Heterogeneous Network Representation Learning: Survey, Benchmark, Evaluation, and Beyond

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ABSTRACT

Since real-world objects and their interactions are often multi-modal and multi-typed, heterogeneous networks have been widely used as a more powerful, realistic, and generic superclass of traditional homogeneous networks (graphs). Meanwhile, representation learning (a.k.a. embedding) has recently been intensively studied and shown effective for various network mining and analytical tasks. Since there has already been a broad body of heterogeneous network embedding (HNE) algorithms but no dedicated survey, as the first contribution of this work, we pioneer in providing a unified paradigm for the systematic categorization and analysis over the merits of various existing HNE algorithms. Moreover, existing HNE algorithms, though mostly claimed generic, are often evaluated on different datasets. Understandable due to the natural application favor of HNE, such indirect comparisons largely hinder the proper attribution of improved task performance towards effective data preprocessing and novel technical design, especially considering the various ways possible to construct a heterogeneous network from real-world application data. Therefore, as the second contribution, we create four benchmark datasets with various properties regarding scale, structure, attribute/label availability, and etc, from different sources, towards the comprehensive evaluation of HNE algorithms. As the third contribution, we carefully refactor and amend the implementations of and create friendly interfaces for ten popular HNE algorithms, and provide all-around comparisons among them over multiple tasks and experimental settings.

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By putting all existing HNE algorithms under a general and complete paradigm, we aim to provide a universal reference and guideline for the understanding and development of HNE algorithms. Meanwhile, by open-sourcing all data and code, we envision to serve the community with an easy-to-use benchmark platform to test and compare the performance of existing and future HNE algorithms.

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1. INTRODUCTION

Networks and graphs constitute a canonical and ubiquitous paradigm for the modeling of interactive objects, which has drawn significant research attention from various scientific domains [59, 30, 24, 3, 89, 87]. However, real-world objects and interactions are often multi-modal and multi-typed (e.g., authors, papers, venues and terms in a publication network [69, 63]; users, places, categories and GPS-coordinates in a location-based social network [101, 91, 94]; and genes, proteins, diseases and species in a biomedical network [38, 14]). To capture and exploit such node and link heterogeneity, heterogeneous networks have been proposed and widely used in many real-world network mining scenarios, such as meta-path based similarity search [70, 64, 92], node classification and clustering [18, 20, 11], knowledge base completion [68, 45, 103], and recommendations [23, 106, 31]. In the meantime, current research on graphs has largely focused on representation learning (embedding), especially following the pioneer of neural network based algorithms that demonstrate revealing empirical evidence towards unprecedentedly effective yet efficient graph mining [25, 1, 13]. They aim to convert graph data (e.g., nodes [49, 72, 26, 77]
Labeled attributed net. Particularly, based on a uniform taxonomy the understanding of the critical merits of each mathematical paradigm that generalizes all HNE algorithms, makes it hard to clearly attribute performance gains between supervised inductive learning algorithms, which may introduce various properties regarding scale, structure, attribute/label availability, etc. This diverse set of data, together with a series of different network mining tasks and evaluation metrics, constitute a systematic and comprehensive benchmark resource for future HNE algorithms.

As the second contribution, we deliberately prepare four benchmark heterogeneous network datasets through exhaustive data collection, cleaning, analysis and curation (Section 4). The datasets we come up with cover a wide spectrum of application domains (i.e., publication, recommendation, knowledge base, and biomedicine), which have various properties regarding scale, structure, attribute/label availability, etc. This diverse set of data, together with a series of different network mining tasks and evaluation metrics, constitute a systematic and comprehensive benchmark resource for future HNE algorithms.

As the third contribution, many existing HNE algorithms (including some very popular ones) either do not have a flexible implementation (e.g., hard-coded node and edge types, fixed set of meta-paths, etc.), or do not scale to larger networks (e.g., high memory requirement during training), which adds much burden to novel research (i.e., requiring much engineering effort in correct reimplementation). To this end, we select 10 popular HNE algorithms, where we carefully refactor and scale up the original authors’ hustled implementations and apply additional interfaces for plug-in input of our prepared datasets (Section 5). Based on these easy-to-use and efficient implementations, we then conduct all-around empirical evaluations of the algorithms, and report their benchmark performances. The empirical results, while providing much insight into the merits of different models that are consistent with the conceptual analysis in Section 3, also serve as the example utilization of our benchmark platform that can be followed by future studies on HNE.

Note that, although there have been several attempts to survey or benchmark heterogeneous network models (including some very popular ones) either do not have a flexible implementation (e.g., hard-coded node and edge types, fixed set of meta-paths, etc.) or do not scale to larger networks (e.g., high memory requirement during training), which makes them only available to the semi-supervised inductive learning algorithms, which may introduce even more bias. Eventually, it is often hard to clearly attribute performance gains between technical novelty and data tweaking.

In this work, we first formulate a unified yet flexible mathematical paradigm that generalizes all HNE algorithms, easing the understanding of the critical merits of each model (Section 2). Particularly, based on a uniform taxonomy that clearly categorizes and summarizes the existing models (and likely future models), we propose a generic objective function of network smoothness, and reformulate all existing models into this uniform paradigm while highlighting their individual novel contributions (Section 3). We envision this paradigm to be helpful in guiding the development of future novel HNE algorithms, and in the meantime facilitate their conceptual contrast towards existing ones.

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2. GENERIC PARADIGM

2.1 Problem Definitions

We first give formal definitions of concepts closely related to HNE, starting from network embedding.

**Definition 2.1. Network embedding.** For a given network $G = (V, E)$, where $V$ is the set of nodes (vertices) and $E$ is the set of links (edges), a network embedding is a mapping function $\Phi : V \rightarrow \mathbb{R}^{d}$, where $d \ll |V|$. This mapping $\Phi$ defines the latent representation (a.k.a. embedding) of each node $v \in V$, which captures network topological information in $E$.

In most cases, network proximity is the major topological information to be captured. For example, DeepWalk [49] captures the random-walk based node proximity and illustrates the 2-dim node representations learned on the famous Zachary’s Karate network of small groups, where a clear correspondence between the node position in the input graph and learned embedding space can be observed. Various follow-up works have improved or extended DeepWalk, while a complete coverage of them is beyond the scope of this work. In this work, we focus on the embedding of heterogeneous networks.

**Definition 2.2. Heterogeneous network.** A heterogeneous network $H = \{V, E, \phi, \psi\}$ is a network with multiple types of nodes and links. Particularly, within $H$, each node $v_i \in V$ is associated with a node type $\phi(v_i)$, and each link $e_{ij} \in E$ is associated with a link type $\psi(e_{ij})$. It is worth noting that the type of a link $e_{ij}$ automatically defines the types of nodes $v_i$ and $v_j$ on its two ends.

Heterogeneous networks have been intensively studied due to its power of accommodating multi-modal multi-typed interconnected data. Besides the classic example of DBLP data used in most existing works as well as Figure 1 consider a different yet illustrative example from NYT in Figure 2. Nodes in this heterogeneous network include news articles, categories, phrases, locations, and datetimes. To illustrate the power of heterogeneous networks, we introduce the concept of meta-path, which has been leveraged by most existing works on heterogeneous network modeling [69, 65].

