Meta-node: A Concise Approach to Effectively Learn Complex Relationships in Heterogeneous Graphs

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Abstract

Existing message passing neural networks for heterogeneous graphs rely on the concepts of meta-paths or meta-graphs due to the intrinsic nature of heterogeneous graphs. However, the meta-paths and meta-graphs need to be pre-configured before learning and are highly dependent on expert knowledge to construct them. To tackle this challenge, we propose a novel concept of meta-node for message passing that can learn enriched relational knowledge from complex heterogeneous graphs without any meta-paths and meta-graphs by explicitly modeling the relations among the same type of nodes. Unlike meta-paths and meta-graphs, meta-nodes do not require any pre-processing steps that require expert knowledge. Going one step further, we propose a meta-node message passing scheme and apply our method to a contrastive learning model. In the experiments on node clustering and classification tasks, the proposed meta-node message passing method outperforms state-of-the-arts that depend on meta-paths. Our results demonstrate that effective heterogeneous graph learning is possible without the need for meta-paths that are frequently used in this field.

Introduction

Graph Neural Networks (GNNs) (Gori, Monfardini, and Scarselli 2005; Gilmer et al. 2017; Kipf and Welling 2017; Hamilton, Ying, and Leskovec 2017; Velickovic et al. 2018; Xu et al. 2018) have become the de facto standard for representation learning on graph-structured data. Among the differing architectures for GNNs, Message Passing Neural Networks (MPNNs) (Gilmer et al. 2017; Morris et al. 2019) in which nodes exchange messages (i.e., representations) along edges, are considered well-known and effective mechanisms. Since GNNs were first proposed (Gori, Monfardini, and Scarselli 2005), the majority of efforts in this field have been aimed at learning representations for homogeneous graphs with a single type of nodes and a single type of edges (i.e., relationships).

However, graph-structured datasets in real-world applications are not limited to a single type of nodes and edges. For instance, in the movie network of Figure 1(a), there exist multiple types of nodes (movies, actors, directors, and producers) and multiple types of edges (acting, filming, and producing). This kind of graph that has multiple types of nodes and edges is called heterogeneous graph (Wang et al. 2020; Yang et al. 2020). To capture complex relations in heterogeneous graphs, the representation learning model must consider the distinct nature of multiple types of nodes and edges. Thus simply plugging heterogeneous graphs into conventional MPNNs is inadequate because the MPNNs cannot distinguish multiple node and edge types. To deal with this problem, recently, Heterogeneous Graph Neural Networks (HGNNs) (Schlichtkrull et al. 2018; Zhang et al. 2019; Wang et al. 2019; Kim et al. 2019; Yun et al. 2019; Wang et al. 2021; Ren et al. 2020; Hu et al. 2020) have been proposed to extract useful knowledge from heterogeneous graphs by leveraging the power of GNNs.

To learn complex relational knowledge from heterogeneous graphs, most HGNNs rely on the node compositions constructed before training. This dependency on pre-processing steps of HGNNs is from the unique characteristics of heterogeneous graphs. As an example in Figure 1 the nature of k-partite graphs, all that is given are sparse inter-type
Table 1: Predefined meta-paths of real-world datasets. In this table, it can be noticed that most of $R$ are inter-type relations and $P$ target on intra-type relations by setting the same type of nodes at both ends of $P$.

| Dataset  | $A$ | $R$ | $P$ |
|----------|-----|-----|-----|
| DBLP     | A, P, T, C | A-P, P-T, P-C | APA, APCPA, APTPA |
| IMDB     | M, D, A | M-D, M-A | MDM, MAM |
| ACM      | P, A, S | P-A, P-S | PAP, PSP |
| AMiner   | P, A, R | P-A, P-R | PAP, PRP |
| Freebase | M, D, A, P | M-D, M-A, M-P | MM, MDM, MPM |
| Last.FM  | U, A, T | U-U, U-A, A-T | UU, UAU, UATAU, AU, AUUA, ATA |
| Yelp     | U, B, Co, Ci, Ca | U-U, U-B, U-Co, B-Ci, B-Ca | UB, UCoB, UCiBU, UBcBU, BUB, BCiB, BCaB, BCaUB |
| Douban   | U, M, G, L, D, A, T | U-U, U-G, U-M, U-L, M-D, M-T, M-A | MUM, MTM, MDM, MAM, UMU, UMAMU, UMDMU, UMTMU |

relations (i.e., edges between different types of nodes). However, using only these inter-type relations is not enough to extract useful knowledge from the intricate relations in the data. To resolve this problem, most HGNNs rely on additional predefined relational information, and the most commonly used methods are meta-path (Sun et al. 2011) and meta-graph (Fang et al. 2016; Wang et al. 2016), each of which are a composition of different types of nodes and multiple meta-paths as shown in Figure 1(c) and (d). As we will show later, nearly all meta-paths implicitly derive intra-type relations (i.e., relations between the same type of nodes) by manipulating given inter-type relations.

