Structure-Aware Hard Negative Mining for Heterogeneous Graph Contrastive Learning

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ABSTRACT

Recently, heterogeneous Graph Neural Networks (GNNs) have become a de facto model for analyzing HGs, while most of them rely on a relative large number of labeled data. In this work, we investigate Contrastive Learning (CL), a key component in self-supervised approaches, on HGs to alleviate the label scarcity problem. We first generate multiple semantic views according to metapaths and network schemas. Then, by pushing node embeddings corresponding to different semantic views close to each other (positives) and pulling other embeddings apart (negatives), one can obtain informative representations without human annotations. However, this CL approach ignores the relative hardness of negative samples, which may lead to suboptimal performance. Considering the complex graph structure and the smoothing nature of GNNs, we propose a structure-aware hard negative mining scheme that measures hardness by structural characteristics for HGs. By synthesizing more negative nodes, we give larger weights to harder negatives with limited computational overhead to further boost the performance. Empirical studies on three real-world datasets show the effectiveness of our proposed method. The proposed method consistently outperforms existing state-of-the-art methods and notably, even surpasses several supervised counterparts.

1 INTRODUCTION

Many real-world complex interactive objectives can be represented in Heterogeneous Graphs (HG) or heterogeneous information networks. Recent development in heterogeneous Graph Neural Networks (GNNs) has achieved great success in analyzing heterogeneous structure data \cite{16, 17}. However, most existing models require a relatively large amount of labeled data for proper training \cite{6, 11, 22, 23, 24}, which may not be accessible in reality. As a promising strategy of leveraging abundant unlabeled data, Contrastive Learning (CL), as a case of self-supervised learning, is proposed to learn representations by distinguishing semantically similar samples (positives) over dissimilar samples (negatives) in the latent space \cite{2-4, 6, 7, 19}.

Most existing CL work follows a multiview paradigm, where multiple views of the input data are constructed via semantic-preserving augmentations. In the HG domain, since multiple types of nodes and edges convey abundant semantic information, it is straightforward to construct views based on HG semantics such as metapaths and schemas. In this way, for one anchor node, its embeddings in different semantic views constitute positives and all other embeddings are naturally regarded as negative examples.

However, the previous scheme assumes that all negative samples make equal contribution to the CL objective. Previous research in metric learning \cite{14} and visual representation learning \cite{1, 24} has established that the hard negative sample is of particular concern in effective CL. To be specific, the more similar a negative sample to its anchor, the more helpful it is for learning effective representatives. Therefore, a natural question arises: whether could we make use of hard negatives in HGCL? To this end, we propose to investigate the relative hardness of different negative samples in HGs and reweight hard negatives to further boost performance of CL in HGs.

In visual CL studies, the hardness of one image is defined to be its semantic similarity to the anchor, e.g., inner product of two normalized vectors in the embedding space. When dealing with HGs, due to the neighborhood aggregation scheme in each semantic view \cite{23}, heterogeneous GNN produces similar embeddings within ego networks; embeddings of neighboring nodes sharing the same label with the anchor node thus tend to be similar to the anchor, as shown in Figure 1(a). We further plot pairwise similarities of negative nodes with one arbitrary author node in a real-world DBLP network in Figure 1(b). With the similarity of negative node to the anchor (the hardness) increasing, there are more positive samples...
Heterogeneous graph neural networks. Most heterogeneous GNNs learn node representations under different semantic views and then aggregates them using attention networks. We first generate multiple semantic views, each corresponding to one metapath that encodes one aspect of semantic information. Then, we leverage an attentive network to compute semantic-specific embedding \( h^p_i \) for node \( v_i \) under metapath \( p \) as

\[
 h^p_i = \sigma \left( \sum_{v_j \in N_p(v_i)} \alpha^p_{ij} W^P x_j \right),
\]

where \( \| \) concatenates \( K \) standalone node representations in each attention head, \( N_p(v_i) \) defines the neighborhood of \( v_i \) that is connected by metapath \( p \), \( W^P \in \mathbb{R}^{d \times m} \) is a linear transformation matrix for metapath \( p \), and \( \sigma(\cdot) \) is the activation function, such as ReLU(\( \cdot \)) = max(0, \( \cdot \)). The attention coefficient \( \alpha^p_{ij} \) can be computed by a softmax function

\[
 \alpha^p_{ij} = \frac{\exp(\sigma(a^p_{ij} | h^p_i \| h^p_j))}{\sum_{k \in N_p(v_i)} \exp(\sigma(a^p_{ij} | h^p_i \| h^p_k))},
\]

where \( a^p_{ij} \in \mathbb{R}^{2d} \) is a trainable semantic-specific linear weight vector.