**Definition 2.3. Meta-path.** A meta-path is a path defined on the network schema denoted in the form of $o_1 \xrightarrow{l_1} o_2 \xrightarrow{l_2} \cdots \xrightarrow{l_m} o_{m+1}$, where $o$ and $l$ are node types and link types, respectively.

Each meta-path captures the proximity among the nodes on its two ends from a particular semantic perspective. Continue with our example of heterogeneous network from news data in Figure 2. The meta-path of article $\xrightarrow{\text{category}}$ article carries different semantics from article $\xrightarrow{\text{mention}}$ location $\xrightarrow{\text{mentioned by}}$ article. Thus, the leverage of different meta-paths allows heterogeneous network models to compute the multi-modal multi-typed node proximity and relation, which has been shown beneficial to many real-world network mining applications [64, 36, 31].

Now we define the main problem of focus in this work, heterogeneous network embedding (HNE), which lies in the intersection between Def 2.1 and Def 2.2.

Figure 2: Toy example of a heterogeneous network constructed from the news data.

**Definition 2.4. Heterogeneous network embedding.** For a given heterogeneous network $H$, a heterogeneous network embedding is a set of mapping functions $\{\Phi_k : V_k \rightarrow \mathbb{R}^{d} \}_{k=1}^{K}$, where $K$ is the number of node types, $\forall v_i \in V_k$, $\phi(v_i) = k$, $d \ll |V|$. Each mapping $\Phi_k$ defines the latent representation (a.k.a. embedding) of all nodes of type $k$, which captures the network topological information regarding the heterogeneous links in $E$.

Compared with homogeneous networks, the definition of topological information in heterogeneous networks is even more diverse. As we will show in Section 3, the major distinctions among different HNE algorithms mostly lie in their different ways of capturing such topological information. Particularly, the leverage of meta-paths as in Def 2.3 often plays an essential role, since many popular HNE algorithms exactly aim to model the different proximity indicated by meta-paths [16, 22, 33, 7, 99, 82, 104, 63].

2.2 Proposed Paradigm

In this work, we stress that one of the most important principles underlying HNE (as well as most other scenarios of network modeling and mining) is homophily [43]. Particularly, in the network embedding setting, homophily can be translated as ‘nodes close on a network should have similar embeddings’, which matches the requirement of Def 2.1. In fact, we further find intrinsic connections between the well-perceived homophily principle and widely-used smoothness enforcement technique on networks, which leads to a generic mathematical paradigm covering most existing and likely many future HNE algorithms.

Based on earlier well-established concepts underlying network modeling and embedding learning [73, 56, 2, 110, 111], we introduce the following key objective function of network smoothness enforcement as follows

$$J = \sum_{u, v \in V} w_{uv} d(e_u, e_v) + J_R,$$

where $e_u = \Phi(u)$ and $e_v = \Phi(v)$ are the node embedding vectors to be learned. $w_{uv}$ is the proximity weight, $d(\cdot, \cdot)$ is the embedding distance function, and $J_R$ denotes possible additional objectives such as regularizers, all three of which can be defined and implemented differently by the particular HNE algorithms.
3. ALGORITHM TAXONOMY

In this section, we find a universal taxonomy for existing HNE algorithms with three categories based on their common objectives, and elaborate in detail how they all fit into our paradigm of Eq. (1). The main challenge of instantiating Eq. (1) on heterogeneous networks is the consideration of complex interactions regarding multi-typed links and higher-order meta-paths. In fact, our Eq. (1) also readily generalizes to homogeneous networks, though that is beyond the scope of this work.

3.1 Proximity-Preserving Methods

As mentioned above, one basic goal of network embedding is to capture network topological information. This can be achieved by preserving different types of proximity among nodes. There are two major categories of proximity-preserving methods in HNE: random walk-based approaches (inspired by DeepWalk [49]) and first/second-order proximity-based ones (inspired by LINE [72]).

3.1.1 Random Walk-Based

metapath2vec [16]. Following homogeneous network embedding [49,29], metapath2vec utilizes the node paths traversed by meta-path guided random walks to model the context of a node regarding heterogeneous semantics. Formally, given a meta-path \( M = a_1 \xrightarrow{l_1} a_2 \xrightarrow{l_2} \cdots \xrightarrow{l_{m-1}} a_m \), the transition probability at step \( i \) is defined as

\[
p(u_{i+1}|v_i, M) = \begin{cases} 
\frac{1}{|N_i(v_i)|} & \phi(v_{i+1}) = a_{i+1}, \\
0 & \text{otherwise}
\end{cases}
\]

where \( N_i(v) = \{u|\psi(u,v) = i\} \) denotes the neighbors of \( v \) associated with edge type \( l_i \). Assume \( \mathcal{P} = \{\mathcal{P}_1, \ldots, \mathcal{P}_M\} \) is the set of generated random walk sequences. The objective of metapath2vec is

\[
\mathcal{J} = \sum_{u,v \in \mathcal{V}} \sum_{u \in \mathcal{C}(v)} \log \frac{\exp(e_u^T e_v)}{\sum_{u' \in \mathcal{V}} \exp(e_{u'}^T e_v)},
\]

(3)

where \( \mathcal{C}(v) \) is the contexts (i.e., skip-grams) of \( v \) in \( \mathcal{P} \). For example, if \( \mathcal{P}_1 = v_1 v_2 v_3 v_4 v_7 v_8 \ldots \) and the context window size is 2, then \( \{v_1, v_2, v_3, v_4\} \subseteq \mathcal{C}(v_2) \). Let \( w_{uv} \) be the number of times that \( u \in \mathcal{C}(v) \) is in \( \mathcal{P} \). Eq. (3) can be rewritten as

\[
\mathcal{J} = \sum_{u,v \in \mathcal{V}} w_{uv} \log \frac{\exp(e_u^T e_v)}{\sum_{u' \in \mathcal{V}} \exp(e_{u'}^T e_v)}.
\]

The denominator in this objective requires summing over all nodes and is computationally expensive. In actual computation, it is approximated using negative sampling [44]. In this paper, we still analyze the original objective.

HIN2Vec [22]. HIN2Vec considers the probability that there is a meta-path \( M \) between nodes \( u \) and \( v \). Specifically,

\[
p(\mathcal{M}|u,v) = \sigma \left( 1^T \left( W_{\mathcal{X}}^T u \odot W_{\mathcal{Y}}^T v \odot f_{01}(W_R^T m) \right) \right),
\]

where \( 1 \) is an all-ones vector; \( \odot \) is the Hadamard product; \( f_{01} \) is a normalization function. Here \( e_u = W_{\mathcal{X}}^T u \), \( e_v = W_{\mathcal{Y}}^T v \) and \( e_M = f_{01}(W_R^T m) \) can be viewed as the embeddings of \( u \), \( v \) and \( M \), respectively. Let \( A_M = \text{diag}(e_{M1}, \ldots, e_{M3}) \). We have

\[
p(\mathcal{M}|u,v) = \sigma \left( 1^T (e_u \odot e_v \odot e_M) \right) = \sigma(e_u^T A_M e_v).
\]