However, there exist three major problems with using predefined methods such as meta-paths for heterogeneous graph learning. Firstly, there exist certain limitations on inducing intra-type relations from predefined inter-type relations. When the given inter-type relations are sparse or noisy, induced intra-type relations can also be affected. Secondly, the appropriate composition of nodes and edges (designing meta-paths and meta-graphs) for representation learning requires significant domain-specific knowledge. Thus, it is extremely hard to know which combinations of nodes and edges are suitable for learning useful representations, especially in unsupervised environments. Lastly, although there exist attempts to learn appropriate meta-paths beyond given ones (Yun et al. 2019), several multiplications of the adjacency matrix are required. Due to the high computational cost of multiple matrix multiplications, their method is limited to very small datasets (Lv et al. 2021).

To circumvent the above limitations of current methods, we propose a novel concept of meta-node to construct simple and powerful MPNNs for learning heterogeneous graphs. Meta-nodes are virtual nodes in which one meta-node is added to the graph for each type of node in the heterogeneous graph. Each meta-node is connected to all nodes of each type as illustrated in Figure 1(b). By introducing meta-nodes, message passing is no longer limited to sparse inter-type relations, and every node can directly perform message passing with other nodes of the same type via meta-nodes. To do so, we can enrich the information on the relationship by adding explicit intra-type relations to the given inter-type relations. After introducing the concept of meta-nodes, we propose a message passing scheme via meta-node to learn both intra- and inter-type relations effectively.

Unsupervised representation learning on heterogeneous graphs has become one of the major challenges in graph-structured data learning, as it can pave the way to make use of large amounts of unlabeled multi-modal data. Thus, we validate the proposed message passing scheme by applying it to unsupervised representation learning for graph-structured data. To do so, we apply our meta-node message passing layer to the encoder of Deep Graph Infomax (Veličković et al. 2019) which is one of the most well-known graph contrastive models. Through downstream tasks on four real-world heterogeneous graph datasets, we validate the proposed message passing scheme. We confirm that our meta-node message passing layer learns rich relational information and shows competitive performance compared to existing state-of-the-art HGNNs even without any meta-paths.

**Related Work**

**Meta-path.** A meta-path (Sun et al. 2011) $P$ is defined as a path that has a form of $A_1 \xrightarrow{R_1} A_2 \xrightarrow{R_2} \cdots \xrightarrow{R_l} A_{l+1}$ (abbreviated as $A_1 A_2 \cdots A_{l+1}$) which describes relations between $A_1$ and $A_{l+1} \in A$ with a composition of relations $R_1, R_2, \ldots, R_l \in R$, where $A$ and $R$ denote sets of node types and edge types of heterogeneous graphs, respectively. Each meta-path can describe a semantic relation between nodes at both ends of the meta-path. For instance, in Figure 1(c), the meta-path of movie-director-movie can describe the relationship between two movies by which the director filmed them. Nearly all meta-paths of the real-world datasets (Wang et al. 2019; Fu et al. 2020; Wang et al. 2020, 2021) are implicitly composed for intra-type relations by setting the same type of nodes at both ends of $P$ using given inter-type relations $R$ as shown in Table 1.

**Representation Learning for Heterogeneous Graphs.** For several past years, there have been many efforts to learn representations of heterogeneous graphs based on random-walk-based methods (Dong, Chawla, and Swami 2017; Fu, Lee, and Lei 2017; Jeong et al. 2020; He et al. 2019) or GNNs methods (Schlichtkrull et al. 2018; Shi et al. 2018; Zhang et al. 2019; Yun et al. 2019; Wang et al. 2019; Zhao et al. 2020; Fu et al. 2020; Hu et al. 2020; Zhao et al. 2021). Nowadays, HGNNs leveraging the power of GNNs show a remarkable ability to learn intricate relations between multiple types of nodes and edges both in semi-supervised and unsupervised conditions. For instance, in semi-supervised learning, HAN (Zhang et al. 2019) proposed attention-based MPNNs using meta-paths to take each semantic meaning of
meta-paths into account. Further, MAGNN (Fu et al. 2020) considered all the nodes constituting each meta-path to respect intermediate semantic information. GTN (Yun et al. 2019) is an advanced method to learn new relations (meta-paths) in heterogeneous graphs by several multiplications of the adjacency matrix. In unsupervised learning, HetGNN (Zhang et al. 2019) learns a fixed size of correlated neighbors using random walks with restart. NSHE (Zhao et al. 2020) samples subgraphs and learns via multi-task learning to preserve relations in heterogeneous graphs.