Finally, we combine node representation in each view to an aggregated representation. We employ another attentive network to obtain the semantic-aggregated representation \( h_i \) that combines information from every semantic space as given by

\[
 h_i = \sum_{p=1}^{\lvert \mathcal{P} \rvert} \beta^p h^p_i.
\]

The coefficients are given by

\[
 \beta^p = \frac{\exp(w^p)}{\sum_{p' \in \mathcal{P}} \exp(w^{p'})},
\]

\[
 w^p = \frac{1}{\lvert \mathcal{V} \rvert} \sum_{v_i \in \mathcal{V}} q^T \cdot \tanh(W h^p_i + b),
\]

where \( q \in \mathbb{R}^{d_m} \) is the semantic-aggregation attention vector, \( W \in \mathbb{R}^{d_m \times d} \), \( b \in \mathbb{R}^{d_m} \) is the weight matrix and the bias vector respectively, and \( d_m \) is a hyperparameter.

The above data analysis motivates us to discover hard negatives for HGs from structural aspects. Specifically, we propose to select hard negative nodes according to structural measures and synthesize more negatives by randomly mixing up these selected negatives, so as to give larger weights to harder negatives. Moreover, measuring hardness through structural characteristics enjoys another benefit that being irrespective of training progress, which can be used in supplement to poor representations in the initial training stage. We term the resulting CL framework for HGs as Heterogeneous gRAPh Contrastive learning with structure-aware hard negative mining, HORACE for brevity (Figure 2). The HORACE works by constructing multiple semantic views from the HG at first. Then, we learn node embeddings within each semantic view and combine them into an aggregated representation. Thereafter, we train the model with a contrastive aggregation objective to adaptively distill information from each semantic view. Finally, the proposed structure-aware scheme enriches the selection of negatives with structure embeddings, which yields harder negative samples in the context of HGs.

The main contribution of this work is twofold.

- We present a CL framework that enables self-supervised training for HGs from both semantic and structural aspects, where we propose to enrich the contrastive objective with structurally hard negatives to improve the performance.
- Extensive experiments on three real-world datasets from various domains demonstrate the effectiveness of the proposed method. Particularly, our HORACE method outperforms representative unsupervised baseline methods, achieves competitive performance with supervised counterparts, and even exceeds some of them.

2 THE PROPOSED METHOD: HORACE

2.1 Preliminaries

Problem definition. We denote a HG with multiple types of nodes and edges by \( \mathcal{G} = (\mathcal{V}, \mathcal{E}, X, \phi, \varphi) \), where \( \mathcal{V}, \mathcal{E} \) denote the node set and the edge set respectively. The type mapping function \( \phi \) and \( \varphi \) associates each node and edge with a type respectively. We further denote the set of all considered metapaths as \( \mathcal{P} \), where a metapath \( p \in \mathcal{P} \) defines a path on the network schema that captures the proximity between the two nodes from a particular semantic perspective. Given a HG \( \mathcal{G} \), the problem of HG representation learning is to learn node representations \( H \in \mathbb{R}^{\lvert \mathcal{V} \rvert \times d} \) that encode both structural and semantic information, where \( d \ll \lvert \mathcal{V} \rvert \) is the hidden dimension.

Heterogeneous graph neural networks. Most heterogeneous GNNs learn node representations under different semantic views and then aggregates them using attention networks. We first generate multiple semantic views, each corresponding to one metapath that encodes one aspect of semantic information. Then, we leverage
2.2 Heterogeneous Graph Contrastive Learning

Existing graph CL follows a multiview framework [8, 25–27], which maximizes the agreement among node representations under different views of the original graph and thus enables the encoder to learn informative representations in a self-supervised manner.

In HGs, since multiple views are involved, to implement the CL objective, we resort to maximizing the agreement between node representations under a specific semantic view and the aggregated representations. The resulting contrastive aggregation objective can be mathematically expressed as

\[
\max \frac{1}{|V|} \sum_{v \in V} \left[ \frac{1}{|P|} \sum_{p \in P} \frac{1}{2} \left( l(h_i^p; h_i) + l(h_i; h_i^p) \right) \right].
\] (6)

The proposed objective Eq. (6) conceptually relates to contrastive knowledge distillation [18], where several teacher models (semantic views) and one student model (the aggregated representation) are employed. By forcing the embeddings between several teachers and a student to be the same, these aggregated embeddings adaptively collects information of all semantic relations.