\( \sigma \) is the sigmoid function, so we have

\[
1 - p(\mathcal{M}|u,v) = 1 - \sigma(e_u^T A_M e_v) = \sigma(-e_u^T A_M e_v).
\]

HIN2Vec generates positive tuples \((u, v, M)\) (i.e., \( u \) connects with \( v \) via meta-path \( M \)) using homogeneous random walks [49] regardless of node/link types. For each positive tuple \((u, v, M)\), it generates several negative tuples by replacing \( u \) with a random node \( u' \). Its objective is

\[
J_0 = \sum_{(u,v,M)} \log p(\mathcal{M}|u,v) + \sum_{(u',v,M)} \log(1 - p(\mathcal{M}|u,v))
= \sum_{(u,v,M)} \left( \log \sigma(e_u^T A_M e_v) + \sum_{u'} \log \sigma(-e_u^T A_M e_v) \right).
\]

This is actually the negative sampling approximation of the following objective

\[
\mathcal{J} = \sum_{u,v \in \mathcal{V}} w_{uv} \log \frac{\exp(e_u^T A_M e_v)}{\sum_{u' \in \mathcal{V}} \exp(e_{u'}^T A_M e_v)},
\]

where \( w_{uv} \) is the number of path instances between \( u \) and \( v \) following meta-path \( M \).

SHNE [99]. SHNE improves metapath2vec by incorporating additional node information. It assumes that some types of nodes may have additional text information (denoted as \( x_v \)). It proposes a deep encoder \( f_{\text{ENC}} \) based on GRU [12]. Namely, if \( v \) has text information, \( e_v = f_{\text{ENC}}(x_v) \); otherwise, \( e_v \) represents typical learnable node embeddings. The objective of SHNE is the same as that of metapath2vec, and it is straightforward to extend it to incorporate other types of node information like categorical attributes, images, etc. by leveraging domain-specific deep encoders, which is also considered in HINE [8].

Other random walk-based approaches are summarized in Table I. To be specific, MRWNN [85] incorporates content priors into DeepWalk embedding; HINE [83] extends metapath2vec to the hyperbolic space; GHE [11] proposes a semi-supervised meta-path weighting technique; MNE [100] conducts random walks separately for each view in a multi-view network; JUST [85] proposes Jump/Stay random walks that do not rely on pre-defined meta-paths.

3.1.2 First/Second-Order Proximity-Based

PTE [71]. PTE proposes to decompose a heterogeneous network into multiple bipartite networks, each of which describes one edge type. Its objective is the sum of log-likelihoods over all bipartite networks:

\[
\mathcal{J} = \sum_{l \in \mathcal{T}_E} \sum_{u,v \in \mathcal{V}} w_{uv}^l \log \frac{\exp(e_u^T e_v)}{\sum_{u' \in \mathcal{V}_l(u)} \exp(e_{u'}^T e_v)}
\]

Here \( \mathcal{T}_E \) is the set of edge types; \( w_{uv}^l \) is the type-\( l \) edge weight of \((u,v)\) (if there is no edge between \( u \) and \( v \) with type \( l \), then \( w_{uv}^l = 0 \)); \( w_{uv} = \sum_l w_{uv}^l \) is the total edge weight between \( u \) and \( v \).

AspEm [66]. AspEm assumes that each heterogeneous network has multiple aspects, and each aspect is defined as a subgraph of the network schema [70]. An incompatibility
measure is proposed to select appropriate aspects for embedding learning. Given an aspect \(a\), its objective is

\[
\mathcal{J} = \sum_{l \in \mathcal{T}_E} \sum_{u,v \in V} w_{uv}^l \log \frac{\exp(e_{uv}^T a_{uv})}{\sum_{u',v' \in V_{\mathcal{G}(u)}} \exp(e_{u',v'}^T a_{u',v'})},
\]

where \(\mathcal{T}_E^l\) is the set of edge types in aspect \(a\); \(Z_l = \sum_{u,v} w_{uv}^l\) is a normalization factor; \(a_{uv}\) is the aspect-specific embedding of \(u\) and \(v\).

**HEER** \([67]\). HEER extends PTE by considering *typed closeness*. Specifically, each edge type \(l\) has an embedding \(\mu_l\), and its objective is

\[
\mathcal{J} = \sum_{l \in \mathcal{T}_E} \sum_{u,v \in V} w_{uv}^l \log \frac{\exp(\mu_l^T g_{uv})}{\sum_{(u',v') \in \mathcal{P}_{l}(u,v)} \exp(\mu_l^T g_{u',v'})},
\]

where \(g_{uv}\) is the edge embedding of \((u, v)\); \(\mathcal{P}_l(u,v) = \{(u',v')| \psi(u',v') = l\} \cup \{(u,v)| \psi(u,v) = l\}\). In \([67]\), \(g_{uv}\) has different definitions for directed and undirected edges based on the Hadamard product. To simplify our discussion, we assume \(g_{uv} = e_u \otimes e_v\). Let \(A_l = \text{dia}(\mu_{l1}, \ldots, \mu_{ld})\). We have \(\mu_l^T g_{uv} = e_u^T A_l e_v\), and

\[
\mathcal{J} = \sum_{l \in \mathcal{T}_E} \sum_{u,v \in V} w_{uv}^l \log \frac{\exp(e_u^T A_l e_v)}{\sum_{(u',v') \in \mathcal{P}_{l}(u,v)} \exp(e_{u'}^T A_l e_{v'})}.
\]

Other first/second-order proximity-based approaches are summarized in Table 1. To be specific, Chang et al. \([8]\) introduce a node type-aware content encoder: CMF \([108]\) performs joint matrix factorization over the decomposed bipartite networks; HEBE \([27]\) preserves proximity regarding each meta-graph; Phine \([31]\) combines additional regularization towards semi-supervised training; MVE \([53]\) proposes an attention-based framework to consider multiple views of the same nodes.

There are also studies adopting other forms of objectives to characterize first/second-order proximities. For example, SHINE \([78]\) uses reconstruction loss of autoencoders inspired by SDNE \([76]\); DRL \([52]\) proposes to learn one type of edges at each step and uses deep reinforcement learning approaches to select the edge type for the next step; HINSE \([90]\) adopts spectral embedding based on adjacency matrices with different meta-graphs; HeGAN \([32]\) proposes an adversarial framework with a relation type-aware discriminator.

