Metapaths-guided Neighbors-aggregated Network for Heterogeneous Graph Reasoning

Bang Lin  
Alibaba Group  
linbang.lb@alibaba-inc.com

Xiuchong Wang  
Alibaba Group  
xiuchong.wxc@alibaba-inc.com

Yu Dong  
Alibaba Group  
dongyu.dy@alibaba-inc.com

Chengfu Huo  
Alibaba Group  
chengfu.huocf@alibaba-inc.com

Weijun Ren  
Alibaba Group  
afei@alibaba-inc.com

Chuanyu Xu  
Alibaba Group  
tracy.xcy@alibaba-inc.com

ABSTRACT

Most real-world datasets are inherently heterogeneous graphs, which involve a diversity of node and relation types. Heterogeneous graph embedding is to learn the structure and semantic information from the graph, and then embed it into the low-dimensional node representation. Existing methods usually capture the composite relation of a heterogeneous graph by defining metapath, which represent a semantic of the graph. However, these methods either ignore node attributes, or discard the local and global information of the graph, or only consider one metapath. To address these limitations, we propose a Metapaths-guided Neighbors-aggregated Heterogeneous Graph Neural Network (MHN) to improve performance. Specially, MHN employs node base embedding to encapsulate node attributes, BFS and DFS neighbors aggregation within a metapath to capture local and global information, and metapaths aggregation to combine different semantics of the heterogeneous graph. We conduct extensive experiments for the proposed MHN on three real-world heterogeneous graph datasets, including node classification, link prediction and online A/B test on Alibaba mobile application. Results demonstrate that MHN performs better than other state-of-the-art baselines.

CCS CONCEPTS

• Mathematics of computing → Graph algorithms; • Computing methodologies → Machine learning.

KEYWORDS

Heterogeneous graph; Deep learning; Graph embedding

1 INTRODUCTION

Real-world datasets usually exist in the form of graph structure, such as social networks[1], citation networks[2], knowledge graphs[3], especially recommendation systems[4] where nodes and edges represent objects and relationships, respectively. Taking an example, users and items in recommendation system can be represented as nodes while relationships such as purchases and clicks can be represented as edges, so that we can turn the recommendation dataset into a graph structure. Because graph is a high-dimensional non-Euclidean structure, it is difficult to model by traditional machine learning methods. Therefore, it is helpful to represent nodes by low-dimensional dense vectors, which can be the input of other machine learning models.

There have been many graph embedding methods, which are divided into two different solutions generally. For methods based on random walk, such as Deepwalk[5], Node2vec[6] and so on, sequences generated by random walk are fed into the skip-gram model to learn node embedding. However, with the rapid development of neural networks, methods based on graph neural network(GNN) have become more widely used, which learn the node embedding using specially designed neural layers. Methods like GCN[7], GAT[8], GraphSAGE[9] and other variants, they perform convolution operations on the graph or apply attention mechanism to generate more reasonable node representations.

Although the above methods have achieved state-of-the-art results in graph embedding learning, their input is homogeneous graph, which consist one edge type and one node type. Many real-world datasets are heterogeneous graphs, which consist of various types of nodes and edges. For example, an E-commerce recommendation graph consists at least two types of nodes, namely user and item. At the same time, different types of nodes have different attributes. Attributes of user node may include age, sex and address while item node attributes may consist of price, brand, category, and so on. Due to the heterogeneity of graphs, it is a challenge for GNNs to encoder the complex information into low-dimensional vectors.

Since metapath can extract relations between different types of nodes in heterogeneous graphs, most of heterogeneous graph embedding methods are based on metapath. Metapath is an ordered sequence of node and edge types, which represents a semantic space of the graph. For example, in E-commerce recommendation graph, metapath user-item-user means the User-based collaborative filtering, while item-user-item means the Item-based collaborative filtering. Also, metapath can guide the way to sample the heterogeneous graph and obtain neighbors.

Currently, there are many methods using metapath to generate node representation of heterogeneous graph, but they still have some limitations. (1) Some methods do not make use of the attributes of nodes, resulting in the lack of rich information, such as Metapath2vec[10], HERec[11]. (2) Some methods do not consider local and global information of nodes, which are important to the generation of node embedding(e.g. HAN[12], GATNE[13]). (3) Although nodes in different semantics have different meanings, some methods adopt one metapath to embed the heterogeneous graph, ignoring the importance of multiple semantic spaces(e.g. Metapath2vec[10], EGES[14]).
In order to address these limitations, we propose a Metapath-guided Neighbors-aggregated Heterogeneous Graph Neural Network (MHN) model for heterogeneous graph embedding learning. Through applying node base embedding by attributes transformation, aggregation within one metapath and aggregation among metapaths, MHN can address these limitations. Specifically, MHN first adopts type-specific linear transformations to project attributes of different types of nodes, aiming to transform them into the same latent vector space. Then, MHN applies metapath-guided neighbors aggregation for each metapath. During extracting local information from BFS neighbors and global information from DFS neighbors, MHN weighted sums them and obtains the representation of target node under the current semantic. In this way, MHN can learn the comprehensive semantics in the heterogeneous graph.