Contrastive Methods. Starting from a pioneering work of contrastive learning for homogeneous graphs (Velickovic et al. 2019), there are some efforts to learn heterogeneous graphs through contrastive methods. HDMI (Jing, Park, and Tong 2021) utilizes higher-order mutual information via considering relations of raw features of nodes, learned representations, and global summary vectors. HDGI (Ren et al. 2020) is a contrastive model whose encoder is meta-path-based neighborhood aggregation and contrasts between an original graph and a corrupted graph. HeCo (Wang et al. 2021) is another contrastive model that contrasts local representation results of direct heterogeneous neighborhood aggregation and the representation to those of meta-path-based neighborhood aggregation.

Limitations of Existing Works. Whether the target condition of models is semi-supervised or unsupervised, it can be noticed that many heterogeneous graph learning models rely on predefined meta-paths or meta-graphs. However, depending on predefined meta-paths is undesirable since the results of meta-paths based message passing cannot directly leverage the relationships between nodes of the same type. Also, it is difficult to know whether meta-paths given in advance are conducive to effective learning. Thus, the question of how to effectively learn node representations of heterogeneous graphs without any predefined relational knowledge is one of the major challenges to be solved.

Proposed Method

In this section, we present the meta-node concept, a meta-node message passing layer (MN-MPL), and a contrastive model for heterogeneous graphs. The encoder of the contrastive model adopts a MN-MPL. The graphical descriptions of the meta-node, MN-MPL, and the contrastive model are illustrated in Figures 2 and 3.

Definitions

Definition 1. Heterogeneous graph. A heterogeneous graph $G = (\mathcal{V}, \mathcal{E}, \mathcal{A}, \mathcal{R}, \phi, \psi)$ is a network with multiple types of nodes and edges, where $\mathcal{V}$ and $\mathcal{E}$ denote the node set and edge set, respectively. Each node $v \in \mathcal{V}$ and edge $e \in \mathcal{E}$ are associated with a node type mapping function $\phi(v) : \mathcal{V} \to \mathcal{A}$ and an edge type mapping function $\psi(e) : \mathcal{E} \to \mathcal{R}$, where $\mathcal{A}$ and $\mathcal{R}$ denote sets of node types and edge types with $|\mathcal{A}| + |\mathcal{R}| > 2$, respectively. $\mathcal{V}_j$ denotes the node set having $j$-th node type, that is, $\bigcup_{j=1}^{|\mathcal{A}|} \mathcal{V}_j = \mathcal{V}$.

Definition 2. Meta-node. Meta-nodes $\{v_j\}_{j=1}^{|A|}$ are additional nodes whereby one node is introduced for each node type in $G$. Each meta-node $v_j$ is connected to all nodes in $\mathcal{V}_j$ via added edges that connect each meta-node and the nodes in each node type. The added edges enable message passing between each meta-node $v_j$ and all nodes in $\mathcal{V}_j$.

We illustrate an example of a heterogeneous graph introducing meta-nodes in Figure 2(a). Introducing the concept
of meta-nodes enables explicit modeling of intra-type relations that is otherwise hard to infer due to the $k$-partite structural characteristics of heterogeneous graphs. Compared to conventional methods of using meta-paths or meta-graphs that infer intra-type relations from given inter-type relations indirectly, meta-nodes can directly establish intra-type relations. Also, unlike meta-paths or meta-graphs that are predefined before learning, meta-nodes do not require any prior domain knowledge or predefined steps.

**MN-MPL: Meta-node Message Passing Layer**

We now propose a novel message passing layer using meta-nodes. The proposed layer takes three components as input: the representation of the previous layer, the meta-node representation, and aggregated messages from direct heterogeneous neighbors as shown in Figure 2(b). For a node $v_i \in \mathcal{V}$ who has $R$ different types of immediate neighbors, the meta-node message passing layer (MN-MPL) can be expressed as

$$h_i^{(l+1)} = \text{COM} \left( h_i^{(l)} , h_{\phi(v_i)}^{(l)} \sum_{l=1}^{R} h_{i,t}^{(l)} \right),$$