Based on the above discussions, the objective of most proximity-preserving methods can be unified as

\[
\max_{l \in \mathcal{T}_E} \mathcal{J} = \sum_{u,v} w_{uv} \log \frac{\exp(s(u,v))}{\sum_{u,v} \exp(s(u',v'))} + \mathcal{J}_{R0}
\]

\[
= \sum_{u,v} w_{uv} s(u,v) - \sum_{u,v} \sum_{u',v'} w_{uv} \log \sum_{u'} \exp(s(u',v')) + \mathcal{J}_{R0}
\]

\[
(4)
\]

Here, \(w_{uv}\) can be specific to a meta-path \(M\) or an edge type \(l\) (denoted as \(w_{uv}^M\) or \(w_{uv}^l\) accordingly); \(\mathcal{J}_{R0}\) is an algorithm-specific regularizer (which is summarized in Table 1); \(s(u,v)\) is the proximity function between \(u\) and \(v\). Note that in most cases, we can write \(s(u,v) = f(e_u)^T f(e_v)\). For example, \(f(e_u) = e_u\) in metapath2vec, PTE, etc.; \(f(e_u) = \sqrt{A_M e_u}\) in HIN2Vec; \(f(e_u) = \sqrt{A_e} e_u\) in HEER. In these cases,

\[
\mathcal{J} = \sum_{u,v} w_{uv} f(e_u)^T f(e_v) - \sum_{u,v} w_{uv} \log \sum_{u',v'} \exp(s(u',v')) + \mathcal{J}_{R0}
\]

\[
= \sum_{u,v} w_{uv} \cdot \frac{1}{2} \left( ||f(e_u)||^2 + ||f(e_v)||^2 - ||f(e_u) - f(e_v)||^2 \right)
\]

\[
- \sum_{u,v} w_{uv} \log \sum_{u'} \exp(s(u',v')) + \mathcal{J}_{R0}.
\]

The second step holds because \(||x - y||^2 = (x - y)^T (x - y) = ||x||^2 + ||y||^2 - 2 x^T y\). Therefore, our goal is equivalent to

\[
\min -\mathcal{J} = \sum_{u,v} w_{uv} \frac{1}{2} \left( ||f(e_u)||^2 + ||f(e_v)||^2 \right) - \mathcal{J}_{R1}
\]

\[
- \sum_{u,v} w_{uv} \log \sum_{u'} \exp(s(u',v')) + \mathcal{J}_{R2}.
\]

Here \(\mathcal{J}_{R1}\) and \(\mathcal{J}_{R2}\) are two regularizers. Without \(\mathcal{J}_{R1}\), \(d(e_u, e_v)\) can be minimized by letting \(||f(e_u)|| \rightarrow 0\); without \(\mathcal{J}_{R2}\), \(d(e_u, e_v)\) can be minimized by letting \(e_u \equiv e_v \forall (u \in V)\).

\(\mathcal{J}_{R1}\) in Eq. (1) is then the summation of the algorithm-specific regularizer \(-\mathcal{J}_{R0}\) and \(-\mathcal{J}_{R1}\), \(\mathcal{J}_{R2}\), which are commonly shared across most HNE algorithms in the proximity-preserving group. We summarize the choices of \(w_{uv}\), \(d(e_u, e_v)\) and \(\mathcal{J}_{R0}\) in Table 4.

### 3.2 Message-Passing Methods

Each node in a network can have attribute information represented as a feature vector \(x_u\). Message-passing methods aim to learn node embeddings \(e_u\) based on \(x_u\) by aggregating the information from \(u\)’s neighbors. In recent studies, Graph Neural Networks (GNNs) \([37]\) are widely adopted to facilitate this aggregation/message-passing process.

**R-GCN** \([57]\). R-GCN has \(K\) convolutional layers. The initial node representation \(h_u^{(0)}\) is just the node feature \(x_u\).

In the \(K\)-th convolutional layer, each representation vector is updated by accumulating the vectors of neighbors through a normalized sum.

\[
h_u^{(k+1)} = \sigma \left( \sum_{l \in \mathcal{T}_E} \sum_{v \in N_l(u)} \frac{1}{|N_l(u)|} W_l^{(k)} h_v^{(k)} + W_0^{(k)} h_u^{(k)} \right).
\]

Different from regular GCNs \([37]\), R-GCN considers edge heterogeneity by learning multiple convolution matrices \(W\)’s, each corresponding to one edge type. During message passing, neighbors under the same edge type will be aggregated and normalized first. The node embedding is the output of the \(K\)-th layer (i.e., \(e_u = h_u^{(K)}\)).

In unsupervised settings, message-passing approaches use link prediction as their downstream task to train GNNs. To be specific, the likelihood of observing edges in the heterogeneous network is maximized. R-GCN uses negative sampling and cross-entropy loss, which is the approximation of the following objective.

\[
\mathcal{J} = \sum_{l \in \mathcal{T}_E} \sum_{u,v \in V} w_{uv}^l \log \frac{\exp(e_u^T A_l e_v)}{\sum_{u' \in V} \exp(e_{u'}^T A_l e_v)},
\]

where \(w_{uv}^l = 1_{(u,v) \in E_l}\).
Table 1: A summary of proximity-preserving based HNE algorithms. (Additional notations: $f_{\text{ENC}}$: a function to encode text/image/attribute information; $d_0$: distance between two points in the Poincaré ball.)

| Algorithm   | $w_{uv} / w^M_{uv} / w^M_{uv}$ | $d(e_u, e_v)$ | $J_{R0}$ | Applications                  |
|-------------|--------------------------------|--------------|----------|-------------------------------|
| MRWNN       | number of times that $u \in C(v)$ in homogeneous random walks | $\|e_u - e_v\|^2$ | $-\sum_v \|e_v - f_{\text{ENC}}(X_v)\|^2$ | image retrieval               |
| meta2vec    | number of times that $u \in C(v)$ in heterogeneous random walks following $\mathcal{M}$ (Eq. (2)) | $\|e_u - e_v\|^2$, $e_u = f_{\text{ENC}}(x_u)$ | $d_0(e_u, e_v)$ | classification, clustering, link prediction and recommendation |
| SHNE        | number of times that meta-path $\mathcal{M}$ instances between $u$ and $v$ following $\mathcal{M}$ | $\|e_u - e_v\|^2$ | $N/A$ | author identification         |
| HHNE        | number of times that $u \in C(v)$ in homogeneous random walks | $\|e_u - e_v\|^2$ | $N/A$ | classification, clustering, link prediction and recommendation |
| GHE         | number of meta-path | $\|\sqrt{A_{\mathcal{M}}(e_u - e_v)}\|^2$ | $N/A$ | text classification and image retrieval |
| HIN2vec     | number of times that $u \in C(v)$ in homogeneous random walks in $(V, E_l)$ | $\|e_u - e_v\|^2$ | $N/A$ | text classification           |
| MNE         | number of times that $u \in C(v)$ in Jumpr/Stay random walks | $\|e_u - e_v\|^2$ | $N/A$ | relatedness measurement of Wikipedia entities |
| JUST        | number of times that $u \in C(v)$ | $\|e_u - e_v\|^2$ | $-\sum_v \|e_v\|^2$ | event embedding               |
| HNE         | $1_{(u,v)\in E}$ | $\|e_u - e_v\|^2$, $e_u = A_{\mathcal{M}}(u)x_u$ | $-\sum_{o\in T_v} \|A_o\|^2_F$ | text classification and image retrieval |
| PTE         | edge weight of $(u, v)$ | $\|e_u - e_v\|^2$ | $N/A$ | supervised loss $\sum [y - y']^2$ | user rating prediction         |
| CMF         | edge weight of hyperedge $(u, C)$ | $\|e_u - e_C\|^2$, $e_C = \sum_{o\in C} e_{o}/|C|$ | $N/A$ | classification and link prediction |
| HEE        | number of times that $u$ and $v$ co-occur in a semantic pattern | $\|e_u - e_v\|^2$ | $N/A$ | aspect mining                 |
| Phine       | edge weight of $(u, v)$ with type $l$ | $\|e_{u,l} - e_v\|^2$ | $-\sum_{v, l} \sum_{v,l}(e_{v,l} - e_v)^2$ | relation prediction in knowledge graphs |
| MVE         | edge weight of $(u, v)$ with type $l$ | $\|e_{u,l} - e_v\|^2$ | $-\sum_{v, l} \sum_{v,l}(e_{v,l} - e_v)^2$ | relation prediction in knowledge graphs |
| AspEm       | edge weight of $(u, v)$ with type $l$ | $\|e_{u,a} - e_v\|^2$, $a$: aspect | $N/A$ | relation prediction in knowledge graphs |
| HEER        | edge weight of $(u, v)$ with type $l$ | $\|e_{u,a} - e_v\|^2$, $a$: aspect | $N/A$ | relation prediction in knowledge graphs |

