

Learning Bi-typed Multi-relational Heterogeneous Graph via Dual Hierarchical Attention Networks

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Abstract—Bi-type multi-relational heterogeneous graph (BMHG) is one of the most common graphs in practice, for example, academic networks, e-commerce user behavior graph and enterprise knowledge graph. It is a critical and challenge problem on how to learn the numerical representation for each node to characterize subtle structures. However, most previous studies treat all node relations in BMHG as the same class of relation without distinguishing the different characteristics between the intra-class relations and inter-class relations of the bi-typed nodes, causing the loss of significant structure information. To address this issue, we propose a novel **Dual Hierarchical Attention Networks** (DHAN) based on the bi-typed multi-relational heterogeneous graphs to learn comprehensive node representations with the intra-class and inter-class attention-based encoder under a hierarchical mechanism. Specifically, the former encoder aggregates information from the same type of nodes, while the latter aggregates node representations from its different types of neighbors. Moreover, to sufficiently model node multi-relational information in BMHG, we adopt a newly proposed hierarchical mechanism. By doing so, the proposed dual hierarchical attention operations enable our model to fully capture the complex structures of the bi-typed multi-relational heterogeneous graphs. Experimental results on various tasks against the state-of-the-arts sufficiently confirm the capability of DHAN in learning node representations on the BMHGs.

Index Terms—Bi-typed Multi-relational Heterogeneous Graph, Graph Learning, Dual Hierarchical Attention Networks, Graph Neural Networks

1 INTRODUCTION

BI-TYPED multi-relational heterogeneous graph (BMHG) typically consists of two different types of nodes and multiple intra-class/inter-class relations among them, which are ubiquitous in the real-world scenarios [1], such as academic social networks [2], [3], e-commerce user behavior graph [4], [5], and enterprise knowledge graph [6], [7]. These graphs have rich and valuable heterogeneous information that is worth deep mining. For more clarity, we formally define the BMHG in Definition 1. Without loss of generality, let us take OAG dataset [3] as an example of the BMHG, which consists of two types of nodes, i.e. *authors* and *papers*, and multiple relationships, i.e. *colleague*, *cite*, *is_ordinary_author_of*, etc, as shown in Figure 1.

Definition 1. Bi-typed Multi-relational Heterogeneous Graph. A bi-typed multi-relational heterogeneous graph is defined as a connected graph $\mathcal{BMHG} = (\mathcal{V}, \mathcal{L}, \mathcal{T}, \mathcal{R})$. \mathcal{V} denotes the node set, and \mathcal{L} denotes a link set. They are associated with two

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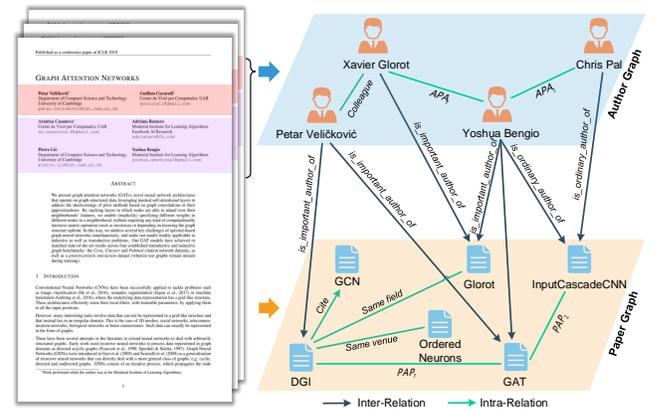


Fig. 1. A toy example of bi-typed multi-relational heterogeneous graph (BMHG) in the academic networks. This graph consists of two types of nodes, i.e. *authors* and *papers*. Their links could be divided into two classes: (1) node intra-class relations, such as "colleague" between authors, "cite" and "same venue" between papers; (2) node inter-class relations, such as "is_important_author_of", "is_ordinary_author_of". Table 2 reports a detailed statistics of the graph.

functions: (i) a node type mapping function $\varphi : \mathcal{V} \rightarrow \mathcal{T}$, $|\mathcal{T}| = 2$. $\mathcal{V} = \{\mathcal{V}_1, \mathcal{V}_2\}$, $\mathcal{V}_1 \cap \mathcal{V}_2 = \emptyset$. Each node $v \in \mathcal{V}$ belongs to one particular node type in the node type set \mathcal{T} : $\varphi(v) \in \mathcal{T}$. (ii) a link class mapping function $\psi : \mathcal{L} \rightarrow \mathcal{R}$. $\forall l_1, l_2 \in \mathcal{L}$, $\psi(l_1) \in \mathcal{R}_{intra}$ and $\psi(l_2) \in \mathcal{R}_{inter}$ denote the node intra-class relationships and the node inter-class relationships, respectively. BMHG has multiple relationships, i.e., $|\mathcal{R}_{inter}| > |\mathcal{T}| - 1 > 0$ and $|\mathcal{R}_{intra}| > 1$.

TABLE 1
Comparison between several SOTA methods and the proposed model in terms of nodes heterogeneity and edges heterogeneity.

Models		Graph Heterogeneity		
Name	Main ideas	Bi-typed $ \mathcal{T} = 2$	Inter-class multi-relations $ \mathcal{R}_{\text{inter}} > 1$	Intra-class multi-relations $ \mathcal{R}_{\text{intra}} > 1$
GCN [8]	• Average message passing	✗	✗	✗
GAT [9]	• Attention based message passing	✗	✗	✗
RGCN [10]	• Multi-relations • Hierarchical weighting message passing	✗	✗	✓
GTN [11]	• Multi-relations • Self-adaption weighting message passing	✗	✓	✗
HAN [12]	• Meta-path relations • Hierarchical attention based message passing	✗	✓	✗
HetGNN [3]	• Heterogeneous features of nodes • Attention based message passing	✓	✗	✗
HGT [13]	• Self-attention based message passing • Node-balanced graph sampling • Time encoding	✗	✓	✓
HGConv [14]	• Multi-relations • Hierarchical attention based message passing	✗	✓	✗
ie-HGCN [15]	• Meta-path based relations • Hierarchical attention based message passing	✗	✓	✗
DHAN (Ours)	• Distinguish inter-class relationship and intra-class relationship • A newly proposed global-local hierarchical mechanism	✓	✓	✓

In this paper, we focus on how to encode the bi-typed multi-relational heterogeneous graphs, providing an effective and flexible way to use their structural knowledge. The ultimate goal is to pursue perfect low-dimension distributed representations for nodes and relations mainly according to heterogeneous information in BMHG. The learned results are essential for the inference tasks over graph, such as link prediction [16], [17], node classification [18], [19], node clustering [1], and graph classification [20], [21].

Previous heterogeneous graph learning studies attempt to adopt the advanced Graph Neural Networks (GNNs) to learn heterogeneous graph while preserving the heterogeneous structures [3], [10], [12], [13]. However, most previous studies treat all node relations in BMHG as the same class of relation without distinguishing the different characteristics between the intra-class relations and inter-class relations of the bi-typed nodes, which inevitably leads to graph significant structural information loss.