where $h_i^{(l)}$, $h_{\phi(v_i)}^{(l)}$, and $h_{i,t}^{(l)}$ denote the representation of the $i$-th node at the $l$-th layer, the meta-node representation that represents the type of the $i$-th node $\phi(v_i)$, and the aggregated representation from $t$ type neighbors of $v_i$, respectively. For the combination function COM, we apply concatenation $[x_j]_{j=1}^{k}$ or summation $\sum_{j=1}^{k} x_j$. COM includes a nonlinear MLP after concatenation or summation. The meta-node representation $h_{\phi(v_i)}^{(l)}$ is defined by sum pooling: $\sum_{j \in \mathcal{V}_{\phi(v_i)}} h_j^{(l)}$, mean pooling: $\frac{1}{|\mathcal{V}_{\phi(v_i)}|} \sum_{j \in \mathcal{V}_{\phi(v_i)}} h_j^{(l)}$, or max pooling: $\max\{h_j^{(l)}\}_{j \in \mathcal{V}_{\phi(v_i)}}$, where max denotes the element-wise max function. To aggregate messages from $R$ types of direct heterogeneous neighbors of $v_i$, we aggregate messages of each different type of direct neighbors separately first $\{h_{i,1}^{(l)}, \ldots, h_{i,R}^{(l)}\}$, then sum them to make a single vector representation: $\sum_{r=1}^{R} h_{i,t}^{(l)}$.

**Advantages of MN-MPL**

The proposed MN-MPL has three major advantages over conventional message passing on heterogeneous graphs. Firstly, each node can exchange messages with nodes of the same type by taking the aggregated messages through metanodes as input during the proposed message passing process. Thus, the proposed message passing scheme makes full use of both inter-type relations via direct heterogeneous neighbors and intra-type relations via meta-node representations. Compared to conventional message passing schemes that infer intra-type relations indirectly using predefined meta-paths or meta-graphs, the proposed layer does not require any indirect infer or pre-processing steps before learning. Secondly, through the meta-nodes, each node can easily exchange messages with distant nodes without having to pass through as many layers as the length of the meta-path. With our newly introduced meta-nodes, since each meta-node connects all nodes of each type, nodes within each type can consider the others as one-hop neighbors. Thus, classically distant but informative nodes can be learned with only a small number of MN-MPLs. Lastly, the cost of message passing between intra-type nodes is extremely low. As explained in the previous subsection, the computation of meta-node representations is a simple sum, mean or max pooling operation on the node representations, and infers negligible computational cost. Thus, the computational cost of establishing unseen relations of heterogeneous graphs using meta-nodes is extremely low compared to existing methods such as [Yun et al. 2019] requiring several adjacency matrix multiplications that attempts to do an efficient variant very recently [Yun et al. 2021].

**Contrastive Learning Framework**

We apply MN-MPLs to the contrastive framework of Deep Graph Infomax [Veličković et al. 2019]. At first, because each node type has attributes of different dimensions, we project each different attribute into a common latent space whose dimension is $d$ using one layer transformation network:

$$h_i^{(0)} = \zeta(W_{\phi(v_i)} x_i + b_{\phi(v_i)}),$$

where $x_i \in \mathbb{R}^{d_{\phi(v_i)}}$, $W_{\phi(v_i)} \in \mathbb{R}^{d \times d_{\phi(v_i)}}$, $b_{\phi(v_i)} \in \mathbb{R}^d$, and $\zeta$ denote the node attribute of $v_i$, a transformation matrix, a bias vector for type $\phi(v_i)$, and the nonlinear activation, respectively. For constrastive learning, we apply a corruption function $C$ to generate a negative graph $\tilde{G} = C(G)$. We select the corruption function $C$ as a type-wise random permutation of the node feature matrix. By applying $C$, each node is given the features of other nodes of the same type.

To learn the representation of each node, we apply MN-MPLs as the encoder network. We share the same encoder network for both the original graph and the corrupted graph to learn the representation of each node. $h_i$ and $\tilde{h}_i$ on node $v_i \in \mathcal{V}$ denote the outputs of the encoder network for the original graph and the corrupted graph, respectively. We extract global summary vector $s$ of the original graph by applying mean pooling $s = \sigma(\frac{1}{|\mathcal{V}|} \sum_{i=1}^{|\mathcal{V}|} h_i)$, where $\sigma$ denotes

![Figure 3: Overview of the contrastive model. C, D, E, and s denote a corruption function for generating negative samples, a discriminator function, an encoder network that is composed of our MN-MPL, and a global summary vector, respectively. We referred to the graphical description of Veličković et al. [2019].](image-url)
the logistic sigmoid function. Then, we utilize a contrastive objective with binary cross entropy loss function between positive samples \((h_i, s)\) and negative samples \((\tilde{h}_i, s)\):

\[
L = \frac{1}{2|V|} \left( \sum_{i=1}^{|V|} \mathbb{E}_G[\log D(h_i, s)] + \sum_{i=1}^{|V|} \mathbb{E}_G[\log (1 - D(\tilde{h}_i, s))] \right),
\]

where \(D(h_i, s) = \sigma(h_i^T W s)\) denotes the discriminator function which is a bilinear network \((W)\) is a learnable matrix. Maximizing the objective function \(L\) is equal to maximizing the mutual information between the representation from the original graph \(h_i\) and the global summary vector \(s\) from the original graph. The graphical overview of the contrastive learning framework is illustrated in Figure 3.

