Meta-path Free Semi-supervised Learning for Heterogeneous Networks

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Abstract

Graph neural networks (GNNs) have been widely used in representation learning on graphs and achieved superior performance in tasks such as node classification. However, analyzing heterogeneous graph of different types of nodes and links still brings great challenges for injecting the heterogeneity into a graph neural network. A general remedy is to manually or automatically design meta-paths to transform a heterogeneous graph into a homogeneous graph, but this is suboptimal since the features from the first-order neighbors are not fully leveraged for training and inference. In this paper, we propose a heterogeneous graph of different types of nodes and links still brings great challenges for injecting the heterogeneity into a graph neural network. A general remedy is to manually or automatically design meta-paths to transform a heterogeneous graph into a homogeneous graph. A common remedy is to manually or automatically design meta-paths to transform a heterogeneous graph into a homogeneous graph. A common remedy is to manually or automatically design meta-paths to transform a heterogeneous graph into a homogeneous graph.

Introduction

A large number of real-world graphs are heterogeneous in nature, involving diversity of node types and/or relationships between nodes (Sun and Han 2012). For example, an academic graph denotes multiple types of entities, authors (A), papers (P) and publishing venues (V), and their relations between A-P, P-A, P-V, and V-P. These heterogeneous graphs present unique challenges that cannot be handled by graph neural networks (GNN) that are specifically designed for homogeneous graphs having singular type of nodes and relationships. A common remedy is to manually design meta-paths, which are paths connected with heterogeneous edges, and transform a heterogeneous graph into a homogeneous graph defined by the meta-paths (Zhang et al. [2018], Wang et al. [2019]). For example, a meta-path A-P-A generates another homogeneous graph, where nodes represent authors and edges denote the coauthor relationships between authors. Meanwhile, another meta-path A-P-V-P-A captures the relationship between a pair of authors through their papers published on the common venues. Clearly, mixing a heterogeneous graph through diverse meta-paths can provide new insights about how the same types of distant nodes are implicitly related each other.

Despite their effectiveness, such homogenizing approach based on meta-paths has critical limitations. First of all, meta-paths commonly used in prior work take two-hop or farther neighbors into account graph analysis, ignoring the first-order neighbor in their context. For example, to understand an author node, its surrounding paper nodes can be informative but are sacrificed by meta-paths. These constraints can be a bottleneck to capture properties of heterogeneous graphs. Another commonly known drawback is that it requires domain knowledge to design meta-paths whose quality significantly affects the accuracy of downstream analysis (Yun et al. 2019).

To overcome above drawbacks, our research question is “Do we really need the meta-path scheme to learn GNNs for heterogeneous graphs?”, revisiting the naive approach of excluding the use of meta-paths, that is, ignoring the node/edge types and treating them as in a homogeneous graph where the general GNNs can operate on. For example, graph attention network (GAT) (Velickovic et al. 2018) learns node representations based on attention mechanism, which computes the feature similarity of each neighboring node pair and aggregates the first-order node features according to attention coefficients. However, practically, it is reported that such approach fails to outperform meta-path based approaches. One possible explanation is that a single shared layer is insufficient for diverse heterogeneous node pairs (e.g., A-P, P-A, P-V, and V-P). We call such property “heterogeneity stress”, which can be defined as the number of node/edge types fed into a specific model layer.

In light of these limitations and challenges, we propose to relax the heterogeneity stress with the goal of better using attention mechanism for heterogeneous graphs without meta-paths. First, we present Heterogeneity Relaxation (HER) network that replaces the use of node pair information by using only single node information to compute attention coefficients. Unlike going through the similarity computation in GAT, HER directly deals with neighbor importances in a transductive manner. Such approach can contribute to reducing the heterogeneity stress from edge-level to node-level since node types are less diverse than edge types in general. Second, we extend HER to HER++ network that avoids sharing the same attention layer among heterogeneous edge
types, extremely reducing the heterogeneity stress. Specifically, inspired by negative sampling for the softmax operation in skip-gram model (Mikolov et al. 2013) and meta-path2vec++ (Dong, Chawla, and Swami 2017), different types of edges can be handled by distinct attention layers for the transductive learning, masking all neighbors with heterogeneous edge types.