**HAN** [82]. Instead of one-hop neighbors, HAN utilizes meta-paths to model higher-order proximity. Given a meta-path $\mathcal{M}$, the representation of node $u$ is aggregated from its meta-path based neighbors $N_{\mathcal{M}}(u) = \{u\} \cup \{v\mid v \text{ connects with } u \text{ via meta-path } \mathcal{M}\}$. HAN proposes an attention mechanism to learn the weights of different neighbors:

$$a_{\mathcal{M}}^u = \exp\left(\sigma(a_{\mathcal{M}}^u[x_u||x'_u])\right) \sum_{v \in N_{\mathcal{M}}(u)} \exp\left(\sigma(a_{\mathcal{M}}^u[x_u||x'_u])\right).$$

$$h_u^\mathcal{M} = \sigma\left(\sum_{v \in N_{\mathcal{M}}(u)} a_{\mathcal{M}}^u h_v^\mathcal{M}\right).$$

where $a_{\mathcal{M}}^u$ is the node-level attention vector of $\mathcal{M}$; $x'_u = M_{\mathcal{M}}(u)x_u$ is the projected feature vector of node $u$; $||$ is the concatenation operator.

Given meta-path specific embedding $h_u^\mathcal{M}$, HAN uses a semantic-level attention to weigh different meta-paths:

$$\beta_\mathcal{M} = \frac{\exp\left(\frac{1}{q^T} \sum_{v \in V} q^T \tanh(W h_u^\mathcal{M} + b)\right)}{\sum_{\mathcal{M}' \in M} \exp\left(\frac{1}{q^T} \sum_{v \in V} q^T \tanh(W h_v^\mathcal{M}' + b)\right)},$$

$$e_u = \sum_{\mathcal{M}} \beta_\mathcal{M} h_u^\mathcal{M}.$$

where $q$ is the semantic-level attention vector.

Very recently, [54] proposed HDGI to improve unsupervised training based on HAN, and [53] proposed HGT to enable temporal encoding for dynamic networks and minibatch sampling for scalable training. Since HAN is mainly designed for semi-supervised node classification, when we learn node embeddings in unsupervised settings (like many proximity-preserving methods), we adopt the widely used link prediction loss in R-GCN and GraphSAGE [28].

**HetGNN** [98]. HetGNN assumes that each node is associated with different features (e.g., categorical, textual and visual). It first encodes the content of each node to a vector $h_u^\mathcal{M}$, and then adopts a node type-aware aggregation function to collect information from neighbors:

$$h_u^\mathcal{M} = f_{\text{ENC}}(x_u), h_v^\mathcal{M} = f_{\text{AGG}}(\{h_v^\mathcal{M}||v \in N_{\text{RWWR}}(u), \delta(v) = o\})$$

where $N_{\text{RWWR}}(v)$ is the neighborhood of $v$ defined through random walk with restart [27]. Then HetGNN uses attention over neighborhood node types to get the final embedding, which share the same spirits as HAN:

$$a_u^o = \frac{\exp(\text{LeakyReLU}(a^T[h_v^\mathcal{M}||h_u^\mathcal{M}])))}{\sum_{o' \in T \cup \{s\}} \exp(\text{LeakyReLU}(a^T[h_v^\mathcal{M}||h_u^\mathcal{M}])))},$$

$$e_u = \sum_{o \in T \cup \{s\}} a_u^o h_u^o.$$
Table 2: A summary of message-passing based HNE algorithms. (Additional notations: $N_u$: neighbors of $u$ with edge type $l$; $N_\alpha(u)$: neighbors of $u$ with node type $\alpha$; $f_{\text{agg}}$: a function to aggregate information from neighbors. For HAN, we assume it adopts the unsupervised loss in GraphSAGE [28]. For GATNE, we show the transductive version.)

| Algorithm | $w_{uv}$ / $w'_{uv}$ | $d(e_u, e_v)$ | Aggregation Function | Applications |
|-----------|----------------------|---------------|----------------------|--------------|
| R-GCN [57] | $1_{(u,v)\in E}$ | $||\sqrt{\mathcal{A}}(e_u - e_v)||^2$ | $h_u^{(k+1)} = \sigma\left(\sum_{l\in T_G}\sum_{e \in N_\alpha(u)}\frac{1}{N_\alpha(u)} W_l^{(k)} h_v^{(k)} + W_0^{(k)} h_u^{(k)}\right)$ | entity classification and KB completion |
| HEP [109] | $1_{(u,v)\in E}$ | $||\sqrt{\mathcal{A}}(e_u - e_v)||^2$ | $h_u = \sigma\left(W_0\left(\sum_{l\in T_G}\sum_{e \in N_\alpha(u)} a_u e_v + b_0(u)\right)\right)$ | user alignment |
| HAN [82] | edge weight of $(u,v)$ | $||e_u - e_v||^2$ | $e_u = \sum_{M} \Phi^M(\sum_{e \in N_\alpha(u)} a_u^M M_{e\alpha}(u))$ | node classification, node clustering, link prediction and recommendation |
| HetGNN [98] | number of times that $u \in C \in V$ in random walks in $(V, E_G)$ | $||e_u,l - e_v||^2$ | $h_u^{(k+1)} = f_{\text{agg}}(k^{(k)} v \in N_\alpha(u))$, $h_u^{(0)} = x_u$ | |
| GATNE [7] | | | | |

Within this group of algorithms, only HEP has an additional reconstruction loss $\mathcal{J}_{R_0} = \sum_{e} ||e_u - h_u||^2$, while all other algorithms have $\mathcal{J}_{R_0} = 0$. We summarize the choices of $w_{uv}$, $d(e_u, e_v)$ and the aggregation function in Table 2.

3.3 Relation-Learning Methods

Each edge in a heterogeneous network can be viewed as a triplet $(u, l, v)$ composed of two nodes $u, v \in V$ and an edge type $l \in T_G$ (i.e., entities and relations, in the terminology of KG). The goal of relation-learning methods is to learn a scoring function $s_l(u, v)$ which evaluates an arbitrary triplet and outputs a scalar to measure the acceptability of this triplet. This idea is widely adopted in KB embedding. Since there are surveys of KB embedding algorithms already [81], we only cover the most popular approaches here and highlight their connections to HNE.