Experiments

To verify the validity of the proposed meta-node message passing scheme, we applied the contrastive model with MN-MPL to node classification and node clustering tasks on the target node type of each dataset. Further, we analyzed the quality of the learned representation of nodes and the effectiveness of the proposed method via additional analysis.

Experimental Settings

Datasets. We validated the contrastive learning model based on our MN-MPL using four real-world heterogeneous graph datasets. The statistics of datasets are presented in Table 2. The details and download links of datasets are presented in the supplementary material.

Compared Methods. We compared our method with graph representation learning methods in three categories: i) unsupervised homogeneous models: n2vec (Grover and Leskovec 2016), SAGE (Hamilton, Ying, and Leskovec 2017), GAE (Kipf and Welling 2016), DGI (Veličković et al. 2019), ii) unsupervised heterogeneous models: mp2vec (Dong, Chawla, and Swami 2017), HeCo (Wang et al. 2021), and iii) semi-supervised heterogeneous model: HAN (Wang et al. 2019). The brief explanation and the download link of each compared method are presented in the supplementary material.

Implementation Details. In the settings of our method, we did not use any meta-paths or meta-graphs. For COM in Eq. (1), we used summation for DBLP and ACM, and concatenation for AMiner and Freebase. For the direct heterogeneous neighbor aggregation in Eq. (1), we assigned GraphSAGE (Hamilton, Ying, and Leskovec 2017) modules as many numbers as the edge types in the dataset to compute \(h_{i_1}, \ldots, h_{i_R}\). When computing the vector representation of meta-nodes \(h_{\phi(v)}^{(t)}\) in Eq. (1), every node message in each node type was aggregated. However, aggregating all the information about each node type into one fixed-size vector can lead to over-squashing issues and lose its intended meaning (Alon and Yahav 2020; Topping et al. 2021). To solve this issue, for each training epoch, we randomly connect only \(r\%\) nodes in each node type to each meta-node, where \(r \in \{40, 50, 60, 70, 80, 90\}\). The choice of hyper-parameter and further implementation details are described in the supplementary material for reproducibility.

Node Classification

We conducted node classification to see how useful the learned representation from the meta-node message passing encoder of contrastive learning is. For each dataset, we selected 20, 40, 60 nodes per class for training set, 1,000 nodes for validation set, and 1,000 nodes for test set. We trained and tested a single layer of logistic regression classifier, and used Macro-F1, Micro-F1, and AUC for evaluation metrics. The average value and standard deviation after executing each model 10 times are reported in Table 3. The results demonstrate that our method (MN) can achieve outstanding results compared to the existing homogeneous models and heterogeneous models even without any predefined composition of heterogeneous nodes such as meta-paths. Especially, in most cases, the proposed method shows outperforming results compared to state-of-the-art heterogeneous models (mp2vec, DMGI, HeCo, etc.) that rely on the pre-configured meta-paths. Also, it can be seen that our method shows outstanding performances compared to contrastive learning models including DGI, DMGI, and HeCo. We have also observed that, for AMiner and Freebase datasets where the node feature does not have proper information about the semantics of the node, homogeneous models can achieve similar performances to heterogeneous models. Specifically, n2vec and GAE show classification performances close to those of several heterogeneous models such as mp2vec, HERec, HetGNN. We conjecture that the node feature with rich semantics plays an important role in distinguishing different types of nodes of heterogeneous graphs.

Node Clustering

We conducted node clustering by applying k-means clustering algorithm to the learned representation of each model. The clustering performance is measured by Normalized Mu-
of the movie genres. Every movie can have multiple genres, but for the classification task, only one genre was selected as a label among them. As evidence for this conjecture, we found that another paper (Li et al., 2016) used different movie genres, Action, Adventure, and Crime for the Freebase dataset, while in our experiments, we used Action, Comedy and Drama labels.

Table 3: Summary of node classification results (% ± σ).

| Datasets | Metric | split | n2vec | SAGE | GAE | mp2vec | HERec | HetGNN | HAN | DGI | DMGI | HeCo | MN (ours) |
|----------|--------|-------|-------|------|-----|--------|-------|-------|-----|-----|------|------|------------|
| DBLP     |        |       |       |      |     |        |       |       |     |     |      |      | 78.39 | 83.02 | 63.56 | 67.35 | 37.69 | 29.05 | 17.13 | 18.39 |
| ACM      |        |       |       |      |     |        |       |       |     |     |      |      | 68.51 | 64.46 | 58.60 | 54.42 | 42.37 | 35.05 | 29.40 | 24.88 |
| AMiner   |        |       |       |      |     |        |       |       |     |     |      |      | 50.68 | 44.60 | 37.80 | 33.74 | 27.74 | 21.84 | 18.27 | 14.87 |
| Freebase |        |       |       |      |     |        |       |       |     |     |      |      | 42.97 | 38.51 | 33.54 | 30.56 | 25.53 | 20.54 | 17.28 | 14.03 |