We conduct extensive experiments to evaluate the performance of the proposed models on six different benchmark datasets. The results show the superiority of the proposed models by comparing with the state-of-the-art models. More importantly, by carefully analyzing learning issues such as generality and scalability, HER and HER++ demonstrate their potentially good balance between reducing the heterogeneity stress and increasing the parameter size.

Background
Graph can be formalized as $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V}$ is a set of nodes, $\mathcal{E}$ is a set of edges. Let $\mathcal{T}$ be an union set of a node type set $\mathcal{T}^{\mathcal{V}}$ and an edge type set $\mathcal{T}^{\mathcal{E}}$ on $\mathcal{G}$. When $|\mathcal{T}^{\mathcal{V}}| = 1$ and $|\mathcal{T}^{\mathcal{E}}| = 1$, $\mathcal{G}$ becomes a homogeneous graph, otherwise heterogeneous graph (i.e., $|\mathcal{T}| > 2$). Each node $v_i \in \mathcal{V}$ and each edge $e_{ij} \in \mathcal{E}$ have one node and edge type, respectively, where the types are captured by the type mapping function $\phi : (v_i \text{ or } e_{ij}) \rightarrow t \in \mathcal{T}$.

Following (Yun et al. 2019), we consider the task of classifying nodes in a heterogeneous graph. Given a set $\mathcal{V}$ of $N$ nodes, we have a feature matrix $X \in \mathbb{R}^{N \times F}$ meaning that the $F$-dimensional input feature is given for each node, but labels are only available for a small subset of $\mathcal{V}$. This task can be framed as graph-based semi-supervised learning (i.e., transductive learning). We thus start by describing each single layer for related GNNs. Generally, the input to one layer is a set of node features, $H = [\vec{h}_1, \vec{h}_2, \ldots, \vec{h}_N]$ (initially $X$) where $\vec{h}_i \in \mathbb{R}^F$ is a feature vector of $v_i$. The layer produces a new set of node features (of potentially different cardinality $F'$), $H' = \{\vec{h}'_1, \vec{h}'_2, \ldots, \vec{h}'_N\}$, $\vec{h}'_i \in \mathbb{R}^{F'}$, as its output.

General Graph Neural Networks
As homogeneous graph contains a singular type of nodes and edges, it is handled by general graph neural networks such as Graph Convolutional Networks (GCN) and GAT.

GCN (Kipf and Welling 2017) employs convolutional operator to encode the node features $H \in \mathbb{R}^{N \times F}$ into higher-level features $H' \in \mathbb{R}^{N \times F'}$ by aggregating feature information of the first-order neighboring nodes with the following layer-wise propagation rule:

$$H' = \text{ReLU} \left( \tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2} HW^T \right)$$  \hspace{1cm} (1)

Here, $\tilde{A} = A + I$ is the adjacency matrix, $A \in \mathbb{R}^{N \times N}$ of graph $\mathcal{G}$ with the added identity matrix $I$ (i.e., self-connections), and $\tilde{D}$ is the degree matrix of $\tilde{A}$ for normalization. $W \in \mathbb{R}^{F \times F'}$ is a layer-specific trainable weight matrix. In GCN, all nodes of a same neighborhood are equally considered for the their convolutional operation.

GAT (Velickovic et al. 2018) allows for assigning different importances to neighbor nodes by self-attention mechanism. The attention mechanism $f$ in GAT is a single-layer feed forward neural network, parameterized by a weight vector $\hat{a} \in \mathbb{R}^{2F}$ with nonlinearity. Specifically, to support both scenarios of transductive and inductive learning, attention coefficients can be computed as the importance of node $f$’s features to node $i$ as follows:

$$s_{ij} = f(e_{ij}) = \text{LeakyReLU} \left( \hat{a}^T [W_i h_i || W_j h_j] \right)$$  \hspace{1cm} (2)

where $\|\|$ is the concatenation operation. To inject the graph structure into the mechanism, GAT only uses $s_{ij}$ for each node $v_j \in \mathcal{N}_i$, where $\mathcal{N}_i$ is the first-order neighbors of $v_i$ (including $v_i$), i.e., $\tilde{A}(i, j) = 1$, and normalizes the attention coefficients by the softmax function:

$$\alpha_{ij} = \text{softmax}(s_{ij}, \mathcal{N}_i) = \frac{\exp(s_{ij})}{\sum_{k \in \mathcal{N}_i} \exp(s_{ik})}$$  \hspace{1cm} (3)