To address the issue, we propose a novel **Dual Hierarchical Attention Networks (DHAN)** to learn comprehensive node representations based on the bi-typed multi-relational heterogeneous graph with the intra-class and inter-class attention-based encoder under a hierarchical mechanism. Specifically, the former encoder model aggregates information from the same type of nodes (Section 3.1), while the latter encoder aggregates node representations from its different types of neighbors (Section 3.2). Moreover, to sufficiently learn node multi-relational information in BMHG, we adopt a newly proposed hierarchical mechanism. By doing so, the proposed dual hierarchical attention operations enable our model to fully capture the complex structures of the bi-typed multi-relational heterogeneous graphs. The comparison between previous existing methods with our proposed DHAN in terms of nodes heterogeneity and edges heterogeneity is shown in Table 1.

To evaluate the effectiveness of our proposed model, we generate three different kinds of datasets according to the popular Open Academic Graph (OAG) [3] with various paper citation thresholds,

including *OAG1Y*, *OAG2Y* and *OAG10Y*. We conduct extensive experiments on these datasets with author disambiguation and paper classification task against the state-of-the-art methods, which sufficiently demonstrate the better capability of our proposed DHAN in learning node representations in the bi-typed multi-relational heterogeneous graphs.

The contributions of our work are summarized as follows:

- In this paper, we focus on embedding the bi-typed multi-relational heterogeneous graphs. To the best of our knowledge, no one attempts to deal with the task before. This paper is expected to further facilitate the bi-typed heterogeneous graph-involved applications, such as academic network mining [13], recommendation system [22], enterprise knowledge graph embedding [23], etc.
- To tackle the bi-typed multi-relational heterogeneous graph learning task, we propose a novel dual hierarchical attention networks (DHAN). Specifically, we equipped DHAN with the intra-class and inter-class attention networks under a newly proposed hierarchical mechanism, which enables the proposed model to sufficiently capture the complex structural knowledge in the BMHG.
- We conduct extensive experiments to evaluate the performance of the proposed model. The results demonstrate the superiority of the proposed model against the SOTA methods for learning node representations on bi-typed multi-relational heterogeneous graphs. The source code and data of this paper can be obtained from: <https://github.com/superweisp/DHAN2022>.

The rest of the paper is organized as follows. In Section 2, we summarize and compare the related work. Section 3 introduces the details of DHAN. Extensive experiments are conducted to evaluate the effectiveness of the proposed model in Section 4. Finally, we conclude the paper in Section 5.

2 RELATED WORK

2.1 Graph Learning

Recent years have witnessed a growing interest in developing graph learning algorithms [24], [25], [26], [27] since most real-world data can be represented by graphs conveniently. Classical graph learning methods aim to reduce the dimension of graph data into low-dimensional representations, such as the linear method PCA [28] and the non-linear method LLE [29]. Inspired by the basic idea from probabilistic language models such as skip-gram [30] and bag-of-words [31], some random walk-based methods are proposed to learn node representations, such as DeepWalk [25] and its advanced extension Node2Vec [26]. DeepWalk is a popular random walk-based graph learning method, which uses local information obtained from truncated random walks to learn node representations. There are also some matrix factorization-based methods for graph learning tasks [32], [33]. We refer the readers to [34] for more surveys on graph learning.

2.2 Graph Neural Networks

Graph Neural Networks (GNNs) develop a deep neural network to deal with arbitrary graphs for representation learning [13], [35], [36], [37], [38]. GNNs have been successfully applied to various tasks over graphs [9], [39], such as graph classification [20], [21], link prediction [16], and node classification [18], [19]. The Graph Convolutional Networks (GCNs), as a representative GNN model, generalize convolutional operation on the graph-structured data [4], [10], [40], [41]. Graph Attention Networks (GATs) learn from the underlying graph structure by incorporating attention mechanism into GCNs [40], [41], where the hidden representation of each node is computed by recursively aggregating and attending over its corresponding local neighbors' features, and the weighting coefficients are calculated inductively with self-attention strategy [42], [43]. We refer the readers to [35] for more references of GNNs. Despite the success of the above methods, they are constrained to perform only on homogeneous graphs, which thus could not handle the rich information in heterogeneous graphs.

2.3 Heterogeneous Graph Neural Networks

Heterogeneous graphs contain different types of nodes and edges [3], [12], [44], [45], which have rich and valuable heterogeneous information. Heterogeneous graph modeling methods are useful for various task, such as short text classification [45], spam review detection [46], recommendation system [47], node and graph classification [20], conversation generation [48], sentiment analysis [49]. To deal with heterogeneous graphs, Wang et al. [12] proposed heterogeneous graph attention networks (HAN), which mainly concentrate on the different meta-paths. Zhang et al. [3] proposed HetGNN that uses specialized Bi-LSTM to integrate the heterogeneous node attributes and neighbors. Schlichtkrull et al. [10] proposed RGCN to learn knowledge graphs [50] by employing relation-specific transformation matrices. Busbridge et al. [50] proposed RGAT by extending non-relational GATs to incorporate relational information, but with poor performance. Hu et al. [13] proposed heterogeneous graph transformer (HGT) to model web-scale heterogeneous graphs, which considers graph heterogeneity, dynamic nature and efficient training for large-scale graph.

Despite their success, to the best of our knowledge, no one focuses on bi-typed multi-relational heterogeneous graph learning.

Previous methods usually ignore the heterogeneous characteristics of inter-class and inter-class relationships of bi-typed nodes in BMHG. Different from the conventional heterogeneous GNNs, this paper concentrates on the bi-typed heterogeneous graph learning task and attempts to design dual hierarchical graph attention networks to learn comprehensive node representations. Table 1 summarizes the key advantages of our model in terms of modeling graph heterogeneity, compared with a variety of state-of-the-art heterogeneous GNNs models.

3 METHODOLOGY

This section introduces the framework of the overall architecture, as shown in Figure 2. (1) Node Representation Initialization. We firstly initialize paper node representations through a pre-trained XLNet with their titles. Then we calculate author node representations by averaging their corresponding paper nodes' representations. (2) Dual Hierarchical Attention Networks (DHAN). The proposed DHAN consists of two submodules: intra-class attention-based encoder and inter-class attention-based encoder, which aim to fully capture the structural knowledge of BMHG. To model node multi-relational information in BMHG, we will introduce a newly proposed hierarchical mechanism, as shown in Figure 3. Next, we gives the details of DHAN.