The contribution of this paper lies in three aspects:

- We propose an end-to-end model MHN for heterogeneous graph embedding, which is a novel metapath aggregated graph neural network.
- MHN extracts local and global information under the guidance of a single metapath, and applies attention mechanism to fuse different semantic vectors. MHN supports both supervised and unsupervised learning.
- We conduct extensive experiments on the DBLP dataset for node classification task, as well as on the Amazon and Alibaba datasets for link prediction task to evaluate the performance of the proposed model. Moreover, we conduct online A/B test on Alibaba mobile application. Results show that representations generated by MHN performs better than other state-of-the-art methods consistently.

The rest of this paper is organized as follows. Section 2 introduces the related work. Section 3 describes some preliminary knowledge. Then we proposed the heterogeneous graph embedding method in Section 4. Experiments and analysis are shown in Section 5. Finally, we conclude the paper in Section 6.

2 RELATED WORK

In this section, we will review the related studies about graph representation learning related to the proposed model. These methods are organized into four subsections: Homogeneous Graph Embedding methods, Homogeneous GNN methods, Heterogeneous Graph Embedding methods and Heterogeneous GNN methods.

**Homogeneous Graph Embedding methods.** The goal of these methods is to learn a low-dimensional representations for each node from homogeneous graph, which can be used for many downstream tasks directly. DeepWalk[5] is a model for learning latent representation, which applies random walk to obtain node sequences and feeds them into skip-gram model to generate representations. LINE[15] learns node representations on large-scale graph, which summaries local and global information through first-order and second-order proximities. Node2vec[6] designs a biased random walk to explore diverse neighborhoods and maximize the likelihood of preserving network neighborhoods of nodes. SDNE[16] applies an autoencoder structure to optimize both the first-order and second-order similarities.

**Homogeneous GNN methods.** These methods are mainly built by homogeneous graph convolution and can be used for both supervised and unsupervised learning. GCN[7] generates the node embedding by graph convolution, which is performed in the graph Fourier domain. GAT[8] introduces the attention mechanism into the graph convolution, and assigns different weights to neighboring nodes to update the node representation. GraphSage[9] is an inductive learning method. By training the aggregation function, it can merge features of neighborhoods and generate the target node embedding.

**Heterogeneous Graph Embedding methods.** Unfortunately, most of above studies focus on the homogeneous graph and cannot be used directly in heterogeneous graph. Nowadays, there are more and more studies about heterogeneous graph embedding. Metapath2vec[10] proposes to use metapath guided random walk to sample the heterogeneous graph and obtain several node sequences. EGES[14] is proposed to solve above problem. Through attention mechanism, it can merge attribute information into node embedding, which have achieved good improvement in CTR prediction task. HIN2vec[17] captures the rich semantics embedded in heterogeneous graph by predicting whether there is a metapath between nodes.

**Heterogeneous GNN methods.** Due to the complexity of heterogeneous graph, homogeneous GNN methods cannot be applied directly. There are many researches on how to introduce graph convolution into heterogeneous graph. HAN[12] proposes a node-level attention layer to aggregate neighbors of target node features and a semantic-level attention layer to merge different semantic representations. GATNE[13] solves the problem of embedding learning for the heterogeneous graph with attributes. HERec[11] proposes an embedding method for heterogeneous graph and applies to the recommendation scene by matrix factorization.

However, heterogeneous graph embedding methods introduced above have the limitation of ignoring the local and global information. Although they have achieved some results in several datasets, we believe that there is still room for improvement by fully utilizing the information, which promotes us to study the optimal method of embedding for heterogeneous graph.

3 PRELIMINARIES

In this section, we give definitions of important terms related to heterogeneous graph and show them in Figure 1.

**Definition 3.1 Heterogeneous graph[18].** A heterogeneous graph is denoted as a graph $G = (\mathcal{V}, \mathcal{E})$, consisting of a node set $\mathcal{V}$ and a link set $\mathcal{E}$, which is also associated with a node type mapping function $\varphi : \mathcal{V} \rightarrow \mathcal{A}$ and a link type mapping function $\psi : \mathcal{E} \rightarrow \mathcal{R}$. $\mathcal{A}$ and $\mathcal{R}$ denote the sets of predefined node types and link types, where $|\mathcal{A}| + |\mathcal{R}| > 2$.

**Example.** As shown in Figure 1(a), we construct a heterogeneous graph to model the E-commerce. It consists of two type of nodes (User($U$) and Item($I$)) and two relations, which are user click item relation(u-i) and the similarity of items relation(i-i).
Definition 3.2 Metapath[19]. A metapath \( p \) is defined as a path in the form of \( p = A_1 \circ A_2 \circ A_3 \cdots \circ A_{L+1} \), which describes a composite relation \( R = R_1 \circ R_2 \cdots \circ R_L \) between objects \( A_i \) and \( A_{i+1} \), where \( \circ \) denotes the composition operator on relations. Different metapaths represent different semantics.

Definition 3.3 Metapath instance[21]. Given a metapath \( p \) of a heterogeneous graph, we can sample the graph under the guidance of \( p \) and obtain several node sequences, which is defined as metapath instance.

Example. As is shown in Figure 1(c), under the guidance of metapath \( p = \{U-I-I-U\} \), we can sample the graph and get two metapath instances \( user1-item1-item2-user2 \) and \( user1-item3-item1-user3 \).

Definition 3.4 Metapath based BFS Neighbors. Given a node \( u \) and a metapath \( p \) in a heterogeneous graph, we can sample the the metapath and obtain metapath instance for \( u \), which is denoted as \( P(u) \). Metapath based BFS Neighbors \( N^p_{\text{BFS}} \) of node \( u \) is defined as the set of nodes which connect to the node \( u \) directly from \( P(u) \). Note that the node’s BFS neighbors does not include itself.