Following previous work [9, 20], to implement the objective in Eq. (6), we empirically choose the InfoNCE estimator. Specifically, for node representation \( h_i^p \) in one specific semantic view, we construct its positive sample as the aggregated representation, while embeddings of all other nodes in the semantic and the aggregated embeddings are considered as negatives. The contrastive loss can be expressed by

\[
l(h_i^p; h_i) = -\log \frac{e^{\theta(h_i^p; h_i)/\tau}}{e^{\theta(h_i^p; h_i)/\tau} + \sum_{j \neq i} e^{\theta(h_i^p; h_j)/\tau} + e^{\theta(h_i; h_j)/\tau}},
\] (7)

where \( \tau \in \mathbb{R} \) is a temperature parameter. We define the critic function \( \theta(\cdot, \cdot) \) by

\[
\theta(h_i; h_j) = \frac{g(h_i)^T g(h_j)}{||g(h_i)|| ||g(h_j)||}
\]

where \( g(\cdot) \) is parameterized by a non-linear multilayer perceptron to enhance expressive power [3].

2.3 Structure-Aware Hard Negative Mining

As with previous studies [1, 14, 24], CL benefits from hard negative samples, i.e. samples close to the anchor node such that cannot be distinguished easily. In the context of HGs, we observe that semantic-level node representations are not sufficient to calculate the hardness of each negative pair. Therefore, in this work, to effectively measure hardness of each sample with respect to the anchor, we propose to explore the hardness of negative samples in terms of their structural similarities. The proposed structure-aware hard negative mining scheme is illustrated in Figure 3.

We first introduce a structure-aware metric \( s(i, j, p) \) representing distance measure of a negative node \( v_i \) to the anchor node \( v_j \) given a semantic view \( p \), which can be regarded as the hardness of the negative node \( v_i \). Note that in order to empower the model with inductive capabilities, we prefer a local measure to a global one. In this paper, we propose two model variants HORACE-PPR and HORACE-PE, which use Laplacian positional embeddings and personalized PageRank scores for structure-aware hard negative mining respectively.

- The Personalized PageRank (PPR) score [10, 12] of node \( v \) is defined as the stationary distribution of a random walk starting from and returning to node \( v \) at a probability of \( c \) at each step. Formally, the PPR vector of node \( v \) under semantic view \( p \) satisfies the following equation

\[
s_c^p = (1 - c)A^p s^p + c p_v,
\] (8)

where \( c \) is the returning probability and \( p_v \) is the preference vector with \( (p_v)_i = 1 \) when \( i = v \) and all other entries set to 0. \( A^p \) denotes the adjacency matrix generated by metapath \( p \). The structural similarity between node \( v \) and \( k \) can be represented by the PPR score of node \( k \) with respect to node \( v \), i.e. \( s_c^k \).

- The Laplacian positional embedding of one node is defined to be its \( k \) smallest non-trivial eigenvectors [5]. We simply define the structure similarity as the inner product between \( s_c^i \) and \( s_c^j \).

After that, we perform hard negative mining by giving larger weights to harder negative samples. Specifically, we sort negatives according to the hardness metric and pick the top-\( T \) negatives to form a candidate list for semantic view \( p \). Then, we synthesize \( M \ll |V| \) samples by creating a convex linear combination of them. The generated sample \( \tilde{h}_i^p \) is mathematically expressed as

\[
\tilde{h}_i^p = \alpha_m h_i^p + (1 - \alpha_m) h_j^p,
\] (9)

where \( h_i^p, h_j^p \in \mathbb{B}^p \) are randomly picked from the memory bank, \( \alpha_m \sim \text{Beta}(\alpha, \alpha) \), and \( \alpha \) is a hyperparameter, fixed to 1 in our experiments. These interpolated samples will be added into negative bank when estimating mutual information \( l(h_i^p; h_i) \), as shown in Figure 3.

\[
\mathcal{L}(h_i^p; h_i) = -\log \frac{e^{\theta(h_i^p; h_i)/\tau}}{e^{\theta(h_i^p; h_i)/\tau} + \sum_{h \in \mathbb{B}^p} e^{\theta(h_i^p; h_i)/\tau} + e^{\theta(h_i; h_i)/\tau}},
\] (10)

where the negative bank

\[
\mathbb{B}^p = \{h_j^p\}_{j \neq i} \cup \{h_j\}_{j \neq i} \cup \{\tilde{h}_i^p\}_{i=1}^M
\] (11)

consists of all inter-view and intra-view negatives as well as synthesized hard negatives. The contrastive objective \( l(h_i; h_i^p) \) for the aggregated node representation \( h_i \) can be defined similarly as
Table 1: Performance comparison on three datasets. Node classification performance is in terms of Macro-F1 (Ma-F1) and Micro-F1 (Mi-F1). The highest performance of unsupervised and supervised models is boldfaced and underlined, respectively.