3.1 Intra-class Attention-based Encoder

The intra-class attention networks aim to learn the node embeddings by aggregating node information from their same type of neighbors, as shown in Figure 2 (a). Given a set of nodes with the same type $\mathcal{V}_a \in \{\mathcal{V}_1, \mathcal{V}_2\}$, and a node pair $(v_i, v_j) (\in \mathcal{V}_a)$ that are connected via node intra-class relationship $\Phi_k \in \mathcal{R}_{\text{intra}}^{(a)}$, we firstly perform transformation based on node type to project original node representation into \mathbb{R}^d latent space as follow:

$$\mathbf{H}^{(a)} = \mathbf{W}^{(a)} \mathbf{H}^{(a)}, \quad (1)$$

where $\mathbf{W}^{(a)} \in \mathbb{R}^{d \times d'}$ are a trainable weight matrix related to a corresponding node type. $\mathbf{H}^{(a)} \in \mathbb{R}^{|\mathcal{V}_a| \times d}$ and $\mathbf{H}'^{(a)} \in \mathbb{R}^{|\mathcal{V}_a| \times d'}$ is the original and transformed node representations, respectively.

For node v_i , different types of intra-class relationships contribute different semantics to its embeddings, and so do different nodes with the same relationship. Hence, we then employ attention mechanism here in node-level and relation-level to hierarchically aggregate signals from the same types of neighbors to target node v_i . We first perform self-attention on the nodes to formulate the importance $e_{ij}^{\Phi_k}$ of a specific-relation based node pair (v_i, v_j) :

$$e_{ij}^{\Phi_k} = \text{att}_{\text{local}}(\mathbf{h}'_i, \mathbf{h}'_j; \Phi_k) = \text{LeakyRelu}(\mathbf{a}_{\Phi_k}^\top \cdot [\mathbf{h}'_i \| \mathbf{h}'_j]), \quad (2)$$

where $\mathbf{h}'_i \in \mathbb{R}^{d'}$, $\mathbf{h}'_j \in \mathbb{R}^{d'}$ are transformed hidden representations of the node v_i and v_j , respectively. $\|$ denotes the concatenate operation. $\mathbf{a}_{\Phi_k}^\top \in \mathbb{R}^{2d' \times 1}$ is the shared node-level attention weight vector under relation Φ_k . LeakyReLU is a nonlinearity activation function.

Based on Eq. (2), we calculate the $e_{ij}^{\Phi_k}$ for all nodes $v_j \in \mathcal{N}_{\text{intra}}^{\Phi_k}(v_i)$, where $\mathcal{N}_{\text{intra}}^{\Phi_k}(v_i)$ denotes specific relation-based neighbors of v_i . To make importance easily comparable across different nodes, we normalize them across all choices of v_j using the softmax function:

$$\alpha_{ij}^{\Phi_k} = \text{softmax}_j(e_{ij}^{\Phi_k}) = \frac{\exp(e_{ij}^{\Phi_k})}{\sum_{v_p \in \mathcal{N}_{\text{intra}}^{\Phi_k}(v_i)} \exp(e_{ip}^{\Phi_k})}, \quad (3)$$

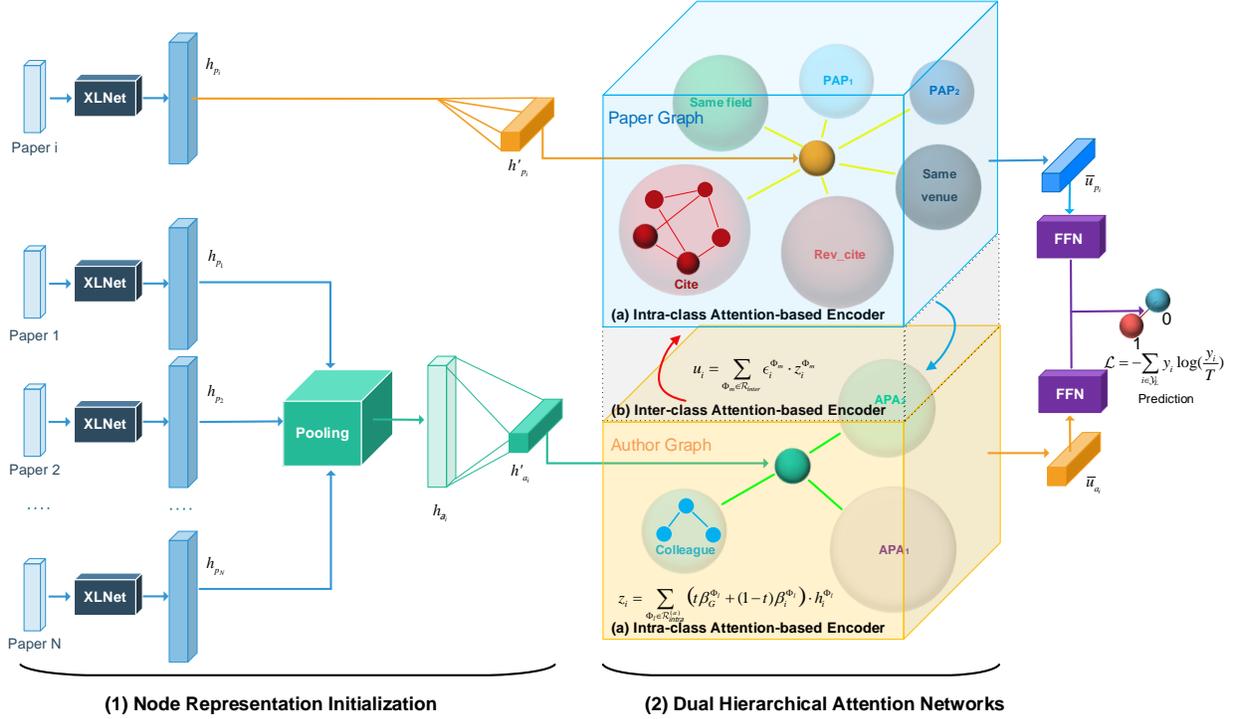


Fig. 2. The overall architecture of the proposed method. (1) **Node Representation Initialization** We utilize a pretrained XLNet to retrieval papers' representations from their titles. Authors' representations are calculated by averaging their published papers' information. (2) **Dual Hierarchical Attention Networks**: (a) **Intra-class Attention-based Encoder** aims to aggregate different types of intra-class relationships with our novel hierarchical mechanism. For each type of node, the intra-class hierarchical attention module shares the same structure but with different parameters; (b) **Inter-class Attention-based Encoder** is designed for updating information between two types of nodes. Each type of node incorporates their inter-class neighbors' information with different weights according to different relationships and node pairs.