TransE [3]. TransE assumes that the relation induced by $l$-labeled edges corresponds to a translation of the embedding (i.e., $e_u + e_l \approx e_v$) when $(u, l, v)$ holds. Therefore, the scoring function of TransE is defined as $s_l(u, v) = -||e_u + e_l - e_v||_p$, where $p = 1$ or $2$. The objective is to minimize a margin-based ranking loss.

$$J = \sum_{(u, l, v) \in T} \sum_{(u', l', v') \in T'} \max(0, \gamma - s_l(u, v) + s_l(u', v'))$$

where $T$ is the set of positive triplets (i.e., edges); $T'_{(u, l, v)}$ is the set of corrupted triplets, which are constructed by replacing either $u$ or $v$ with an arbitrary node. Formally, $T'_{(u, l, v)} = \{(u', l, v)| u' \in V\} \cup \{(u, l, v')| v' \in V\}$.

TransE is the most representative model using “a translation distance” to define the scoring function. Its extensions include TransH [84], TransR [40], RHINE [41], etc.

DistMult [88]. In contrast to translational distance models [3] [84] [40], DistMult exploits a similarity-based scoring function. Each relation is represented by a diagonal matrix $A_l = \text{diag}(e_1, ..., e_d)$, and $s_l(u, v)$ is defined using a bilinear function:

$$s_l(u, v) = e_u^T A_l e_v$$

Note that $s_l(u, v) = s_l(v, u)$ for any $u$ and $v$. Therefore, DistMult is mainly designed for symmetric relations.

Besides DistMult, RESCAL [46] also uses a bilinear scoring function, but $A_l$ is no longer restricted to be diagonal.

ConVe [15]. ConvE goes beyond simple distance or similarity functions and proposes deep neural models to score a triplet. The score is defined by a convolution over 2D shaped embeddings. Formally,

$$s_l(u, v) = \log \left(\frac{\exp(s_l(u, v))}{\sum_{(u', l', v')} \exp(s_l(u', v'))}\right) + \mathcal{J}_{R_0}.$$

For translational distance models [3] [84] [40] [41], where $s_l(u, v)$ is described by distance, this is equivalent to

$$\min_{s_l(u, v)} \frac{1}{2} ||e_u + e_l - e_v||_p^2 + \mathcal{J}_{R_0}.$$

In [41], Qiu et al. point out that the margin-based loss shares a similar form as the following negative sampling loss:

$$\sum_{(u, l, v) \in T} \left(\log(s_l(u, v)) - b\mathbb{E}_{(u', l', v')} \left[\log(s_l(u', v'))\right]\right).$$

Following [41], if we use use negative sampling loss to rewrite Eq. (7), we are approximately maximizing

$$J = \sum_{(u,l,v)} w_{uv} \log \left(\frac{\exp(s_l(u,v))}{\sum_{(u',l',v')} \exp(s_l(u',v'))}\right) + \mathcal{J}_{R_0}.$$

In this case, we can write $\mathcal{J}_R$ as $-\mathcal{J}_{R_0} + \mathcal{J}_{R_1}$.

For neural triplet scorers [15] [68] [48] [60], the forms of $s_l(u, v)$ are more complicated than the inner product or distance. In these cases, since distance and proximity can be viewed as reverse metrics, we define $d(e_u, e_v)$ as $C - s_l(u, v)$, where $C$ is an constant upper bound of $s_l(\cdot)$. Then the derivation of the loss function is similar to that of Eq. (5), and we will have $\mathcal{J}_R = -\mathcal{J}_{R_0} + \mathcal{J}_{R_1}$.

We summarize the choices of $w_{uv}$, $d(e_u, e_v)$ and $\mathcal{J}_{R_0}$ in Table 3. Note that for relation learning methods, $d(\cdot, \cdot)$ may not be a distance metric. For example, $d(e_u, e_v) \neq d(e_u, e_v)$ in most translational distance models. This is intuitive because $(u, l, v)$ and $(v, l, u)$ often express different meanings.
Table 3: A summary of relation-learning based HNE algorithms. (Additional notations: $f$: a non-linear activation function; $[x]^+ = \max\{x, 0\}$; $\Theta$: the set of learned parameters; $E_u$, $E_v$: 2D reshaping matrices of $e_u$ and $e_v$, (14); $M(e_u, e_v)$: a matrix aligning the output vectors from the convolution with all kernels (60).)

| Algorithm | $w_{ij, kl}$ | $d(e_u, e_v)$ | $f_{bs}$ | Applications |
|-----------|--------------|---------------|----------|--------------|
| TransE 3 | $1_{(u, v) \in E_i}$ | $\|e_u + e_i - e_v\|^2$, $e_{ui} = e_u - w_i^l e_v w_l$ | $\sum_{i} [\|e_u\| - 1] + \sum_{i} [\|e_v\| - 1] + \sum_{i} [\|e_i\| - 1] + \sum_{i} [\|A_i e_u\| - 1] + \sum_{i} [\|A_i e_v\| - 1]$ | KB completion and relation extraction from text |
| TransH 84 | $1_{(u, v) \in E_i}$ | $\|e_u + e_i - e_v\|^2$, $e_{ui} = e_u - w_i^l e_v w_l$ | $\sum_{i} [\|e_u\| - 1] + \sum_{i} [\|e_i\| - 1] + \sum_{i} [\|A_i e_u\| - 1] + \sum_{i} [\|A_i e_v\| - 1]$ | KB completion and node classification |
| RHINE 41 | edge weight of $(u, v)$ with type $t$ | $\|e_u - e_v\|^2$ if $l$ models affiliation, $\|e_u + e_i - e_v\|$ if $l$ models interaction | N/A | link prediction and text classification |
| DistMult 88 | $\|\sqrt{A(e_u - e_v)}\|^2$ | $\|\sum_{i} [\|e_u\| - 1] + \sum_{i} [\|e_i\| - 1] + \sum_{i} [\|A_i e_u\| - 1] + \sum_{i} [\|A_i e_v\| - 1]$ | N/A | KB completion and rule extraction |
| NTN 68 | $C - e_u^T \tanh(e_u^T M e_v + M_2 e_u + M_3 e_v + b)$ | $\|f\|^2$ | triplet classification |
| ConvE 49 | $C - f(e_u \sigma(w_u \odot e_u + w_v \odot e_v + b) + b)$ | $\|f\|^2$ | KB completion and triplet classification |
| SACN 69 | $C - f(\text{vec}(e_u + e_v))^T W e_u$ | N/A | KB completion |
| NKGE 79 | $C - f(\text{vec}(M(e_u, e_v))) W e_u$ | $\|f\|^2$ when using the TransE objective | N/A | KB completion |

4. BENCHMARK

4.1 Dataset Preparation

Towards off-the-shelf evaluation of HNE algorithms in a systematic and comprehensive manner, in this work, we spare no effort to collect, process, analyze, and publish four real-world heterogeneous network datasets from different domains, which we aim to set up as a benchmark for existing and future HNE algorithms.

DBLP. We construct a network of authors, papers, venues, and phrases from DBLP. Phrases are extracted by the popular AutoPhrase [61] algorithm from paper texts and further filtered by human experts. We compute word2vec [44] on all paper texts and aggregate the word embeddings to get 300-dim paper and phrase features. Author and venue features are the aggregations of their corresponding paper features. We further manually label a relatively small portion of authors into 12 research groups from four research areas by crawling the web. Each labeled author has only one label.