Once the normalized attention coefficient $\alpha_{ij}$ is obtained, GAT aggregates neighbor node features to update each node feature by using $\alpha_{ij}$ and an ELU nonlinearity:

$$\vec{h}'_i = \text{ELU} \left( \sum_{v_j \in \mathcal{N}_i} \alpha_{ij} \vec{h}_j \right)$$  \hspace{1cm} (4)

Meta-path based Graph Neural Networks
A straightforward way to handle heterogeneous graph is to leverage meta-paths (Sun et al. 2011), which are paths connected with heterogeneous edges, and transform a heterogeneous graph into a homogeneous graph defined by the meta-paths. Many classes of GNNs adopt such homogenizing strategy, for example, heterogeneous graph attention network (HAN) (Wang et al. 2019) uses manual and multiple meta-paths designed by domain experts and extends the architecture of GAT to aggregate features from different sets of meta-path based neighbors.

GTN (Yun et al. 2019) learns to automatically generate meta-paths from a heterogeneous input graph without hand-crafted meta-paths. Formally, a new graph structure $\hat{A}$ in GTN is modeled based on composite relations connected with softly chosen edge types as follows:

$$\hat{A} = \left( \sum_{t \in T} \beta_t^{(1)} A_t \right) \left( \sum_{t \in T} \beta_t^{(2)} A_t \right) \cdots \left( \sum_{t \in T} \beta_t^{(l)} A_t \right)$$  \hspace{1cm} (5)

where $A_t$ denotes the adjacency matrix of edge type $t$ and $\beta_t^{(l)}$ is the (trainable) weight for edge type $t$ at the $l$th GTN layer. GTN learns the machine-generated adjacency matrix $\hat{A}$ by feeding $\hat{A}$ into the subsequent convolutional layer (e.g., a variant of Eq (1)) in an end-to-end fashion.

Proposed Models
This section presents simple and effective learning of GNN on heterogeneous graphs but excluding the use of the meta-path scheme. Our ultimate goal is to leverage the useful information of both the first-order and multi-hop neighbors based on graph convolutional operator and self-attention mechanism without the meta-path constraints, while capturing meaningful implicit relations on the input heterogeneous graph without the meta-path guidance.
Model I: HER

We, first, revisit self-attention mechanism in GAT. Although GAT is designed to handle homogeneous graphs, we believe that the multiple and parallel attention heads of GAT may be capable of overcoming the heterogeneity, which is the intrinsic property from various node and edge types. Empirically, [1] reports the promising performance of GAT, which is comparable with the state-of-the-arts on heterogeneous graphs. Nevertheless, we argue that GAT fails to control the stress level of heterogeneity (SLH) (Def. 1) on its graph attentional layer.

Definition 1 Stress Level of Heterogeneity (SLH): Given an attention function \( f(\cdot) \) and the overall set \( Z \) of node or edge information fed into \( f(\cdot) \) for training. SLH is defined as the cardinality of node or edge types in \( Z \). For example, in the aforementioned academic graph, SLH is 4 in GAT as \( f(e_{ij}) \) covers 4 edge types, i.e., \{AP, PA, PV, VP\}.