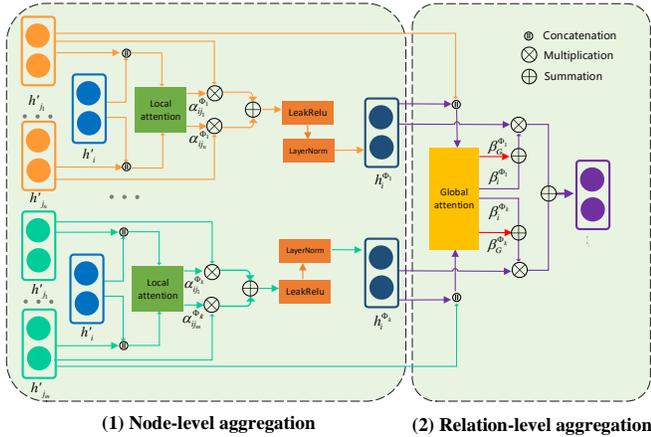


Fig. 3. The proposed hierarchical attention mechanism. (1) **Node-level aggregation** aims to capture neighbor nodes' importance $\alpha_{ij}^{\Phi_k}$ under a specific type of relation Φ_k . Then relation representations $\mathbf{h}_i^{\Phi_k}$ are aggregated by weighting and summing the target node's Φ_k based neighbors' information. (2) **Relation-level aggregation** firstly assigns relation importance utilizing attention mechanism based on target node embedding and relation representations. Then relation representations are aggregated to get comprehensive neighbor information \mathbf{z}_i with final importance, which consists of global relation weight $\beta_G^{\Phi_k}$ and local relation weight $\beta_i^{\Phi_k}$.

Then, the embedding $\mathbf{h}_i^{\Phi_k}$ of node v_i under given relation Φ_k is calculated by aggregating its intra-class neighbors' projected representations with the corresponding coefficients as follows:

$$\mathbf{h}_i^{\Phi_k} = \text{LeakyRelu} \left(\text{Norm}_{\Phi_k} \left(\sum_{v_j \in \mathcal{N}_{\text{intra}}^{\Phi_k}(v_i)} \alpha_{ij}^{\Phi_k} \cdot \mathbf{h}'_j \right) \right), \quad (4)$$

where Norm_{Φ_k} denotes relation-specific layer normalization operation. Since the attention coefficient $\alpha_{ij}^{\Phi_k}$ is computed for a particular relationship, $\mathbf{h}_i^{\Phi_k}$ is semantic-specific and capable of capturing one kind of semantic information.

To learn more comprehensive node representations, we fuse different relation-specific aggregated information of nodes. Different from previous methods that either consider relation global importance [12] or local importance [14], we take advantage of both of the two factors in relation-level attention, considering both the heterogeneity with regard to different nodes and the common information that a type of relation has among all nodes. Firstly, we calculate the local importance $g_i^{\Phi_k}$ of relation Φ_k with respect to node v_i as follows:

$$g_i^{\Phi_k} = \mathbf{q}^\top (\mathbf{h}'_i \parallel \mathbf{h}_i^{\Phi_k}), \quad (5)$$

where $\mathbf{q} \in \mathbb{R}^{2d' \times 1}$ is a trainable parameter. Then, we implement the softmax function to normalize the node-relation specific local importance across different relations.

$$\beta_i^{\Phi_k} = \text{softmax}_k(g_i^{\Phi_k}) = \frac{\exp(g_i^{\Phi_k})}{\sum_{\Phi_l \in \mathcal{R}_{\text{intra}}^{(\alpha)}} \exp(g_i^{\Phi_l})}, \quad (6)$$

where $\beta_i^{\Phi_k}$ indicates how important relation Φ_k is for node v_i , which measures local importance of intra-relation Φ_k . Secondly, to prevent model from local optimum and alleviate effects of noisy links, we design a relation global importance $\beta_G^{\Phi_l}$, which denotes how important intra-class Φ_l is for all nodes $v_i \in \mathcal{V}_a$. Finally, as shown in 3, we fuse different relation-specific aggregated information of nodes in both local and global view, as follow:

$$\mathbf{z}_i = \sum_{\Phi_l \in \mathcal{R}_{intra}^{(a)}} \left(t\beta_G^{\Phi_l} + (1-t)\beta_i^{\Phi_l} \right) \cdot \mathbf{h}_i^{\Phi_l}, \quad (7)$$

where $\mathbf{z}_i \in \mathbb{R}^{d'}$ is the learned representation of node v_i , which contains global and local information. $\mathbf{h}_i^{\Phi_l}$ denotes aggregated information for node v_i under intra-class relation Φ_l . t is a smooth parameter to balance the global and local importance of intra-class relation Φ_l . $\beta_G^{\Phi_l}$ and t can be learned from training.

3.2 Inter-class Attention-based Encoder

Different from the above intra-class attention networks, the inter-class attention-based encoder aims to deal with the interaction between different types of nodes. We set $v_i^{(1)} \in \mathcal{V}_1$ and $v_j^{(2)} \in \mathcal{V}_2$. $\mathbf{z}_i^{(1)}, \mathbf{z}_j^{(2)}$ are the learned representations of the node $v_i^{(1)}$ and $v_j^{(2)}$ by intra-class attention networks, respectively.

We calculate the node-level importance $c_{ij}^{\Phi_m}$ for all nodes $v_j \in \mathcal{N}_{inter}^{\Phi_m}(v_i)$, where $\mathcal{N}_{inter}^{\Phi_m}(v_i)$ denotes the neighbors of node v_i under specific inter-relation Φ_m . We normalize them across all choices of v_j using the softmax function:

$$\begin{aligned} c_{ij}^{\Phi_m} &= att_{node}(\mathbf{z}_i, \mathbf{z}_j; \Phi_m) \\ &= \text{LeakyRelu}(\mathbf{a}_{\Phi_m}^\top \cdot [\mathbf{W}^{(1)}\mathbf{z}_i \parallel \mathbf{W}^{(2)}\mathbf{z}_j]), \end{aligned} \quad (8)$$

$$\gamma_{ij}^{\Phi_m} = \text{softmax}_j(c_{ij}^{\Phi_m}) = \frac{\exp(c_{ij}^{\Phi_m})}{\sum_{v_k \in \mathcal{N}_{inter}^{\Phi_m}(v_i)} \exp(c_{ik}^{\Phi_m})}, \quad (9)$$

where $\mathbf{W}^{(1)}, \mathbf{W}^{(2)} \in \mathbb{R}^{d' \times d'}$ are two type-specific matrices to map their features $\mathbf{z}_i, \mathbf{z}_j$ into a common space. $\mathbf{a}_{\Phi_m} \in \mathbb{R}^{2d'}$ is a trainable weight vector. Then, as shown in Figure 2, the relation representation of node $v_i^{(1)}$ can be aggregated by its different types of neighbors' representations with the corresponding coefficients as follows:

$$\mathbf{z}_i^{\Phi_m} = \text{LeakyRelu} \left(\text{Norm}_{\Phi_m} \left(\sum_{v_j \in \mathcal{N}_{inter}^{\Phi_m}(v_i)} \gamma_{ij}^{\Phi_m} \mathbf{W}^{(2)}\mathbf{z}_j \right) \right), \quad (10)$$

where Norm_{Φ_m} indicates layer normalization operation related to the inter-class relation.

