graphs with high average degree, i.e. the publication source and topic-based subgraphs; nodes with high degree aggregate more information from their neighbors, increasing the likelihood of homogenization as network depth increases.
Table 2: Ablation study for both datasets, 3-run average test accuracy with a 2-layer GCN. The best results are highlighted in bold. Note the table feature differences (Venue, FoS, and Skip-Gram for ogbn-arxiv, Journal, MeSH, and Bag-of-Words for PubMed).

<table>
<thead>
<tr>
<th>References</th>
<th>Authorship</th>
<th>Venue / Journal</th>
<th>FoS / MeSH</th>
<th>ogbn-arxiv</th>
<th>PubMed</th>
</tr>
</thead>
<tbody>
<tr>
<td>✓</td>
<td></td>
<td></td>
<td></td>
<td>SkipGram</td>
<td>SciBERT</td>
</tr>
<tr>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td>0.6858 ± 0.0008</td>
<td>0.7177 ± 0.0024</td>
</tr>
<tr>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td>0.6795 ± 0.0008</td>
<td>0.7136 ± 0.00036</td>
</tr>
<tr>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td>0.6995 ± 0.0009</td>
<td>0.7334 ± 0.0008</td>
</tr>
<tr>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td>0.7145 ± 0.0024</td>
<td>0.7383 ± 0.0003</td>
</tr>
<tr>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td>0.7094 ± 0.0011</td>
<td>0.7327 ± 0.0004</td>
</tr>
</tbody>
</table>

*Indicates (significant) oversmoothing.

3.2 Optimal Configuration

Results with the optimal configuration identified from the ablation study on ogbn-arxiv and PubMed are listed in Tables 3 and 4, respectively. Note that the actual performance gains may vary slightly since the third-party benchmarks were used with directed References graphs and differently-tuned hyperparameters.

Table 3: Results on the best ogbn-arxiv configuration (References, Authorship, Fields of Study subgraphs, and SciBERT embeddings) with hyperparameters described in Appendix 4. The baseline results on the unmodified dataset and the improvement over the baseline (test acc. minus baseline acc.) are also displayed. For GCN, GCN+JK, and SAGE, these are taken from the official leaderboard. The SGC baseline was obtained by using the (undirected) References subgraph and provided SkipGram features.

<table>
<thead>
<tr>
<th>Model</th>
<th>Validation Accuracy</th>
<th>Test Accuracy</th>
<th># Params</th>
<th>Baseline Accuracy</th>
<th>Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>GCN</td>
<td>0.7586 ± 0.0012</td>
<td>0.7461 ± 0.0006</td>
<td>621,944</td>
<td>0.7174 ± 0.0029</td>
<td>+2.87%</td>
</tr>
<tr>
<td>GCN+JK</td>
<td>0.7629 ± 0.0007</td>
<td>0.7472 ± 0.0024</td>
<td>809,512</td>
<td>0.7219 ± 0.0021</td>
<td>+2.53%</td>
</tr>
<tr>
<td>SAGE</td>
<td>0.7605 ± 0.0007</td>
<td>0.7461 ± 0.0013</td>
<td>1,242,488</td>
<td>0.7149 ± 0.0027</td>
<td>+3.12%</td>
</tr>
<tr>
<td>SGC</td>
<td>0.7515 ± 0.0005</td>
<td>0.7419 ± 0.0004</td>
<td>92,280</td>
<td>0.6855 ± 0.0002</td>
<td>+5.64%</td>
</tr>
</tbody>
</table>

The results demonstrate that the additional structural information provided by edge heterogeneity consistently improves final performance of a variety of hetero-transformed GNN frameworks compared to their homogeneous counterparts on both datasets, when making optimal subgraph choices (though, suboptimal choices can still situationally improve performance). These improvements are independent of the tested textual embedding methods, and can occur even when the added subgraphs possess suboptimal graph properties, e.g. lower edge homophily ratio and presence of isolated nodes, compared to the starting References graph. SGC with ogbn-arxiv shows the strongest improvement over the baseline. Most likely, the linear classifier relies less on graph structures, and hence benefits more from the deeper textual semantics captured by SciBERT. Notably, the best results are competitive with the SOTA, while operating on a limited compute budget and low level of complexity (simple 2-layer GNN model pipelines with comparatively few tunable parameters). On ogbn-arxiv, we achieve a top-15 result with the GCN backbone, being the highest-scoring solution with sub-1 million parameters. On PubMed with the aforementioned splitting strategy, we closely trail the best
Table 4: Results on the best PubMed configuration (References and Authorship subgraphs, and default Bag-of-Words vectors) with hyperparameters given in Appendix 4. The GCN and GCN+JK baselines are from Chen et al. [2020] (no standard deviations reported), and the others were obtained by using only the (undirected) References subgraph and provided Bag-of-Words features.