Yelp. We construct a network of businesses, users, locations, and reviews from Yelp[4] Nodes are not associated with any feature, but a large portion of businesses are labeled into sixteen categories. Each labeled business has one or multiple labels.

Freebase. We construct a network of books, films, music, sports, people, locations, organizations, and businesses from Freebase[8] Nodes are not associated with any features, but a large portion of books are labeled into eight genres of literature. Each labeled book has only one label.

PubMed. We construct a network of genes, diseases, chemicals, and species from PubMed[9] All nodes are extracted by AutoPhrase [61], typed by AutoNER [62], and further filtered by human experts. We compute word2vec [44] on all PubMed papers and aggregate the word embeddings to get 200-dim features for all types of nodes. We further label a relatively small portion of diseases into eight categories. Each labeled disease has only one label.

5https://www.ncbi.nlm.nih.gov/pubmed/
Table 4: A summary of the statistics on four real-world heterogeneous network datasets.

| Dataset | #node type | #node   | #link type | #link   | #attributes | #attributed nodes | #labels | #labeled node |
|---------|------------|---------|------------|---------|-------------|------------------|---------|---------------|
| DBLP    | 4          | 1,989,077 | 6          | 275,940,913 | 300         | ALL              | 13      | 618           |
| Yelp    | 4          | 82,455   | 4          | 30,542,675  | N/A         | N/A              | 16      | 7,417         |
| Freebase| 8          | 12,164,768 | 10        | 244,986    | 200         | 200              | 8       | 47,190        |
| PubMed  | 4          | 64,119   | 10         | 244,986    | 200         | ALL              | 8       | 47,190        |

Figure 3: Portion of different node types in four real-world heterogeneous network datasets.

Figure 4: Degree distribution of different node types in four real-world heterogeneous network datasets.

Figure 5: Local clustering coefficient of different node types in four real-world heterogeneous network datasets.

Figure 6: Number of five most frequent 2-hop meta-paths in four real-world heterogeneous network datasets.
semi-supervised HNE, we also conduct additional experiments for them in the corresponding settings. Particularly, due to the nature of the datasets, we evaluate attributed HNE on DBLP and PubMed datasets where node attributes are available, and semi-supervised HNE on Yelp and Freebase where node labels are abundant. We always test the computed network embeddings on two standard network mining tasks of node classification and link prediction. We set the embedding size of all algorithms to 50 by default, and tune other hyperparameters following the original papers through standard five-fold cross validation on all datasets.

For the standard unattributed unsupervised HNE setting, we first randomly hide 20% links and train all HNE algorithms with the remaining 80% links. For node classification, we then train a separate linear Support Vector Machine (LinearSVC) [21] based on the learned embeddings on 80% of the labeled nodes and predict on the remaining 20%. We repeat the process for five times and compute the average scores regarding macro-F1 (across all labels) and micro-F1 (across all nodes). For link prediction, we use the Hadamard function to construct feature vectors for node pairs, train a two-class LinearSVC on the 80% training links and evaluate towards the 20% held out links. We also repeat the process for five times and compute the two metrics of AUC (area under the ROC curve) and MRR (mean reciprocal rank). AUC is a standard measure for classification, where we regard link prediction as a binary classification problem, and MRR is a standard measure for ranking, where we regard link prediction as a link retrieval problem. Since exhaustive computation over all node pairs is too heavy, we always use the two-hop neighbors as the candidates for all nodes.

For attributed HNE, node features are used during the training of HNE algorithms, while for semi-supervised HNE, certain amounts of node labels are used (80% by default).

5. EXPERIMENTAL EVALUATIONS

5.1 Algorithms and Modifications

We amend the implementations of 10 popular HNE algorithms for seamless and efficient experimental evaluations on our prepared datasets. The algorithms we choose and the modifications we make are as follows

- **metapath2vec** [16]: Since the original implementation contains a large amount of hard-coded data-specific settings such as node types and meta-paths, and the optimization is unstable and limited as it only examines one type of meta-path based context, we completely reimplement the algorithm. In particular, we first run random walks to learn the weights of different meta-paths based on the number of sampled instances, and then train the model using the unified loss function, which is a weighted sum over the loss functions of individual meta-paths. Both the random walk and meta-path-based embedding optimization are implemented with multi-threads in parallel.

- **PTE** [71]: Instead of accepting labeled texts as input and working on text networks with the specific three types of nodes (word, document, and label) and three types of edges (word-word, document-word, and label-word), we revise the original implementation and allow the model to consume heterogeneous networks directly with arbitrary types of nodes and edges.

- **DistMult** [88]: We remove the hard-coded data-specific settings and largely simplify the data preprocessing step in the original implementation.

- **ConvE** [15]: Same as for DisMult.

- **R-GCN** [80]: The existing implementation from DGL is only scalable to heterogeneous networks with thousands of nodes, due to the requirement putting the whole graphs into memory during graph convolutions. To scale up R-GCN, we perform fixed-sized node and edge sampling for batch-wise training following the framework of GraphSage.

- **HAN** [82]: Since the original implementation of HAN contains a large amount of hard-coded data-specific settings such as node types and meta-paths, and is unfeasible for large-scale datasets due to the same reason as R-GCN, we completely reimplement the HAN algorithm based on our implementation of R-GCN. In particular, we first automatically construct meta-path based adjacency lists for the chosen node type, and then sample the neighborhood for the seed nodes during batch-wise training.

- **HEER** [67]: We remove the hard-coded data-specific settings and largely simplify the data preprocessing step in the original implementation.

- **HIN2Vec** [22]: We remove unnecessary data preprocessing codes and modify the original implementation so that the program first generates random walks, then trains the model and finally outputs node embeddings only.

- **AspEm** [63]: We clean up the hard-coded data-specific settings in the original implementation and write a script to connect the different components of automatically selecting the aspects with the least incompatibilities, as well as learning, matching and concatenating the embeddings based on different aspects.

- **TransE** [3]: We modify the OpenKE implementation so that the model outputs node embeddings only.

We have put the implementation of all compared algorithms in a python package and released them together with the datasets to constitute an open-source easy-to-use HNE benchmark.

5.2 Performance Benchmarks

We provide comprehensive experimental comparisons of the 10 popular state-of-the-art HNE algorithms across our four datasets, on the scenarios of unsupervised unattributed HNE, attributed HNE, and semi-supervised HNE.