Similar to the above hierarchical attention, all relation representations are fused to get the final representations:

$$f_i^{\Phi_m} = \tilde{\mathbf{q}}^\top \left(\mathbf{z}_i \parallel \mathbf{z}_i^{\Phi_m} \right), \quad (11)$$

$$\epsilon_i^{\Phi_m} = \text{softmax}_m(f_i^{\Phi_m}) = \frac{\exp(f_i^{\Phi_m})}{\sum_{\Phi_n \in \mathcal{R}_{inter}} \exp(f_i^{\Phi_n})}, \quad (12)$$

where $\tilde{\mathbf{q}} \in \mathbb{R}^{2d'}$ is a projection vector. $f_i^{\Phi_m}$ denotes the importance of relation embedding $\mathbf{z}_i^{\Phi_m}$ related to node $v_i^{(1)}$. We apply the the softmax function to make relation importance comparable

within inter-class relations. The representation \mathbf{u}_i of node v_i us obtained by fusing these relation-specific representations.

$$\mathbf{u}_i = \sum_{\Phi_m \in \mathcal{R}_{inter}} \epsilon_i^{\Phi_m} \cdot \mathbf{z}_i^{\Phi_m}, \quad (13)$$

where \mathcal{R}_{inter} indicates the set of relations among different types of nodes, i.e., node inter-class links.

In inter-class hierarchical attention, the aggregation of different nodes' embedding is seamlessly integrated, and they are mingled and interactively affected each other in nature, as demonstrated in Figure 2 (b).

3.3 Weighted Residual Connection

For both intra-class encoder and inter-class encoder, we use weighted residual connection and layer normalization to alleviate over-smooth in practice.

$$\bar{\mathbf{z}}_i = \text{Norm} \left(\lambda \sigma(\mathbf{z}_i) + (1-\lambda)\mathbf{h}_i \right), \quad (14)$$

$$\bar{\mathbf{u}}_i = \text{Norm} \left(\tilde{\lambda} \sigma(\mathbf{u}_i) + (1-\tilde{\lambda})\mathbf{z}_i \right), \quad (15)$$

where λ and $\tilde{\lambda}$ are hyperparameters.

3.4 Optimization

We train our model by minimizing the cross-entropy loss. Inspired by [51], we promote the training efficiency by adding Temperature T in the learning.

$$\mathcal{L} = - \sum_{i \in \mathcal{Y}_L} y_i \log \left(\frac{\tilde{y}_i}{T} \right), \quad (16)$$

where \mathcal{Y}_L is the set of labeled nodes. y_i and \tilde{y}_i are the ground truth and the predicted label for node i , respectively.

4 EXPERIMENTS

4.1 Experimental Settings

4.1.1 Datasets

We generate three different kinds of datasets by extracting different sub-graphs from the popular Open Academic Graph (OAG) dataset [3] with various paper citation thresholds, including *OAG1Y*, *OAG2Y* and *OAG10Y*. In *OAG1Y*, we only retain the papers which are cited more than once a year. In *OAG2Y* and *OAG10Y*, we loose the time constraints to 2 years and 10 years, respectively. They contain two types of nodes, i.e., authors and papers, and several preliminary links including (author, *colleague*, author), (author, *is_important_author_of*, paper), (author, *is_ordinary_author_of*, paper), (paper, *cite*, paper). Note that the "important" authorship indicates an author is the first or second author of a paper, and the "ordinary" authorship indicates an author is not the important author of a paper. The basic statistics of all datasets are included in Table 2. The intra-class relations of authors include: *colleague*, *APA1* and *APA2*. *APA1* and *APA2* indicate the co-authorship of important authors and ordinary authors, respectively. The intra-class relations of papers include: *cite*, *rev_cite*, *is_same_venue_of*, *is_same_field_of*. The inter-class relation between author and paper includes: *is_important_author_of* and *is_ordinary_author_of*.

TABLE 2

Statistics of the datasets *OAG1Y*, *OAG2Y* and *OAG10Y*, which are extracted from the popular Open Academic Graph [3] with various citation thresholds.

Datasets		<i>OAG1Y</i>	<i>OAG2Y</i>	<i>OAG10Y</i>
Bi-typed nodes	#Papers	494,051	825,234	1,564,109
	#Authors	480,575	734,451	1,266,569
Author intra-relations	#Colleague	285,393,669	562,821,414	1,400,301,929
	#APA1	369,973	600,344	1,074,851
	#APA2	1,015,964	1,413,447	2,059,826
Paper intra-relations	#Cite/Rev_Cite	4,847,142	7,367,512	22,407,910
	#Same Field	160,283,374,629	440,183,678,370	1,548,687,874,807
	#Same Venue	273,272,355	619,484,732	1,929,963,113
	#PAP1	3,022,137	5,966,848	13,450,631
	#PAP2	4,973,945	9,042,142	17,648,847
Author-Paper inter-relations	#Important author	800,061	1,306,953	2,372,890
	#Ordinary author	661,250	1,019,506	1,687,184
Training data Period		2000 - 2015		
Validation data Period		2015 - 2016		
Testing data Period		2016 - 2019		

4.1.2 Baselines

To demonstrate the effectiveness of our proposed model DHAN, we compare it with three types of SOTA baselines: (1) the homogeneous graph neural networks which do not consider multi-relationships between nodes, such as GCN, GAT; (2) the heterogeneous graph neural networks which take different relationships into consideration, such as RGCN, HGT; (3) the heterogeneous networks which implement a hierarchical mechanism to aggregate different kinds of relations in graphs, such as HAN, HGConv.

Homogeneous models:

- Graph Convolutional Networks (GCN) [8], [52]: a popular model which simply averages neighboring nodes’ representations in aggregation.
- Graph Attention Networks (GAT) [9]: a recent model which takes attention mechanism to align different weights to neighbors during the information aggregating process.

Heterogeneous models:

- Relational Graph Convolutional Networks (RGCN) [10]: an advanced extension of GCN, which takes relation information into consideration by giving different weights for difference relationships.
- Heterogeneous graph neural network (HetGNN) [3]: a multi-modal heterogeneous graph model which utilizes Bi-LSTM to process multi-modding information, then applies attention mechanism in heterogeneous information fusing.
- Graph Transformer Networks (GTN) [11]: a novel heterogeneous graph neural network based on GCN which updates adjacent matrix of different relations during the training process.
- Heterogeneous Graph Transformer (HGT) [13]: a state-of-the-art model which implements on heterogeneous graph with different types of nodes and multiple relations.

Hierarchical models:

- Heterogeneous Graph Attention Network (HAN) [12]: one of the earliest model which implements hierarchical attention on graph neural network based on meta-path.
- Heterogeneous Graph Convolution (HGConv) [14]: an efficient model which utilizes hierarchical mechanism based on different node types and different relations.

- interpretable and efficient Heterogeneous Graph Convolutional Network (ie-HGCN) [15]: a SOTA model which firstly implements object-level aggregation and then aggregates type-level information based on different meta-paths.