Unlike GAT, as illustrated in Fig. 1, our proposed model, HER, replaces feeding edge information (i.e., neighboring node pair) in the attention layer by using only single node information, which contributes to reducing SLH from \(|T^+|\) to \(|T^-|\)[1]. That is, in contrast with the content-based attention function in Eq. (2), we exploit the transductive ability of the self-attention mechanism on graphs. Specifically, in HER, a shared linear transformation parameterized by a weight matrix \( M \in \mathbb{R}^{N \times F} \) is applied to every node with nonlinearity to compute attention coefficients \( \tilde{s}_i = (s_{i1}, s_{i2}, \ldots, s_{i|N|}) \) from solely the target node \( v_i \) as follows:

\[
\tilde{s}_i = f(v_i) = \text{LeakyReLU}(MW\hat{h}_i) \quad (6)
\]

This transductive attention can be viewed as a graph analogue of location-based attention [2], which learns the attention coefficients of fixed time stamps in LSTM. Also, HER can be viewed as a GTN-like approach (but meta-path free), which learns a new graph structure (e.g., \( \hat{A} \sim MHW^T \)) in an end-to-end fashion.

Once \( \tilde{s}_i \) is obtained, HER follows Eq. (3) and (4) to normalize the attention coefficients and inject the graph structure into the attentional layer with the masked softmax function—we only use \( s_{ij} \) for node \( v_j \in N_i \). Note that GAT and HER can be trivially extended to multi-head attention for stabilizing the learning process of self-attention.

Model II: HER++

We further extend HER to the HER++ model, in which SLH is extremely reduced. Our key idea is to divide the heterogeneous graph into multiple sub-graphs with individual edge types and apply different attention layers to each sub-graph. For example, if one sub-graph is of edge type AP, its attention function \( f^{(AP)} \) takes only “from node” (i.e., author) as input, i.e., SLH=1. Formally, given a sub-graph with edge type \( t \), attention coefficients are computed by attention function \( f^t \) parameterized a weighted matrix \( M^t \in \mathbb{R}^{N \times F} \):

\[
(s_{t1}, s_{t2}, \ldots, s_{t|N|}) = f^t(v_i) = \text{LeakyReLU}(M^tW\hat{h}_i) \quad (7)
\]

\[
\alpha_{ij}^t = \text{softmax}(s_{ij}^t, N_i^t) = \frac{\exp(s_{ij}^t)}{\sum_{k \in N_i^t} \exp(s_{ik}^t)} \quad (8)
\]

where \( N_i^t \) is the neighbors of \( v_i \) with edge type \( t \). To inject the sub-graph structure, HER++ leverages the edge type information in softmax, whereas HER encourages all edge types of neighbors for normalization.

Once attention coefficients of multiple sub-graphs are obtained, HER++ aggregates them in a hierarchical manner.

Finally, we follow the K-multi-head architecture of GAT: node representations are concatenated by Eq. (10) at intermediate layers, and averaged by Eq. (11) at the final layer.

\[
\hat{h}_i^k = \frac{1}{K} \sum_{k=1}^{K} \alpha_{ij}^{(k)}W^{(k)}\hat{h}_j \quad (10)
\]

\[
\hat{h}_i^t = \text{ELU} \left( \frac{1}{K} \sum_{k=1}^{K} \alpha_{ij}^{(k)}W^{(k)}\hat{h}_j \right) \quad (11)
\]

where \( \alpha_{ij}^{(k)} \) is an attention coefficient in \( \hat{h}_i^{(k)} \) computed by the \( k \)-th attention mechanism, and \( W^{(k)} \) is the corresponding input linear transformation’s weight matrix.
Comparisons to Related Work

Here, we discuss several issues present in prior approaches:

- Much literature (Kipf and Welling 2017, Chen et al. 2020) reported that increasing the number of layers cannot contribute to effectively improving the model capacity of GNNs due to overfitting and oversmoothing. Meanwhile, our models enable a leap in the GNN capacity, without making models deeper. In the subsequent section, we perform relevant in-depth analysis, e.g., by reducing the training data size and de-activating the heterogeneity relaxation ability. When it comes to layer depth, similarly to prior work (Velickovic et al. 2018), HER and HER++ have the best performance with 2- or 3-layer architecture.

- The time complexity of a single GAT layer is $O(|V|^2F^2 + |E|F')$ while HER has $O(|V|^2F'F'' + |V|^2F' + |E|F')$ where $|V|$ and $|E|$ are the numbers of nodes and edges in the graph, respectively. Although one possible concern to our models is computational cost in transductive learning, we can collaborate with graph partitioning (Chiang et al. 2019) and sampling (Hu et al. 2020) methods, which enables our models to be parallelized for more scalable scenarios. We empirically demonstrate such complementary property of HER with graph partitioning later.