| Method         | ACM Mi-F1 | ACM Ma-F1 | IMDb Mi-F1 | IMDb Ma-F1 | DBLP Mi-F1 | DBLP Ma-F1 |
|----------------|-----------|-----------|------------|------------|------------|------------|
| DeepWalk       | 76.92     | 77.25     | 46.38      | 40.72      | 79.37      | 77.43      |
| ESim           | 76.89     | 77.32     | 35.28      | 32.10      | 92.73      | 91.64      |
| metapath2vec   | 65.00     | 65.09     | 45.65      | 41.16      | 91.53      | 90.76      |
| HERec          | 66.03     | 66.17     | 45.81      | 41.65      | 92.69      | 91.78      |
| HAN-U          | 82.63     | 81.89     | 43.98      | 40.87      | 90.47      | 89.65      |
| DGI            | 89.15     | 89.09     | 48.86      | 45.38      | 91.30      | 90.69      |
| GRACE          | 88.72     | 88.72     | 46.64      | 42.41      | 90.88      | 89.76      |
| HORACE-PE      | 90.76     | 90.72     | 58.98      | 54.48      | 92.81      | 92.33      |
| HORACE-PFR     | 90.75     | 90.70     | 58.96      | 54.47      | 92.78      | 92.30      |
| GCN            | 86.77     | 86.81     | 49.78      | 45.73      | 91.71      | 90.79      |
| GAT            | 86.01     | 86.23     | 55.28      | 49.44      | 91.96      | 90.97      |
| HAN            | 89.22     | 89.40     | 54.17      | 49.78      | 92.05      | 91.17      |

Eq. (10). The final objective is an average of the losses from all contrastive pairs, formally given by

\[
J = \frac{1}{|V|} \sum_{i \in V} \left[ \frac{1}{|P|} \sum_{p \in P} \frac{1}{2} \left( L(h_i^p; h_i) + L(h_i; h_i^p) \right) \right]. \tag{12}
\]

2.4 Complexity Analysis

Most computational burden of the HORACE framework lies in the contrastive objective, which involves computing \((|V|^2|P|)\) node embedding pairs. For structure-aware hard negative mining, the synthesized samples incur an additional computational cost of \(O(|M||V||P|)\), which is equivalent to increasing the memory size by \(M \ll |V|\). The construction of the candidates list of hard negatives only depends on graph structures of each semantic view, and thus it can be regarded as a preprocessing process.

3 EXPERIMENTS

We evaluate the effectiveness of our proposed HORACE in this section. The purpose of empirical studies is to answer the following questions.

- **RQ1.** How does our proposed HORACE outperform other representative baseline algorithms?
- **RQ2.** How does the proposed structure-aware hard negative mining scheme affect the performance of HORACE?

3.1 Experimental Configurations

3.1.1 Datasets. To achieve a comprehensive comparison, we use three widely-used heterogeneous datasets from different domains: DBLP, ACM, and IMDb, where DBLP and ACM are two academic networks, and IMDb is a movie network.

- **DBLP** is a subset of an academic network extracted from DBLP, consisting of four kinds of nodes: authors, papers, conferences, and topics. Each author is labeled with their research area.
- **ACM** is an academic network from ACM. We construct a heterogeneous graph with nodes of three types: papers, authors, and subjects. Papers are labeled by their research topic.
- **IMDb** is a subset of the movie network IMDb, where nodes represent movies, actors, or directors. We categorize movies into three classes according to their genre.

3.1.2 Baselines. We compare the proposed HORACE against a comprehensive set of baselines, including both representative traditional and deep graph representation learning methods. These baselines include (1) DeepWalk [13], DGI [21], GRACE [26], GCN [11], and GAT [22], designed for homogeneous graphs, and (2) ESim [15], HERec [16], and HAN [23] for heterogeneous graphs. Among them, DeepWalk, ESim, metapath2vec, and HERec only utilize metapaths for multiple views for training. HAN and DGI further use associated node features (if any) for learning representations. Furthermore, we also include three representative supervised baselines GCN, GAT, and HAN for reference. Following HAN [23], for DeepWalk, we simply discard node and edge types, and treat the heterogeneous graph as a homogeneous graph; for DGI, GRACE, GCN, and GAT, we generate homogeneous graphs according to all metapaths, and report the best performance.