Example. Taking Figure 1(d) as an example, given the metapath \( p = \{U-I-I-U\} \), the metapath based BFS neighbors of \( user1 \) is \{item1, item3\} because we can get two metapath instances. Obviously, metapath based BFS neighbors can exploit the local information of the graph because these neighbors connect to target node directly.

Definition 3.5 Metapath based DFS Neighbors. Given a node \( u \) and a metapath \( p \) in a heterogeneous graph, after sampling the graph and get metapath instance \( P(u) \), we can randomly choose a node sequence \( t \in P(u) \). Metapath based DFS Neighbors \( M^p_{\text{DFS}} \) of node \( u \) is defined as the set of nodes that appears on node sequence \( t \). Note that the node’s DFS neighbors does not include the first two nodes.

Example. Taking Figure 1(d) as an example, given the metapath \( p = \{U-I-I-U\} \), we can randomly choose a node sequence \( \{user1-item1-item2-user2\} \) from metapath instances. According to the definition, we remove the first two nodes and obtain the metapath based DFS neighbors of \( user1 \) is \{item2, user2\}. Compared with BFS neighbors, DFS neighbors focus on the global information.

Definition 3.6 Heterogeneous Graph Embedding. Given a heterogeneous graph \( G = (\mathcal{V}, \epsilon) \), heterogeneous graph embedding is the task to learn the \( d \)-dimensional node representations \( z_u \in \mathbb{R}^d, \forall u \in \mathcal{V} \), which can capture the structural and semantic information of the heterogeneous graph, where \( d \ll |\mathcal{V}| \).

## 4 THE PROPOSED MODEL

In this section, we present a metapath guided Heterogeneous Graph Embedding Method, called MHN.

In order to make full use of node attributes and structure information of HIN, the proposed MHN model consists of three major components as is shown in Figure 2. Firstly, we propose a node embedding representation method combining node attributes. Then, we propose an attention based method to aggregate local and global information of HIN under a single semantic space. Finally, we propose a fusion model to merge the node embeddings under multiple semantics. We will present detailed illustration of the proposed model next.

### 4.1 Node Base Embedding

For large-scale networks, node id represents the node directly, which has a great impact on the node embedding. For example, Deepwalk[5] and Metapath2vec[10] feed node id into network to learn node embedding directly. Therefore, we apply an embedding lookup layer to get embedding from id. We have

\[
h^d_u = W_u \cdot u
\]

where \( W_u \in \mathbb{R}^{1 \times d} \) is the parameter matrix, \( u \) is the id of node, \( h^d_u \) is the latent vector of the node. The role of this layer is to obtain the corresponding vector according to the node id. The parameter matrix \( W_u \) is updated during the training process.

In real world graph, nodes are commonly attributed. Because attributes represent the information of node, so it is important for heterogeneous graph. For example, the information of item contains characteristics such as brand, price, etc, which need to be reflected in node embedding. However, different kinds of node may have unequal feature dimension. Even for different types of nodes with the same feature dimension, their features have different meanings. So we can not simply use a matrix to transform attributes. Therefore, we need to design a method to map different types of node features into the same vector space.

In MHN, we multiple transformation matrices to map different types of node attributes into the same space. For node \( u \in \mathcal{V}_\Lambda \), we have

\[
h^{att}_u = W_A \cdot x_u
\]

where \( W_A \) is the parametric weight matrix for type \( \Lambda \)’s nodes, \( x_u \) is the feature vector of node \( u \), \( h^{att}_u \) is the attribute transformed latent vector of node \( u \).

Considering id and attributes, we can finally obtain the representation of the node by average these two vectors:

\[
h_u = \text{pooling}(h^d_u, h^{att}_u)
\]

After applying these options, we can get the node latent vector containing id and attribute information in the same dimension. Then we will explore how to aggregate under the guidance of metapath.

### 4.2 Aggregation Within Metapath

Given a single metapath \( p_i \in \mathcal{P} \), the aggregation within metapath learns the local and global information through sampling the target node \( u \) by BFS and DFS. Firstly, we sample the heterogeneous graph under the guidance of \( p_i \) and get some paths started from \( u \). Then, we let \( N^p_{\text{BFS}} \) denote the BFS neighbors of \( u \) under the metapath \( p_i \). Through the function \( f_0 \), we can encode the neighbors and obtain the \( h^\text{BFS}_{u,p_i} \).

\[
h^\text{BFS}_{u,p_i} = f_0(h_u, v \in N^p_{\text{BFS}})
\]

where \( f_0 \) is the encoder function. We exam three functions:

- **MEAN encoder** This function takes the mean of all the neighbors, thinking that all neighbors have the same contribution.

\[
h^\text{BFS}_{u,p_i} = \text{MEAN}(h_u, v \in N^p_{\text{BFS}})
\]
• **Weighted encoder** This function assigns different weights to neighboring nodes through β.

\[ h_{u,\beta}^{BFS} = SUM(\beta \cdot [h_v, v \in N_u^\beta]) \]  

(6)

• **Non-linear encoder** The above two functions focus on the linear aggregation, which has limited expressive power in modeling complex relations. So we propose a non-linear function to enhance the representation of the relations through parameter matrix \( W \in \mathbb{R}^{h \times h} \), which is updated during the process of training.

\[ h_{u,\alpha}^{BFS} = \sigma(W \cdot [h_v, v \in N_u^\alpha]) \]  

(7)

Where \( \sigma() \) is non-linear function, i.e., sigmoid or relu.