Table 4: Summary of node clustering results (% ± σ).

| Datasets | Metric | split | n2vec | SAGE | GAE | mp2vec | HERec | HetGNN | DGI | DMGI | HeCo | MN (ours) |
|----------|--------|-------|-------|------|-----|--------|-------|-------|-----|------|------|------------|
| DBLP     |        |       |       |      |     |        |       |       |     |     |      |      | 62.89 | 58.80 | 54.06 | 50.02 | 46.56 | 43.00 | 39.54 | 35.08 | 31.28 |
| ACM      |        |       |       |      |     |        |       |       |     |     |      |      | 64.74 | 64.31 | 66.07 | 71.60 | 74.50 | 78.40 | 82.40 | 86.40 | 91.28 |
| AMiner   |        |       |       |      |     |        |       |       |     |     |      |      | 70.96 | 76.80 | 84.81 | 75.11 | 83.16 | 86.88 | 90.04 | 94.18 | 98.39 |
| Freebase |        |       |       |      |     |        |       |       |     |     |      |      | 83.33 | 84.74 | 78.91 | 74.73 | 80.64 | 84.58 | 89.33 | 93.78 | 98.62 |

Effectiveness of Meta-nodes

If there are few inter-type relations, then existing heterogeneous models cannot learn the intra-type relations well due to the limited number of meta-paths that are composed of inter-type relations. To show the effectiveness of meta-nodes compared to meta-paths, we make the graphs of ACM, DBLP, and AMiner sparse by randomly removing a fraction of the edges. Then, we measured the classification performance of three models: i) the proposed model (MN), ii) aggregating only messages of each node and direct heterogeneous neighbors without using meta-node representation (without MN), and iii) HeCo which relies on meta-paths. The results are presented in Figure 9 in the results of ACM and DBLP, by comparing MN and without MN, it can be noticed that the proposed meta-node message passing scheme enables learning enriched relational knowledge by leveraging both inter- and intra-type relations effec-
Figure 4: The classification results of sparse graphs when the training set is composed of 40 nodes per each class. MN (blue line), without MN (green line), and HeCo (red line) denote the proposed message passing scheme, the message passing that only considers the message of each node and the aggregated messages from heterogeneous neighbors, and the message passing scheme that relies on the meta-paths. For instance, 0.2 of the sparsity of graph indicates there exists only 20% of original edges.

Qualitative Analysis
For qualitative analysis of the proposed method, we projected the learned representation of the target node type of each dataset. By using t-SNE [Van der Maaten and Hinton 2008], we obtained 2D projections of learned representations. The projection results are shown in Figure 5. Nodes of the same color share the same label. To measure the quality of projected representations of each model, we measured a silhouette score [Rousseeuw 1987]. Our method can distinguish node classes better than comparison methods. The projected representations of n2vec overlap a lot among other classes due to the limited learning ability of homogeneous models. The projected representations of HeCo show discriminability among classes. However, these results can only be achieved with well-configured meta-paths in advance.

Conclusions
In order to comprehensively learn complex relations in heterogeneous graphs, we proposed a concise and powerful concept of meta-node from the understanding of the unique structural characteristics of heterogeneous graphs. By introducing meta-nodes, each node can take into account information both of heterogeneous neighbors and its corresponding node type by explicit modeling of intra-type relations. Then, we proposed a meta-node message passing layer (MN-MPL) and applied MN-MPL to the contrastive learning model. The proposed method was validated qualitatively and quantitatively on real-world heterogeneous graphs. Unlike meta-paths and meta-graphs, the proposed meta-node does not require expert knowledge to construct, does not need to be designed before learning, and can learn well enough even if there are only a small number of edges. Our results shed light on the possibility of accurate heterogeneous graph learning even without meta-paths or meta-graphs which are frequently used in this field. In the future, we will take one step further about message passing using meta-nodes. Through meta-node message passing, messages can be received from nodes of the same type, but not all of the same type have the same importance. Thus, computation of importance among nodes of the same type by self-attention mechanism or shortest path distance is one of the promising directions.
References

Alon, U.; and Yahav, E. 2020. On the Bottleneck of Graph Neural Networks and its Practical Implications. In International Conference on Learning Representations 2021.

Dong, Y.; Chawla, N. V.; and Swami, A. 2017. Metapath2vec: Scalable Representation Learning for Heterogeneous Networks. In Proceedings of the 23rd ACM SIGKDD Conference on Knowledge Discovery & Data Mining, 135–144.