- As opposed to GCN, our models allow for assigning different importances to nodes of a same neighborhood, which may lead to benefits in interpretability (Velickovic et al. 2018), as was the case in NLP domain (Wiegrefe and Pinter 2019, Serrano and Smith 2019). Furthermore, by our trained models to meta-path based models such as HGCN (Yang et al. 2020), HAN (Wang et al. 2019) and GTN (Yun et al. 2019), it may be possible to transfer our classification results to another sense of interpretations (Ribeiro, Singh, and Guestrin 2016). We leave this as promising future work.

- The recently published meta-path free method of Zhang et al. 2019 adopts a two-phase pipeline of sequentially learning pre-trained heterogeneous node representations and ultimate task-dependent representations, i.e., not fully end-to-end learning. As reported in (Hu et al. 2020), it does not outperform HAN (and implicitly GTN), which are the state-of-the-arts of meta-path based GNNs. We are the first end-to-end model to outperform GTN. Another meta-path free approach (Wang et al. 2020) is irrelevant to our work because it aims at similarity search task.

Table 1: Dataset statistics

| Dataset | # Nodes | # Edges | # Features | # Classes | # Node type | # Edge type | # Training | # Validation | # Test |
|---------|---------|---------|------------|-----------|-------------|-------------|------------|--------------|-------|
| DBLP    | 18405   | 67946   | 334        | 4         | 3           | 4           | 800        | 400          | 2857   |
| ACM     | 8994    | 25922   | 1902       | 3         | 3           | 4           | 600        | 300          | 2125   |
| IMDB    | 12772   | 37288   | 1256       | 3         | 3           | 4           | 300        | 300          | 2339   |
| Cora    | 2708    | 5429    | 1433       | 7         | 1           | 1           | 140        | 500          | 1000   |
| Citeseer| 3327    | 4732    | 3703       | 6         | 1           | 1           | 120        | 500          | 1000   |
| NELL    | 65755   | 266144  | 5414       | 210       | -           | -           | 105        | 500          | 969    |

Experiments

Experimental Setup

Datasets Following (Yun et al. 2019), we use three benchmark datasets of heterogeneous graph (DBLP, ACM, and IMDB). Moreover, to simulate the scenarios that do not benefit from SLH relaxation for analytic purpose, we use two benchmark datasets of homogeneous graph (Cora and Citeseer) and one knowledge graph dataset (NELL).

- Heterogeneous Graph: DBLP (academic network) contains three types of nodes (papers (P), authors (A), venues (V)), four types of edges (PA, AP, PV, VP), and research fields of authors as labels. ACM (academic network) contains three types of nodes (papers (P), authors (A), subject (S)), four types of edges (PA, AP, PS, SP), and research fields of papers as labels. On the other hand, IMDB (movie network) contains three types of nodes (movies (M), actors (A), and directors (D)) and four types of edges (MD, DM, MA, AM), and labels are genres of movies. Each node in the three datasets is represented as a sparse feature vector, which is a bag-of-words of keywords.

- Homogeneous Graph: In Cora and Citeseer (citation networks), nodes and edges correspond to documents and (undirected) citations, respectively. Every node has a class label and a bag-of-words input feature for each document. We follow the same setting in (Kipf and Welling 2017) to select training (20 labels per class), validation, and test samples.