Similarity, with the DFS neighbors of \( u \) under the metapath \( p_i \), we can encode \( v \in M_u^p \) and obtain \( h_{u,\beta}^{DFS} \).

After encoding the BFS and DFS information into vector representations, we adopt a simple attention mechanism to weight sum two vectors related to target node \( u \). The key idea is that BFS neighbors and DFS neighbors have different impacts on node representation. We can model this by learning a normalized importance weight \([\alpha_1, \alpha_2]\):

\[
\begin{align*}
\alpha_1, \alpha_2 &= \frac{e^{\alpha_1}}{e^{\alpha_1} + e^{\alpha_2}}, \frac{e^{\alpha_2}}{e^{\alpha_1} + e^{\alpha_2}} \\
h_{u,\alpha}^{BFS} &= \alpha_1 \cdot h_{u,\alpha}^{BFS} + \alpha_2 \cdot h_{u,\alpha}^{DFS}
\end{align*}
\]  

(8)

where \( h_u \) is the representation of node \( u \), \( \alpha_1 \) and \( \alpha_2 \) represents the relevance of target node between BFS information and DFS information.

In general, given the heterogeneous graph \( G = (\mathcal{V}, \mathcal{E}) \), node attributes \( x_u, \forall u \in \mathcal{V} \) and a set of metapaths \( \mathcal{P} = \{p_1, \ldots, p|\mathcal{P}|\} \), aggregation within metapath of MHN generates \( M \) metapath guided vectors for target node \( u \), denoted as \( [h_u^{p_1}, \ldots, h_u^{p_M}] \). Each \( h_u^{p_i} \) can be interpreted as the representation of \( p_i \) metapath instance of node \( u \), which reflects the semantic information of node \( u \) under the metapath \( p_i \).

### 4.3 Aggregation Among Metapaths

After aggregating DFS and BFS information to generate the final representation under a single metapath, we need to merge these different semantic information revealed by metapaths into a embedding vector. For \( \forall u \in \mathcal{V} \), we have \( |M| \) latent embeddings \( [h_{u}^{p_1}, \ldots, h_{u}^{p_M}] \), where \( M \) is the number of metapaths and \( M = |\mathcal{P}| \). In order to obtain the final embedding, we assign different weights to different metapaths through the attention mechanism. The operation is reasonable because the optimization object may focus on different semantics.

We apply the attention mechanism to merge embeddings of node \( u \) under different semantics as follows:

\[
\begin{align*}
\epsilon_{p_i} &= q^T \cdot h_u^{p_i} \\
\beta_{p_i} &= \frac{\epsilon_{p_i}}{\sum_{p \in \mathcal{P}} \epsilon_p} \\
h_u &= \sum_{p_i \in \mathcal{P}} \beta_{p_i} \cdot h_u^{p_i}
\end{align*}
\]  

(9)

where \( q \) is the parameterized attention vector which is updated in backpropagation, \( \beta_{p_i} \) be interpreted as the importance of metapath \( p_i \).

Attention mechanism can also be extended to multi-heads self attention, which helps to stabilize the learning process and reduce the high variance. We first form all the embeddings of node \( u \) into matrix \( H_u \) of shape \( [M, d] \), where \( M \) is the number of embeddings and \( d \) is the embedding dimension. Then we calculate self-attention output under each head. Finally, we concatenate the output of each head as the embedding of node. Taking head 1 as an example, the
When using methods based on metapaths for heterogeneous graph reasoning, we need to design an attention mechanism to calculate normalized attention weights for each metapath and generate embedding of node $u$.

The calculation process is as follows:

$$h_u = \text{softmax} \left( \frac{Q_1 \cdot K_1}{\sqrt{d}} \right) \cdot V_1$$

where $Q_1, K_1, V_1 \in \mathbb{R}^{d \times K}$, $K$ is the number of heads, and $\text{softmax} = e^i / \sum_j e^j$, $d$ is the embedding size.

At last, we apply a fully connected layer to enhance the nonlinear fitting ability of the network and the output is the final embedding of node $u$:

$$z_u = \sigma(W \cdot h_u)$$

### 4.4 Metapaths Generation

When using methods based on metapaths for heterogeneous graph embedding, we usually need to handcraft some metapaths which are adopted to sample the graph. However, it is not trivial for human to find useful metapaths in a complex heterogeneous graph with multiple node or edge types. Therefore, we need to design an automatic generation method of metapath that does not rely on human intervention, which can generate the most useful metapaths and sample as many nodes as possible.

MST[25] is proposed to select metapaths by using maximal spanning tree, which is instructive but ignore the applicability of metapaths. We propose a three stage approach to generate reasonable metapaths from heterogeneous graph automatically. In the first stage, we perform random walks on heterogeneous graph under a certain length and obtain lots of metapaths instances. Secondly, through node type mapping and rule constraints, we can get hundreds of metapaths. According to unique demand, we can design scoring function and rank these metapaths to get the top K highest.