3.1.3 Evaluation protocols. For comprehensive evaluation, we follow HAN [23] and perform experiments on the node classification task. For node classification, we run a k-NN classifier with \(k = 5\) on the learned node embeddings. We report performance in terms of Micro-F1 and Macro-F1 for evaluation of node classification. For dataset split, we randomly pick 20% nodes in each dataset for training and the remaining 80% for test. Results from 10 different random splits are averaged for the final report.

3.2 Performance Comparison (RQ1)

Experiment results are presented in Table 1. Overall, our proposed HORACE achieves the best unsupervised performance on almost all datasets. It is worth mentioning that our HORACE is competitive to and even better than several supervised counterparts.

Compared with traditional approaches based on random walks and matrix decomposition, our proposed GNN-based HORACE outperforms them by large margins. Particularly, HORACE improves metapath2vec and HERec by over 25% on ACM, which demonstrates the superiority of GNN that can leverage rich node attributes to learn high quality node representations for heterogeneous graphs.

For deep unsupervised learning methods, our HORACE achieves promising improvements as well. For the unsupervised version HAN-U that is trained with a simple reconstruction loss, its performance is even inferior to HERec on IMDb and DBLP despite its utilization of node attributes. This indicates that the reconstruction loss is insufficient to fully exploit the structural and semantic information for node-centric tasks such as node classification and clustering. Compared to DGI, a homogeneous contrastive learning method, HORACE accomplishes excellent performance on all datasets and evaluation tasks, especially on ACM and IMDb dataset, where large
improvements on both tasks are achieved. This validates the effectiveness of our proposed view-to-aggregation contrastive objective and structure-aware hard negative mining strategy.

Furthermore, experiments show that HORACE even outperforms its supervised baselines on ACM and IMDb datasets. It remarkably improves HAN by over 4% in terms of node classification Micro-F1 score on IMDb. This outstanding performance of HORACE certifies the superiority of our proposed heterogeneous graph contrastive learning framework such that it can distill useful information from each semantic view.

### 3.3 Close Inspections on Structure-Aware Hard Negative Mining Module (RQ2)

#### 3.3.1 Effectiveness of the module

We modify the negative bank in our contrastive objective to study the impact of structure-aware hard negative mining component. HORACE– denotes the model with synthesized harder samples \( \{h^m_j\}_{m=1}^M \) removed, where the negative bank \( B^c = \{h^m_j\}_{j\not\in i} \cup \{h^m_i\}_{j\not\in i} \) consists of only inter-view and intra-view negatives. We also construct a model variant HORACE-Sem, that discovers and synthesizes semantic negative samples using inner product of node embeddings.

The results are presented in Table 2. It is observed that HORACE improves consistently than HORACE– on all datasets for both node classification and clustering tasks. Especially for node clustering task on ACM, the gain reaches up to 15%. This verifies the effectiveness of our synthesizing hard negative sample strategy: giving larger weights to harder negative samples with the delicately designed synthesis term. Furthermore, the outstanding performance of HORACE compared to the model variant HORACE-Sem further justifies the superiority of structural-aware hard negative mining.

#### 3.3.2 Hyperparameters sensitivity analysis

We study how the two key parameters in the hard negative mining module affect the performance of HORACE: the number of synthesized hard negatives \( M \) and the threshold \( T \) in selecting top-\( T \) candidate hard negatives. Results on ACM under different parameter settings are obtained and reported by only varying one specific parameter and keeping all other parameters the same. As is shown in Figure 4a, the performance level of HORACE increases as the number of synthesized negatives \( M \) increases. This indicates that the learning of HORACE benefits from the synthesized hard negatives. For the parameter \( T \), as presented in Figure 4b, the model performance first rises with a larger \( T \), but soon the performance levels off and decreases as \( T \) increases further. We suspect that this is because a larger \( T \) will result in the selection of less hard negatives, reducing the benefits brought by our proposed hard negative sampling strategy.

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**Table 2: Effectiveness of the structure-aware hard negative mining module.**

| Method   | ACM  | IMDb | DBLP |
|----------|------|------|------|
|          | Mi-F1 | Ma-F1 | Mi-F1 | Ma-F1 |
| HORACE–  | 88.62 | 88.43 | 57.94 | 52.97 |
| HORACE-Sem | 90.24 | 90.18 | 58.95 | 52.38 |
| HORACE-PE | 91.40 | 91.45 | 58.96 | 53.73 |

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**Figure 4: Model performance with varied numbers of synthesized hard negatives and candidate hard negative samples \( T \) on the ACM dataset.**

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