- Knowledge Graph: NELL (Carlson et al. 2010) is a bi-partite graph dataset extracted from a knowledge graph with 55,864 relation nodes and 9,891 entity nodes. Although the knowledge graph originally consists of entities connected with directed and labeled edges (relations), we follow the same pre-processing scheme in (Kipf and Welling 2017) to obtain relation nodes, by separating triplet $(e_1, r, e_2)$ into $(e_1, r_1)$ and $(e_2, r_2)$ where $r_1$ and $r_2$ are relation nodes. Entity nodes are described by sparse feature vectors, but we extend the number of features in NELL by assigning a unique one-hot representation for every relation node, resulting in a 61,278-dim sparse feature vector per node. Unlike prior work, we select only 105 labeled nodes as training data (label rate 0.001) to consider the extreme case of no labeled example for several classes in the training data.
Baselines We use three baselines including general GNN models, GCN and GAT, and the state-of-the-art heterogeneous model, GTN. As baseline, we exclude the conventional random walk based embedding models (Perozzi, Al-Rfou, and Skiena 2014; Dong, Chawla, and Swami 2017) such as metapath2vec, and heterogeneous GNNs (Zhang et al. 2019; Wang et al. 2019) before GTN. Reproducibility We apply a two-layer HER model to perform node classification on heterogeneous graph. The HER layers have 256 and 64 hidden features respectively. The negative slope of LeakyReLU is set to 0.2. For classification, we add a softmax layer on top of our two-layer HER model. We train the model with the cross-entropy loss function and Adam optimizer (Kingma and Ba 2014) (a learning rate of 0.0005). We set the number of multi-head $K$ to 3 and the dropout rate to 0.5. We apply $L_2$ regularization with 0.005. For HER++, all the hyper-parameters are set equally to HER. Both models are initialized using Glorot initialization (Glorot and Bengio 2010). For the homogeneous and knowledge graph datasets, we make slight architectural changes in HER. We remove the final softmax layer and use the second HER layer for the classification layer. We make the following changes in hyper-parameters for homogeneous graphs: 8 (number of hidden features), 8 (number of multi-head), 0.6 (dropout rate), and $5 \times 10^{-4}$ ($L_2$ regularization); and for NELL: 64 (number of hidden features), 0.01 (learning rate), 0.1 (dropout rate), and $1 \times 10^{-5}$ ($L_2$ regularization). Code is publicly available[3].

Research Questions We conduct experiments and analysis to answer the following four research questions:

• **RQ1:** Is our model effective on heterogeneous graphs?
• **RQ2:** How do hyper-parameters impact its performance?
• **RQ3:** How does various SLH affect its performance?
• **RQ4:** Is our model applicable to scalable scenarios?

RQ1: Overall Performance

To evaluate the effectiveness of our proposed models on heterogeneous graphs, we compare HER and HER++ with the three baselines. The results on three heterogeneous graphs are summarized in Tab. 2. Honoring the semi-supervised learning scenario, we vary the training ratio ($T_R$), which is a randomly sampled portion of the original training nodes, and report its corresponding label rate over the whole dataset (in brackets). Each reported performance denotes the averaged and best F1 score (in brackets) for 5 repeated runs.

In the table, we can find that our proposed models achieve the state-of-the-art performance across all three heterogeneous graph datasets. More specifically, HER always performs better than GAT, which suggests that reducing SLH can be beneficial. Moreover, HER++ outperforms all other models (including HER) in most cases, further reducing SLH rather than HER. In particular on IMDB dataset, its improvement is the most significant and consistent. One possible explanation is that HER++ takes the best benefit from the heterogeneity relaxation in IMDB since the type distribution of nodes in IMDB is comparably less skewed to a specific node type, which leads to a higher level of heterogeneity (meanwhile the number of venue nodes is only 20 in DBLP with more skewed distributions to other types).

Other than HER and HER++, GTN achieves the best performance in baselines, suggesting that automatically generated meta-paths may be useful. However, HER and HER++ use the original graph structure and yield higher performance compared to GTN. This result suggests that, it is possible to effectively learn heterogeneous node representations to only consider the first-order neighbors not using the meta-path scheme. Also, when $T_R=25\%$ in ACM and IMDB, GTN has lower F1 scores than GAT, as the machine-generated meta-paths may be not accurately learned due to lack of labeled data. Meanwhile, our models perform consistently better than other baselines, when varying $T_R$. These results indicate HER and HER++ well exploit their model capacity against overfitting with sparse labels.