Take Alibaba dataset as an example, we generate 4 million node sequences by setting sequence length to 10 and sampling 5 instances for each node. After filtering through rules, all node types must appear in the node sequence, we get almost 400 candidate metapaths. Due to the goal of training more nodes of video type, we design scoring formula in Eq. (12)

$$\text{score}(i) = \frac{\log(i)}{i.\text{count}(u)/i.\text{count}(v)}$$

where $c(i)$ represents the instances sampled by the $i$'th metapath, $i.\text{count}(u)$ and $i.\text{count}(v)$ means the number of user and item in the $i$'th metapath.

### 4.5 Training

After finishing the above components, we generate the embedding of each node, which can be applied in different downstream tasks. According to whether there are labels of data, we mainly divide the training process into two paradigms, supervised learning and unsupervised learning.

For supervised learning with node labels, we minimize the cross entropy loss and update the network parameters through backpropagation and gradient descent. The cross entropy loss of multi-classification for supervised learning is:

$$L = -\frac{1}{|V|} \sum_{u \in V} \sum_{c=1}^{C} y_{uc} \cdot \log p_{uc}$$

where $V$ is the set of training nodes, $C$ is the number of classes, $y_{uc}$ is 1 if the label of $u$ is $c$ else 0, $p_{uc}$ is the probability that $u$’s label belongs to $c$ obtained by model.

For unsupervised learning without node labels, we can optimize the model by minimizing the following nce-loss function through backpropagation and gradient descent.

$$L = -\frac{1}{|V|} \sum_{u \in V} \sum_{c=1}^{C} y_{uc} \cdot \log p_{uc}$$

where $V$ is the set of training nodes, $C$ is the number of classes, $y_{uc}$ is 1 if the label of $u$ is $c$ else 0, $p_{uc}$ is the probability that $u$’s label belongs to $c$ obtained by model.
negative sampling:

\[ L = - \sum_{(u,v) \in S} \log(z_u^T \cdot z_v) - \sum_{(u',v') \in S^-} \log(-z_{u'}^T \cdot z_{v'}) \]  

(14)

where \( \sigma(\cdot) \) is the sigmoid function, \( S \) is the positive node pairs, \( S^- \) is the negative node pairs.

Through above model, we can not only aggregate the DFS and BFS information within a single metapath of the HIN, but also merge the different semantics represented by metapaths into the final embedding. The algorithm is shown in Algorithm 1.

Algorithm 1 MHN forward propagation

Input: The heterogeneous graph \( G = (V, E) \)
  node features \( \{x_u, \forall u \in V\} \),
  node types \( \mathcal{A} = \{A_1, \ldots, A_{|\mathcal{A}|}\} \),
  metapaths set \( \mathcal{P} = \{P_1, \ldots, P_{|\mathcal{P}|}\} \)
Output: The node embeddings \( \{z_u, \forall u \in V\} \)

1: for each node type \( A \in \mathcal{A} \) do
2: for node \( u \in V_A \) do
3: Get node id information \( h_{id}^u \) and attributes transformation \( h_{att}^u = W_A \cdot x_u \)
4: Calculate node representation \( h_u = mean(h_{id}^u + h_{att}^u) \)
5: for metapath \( P \in \mathcal{P}_A \) do
6: Aggregate nodes in \( N_u^P, M_u^P \) to obtain vectors \( h_{u,p}^{DFS}, h_{u,p}^{BFS} \)
7: Calculate the weight \( \alpha_1, \alpha_2 \) for two vectors
8: Obtain \( h_u^P = \alpha_1 \cdot h_{u,p}^{DFS} + \alpha_2 \cdot h_{u,p}^{BFS} \)
9: end for
10: Calculate the weight \( \beta_p \) for each metapath \( P \in \mathcal{P}_A \)
11: Merge the embeddings from all metapaths:
12: \( z_u = \sum_{p \in \mathcal{P}_A} \beta_p \cdot h_u^P \)
13: end for
14: \( z_u = \sigma(W_0 \cdot h_u), \forall u \in V \)
15: return \( z_u \)

5 EXPERIMENTS

In this section, we present several experiments to demonstrate the effectiveness of the model we proposed in this paper. We verify the model on both offline and online datasets.

5.1 Datasets

In order to evaluate the performance of MHN as compared to state-of-the-art baselines, we adopt two widely used heterogeneous graph datasets and collect a real-world dataset from Alibaba mobile application from Android and iOS online. Specifically, the DBLP dataset is used in the experiments for node classification and visualization. Amazon and Alibaba datasets are used in the experiment for link prediction. The details of these datasets are shown in Table 1.

- **DBLP** is a computer science bibliography website, which we adopt a subset of DBLP extracted by [23]. The heterogeneous graph contains 4057 author nodes, 14328 paper nodes, 20 conference nodes, 19645 pa(paper to author) links and 14328 pc(paper to conference) links. These nodes are divided into four classes(Database, Data Mining, Artificial Intelligence and Information Retrieval). Paper’s feature is made by its terms. Author’s and publication’s feature is described by a bag-of-words representation of their papers’ terms. For supervised learning tasks, we divide author nodes into training, validation, test sets of 3245(80.00%), 406(10.01%), 406(10.01%).
- **Amazon** includes product metadata and links between products. We adopt a subset of Amazon extracted by [24], in which we only use the product metadata of Electronics category. We build a heterogeneous graph including the co-viewing and co-purchasing links between products, and the product attributes include the price, sales-rank, brand and category with one-hot processing. For unsupervised learning tasks, we divide the dataset into training, validation, test sets of 3475(74.46%), 398(8.53%), 794(17.01%).
- **Alibaba** consists of four types of links including user-click-item, user-click-video, similarity relation between items, parallelism relation between item and video with three node types user, item, video, which is sampled from the log of Alibaba mobile application. We build a heterogeneous graph by sampling several active users and their behaviors with items and videos. Under the guidance of section 4.4, we generate three metapaths, who’s sampled nodes can cover 96% all nodes. For unsupervised learning tasks, we divide the dataset into training, validation, test sets of 5800(80.00%), 725(10.00%), 725(10.00%).