Table 5 shows the performance of compared algorithms on unsupervised unattributed HNE, attributed HNE, and semi-supervised HNE. In our implementation of R-GCN, we perform fixed-sized node and edge sampling for batch-wise training following the framework of GraphSage. From the perspective of compared algorithms: (1) Proximity-perserving algorithms often perform well on both tasks under the unsupervised unattributed HNE setting, which explains why proximity-perserving is the most widely used HNE or even general network embedding framework. Among the proximity-preserving methods, HIN2Vec and HEER show competitive results in link prediction but perform not so well in node classification (especially on DBLP and Freebase).
Table 5: Performance comparison (%) under the standard setting of unattributed unsupervised HNE.

| Model       | DBLP (Macro-F1/Micro-F1) | Yelp (Macro-F1/Micro-F1) | Freebase (Macro-F1/Micro-F1) | PubMed (Macro-F1/Micro-F1) | Link prediction (AUC/MRR) |
|-------------|--------------------------|--------------------------|-----------------------------|---------------------------|---------------------------|
| metapath2vec | 43.85/55.07              | 20.55/46.43              | 12.90/15.31                 | 65.26/90.68               | 60.14/78.24               | 69.38/84.79               |
| PTE         | 43.34/54.53              | 5.10/12.27               | 10.25/39.87                 | 57.72/77.51               | 50.32/68.84               | 57.89/78.23               |
| HIN2Vec     | 12.17/25.88              | 17.40/41.92              | 10.93/15.31                 | 53.29/75.47               | 51.64/66.71               | 58.11/81.65               |
| AspEm       | 33.07/43.85              | 23.26/45.42              | 11.19/14.44                 | 67.20/91.46               | 55.80/77.70               | 68.31/87.43               |
| HEER        | 09.72/27.72              | 12.69/37.51              | 11.73/15.29                 | 53.00/72.76               | 73.72/95.92               | 55.78/78.31               |
| R-GCN       | 09.38/13.39              | 10.69/23.24              | 10.54/12.18                 | 50.24/73.10               | N/A                       | 51.50/74.13               |
| HAN         | 07.91/16.98              | 9.60/23.01               | 9.54/12.18                  | 50.24/73.10               | N/A                       | 51.50/74.13               |
| TransE      | 22.76/37.18              | 31.83/52.04              | 11.40/15.16                 | 63.53/86.29               | 69.13/83.66               | 52.84/75.80               |
| DisMult     | 12.42/26.42              | 24.57/47.61              | 13.00/14.49                 | 54.03/75.31               | 78.55/99.70               | 71.81/89.82               |
| ConvE       | 11.42/25.07              | 23.82/45.50              | 11.27/15.79                 | 52.87/74.84               | 89.28/99.73               | 54.91/78.04               |

Figure 7: Performance comparison under controlled experiments with varying emb. sizes and link removals.

Figure 8: Performance comparison under controlled experiments with varying label amount and attr. noise.

In fact, these two methods focus on modeling edge representations in their objectives ($A_M$ in HIN2Vec and $A_l$ in HEER), thus are more suitable for link prediction. (2) Under the unsupervised unattributed HNE setting, message-passing methods perform poorly, especially on node classification. As we discuss before, message-passing methods are known to excel due to their integration of node attributes, link structures and training labels. When neither of node attributes and labels are available, we use random vectors as node features and adopt a link prediction loss, which largely limits the performance of R-GCN and HAN. We will focus our evaluation on the two algorithms in the attributed and semi-supervised HNE settings later. Moreover, the link prediction results of HAN on the Yelp dataset are not available. This is because HAN can only predict the link between two nodes with the same type (e.g., Business-Business), while all edges in Yelp connect different types of nodes (e.g., Business-Location, Business-User). (3) Relation-learning methods perform better on Freebase and PubMed in both tasks, especially on link prediction. In fact, in Table 3 and Figure 5 we can observe that both datasets (especially Freebase) have more link types. Relation-learning approaches, which are mainly designed to embed knowledge graphs (e.g., Freebase), can better capture the semantics of numerous types of direct links simultaneously.

From the perspective of datasets: (1) All approaches have relatively low F1 scores on Yelp and Freebase in node classification, especially Yelp. This is because both datasets have larger numbers of node labels (i.e., 16 in Yelp and 8 in Freebase) as shown in Table 4. Moreover, unlike the case of the other datasets, a node in Yelp can have multiple labels, which makes the classification task more challenging. (2) In Figure 4, we can observe that the degree distribution of Freebase is more skewed. Therefore, when we conduct edge sampling or random walks on Freebase during embedding learning, nodes with lower degrees will be sampled less frequently and their representations may not be learned accurately. This observation may explain why the link prediction metrics on Freebase are in general lower than those on DBLP and Yelp. (3) As we can see in Figure 3, most studied network properties are more balanced on Freebase and PubMed (especially PubMed) across different types of nodes and links. This in general makes both the node classification and link prediction tasks harder for all algorithms, and also makes the gaps among different algorithms smaller.

To provide in-depth performance comparison among various HNE algorithms, we further conduct controlled experiments by varying the embedding sizes and randomly removing links from the training set.
In this work, we present a comprehensive survey on various existing HNE algorithms, and provide benchmark datasets and baseline implementations to ease future research in this direction. While HNE has already demonstrated strong performance across a variety of downstream tasks, it is still in its infancy with many open challenges. To conclude this work and inspire future research, we now briefly discuss the limitation of current HNE and several specific directions potential worth pursuing.

Beyond homophily. As we formulate in Eq. (1), current HNE algorithms focus on the leverage of network homophily. Due to recent research on homogeneous networks that study the combination of positional and structural embedding, it would be interesting to explore how to generalize such design principles and paradigms to HNE. Particularly, in heterogeneous networks, relative positions and structural roles of nodes can both be measured under different meta-paths or meta-graphs, which are naturally more informative and diverse. However, such considerations also introduce harder computational challenges.

Beyond accuracy. Most, if not all, existing research on HNE has primarily focused on the accuracy towards different downstream tasks. It would be interesting to further study the efficiency and scalability (for large-scale networks), temporal adaptability (for dynamic evolving networks), robustness (towards adversarial attacks), explainability, uncertainty, fairness of HNE, and so on.

Beyond node embedding. Graph- and subgraph-level embeddings have been intensively studied on homogeneous networks, but hardly on heterogeneous networks. Although existing works like HIN2Vec study the embedding of meta-paths to improve the embedding of nodes, direct applications of graph- and subgraph-level embeddings in the context of heterogeneous networks remain nascent.

Revisiting KB embedding. The difference between KB embedding and other types of HNE is mainly due to the numbers of node and link types. Direct application of KB embedding to heterogeneous networks fails to consider meta-paths with rich semantics, whereas directly applying HNE to KB is unrealistic due to the exponential number of meta-paths. However, it would still be interesting to study the intersection between these two groups of methods (as well as two types of data). For example, how can we combine the ideas of meta-paths on heterogeneous networks and embedding transformation on KB for HNE with more semantic-aware transformations? How can we devise truncated random walk based methods for KB embedding to include higher-order relations?

Modeling heterogeneous contexts. Heterogeneous networks mainly model different types of nodes and links. However, networks nowadays are often associated with rich contents, which provide contexts of the nodes, links, and sub-networks. Thus, how to model heterogeneous interactions under multi-facet contexts through the integration of multimodal content and structure could be a challenging but rewarding research area.

Understanding the limitation. While HNE (as well as many neural representation learning models) has demonstrated strong performance in various domains, it is worthwhile to understand its potential limits. For example, when do modern HNE algorithms work better compared with traditional network mining approaches (e.g., path counting, subgraph matching, non-neural or linear propagation)? How can we join the advantages of both worlds? Moreover, while there has been intensive research on the mathematical mechanisms behind neural networks for homogeneous network data (e.g., smoothing, low-pass filtering, invariant and equivariant transformations), by unifying existing models on HNE, this work also aims to stimulate further theoretical studies on the power and limitation of HNE.
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