| Datasets | $T_R$ | GCN | GAT | GTN | HER | HER+++ |
|----------|-------|-----|-----|-----|-----|--------|
| DBLP     | 25% (4.9%) | 84.35 (86.52) | 88.62 (89.56) | 92.13 (92.37) | **93.00 (93.87)** | 92.50 (93.56) |
| ACM      | 50% (9.9%) | 88.90 (90.51) | 91.59 (92.70) | 92.64 (93.03) | 93.89 (94.22) | **93.92 (94.55)** |
| IMDB     | 75% (14.8%) | 90.55 (91.42) | 92.46 (92.94) | 93.06 (93.48) | 94.04 (94.39) | **94.11 (94.40)** |
|          | 100% (19.7%) | 92.06 (92.71) | 92.87 (93.13) | 93.19 (93.59) | 93.95 (94.62) | **94.32 (94.59)** |

Table 2: Performance on heterogeneous graphs (F1 score)

3https://github.com/seongjunyun/Graph_Transformer_Networks
4https://github.com/convei-lab/metapath_free
RQ2: Sensitivity Analysis

The hyper-parameters play important roles in our models, as they determine how the node representations will be learned. We conduct experiments to analyze the impacts of three key parameters on only ACM dataset due to space limit.

- **Dimension of the final node representation:** As shown in Fig. 2a, HER and HER++ have appropriate levels of feature dimension to well control model capacity for representation learning, which can be easily tuned by linear search. HER++ is clearly less sensitive than HER, relieving the negative effect on extremely small dimension. This suggests that lower SLH also can contribute to the reliable learning when varying the node dimension.

- **Number of attention head $K$:** In order to check the impact of multi-head attention, we investigate the performance with various number of attention head. As shown in Fig. 2b, we observe that the more number of attention head can improve the performance of HER and HER++, and moreover, multi-head attention can make the training process more stable. However, with the change of attention head, the performance improves slightly.

- **Dropout rate:** Finally, we explore how the dropout rate affects the performance. We apply dropout (Srivastava et al. 2014) on HER layers’ inputs, that is, the attention mechanism is performed on randomly sampled neighbor nodes. As shown in Fig. 2c, we find that such stochasticity in the training process is critical as HER and HER++ achieve the best performance when the dropout rate is set to 0.5. We leave using more sophisticated techniques such as DropMax (Lee et al. 2018) as future work.

For a more intuitive analysis for sensitivity, Fig. 3 shows the visualization of the validation set in ACM dataset, where we utilize t-SNE to layout the heterogeneous graph on a low dimensional space. The color indicates the research field of a paper node as its ground-truth label. In this figure, we can observe that, compared to baseline models, HER and HER++ have larger margins in their latent spaces, especially between blue-labeled and green-labeled nodes. Such visualization is a strong signal of less sensitivity, and furthermore, it demonstrates that the node representations by our models have better discriminative power than those by other baselines such as GAT and GTN. To quantify these results, we perform K-means clustering (Wagstaff et al. 2001) for the same paper nodes ($K=3$). Considering the classification labels as clustering labels, we compute NMI and ARI scores as evaluation measures for node clustering results. As a result, our models yield higher NMI and ARI than GAT and GTN. These NMI and ARI scores support the visualization results in which our models can make distinct discrimination among nodes having different ground-truth labels.

RQ3: Ablation Study

To analyze the effect of heterogeneity relaxation, we test the performance changes when gradually deactivating the capability of our model in terms of SLH. For that, we present variants of HER++ (namely HER*), each of which optionally shares the same attentional layer between different two edge types by edge grouping, as it makes its SLH a moderate level $L$ of HER and HER++, i.e., $1 < L < |T^*|$. 

- **HER*:** A variant of HER++ that groups a pair of edge types, MA and AM, i.e., $T^*=(MD, DM, (MA, AM))$.

- **HER**$^+_{T^*}$: A variant of HER++ that groups a pair of edge types, MD and DM, i.e., $T^*=(MD, DM, (MA, AM))$.

- **HER**$^+_{T^*}$: It groups two pairs of edge types, MA and AM, and MD and DM, i.e., $T^*=(MD, DM, (MA, AM))$. 

Figure 2: Parameter sensitivity of HER and HER++. F1 score on y-axis is averaged over 5 repeated runs.