### Table 1: Datasets Statics

| Dataset      | Node   | Edge   | Metaphath |
|--------------|--------|--------|-----------|
| DBLP         | author(A):4057 | P-A:19645 | APA       |
|              | paper(P):14328 | P-C:14328 | APCPA     |
|              | conference(C):20 |            |           |
| Amazon       | Product(P):3475 | P→P:2683 | P→P:791   |
|              | viewing | P→P:2683 | P→P:791   |
|              | purchasing | P→P:791 | P→P:791   |
|              | P−→P   | P−→P   | P−→P     |
|              | UIU    | UIVIU   | UVU       |
|              | IUI    | IUIVUI  | IVI       |
| Alibaba      | user(U):2785 | U-I:2935 | IUI       |
|              | item(I):2780 | I-V:1380 | IUIVUI    |
|              | video(V):2716 | U-V:2935 | IVI       |
|              |         |         | IIIUVUVUI |
|              |         |         | IVIUIVIUI  |
|              |         |         | IIIUVUVUI  |

5.2 Comparing Methods

We categorize different graph embedding methods into four groups and compare MHN against these methods. The overall embedding size is set to 200.

**Homogeneous Graph Embedding Methods.** The compared methods include Deepwalk[5], LINE[15] and node2vec[6]. As these methods can only deal with Homogeneous graph, so we ignore the heterogeneity of graph and treat datasets as homogeneous.
We conduct experiment on the DBLP dataset to compare the per-
with learning rate set to 0.01. These models are trained for 100
Micro-F1
of different methods in Table 2.
Macro-F1
methods have not trained. We compare the average
from the test set, which both supervised learning and unsupervised
Logistic Regression (LR) classifier with varying training proportions.
node embeddings generated by different learning models into the
dimension to 100.
mechanism, we set the number of attention head to 8 and attention
epochs and early stopping is set to 5. For models with attention
including GCN, GAT, HAN, GATNE, we apply Adam optimization
per node to 20, and number of negative samples to 5. For GNNs,
Metapath2vec, we set the window size to 5, walk length to 10, walks
edges using attention mechanism. We test several GATNE
GATNE
focuses on the combination of different types
from different emtapath.
HAN
uses attention mechanism to combine embeddings
from different metapath-guided graph into one vector, cap-
turing information from different entmapath.
GATNE
focuses on the combination of different types of
dges using attention mechanism. We test several GATNE
variants and choose the best model.

For skip-gram based models, like Deepwalk, LINE, Node2vec,
Metapath2vec, we set the window size to 5, walk length to 10, walks
per node to 20, and number of negative samples to 5. For GNNs,
including GCN, GAT, HAN, GATNE, we apply Adam optimization
with learning rate set to 0.01. These models are trained for 100
epochs and early stopping is set to 5. For models with attention
mechanism, we set the number of attention head to 8 and attention
dimension to 100.

5.3 Node Classification
We conduct experiment on the DBLP dataset to compare the per-
formance of different methods on node classification task. We send
node embeddings generated by different learning models into the
Logistic Regression (LR) classifier with varying training proportions.
In order to ensure fairness, all the data used for comparison comes
from the test set, which both supervised learning and unsupervised
methods have not trained. We compare the average Macro-F1 and
Micro-F1 of different methods in Table 2.

As shown in Table 2, under different training proportions of
DBLP dataset, MHN can achieve the best results over other learning
methods. It is worth noting that, whether it is supervised or unsupervised
learning, the method based on random walk performs better than the these based on GNN. This is because the
DBLP dataset pays more attention to the connections between
nodes, rather than the nodes themselves. Our method not only fully
considers the global information, but also premeditates the local
information, which ensures that the node embedding contains rich
semantic information. The performance gain obtained by MHN
over the best baseline (HAN) is about 0.42%-0.93% absolutely.

5.4 Link Prediction
Link prediction task is widely used to evaluate the quality of graph
embeddings in both academia and industry. We also conduct experi-
ments on the Amazon and Alibaba datasets. We hide a set of edges
as the test set and train on the remaining graph. For unsupervised
learning models, we treat the connected links as positive node pairs
and unconnected links as negative node pairs by minimizing the
objective function described in Equation 14. Given the embedding
z_u and z_v, we calculate the probability that u and v are linked as
following:

\[ p_{u,v} = \sigma(z_u \cdot z_v) \]  

We use some commonly used metrics like the ROC curve (ROC-
AUC), the PR curve (PR-AUC), the average precision (AP) and the F1
score.

From Table 3, we can see that MHN performs better than other comparison algorithms. The strongest traditional method here is
Metapath2vec, which learns embedding from node sequences gen-
erated by random walk guided by one metapath. MHN achieves
better scores than Metapath2vec, proving the importance of multi-
ple semantics of heterogeneous graph. Based on the idea of multi-
semantics fusion, MHN considers the influence of BFS and DSF
neighbors of the target node, which helps achieve a relative im-
provement of around 8% on Alibaba dataset over HAN. This result
supports our claim that local and global information are critical to
the node embeddings.