4.1.3 Model Setting and Training Details

We implement DHAN with PyTorch and PyTorch Geometric (PyG). We use a pre-trained XLNet [53] to initialize the paper nodes’ representations. Then the author nodes’ initial representations are aggregated by averaging their published papers’ embeddings. We set the dropout rate of DHAN among {0.1, 0.2, 0.3, 0.4, 0.5} and the temperature T from {0.01, 0.05, 0.1, 1, 1.5, 10}. The ℓ_2 regularization weight is set from {1e-4, 1e-3, 1e-2, 1e-1}. For the paper field L1 task (PF_L1), we add one more weighted residual connection in inter-class aggregation process without adding any new parameters. All models are trained with AdamW optimizer with the Cosine Annealing Learning Rate Scheduler. For all the baseline models and DHAN, we use 128 hidden dimension. For each model, we run 200 epochs and choose the best which has higher NDCG and lower loss compared with former training processes on validation datasets in order to alleviate the overfitting problem. To obtain the experimental results of all baselines, we run official codes provided by the original papers. Finally, we report the results of each model on the testing datasets.

4.2 Classification and Link Prediction

4.2.1 Evaluation Protocol

We evaluate our model on three tasks, including author disambiguation (AD), paper-venue (PV), paper-field in L1 level (PF_L1) classification and paper-field in L2 level (PF_L2) classification. In the datasets, the fields of papers are divided into several hierarchical levels (such as Operating system/ file system), and lower level means more detailed categories. In other words, L2 (such as ‘file system’) has much more categories than L1 (such as operating system). The author disambiguation task could be treated as a link prediction task which aims to predict the possible link between the same name and their associated papers. Both of the paper-venue and paper-field classifications are multi-classification problem. In paper-venue classification, each paper belongs to only one venue, while each paper may belong to several fields of L1 level and L2 level in paper-field classification tasks. We adopt accuracy (ACC), Normalized Discounted Cumulative Gain(NDCG) and Mean Reciprocal Rank (MRR) as evaluation metrics.

4.2.2 Results and Analysis

The experimental results of the proposed model and SOTA baselines are reported in Table 3. We can observe from Table 3 that our proposed DHAN outperforms all the baselines on all tasks across most of metrics on all datasets. For instance, our model improves the ACC, NDCG and MRR of author disambiguation on *OAG1Y* from 0.6477 to 0.8343, 0.5394 to 0.7828, and 0.3479 to 0.6799 respectively comparing to the state-of-the-art model ie-HGCN, which confirms the capability of DHAN in learning bi-typed multi-relational heterogeneous graph.

Analysis. (1) Compared with homogeneous GNNs, i.e. GCN and GAT, DHAN achieves significant and consistent performance, which indicates that our proposed model can sufficiently capture the heterogeneous information from the data. (2) Compared with heterogeneous GNNs, i.e., RGCN, HetGNN, GTN and HGT, the

TABLE 3
Classification and link prediction results. Evaluation of different methods on three datasets.

Datasets	Tasks	Metrics	GCN [8]	GAT [9]	RGCN [10]	HAN [12]	HetGNN [3]	GTN [11]	HGT [13]	HGConv [14]	ie-HGCN [15]	DHAN
OAG1Y	PV	NDCG	0.2661	0.2750	0.2693	0.2880	0.2375	0.2680	0.2970	0.2885	0.2465	0.2995
		MRR	0.1295	0.1391	0.1335	0.1508	0.1031	0.1300	0.1623	0.1502	0.1069	0.1643
	PF_L1	NDCG	0.7180	0.7271	0.7492	0.7227	0.6587	0.7408	0.7515	0.7476	0.7304	0.7532
		MRR	0.6892	0.6905	0.7220	0.6916	0.6189	0.7088	0.7169	0.7179	0.6996	0.7213
	PF_L2	NDCG	0.3598	0.3678	0.4191	0.3817	0.3059	0.3910	0.4502	0.4209	0.3297	0.4512
		MRR	0.3156	0.3300	0.4311	0.3593	0.2183	0.3725	0.4958	0.4403	0.2528	0.4960
	AD	NDCG	0.7297	0.7915	0.7820	0.7497	0.6430	0.7403	0.8037	0.7715	0.7539	0.8222
		MRR	0.6436	0.7241	0.7120	0.6693	0.5309	0.6567	0.7403	0.6982	0.6749	0.7651
		ACC	0.4627	0.5678	0.5610	0.5002	0.3240	0.4800	0.6040	0.5406	0.5106	0.6394
	OAG2Y	PV	NDCG	0.2604	0.2780	0.2739	0.2899	0.2465	0.2569	0.2947	0.2862	0.1828
MRR			0.1282	0.1445	0.1376	0.1553	0.1137	0.1200	0.1616	0.1496	0.0502	0.1629
PF_L1		NDCG	0.7076	0.7271	0.7410	0.7384	0.6614	0.7284	0.7455	0.7438	0.7195	0.7520
		MRR	0.6838	0.6985	0.7131	0.7069	0.6282	0.6905	0.7075	0.7139	0.6861	0.7177
PF_L2		NDCG	0.3651	0.3737	0.4275	0.3882	0.3075	0.4000	0.4544	0.4265	0.3383	0.4558
		MRR	0.3226	0.3427	0.4429	0.3629	0.2179	0.3955	0.4916	0.4391	0.2694	0.4925
AD		NDCG	0.6726	0.7783	0.7841	0.7509	0.6258	0.7167	0.8040	0.7797	0.6718	0.8332
		MRR	0.5698	0.7073	0.7147	0.6716	0.5099	0.6260	0.7410	0.7093	0.5688	0.7796
		ACC	0.3769	0.5539	0.5584	0.5073	0.2959	0.4330	0.5959	0.5513	0.3599	0.6554
OAG10Y		PV	NDCG	0.2604	0.2718	0.2739	0.2598	0.2515	0.2317	0.2801	0.2655	0.2405
	MRR		0.1282	0.1399	0.1376	0.1225	0.1196	0.0971	0.1445	0.1287	0.1047	0.1476
	PF_L1	NDCG	0.7219	0.7300	0.7520	0.7169	0.6837	0.7339	0.7550	0.7489	0.7222	0.7530
		MRR	0.6902	0.6950	0.7266	0.6834	0.6554	0.6953	0.7196	0.7188	0.6899	0.7197
	PF_L2	NDCG	0.3595	0.3641	0.4205	0.3768	0.3125	0.3892	0.3877	0.4189	0.3342	0.4556
		MRR	0.3081	0.3184	0.4196	0.3385	0.2274	0.3679	0.3735	0.4214	0.2559	0.4868
	AD	NDCG	0.6042	0.7201	0.7685	0.7169	0.5712	0.6804	0.7979	0.7659	0.6477	0.8343
		MRR	0.4841	0.6326	0.6955	0.6284	0.4430	0.5807	0.7338	0.6923	0.5394	0.7828
		ACC	0.2862	0.4645	0.5426	0.4615	0.2476	0.3920	0.5973	0.5471	0.3479	0.6799

TABLE 4
Node clustering results.