<table>
<thead>
<tr>
<th>Model</th>
<th>Validation Accuracy</th>
<th>Test Accuracy</th>
<th># Params</th>
<th>Baseline Accuracy</th>
<th>Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>GCN</td>
<td>0.8954 ± 0.0025</td>
<td>0.8938 ± 0.0040</td>
<td>129,286</td>
<td>0.8813</td>
<td>+1.25%</td>
</tr>
<tr>
<td>GCN+JK</td>
<td>0.8953 ± 0.0046</td>
<td>0.8939 ± 0.0064</td>
<td>34,499</td>
<td>0.8894</td>
<td>+0.45%</td>
</tr>
<tr>
<td>SAGE</td>
<td>0.9017 ± 0.0038</td>
<td>0.8988 ± 0.0047</td>
<td>129,155</td>
<td>0.8921 ± 0.0044</td>
<td>+0.67%</td>
</tr>
<tr>
<td>SGC</td>
<td>0.8715 ± 0.0038</td>
<td>0.8698 ± 0.0049</td>
<td>3,006</td>
<td>0.8607 ± 0.0042</td>
<td>+0.91%</td>
</tr>
</tbody>
</table>

performance reported by GCNII (90.30%) and Geom-GCN (90.05%) [Chen et al., 2020, Pei et al., 2020], by using a GraphSAGE backbone with just the added co-authorship subgraph input (89.88%).

4 Conclusions and Future Work

In this paper, we propose a data transformation methodology leveraging metadata retrieved from citation databases to create enriched edge-heterogeneous graph representations based on various additional signals of document relatedness: co-authorship, publication source, fields of study, and subject headings. We also test the substitution of default node features with SciBERT embeddings to capture higher-dimensionality textual semantics. By nature, the methodology is GNN- and embedding-agnostic. Deploying optimal configurations of the transformed graph with a variety of simple GNN pipelines leads to consistent improvements over the starting data, and enables results on par with the SOTA in full-supervised node classification. Overall, results show that our methodology can be an effective strategy to achieve respectable performance on datasets with readily-available article metadata, without necessitating complex GNN architectures and lengthy (pre-)training procedures.

As the methodology is compatible with any hetero-transformable GNN backbone and node embedding technique, we expect that deploying the transformed data with SOTA GNN frameworks, e.g. RevGAT by [Li et al., 2021] on ogbn-arxiv, will lead to a greater raw performance. Though, the larger memory footprint of the graph may complicate the application of such frameworks.

Refining the edge type definitions, e.g. connect papers that share at least two fields of study and/or remove “generic” fields applicable to a majority of papers in the set, can help de-noising and improving the properties of the respective subgraphs. A custom aggregation scheme could be implemented for the heterogeneous transformation dependent on individual subgraph properties, such as a weighted average based on some metric of subgraph “quality,” e.g. homophily. To mitigate the increased risk of heterogeneity-induced oversmoothing, additional regularization techniques, e.g. DropEdge by [Rong et al., 2020], could be considered. Finally, applying parameter-efficient fine-tuning (PEFT) techniques to the SciBERT model can improve feature separability and thus classification performance [Duan et al., 2023]; the effectiveness of different transformer-based language models can also be investigated.

Acknowledgement

The authors would like to thank prof. Paul Groth for his supervision and consultation throughout the project.

References


Appendix A. Hyperparameters

The parameters for the learning rate scheduler (torch.optim.lr_scheduler.ReduceLROnPlateau) were kept constant in all experimental settings: 0.1 factor, 10 patience, 0.0001 threshold, 0.0001 min_lr, 20 cooldown.

Table 5: Hyperparameters used for reported ogbn-arxiv results in Table 3

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<tbody>
<tr>
<td>GCN</td>
<td>num_layers: 2, hidden_channels: 256, weight_decay: 0.001, lr: 0.01, dropout: 0.2</td>
<td>Existing leaderboard submission.</td>
</tr>
<tr>
<td>GCN+JK</td>
<td>num_layers: 2, hidden_channels: 256, weight_decay: 0.003, lr: 0.01, dropout: 0</td>
<td>Existing leaderboard submission.</td>
</tr>
<tr>
<td>SAGE</td>
<td>num_layers: 2, hidden_channels: 256, weight_decay: 0.001, lr: 0.01, dropout: 0.2</td>
<td>Existing leaderboard submission.</td>
</tr>
<tr>
<td>SGC</td>
<td>K: 2, weight_decay: 0, lr: 0.01</td>
<td>K: 3, weight_decay: 0, lr: 0.1</td>
</tr>
</tbody>
</table>

Table 6: Hyperparameters used for reported PubMed results in Table 4

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<tbody>
<tr>
<td>GCN</td>
<td>num_layers: 2, hidden_channels: 128, weight_decay: 0.005, lr: 0.001, dropout: 0</td>
<td>Existing benchmark from Chen et al. [2020].</td>
</tr>
<tr>
<td>GCN+JK</td>
<td>num_layers: 2, hidden_channels: 32, weight_decay: 0.005, lr: 0.001, dropout: 0</td>
<td>Existing benchmark from Chen et al. [2020].</td>
</tr>
<tr>
<td>SAGE</td>
<td>num_layers: 2, hidden_channels: 128, weight_decay: 0.005, lr: 0.001, dropout: 0</td>
<td>num_layers: 2, hidden_channels: 128, weight_decay: 0.005, lr: 0.001, dropout: 0</td>
</tr>
<tr>
<td>SGC</td>
<td>K: 3, weight_decay: 0, lr: 0.1</td>
<td>K: 3, weight_decay: 0, lr: 0.1</td>
</tr>
</tbody>
</table>