5.5 Parameter Sensitivity
We investigate the sensitivity of hyper-parameter in MHN, mainly
the effect of embedding dimension. Figure 3 illustrates the per-
formance of different methods when the embedding dimension
changes. We can see that as the embedding dimension increases,
the performance of models also increases, but the it drops when
embedding dimension is either too small or too large. It can be
conclude that the performance of MHN is relatively stable within
the range of embedding dimensions. Since the heterogeneous in-
formation cannot be identified, Deepwalk and GCN performs the
worst.

5.6 Visualization
In addition to quantitative analysis of node embedding, we also
adopt visualization method to qualitatively assess node embedding
results. We randomly select four categories from DBLP dataset with
25 items under each category, and then project the embeddings of
these nodes into a 2-dimensional space using t-SNE. We illustrate
Table 2: Performance comparison (%) on DBLP dataset for node classification task

| Dataset | Metrics | Train (%) | Unsupervised | Supervised |
|---------|---------|-----------|---------------|-------------|
|         |         |           | Deepwalk | Node2vec | LINE | Metapath2vec | GCN | GAT | HAN | MHN |
| DBLP    | Micro-F1 | 20        | 84.35    | 89.71    | 88.61 | 89.49 | 89.76 | 90.31 | 91.23 | **92.16** |
|         |          | 40        | 86.35    | 89.85    | 89.12 | 90.31 | 90.43 | 90.91 | 91.75 | **92.48** |
|         |          | 60        | 86.49    | 90.13    | 89.68 | 90.53 | 90.82 | 91.05 | 92.01 | **92.94** |
|         |          | 80        | 86.86    | 90.88    | 89.75 | 91.01 | 90.83 | 91.18 | 92.37 | **93.29** |
|         | Macro-F1 | 20        | 82.49    | 89.27    | 88.36 | 88.97 | 89.61 | 89.68 | 90.75 | **91.37** |
|         |          | 40        | 82.59    | 89.96    | 88.52 | 90.03 | 89.74 | 90.74 | 90.96 | **91.65** |
|         |          | 60        | 82.97    | 90.06    | 89.23 | 90.17 | 90.19 | 89.75 | 91.37 | **92.02** |
|         |          | 80        | 85.27    | 90.25    | 89.42 | 90.62 | 90.56 | 90.69 | 91.89 | **92.31** |

Table 3: Experiment results (%) on Amazon and Alibaba datasets for link prediction task

|         | Amazon | Alibaba |
|---------|---------|---------|
|         | ROC-AUC | PR-AUC | F1 | AP | ROC-AUC | PR-AUC | F1 | AP |
| Deepwalk | 89.01   | 87.35  | 64.76 | 59.28 | 73.69 | 71.11 | 66.46 | 73.14 |
| Node2vec | 88.96   | 87.29  | 66.12 | 57.83 | 73.83 | 72.95 | 67.01 | 71.29 |
| LINE     | 88.83   | 86.49  | 62.28 | 62.75 | 67.18 | 72.93 | 61.98 | 70.56 |
| Metapath2vec | 90.56   | 88.69  | 71.95 | 70.65 | 77.92 | 73.54 | 70.94 | 75.17 |
| GCN      | 87.09   | 86.11  | 67.74 | 66.35 | 76.38 | 72.56 | 67.12 | 73.14 |
| GAT      | 88.73   | 88.64  | 69.91 | 67.33 | 76.84 | 72.26 | 67.54 | 73.87 |
| HAN      | 89.32   | 88.66  | 70.51 | 70.12 | 73.14 | 73.03 | 68.04 | 74.01 |
| GATNE    | 89.27   | 88.04  | 69.79 | 70.06 | 74.11 | 72.89 | 68.23 | 73.91 |
| MNH      | **92.02** | **89.81** | **73.15** | **71.46** | 79.37 | 74.92 | 71.85 | 75.38 |

Figure 3: The performance of different methods on Amazon dataset when changing embedding dimensions.

The visualization results of Deepwalk, Metapath2vec, HAN and MHN in Figure 4, where red and blue points indicate different category respectively.

Through visualization, we can intuitively tell the differences among learning ability of graph embedding methods for heterogeneous graph. As a traditional homogeneous graph representation learning method, Deepwalk cannot effectively divide these nodes into four groups. On the contrary, the heterogeneous model Metapath2vec can roughly distinguish these nodes. Because HAN fuse multiple semantics into node embedding, it achieves better performance. MHN method proposed in paper obtains the best embedding results, in which only a few nodes have errors and most of them are completely separated.

5.7 Online A/B Test

We deploy our inductive model MHN on Alibaba mobile application for it’s recall process of recommendation system. The training dataset has about half a million users and videos, a million items, with 3 million interactions among these nodes. We adopt MHN to generate embedding of each node under several metapaths. For each item, we apply K nearest neighbor (KNN) with Euclidean distance to obtain the top-50 videos that are most similar to the current item. Taking top-50 hit-rate as a goal, we compared the original method based on item-CF, Metapath2vec and MHN. The results demonstrate that MHN improves hit-rate by 2.93% and 6.71% compared to Metapath2vec and item-CF methods, respectively.