Figure 3: Visualization embedding on ACM. Each point indicates one paper and its color indicates the research field.
Table 3: Performance on homogeneous graphs (Accuracy)

|           | Cora               | Citeseer                |
|-----------|--------------------|-------------------------|
|           | $T_R$  | GCN       | GAT      | HER     | $T_R$  | GCN       | GAT      | HER     |
| 25%       | 67.12 (70.80)     | **72.88 (74.10)**      | 71.78 (72.30) | 25%     | 52.24 (55.10) | **55.52 (56.40)** | 55.16 (57.00) |
| 50%       | 76.06 (77.10)     | **78.36 (79.50)**      | 77.56 (78.20) | 50%     | 64.22 (66.90) | **68.12 (68.70)** | 67.02 (67.50) |
| 75%       | 78.52 (78.90)     | **79.60 (80.50)**      | 79.54 (80.40) | 75%     | 70.28 (71.20) | **70.88 (71.70)** | 70.44 (71.30) |
| 100%      | 82.22 (82.90)     | 84.14 (84.60)          | **84.38 (84.70)** | 100%    | 70.92 (71.60) | 72.38 (73.30) | **72.94 (73.60)** |

![Graphs showing performance](image)

(a) Performance with edge type grouping  
(b) Performance with graph partitioning  
(c) Training time with graph partitioning

Figure 4: Various tests with variants of HER and HER++

Fig. 4a reports the averaged F1 scores on IMDB dataset. In this figure, we can see that the performance of HER$^+$ is mostly moderate between that of HER and HER++, which roughly indicates the anticorrelated relation between classification performance and SLH. Consequently, HER++ performs the best with the lowest SLH.

To extremely ablate the effect of heterogeneity relaxation, we also perform the node classification task with no heterogeneity on graphs. For that, in Tab. 3, we compare HER with GCN and GAT on homogeneous graphs such as Cora and Citeseer. Note that, unlike RQ1, we use accuracy as an evaluation metric as conventionally adopted in prior work (Kipf and Welling 2017). As a result, although HER cannot benefit from the heterogeneity relaxation at all in such settings, its accuracy is comparable to that of the general GNNs in both datasets. These results demonstrate that our attention mechanism works well even in general cases, where its capability is not limited to a specific heterogeneous graph but also is further improved with diverse heterogeneity challenges.

RQ4: Scalability Test

Here we examine the possible scalability of our models. For that, we adopt a larger graph dataset, NELL, which contains $\times 7.1$ nodes and $\times 9.4$ edges compared to the average of other five datasets used. Specifically, we first split the NELL graph into multiple disjunct partitions using METIS (Karypis and Kumar 1998), a graph clustering method, then train individual HER models on each partition to perform the node classification. Note that, although the knowledge graph is originally a heterogeneous graph, we transform it to a heterogeneous graph by the pre-processing process used in (Kipf and Welling 2017; Liao et al. 2018).

Fig. 4b and Fig. 4c report the averaged accuracy in (partitioned) test data and the mean wall-clock training time per epoch (forward pass, cross-entropy calculation, backward pass) for 100 epochs in (partitioned) training data, respectively. As shown in Fig. 4b, regardless of varying the number of partitions, HER consistently keeps its performance, which gets even higher accuracy than a single GCN model using the whole graph data in NELL. Meanwhile, as the number of partitions gets larger, Fig. 4c shows the linearly decreasing trend of the training time. These results suggest that the training process of our models can be effectively and efficiently parallelized in a scalable manner.

Conclusion

We have presented novel meta-path free GNNs based on self-attention mechanism for heterogeneous graphs, leveraging the two strategies of relieving the heterogeneity stress. The learnt attention models, HER and HER++, lead to more effective node representation resulting in the state-of-the-art performance, without any human efforts and domain knowledge involved in the meta-path scheme, on all three benchmark heterogeneous graph datasets. We demonstrate, for the first time, that the transductive self-attention is capable of not only addressing key challenges in heterogeneous graph domains but also improving the semi-supervised learning in general graph domains.

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$^4$Our models currently do not support the edge type grouping during the learning process, but results of HER$^+$ show it is necessary to find better matchable edge types in an end-to-end manner.

$^5$CPU implementation with 12-core Intel® CPU i9 @ 3.50GHz
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