Fang, Y.; Lin, W.; Zheng, V. W.; Wu, M.; Chang, K. C.-C.; and Li, X.-L. 2016. Semantic Proximity Search on Graphs with Metagraph-based Learning. In 2016 IEEE 32nd International Conference on Data Engineering. 277–288. IEEE.

Fu, T.-y.; Lee, W.-C.; and Lei, Z. 2017. Hin2vec: Explore Meta-paths in Heterogeneous Information Networks for Representation Learning. In Proceedings of the 26th ACM International Conference on Information and Knowledge Management, 1797–1806.

Fu, X.; Zhang, J.; Meng, Z.; and King, I. 2020. Magnn: Metapath Aggregated Graph Neural Network for Heterogeneous Graph Embedding. In Proceedings of The Web Conference 2020, 2331–2341.

Gilmer, J.; Schoenholz, S. S.; Riley, P. F.; Vinyals, O.; and Dahl, G. E. 2017. Neural Message Passing for Quantum Chemistry. In International Conference on Machine Learning, 1263–1272. PMLR.

Gori, M.; Monfardini, G.; and Scarselli, F. 2005. A New Model for Learning in Graph Domains. In Proceedings. 2005 IEEE International Joint Conference on Neural Networks, 2005, 729–734.

Grover, A.; and Leskovec, J. 2016. Node2vec: Scalable Feature Learning for Networks. In Proceedings of the 22nd ACM SIGKDD Conference on Knowledge Discovery & Data Mining, 855–864.

Hamilton, W. L.; Ying, R.; and Leskovec, J. 2017. Inductive Representation Learning on Large Graphs. In Proceedings of the 31st International Conference on Neural Information Processing Systems, 1025–1035.

He, Y.; Song, Y.; Li, J.; Ji, C.; Peng, J.; and Peng, H. 2019. Hetespacewalk: A Heterogeneous Spacey Random Walk for Heterogeneous Information Network Embedding. In Proceedings of the 28th ACM International Conference on Information and Knowledge Management, 639–648.

Hu, Z.; Dong, Y.; Wang, K.; and Sun, Y. 2020. Heterogeneous Graph Transformer. In Proceedings of The Web Conference 2020, 2704–2710.

Huang, Z.; Zheng, Y.; Cheng, R.; Sun, Y.; Mamoulis, N.; and Li, X. 2016. Meta Structure: Computing Relevance in Large Heterogeneous Information Networks. In Proceedings of the 22nd ACM SIGKDD Conference on Knowledge Discovery & Data Mining, 1595–1604.

Jeong, J.; Yun, J.-M.; Keam, H.; Park, Y.-J.; Park, Z.; and Cho, J. 2020. Div2vec: Diversity-Emphasized Node Embedding. arXiv preprint arXiv:2009.09588.

Jing, B.; Park, C.; and Tong, H. 2021. HDMI: High-order Deep Multiplex Infomax. In Proceedings of The Web Conference 2021, 2414–2424.

Kim, K.-M.; Kwak, D.; Kwak, H.; Park, Y.-J.; Sim, S.; Cho, J.-H.; Kim, M.; Kwon, J.; Sung, N.; and Ha, J.-W. 2019. Tripartite Heterogeneous Graph Propagation for Large-scale Social Recommendation. arXiv preprint arXiv:1908.02569.

Kipf, T. N.; and Welling, M. 2016. Variational Graph Auto-encoders. arXiv preprint arXiv:1611.07308.

Kipf, T. N.; and Welling, M. 2017. Semi-Supervised Classification with Graph Convolutional Networks. In International Conference on Learning Representations 2017.

Li, X.; Kao, B.; Zheng, Y.; and Huang, Z. 2016. On Transductive Classification in Heterogeneous Information Networks. In Proceedings of the 25th ACM International Conference on Information and Knowledge Management, 811–820.

Lv, Q.; Ding, M.; Liu, Q.; Chen, Y.; Feng, W.; He, S.; Zhou, C.; Jiang, J.; Dong, Y.; and Tang, J. 2021. Are We Really Making Much Progress? Revisiting, Benchmarking and Refining Heterogeneous Graph Neural Networks. In Proceedings of the 27th ACM SIGKDD Conference on Knowledge Discovery & Data Mining, 1150–1160.

Morris, C.; Ritzert, M.; Fey, M.; Hamilton, W. L.; Lenssen, J. E.; Rattan, G.; and Grohe, M. 2019. Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks. In Proceedings of the AAAI Conference on Artificial Intelligence, 01, 4602–4609.