6 CONCLUSION

In this paper, we propose a metapaths-guided neighbors-aggregated Heterogeneous Graph Neural Network (MHN) method for heterogeneous graph node embedding learning, which can address three limitations mentioned above. MHN applies node base embedding to transform node attributes and enrich node representation. In addition, aggregation within metapath can merge BFS and DFS neighbors to obtain local and global information of the target node,
Figure 4: Embedding visualization of nodes in DBLP.

respectively. Finally, MHN adopts attention based algorithm in aggregation among metapaths to capture information in different semantics. Especially, we put forward several encode functions for neighbors aggregation and self-attention mechanism for vectors aggregation. In experiments, MHN achieves best results on three real-world datasets in node classification and link prediction task. Parameter sensitivity analysis illustrates the effect of embedding dimension. Visualization analysis shows the quality of node representation obtained by different methods directly. Online test in Alibaba mobile application proves the feasibility and effectiveness of MHN.

For the future work, we will consider about the dynamic heterogeneous graph node representation learning methods to adapt the changes in graph.

REFERENCES

[1] Jagadish S, Parikh J. Discovery of friends using social network graph properties: U.S. Patent 8,744,876[P]. 2014-6-3.
[2] Kipf T N, Welling M. Variational graph auto-encoders[J]. arXiv preprint arXiv:1611.07308, 2016.
[3] Nickel M, Murphy K, Tresp V, et al. A review of relational machine learning for knowledge graphs[J]. Proceedings of the IEEE, 2015, 104(1): 11-33.
[4] Ying R, He R, Chen K, et al. Graph convolutional neural networks for web-scale recommender systems[C]/Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. 2018: 974-983.
[5] Perozzi B, Al-Rfou R, Skiena S. Deepwalk: Online learning of social representations[C]/Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining. 2014: 701-710.
[6] Grover A, Leskovec J. node2vec: Scalable feature learning for networks[C]/Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining. 2016: 855-864.
[7] Kipf T N, Welling M. Semi-supervised classification with graph convolutional networks[J]. arXiv preprint arXiv:1609.02907, 2016.
[8] Veličković P, Cucurull G, Casanova A, et al. Graph attention networks[J]. arXiv preprint arXiv:1710.10903, 2017.
[9] Hamilton W, Ying Z, Leskovec J. Inductive representation learning on large graphs[C]/Advances in neural information processing systems. 2017: 1024-1034.
[10] Dong Y, Chawla N V, Swami A. metapath2vec: Scalable representation learning for heterogeneous networks[C]/Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining. 2017: 135-144.
[11] Shi C, Hu B, Zhao W X, et al. Heterogeneous information network embedding for recommendation[J]. IEEE Transactions on Knowledge and Data Engineering, 2018, 31(2): 357-370.
[12] Wang X, Ji H, Shi C, et al. Heterogeneous graph attention network[C]/The World Wide Web Conference. 2019: 2022-2032.
[13] Cen Y, Zou X, Zhang J, et al. Representation learning for attributed multiplex heterogeneous network[C]/Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. 2019: 1358-1368.
[14] Wang J, Huang P, Zhao H, et al. Billion-scale commodity embedding for e-commerce recommendation in alibaba[C]/Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. 2018: 839-848.
[15] Tang J, Qu M, Wang M, et al. Line: Large-scale information network embedding[C]/Proceedings of the 24th international conference on world wide web. 2015: 1067-1077.
[16] Wang D, Cui P, Zhu W. Structural deep network embedding[C]/Proceedings of the 22nd ACM SIGKDD international conference on Knowledge Discovery and data mining. 2016: 1225-1234.
[17] Fu T, Lee W C, Lei Z. Hin2vec: Explore meta-paths in heterogeneous information networks for representation learning[C]/Proceedings of the 2017 ACM on Conference on Information and Knowledge Management. 2017: 1797-1806.
[18] Zhang C, Song D, Huang C, et al. Heterogeneous graph neural network[C]/Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. 2019: 793-803.
[19] Liu B, Pop M. MetaPath: identifying differentially abundant metabolic pathways in metagenomic datasets[C]/BMIC proceedings. BioMed Central, 2011, 5(2): 1-12.
[20] Du Y, Guo W, Liu J, et al. Classification by multi-semantic meta path and active weight learning in heterogeneous information networks[J]. Expert Systems with Applications, 2019, 123: 227-236.
[21] Fu X, Zhang J, Meng Z, et al. MAGNN: Metapath Aggregated Graph Neural Network for Heterogeneous Graph Embedding[C]/Proceedings of The Web Conference 2020. 2020: 2331-2341.
[22] Cai H, Zheng Y W, Chang K C C. A comprehensive survey of graph embedding: Problems, techniques, and applications[J]. IEEE Transactions on Knowledge and Data Engineering, 2018, 30(9): 1616-1637.
[23] Gao J, Jiang F, Fan W, et al. Graph-based consensus maximization among multiple supervised and unsupervised models[C]/Advances in Neural Information Processing Systems. 2009: 585-593.
[24] Qi L, Zhang X, Dou W, et al. A distributed locality-sensitive hashing-based approach for cloud service recommendation from multi-source data[J]. IEEE Journal on Selected Areas in Communications, 2017, 35(11): 2616-2624.
[25] Wang C, Song Y, Li H, et al. Unsupervised meta-path selection for text similarity measure based on heterogeneous information networks[J]. Data Mining and Knowledge Discovery, 2018, 32(6): 1735-1767.