Datasets	Metrics	GCN [8]	GAT [9]	RGCN [10]	HAN [12]	HetGNN [3]	GTN [11]	HGT [13]	HGConv [14]	ie-HGCN [15]	DHAN
OAG1Y	ARI	0.0340	0.0286	0.0308	0.0337	0.0141	0.0350	0.0636	0.0276	0.0451	0.0728
	NMI	0.6566	0.6477	0.6469	0.6541	0.6231	0.6652	0.6746	0.6489	0.6479	0.6764
OAG2Y	ARI	0.0156	0.0194	0.0109	0.0225	0.0120	0.0176	0.0134	0.0313	0.0090	0.0474
	NMI	0.6577	0.6646	0.6571	0.6666	0.6302	0.6773	0.6740	0.6678	0.4758	0.7012
OAG10Y	ARI	0.0152	0.0286	0.0124	0.0079	0.0135	0.0369	0.0318	0.0337	0.0018	0.0370
	NMI	0.6422	0.6477	0.6510	0.6449	0.6207	0.6706	0.6727	0.6744	0.6491	0.6818

proposed model DHAN outperforms all baselines in link prediction tasks on all datasets and indicators. This is mainly because our model is specially designed for bi-typed multi-relational graphs. Hence, it can sufficiently utilize interactions between two types of nodes, which can not be well captured by general heterogeneous graph neural networks. Besides, the proposed model also achieves comparable results in classification tasks on most of datasets and indicators. The observation confirms that our model is able to distinguish different relations delicately by utilizing the hierarchical mechanism. (3) Compared with the conventional hierarchical attention model HGConv and ie-HGCN, our model performs better on all tasks in all datasets. Our model takes advantage of the two typical hierarchical models by fusing relation

global information and local information. To be more specific, HAN proposed to aggregate different types of relation information with same global importance, which overlooks heterogeneity of different nodes. HGConv aggregates relation information with heterogeneous weight related to different nodes, which neglects common information that a type of relation has among all nodes. In contrast, our model overcomes their limits by incorporating both the merits of relation global information as well as local information. (4) In sum, we believe the better performance is due to the better design of our model. First, DHAN can gain improvements via taking both the node intra-class and inter-class attention into consideration. Second, our model also uses an efficient hierarchical attention mechanism to encode the graph.

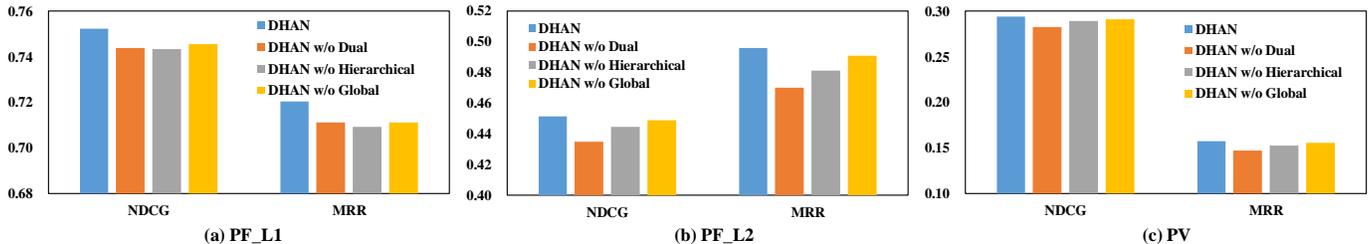


Fig. 4. The ablation study of our model on *OAG1Y*.

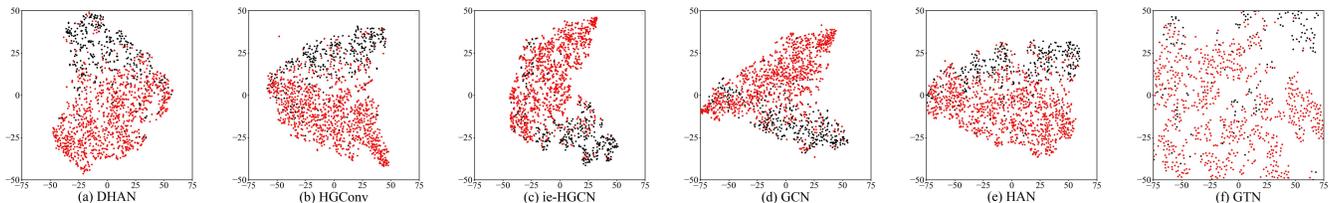


Fig. 5. Visualization of node representation on *OAG1Y*. Each point indicates a paper and its color indicates its publication field.

4.3 Node Clustering

We conduct node clustering based on the paper-venue task on three datasets. Here, we first get node representations via feed forward of each GNN. We then apply K-Means to implement node clustering and evaluate the performance using NMI and ARI based on their ground truth and predicted categories. Since the results tend to be affected by initial centroids, to make performance more stable, we repeat the former process 10 times and report average results in Table 4. Experiments results show that our model outperforms all baselines, e.g. on *OAG1Y*, DHAN outperforms the SOTA model ie-HGCN with a margin as large as 0.0277 on ARI. The results demonstrate the superiority of the learned node representations.

4.4 Ablation Study.

To evaluate the contribution of different model components of DHAN, we conduct an ablation study. We generate variants of DHAN by adjusting the use of its model components and comparing their performance on three tasks on *OAG1Y*. The three ablated variants are as follows: (1) **DHAN w/o dual operation**, which does not distinguish the node intra-class and inter-class relation, and only takes one hierarchical attention. (2) **DHAN w/o hierarchical architecture**, which deletes hierarchical architecture in both intra-class and inter-class encoders. (3) **DHAN w/o global attention**, which deletes the relation global attention.

Figure 4 shows the results of the variants on all three datasets, from which we can observe that removing either dual operation or hierarchical architecture will lead to performance decreasing. Specifically, the proposed model DHAN significantly outperforms **DHAN w/o dual operation**, which confirms the benefits of the dual mechanism. Thus, we highlight the importance of designing a specific model architecture on the bi-typed graphs rather than a general heterogeneous graph model. Compared with **DHAN w/o global attention** and **DHAN w/o hierarchical architecture**, we can find that fusing both global information and local information makes a great contribution to the performance of DHAN. Moreover, we could also observe that **DHAN w/o global**

attention always performs better than **DHAN w/o hierarchical architecture**, which is in line with the fact that **DHAN w/o hierarchical architecture** is also a simplified version of **DHAN w/o global attention** removing local attention mechanism.

4.5 Visualization.

To make a more intuitive comparison, we project the representations of paper nodes into two-dimensional space by t-SNE [54]. The node representations are learned on *OAG1Y* based on PF_L1 tasks. We randomly choose two fields that no papers belongs to both. The color indicates the publishing field of the papers in Figure 5. The less mixed areas the better. We can observe that our model DHAN performs best in visualization as there are more distinct boundaries and fewer mixed nodes. Besides, we also find that those hierarchical heterogeneous models, i.e., ie-HGCN, HGConv, perform better than general heterogeneous graph models, i.e., HAN, GTN.