Park, C.; Kim, D.; Han, J.; and Yu, H. 2020. Unsupervised Attributed Multiplex Network Embedding. In Proceedings of the AAAI Conference on Artificial Intelligence, 04, 5371–5378.

Ren, Y.; Liu, B.; Huang, C.; Dai, P.; Bo, L.; and Zhang, J. 2020. HDGI: An Unsupervised Graph Neural Network for Representation Learning in Heterogeneous Graph. In AAAI Workshop.

Rousseeuw, P. J. 1987. Silhouettes: A Graphical Aid to The Interpretation and Validation of Cluster Analysis. Journal of Computational and Applied Mathematics, 20: 53–65.

Schlichtkrull, M.; Kipf, T. N.; Bloem, P.; Van Den Berg, R.; Titov, I.; and Welling, M. 2018. Modeling Relational Data with Graph Convolutional Networks. In European Semantic Web Conference, 593–607. Springer.

Shi, C.; Hu, B.; Zhao, W. X.; and Philip, S. Y. 2018. Heterogeneous Information Network Embedding for Recommendation. IEEE Transactions on Knowledge and Data Engineering, 31(2): 357–370.

Sun, Y.; Han, J.; Yan, X.; Yu, P. S.; and Wu, T. 2011. Pathsim: Meta path-based Top-k Similarity Search in Heterogeneous Information Networks. Proceedings of the VLDB Endowment, 4(11): 992–1003.

Topping, J.; Di Giovanni, F.; Chamberlain, B. P.; Dong, X.; and Bronstein, M. M. 2021. Understanding Over-squashing and Bottlenecks on Graphs via Curvature. In International Conference on Learning Representations 2022.

Van der Maaten, L.; and Hinton, G. 2008. Visualizing Data using t-SNE. Journal of Machine Learning Research, 9(11).

Velickovic, P.; Cucurull, G.; Casanova, A.; Romero, A.; Li, P.; and Bengio, Y. 2018. Graph Attention Networks. In International Conference on Learning Representations 2018.
Veličković, P.; Fedus, W.; Hamilton, W. L.; Liò, P.; Bengio, Y.; and Hjelm, R. D. 2019. Deep Graph Infomax. In International Conference on Learning Representations 2019.

Wang, X.; Bo, D.; Shi, C.; Fan, S.; Ye, Y.; and Yu, P. S. 2020. A Survey on Heterogeneous Graph Embedding: Methods, Techniques, Applications and Sources. arXiv preprint arXiv:2011.14867.

Wang, X.; Ji, H.; Shi, C.; Wang, B.; Ye, Y.; Cui, P.; and Yu, P. S. 2019. Heterogeneous Graph Attention Network. In Proceedings of The Web Conference 2019, 2022–2032.

Wang, X.; Liu, N.; Han, H.; and Shi, C. 2021. Self-Supervised Heterogeneous Graph Neural Network with Co-Contrastive Learning. In Proceedings of the 27th ACM SIGKDD Conference on Knowledge Discovery & Data Mining, 1726–1736.

Xu, K.; Li, C.; Tian, Y.; Sonobe, T.; Kawarabayashi, K.-i.; and Jegelka, S. 2018. Representation Learning on Graphs with Jumping Knowledge Networks. In International Conference on Machine Learning, 5453–5462. PMLR.

Yang, C.; Xiao, Y.; Zhang, Y.; Sun, Y.; and Han, J. 2020. Heterogeneous Network Representation Learning: A Unified Framework with Survey and Benchmark. IEEE Transactions on Knowledge and Data Engineering.

Yun, S.; Jeong, M.; Kim, R.; Kang, J.; and Kim, H. J. 2019. Graph Transformer Networks. Advances in Neural Information Processing Systems, 32: 11983–11993.

Yun, S.; Jeong, M.; Yoo, S.; Lee, S.; Yi, S. S.; Kim, R.; Kang, J.; and Kim, H. J. 2021. Graph Transformer Networks: Learning Meta-path Graphs to Improve GNNs. arXiv preprint arXiv:2106.06218.

Zhang, C.; Song, D.; Huang, C.; Swami, A.; and Chawla, N. V. 2019. Heterogeneous Graph Neural Network. In Proceedings of the 25th ACM SIGKDD Conference on Knowledge Discovery & Data Mining, 793–803.

Zhao, J.; Wang, X.; Shi, C.; Hu, B.; Song, G.; and Ye, Y. 2021. Heterogeneous Graph Structure Learning for Graph Neural Networks. In Proceedings of the AAAI Conference on Artificial Intelligence, Vol.35, 4697–4705.

Zhao, J.; Wang, X.; Shi, C.; Liu, Z.; and Ye, Y. 2020. Network Schema Preserved Heterogeneous Information Network Embedding. In Proceedings of the 29th International Joint Conference on Artificial Intelligence.