4.6 Variant Analysis

We conduct variant analysis of DHAN on *OAG1Y* with four tasks to show the effectiveness of its architecture. (1) **DAH-N-RGCN** substitutes the proposed hierarchical attention mechanism with RGCN and keeps model structure unchanged. (2) **Inverted Architecture** firstly implements inter-class hierarchical aggregation and then applies intra-class hierarchical aggregation. (3) **Parallel Architecture** conducts intra-class and inter-class hierarchical aggregation simultaneously and concatenates the updated representation of two types of nodes respectively. The results are shown in Figure 6, from which we can observe that all the variants perform worse than DHAN. **DHAN-RGCN** utilizes RGCN rather than our hierarchical module to aggregate different types of relation information, which thus leads to a performance decrease. The proposed DHAN performs better than both **Inverted Architecture** and **Parallel Architecture**, which demonstrates our model structure is a more efficient architecture, i.e., first conducting intra-class relation aggregating then implementing inter-class relation.

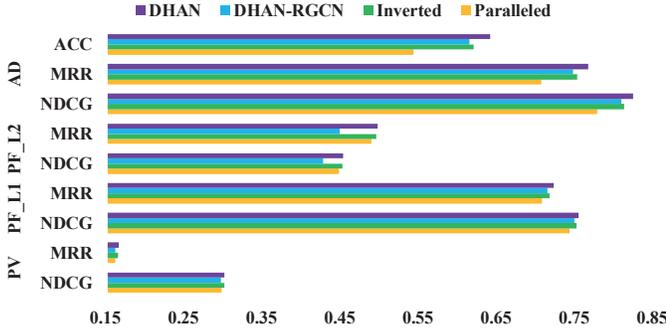


Fig. 6. Variant analysis of DHAN on OAG1Y.

4.7 Interpretability of the Hierarchical Attention

To show the proper interpretability of DHAN, we show the learned attention scores of our model in Figure 7. The global attention is learned parameter for different relations, and the average attention is the finally averaged attention score which is calculated as the sum of global attention score and heterogeneous attention score of all nodes. Here, we show the results of PF_L2 task and AD task on OAG1Y.

Specifically, we can observe from Figure 7 (a) that the learned global attention score of relation *cite* and *rev_cite* gain more weight than other relations in PF_L2 task. This is in line with the fact that those papers which are either cited by or cite target paper contribute much more than other related papers to the target paper while performing paper field tasks. Besides, the “*is_important_author_of*” and “*is_ordinary_author_of*” relationships obtain more significant weight than the “*is_same_venue_of*” and “*is_same_field_of*” relationships, which is also in line with intuition. Moreover, the “*is_important_author_of*” relationship acquires a bit more considerable weight than “*is_ordinary_author_of*”, which confirms the interpretability of our model again. A similar conclusion on AD task is shown in 7 (b). However, different from Figure 7 (a), the global attention weight of “*is_important_author_of*” is the largest one among all relations, which denotes that papers with same important author have much more influence than other related papers in the author disambiguation task. This is mainly because that the author disambiguation task cares more about relations between authors and papers, which is also in line with our intuition. Above all, we can find that the average attention score of each relation is significantly different from global attention weight. Actually, in PF_L2 task, the average attention score of *cite* relation and corresponding standard variance are 0.3293 and 0.0124. In AD task, the average attention score of “*is_important_author_of*” and corresponding standard variance is 0.5682 and 0.0960. The former two facts demonstrate the necessity of combining both global information and local information for aggregation.

4.8 Parameter Analysis

The hyper-parameter plays an vital role in model performance, and one of the most essential hyper-parameter is the dimension of representations. We conduct parameter analysis in the PF_L2 and AD task on the OAG1Y dataset. The results are shown in Figure 8, from which we can observe that the proposed model reaches its best performance when the dimension of output representation

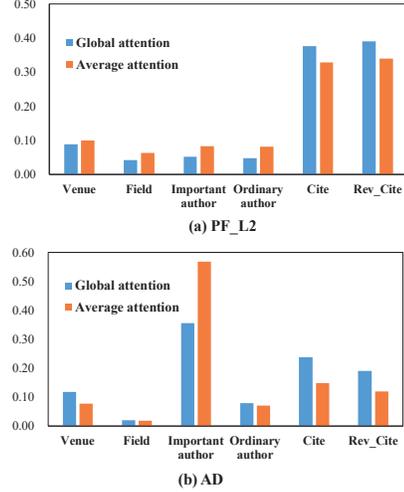


Fig. 7. The presentation of the learned attention scores of DHAN.

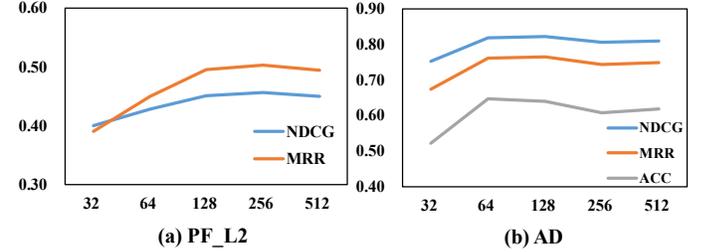


Fig. 8. Parameter sensitivity of DHAN on PF_L2 and AD task with different dimensions in OAG1Y.

is set as 128. Specifically, the performance first rises with the dimension increasing and then reaches its optimal state since the model needs larger dimension to embody rich information. After that, the performance decreases as a result of overfitting.

5 CONCLUSION AND FUTURE WORK

In this paper, we focus on how to learn node efficient representations on bi-typed multi-relational heterogeneous graph. To this end, we propose a novel Dual Hierarchical Attention Networks (DHAN). To the best of our knowledge, we are the first attempt to deal with this task. Specifically, DHAN contains intra-class and inter-class attention-based encoders which enables DHAN to sufficiently leverage not only the node intra-class neighboring information but also the inter-class neighboring information in BMHG. Moreover, we adopt a newly proposed hierarchical mechanism to to sufficiently model node multi-relational information in BMHG. By doing so, the proposed dual hierarchical attention operations enable our model to fully capture the complex structures of the BMHGs. We conduct extensive experiments on various tasks against the state-of-the-arts, which sufficiently confirms the capability of DHAN in learning node comprehensive representations in BMHGs. Interesting future work directions include generalizing DHAN to other BMHG-based applications.

ACKNOWLEDGMENTS

The authors would like to thank all anonymous reviewers in advance. This research has been partially supported by grants from

the National Natural Science Foundation of China under Grant No. 71725001, 71910107002, 61906159, 62176014, U1836206, 71671141, 71873108, 62072379, the State key R & D Program of China under Grant No. 2020YFC0832702, the major project of the National Social Science Foundation of China under Grant No. 19ZDA092. and the Financial Intelligence and Financial Engineering Key Laboratory of Sichuan Province.

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