Heterformer: A Transformer Architecture for Node Representation Learning on Heterogeneous Text-Rich Networks

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ABSTRACT

We study node representation learning on heterogeneous text-rich networks, where nodes and edges are multi-typed and some types of nodes are associated with text information. Although recent studies on graph neural networks (GNNs) and pretrained language models (PLMs) have demonstrated their power in encoding network and text signals, respectively, less focus has been given to deliberately coupling these two types of models on heterogeneous text-rich networks. Specifically, existing GNNs rarely model text in each node in a contextualized way; existing PLMs can hardly be applied to characterize graph structures due to their sequence architecture. In this paper, we propose Heterformer, a \textit{Heterogeneous GNN-nested transformer} that blends GNNs and PLMs into a unified model. Different from previous "cascaded architectures" that directly add GNN layers upon a PLM, our Heterformer \textit{alternately} stacks two modules — a graph-attention-based neighbor aggregation module and a transformer-based text and neighbor joint encoding module — to facilitate thorough mutual enhancement between network and text signals. Meanwhile, Heterformer is capable of characterizing network heterogeneity and nodes without text information. Comprehensive experiments on three large-scale datasets from different domains demonstrate the superiority of Heterformer over state-of-the-art baselines in link prediction, transductive/inductive node classification, node clustering, and semantics-based retrieval.

KEYWORDS

Text-Rich Network, Pretrained Language Model, Graph Neural Network.

1 INTRODUCTION

Networks are ubiquitously utilized to model real-world data such as academic graphs [35], product graphs [7], and social media [48]. Such networks often have two characteristics: (1) \textit{Heterogeneous}: nodes and edges in the network are multi-typed. For example, academic graphs [35] have paper, author, and venue nodes; product graphs [7] have purchase and view edges between users and products. (2) \textit{Text-rich}: some types of nodes are associated with text information. For instance, papers in academic graphs [35] have their titles and abstracts; tweets in social media networks [48] have their tweet contents. In such text-rich networks (Figure 1(a)), to achieve satisfactory performance in tasks such as link prediction [34], node classification [40], and recommendation [46], models need to jointly consider network structures and text semantics.

To encode network structures, representation learning on graphs [9, 41] has been extensively studied. However, early studies on “shallow” node embedding [8, 27] do not consider node attributes, thus cannot utilize text in each node; attributed node embedding methods [3] and graph neural networks (GNNs) [11, 19, 38, 40] assign an attribute vector (e.g., bag-of-words or context-free text embeddings [25]) to each node as its initial feature, but such context-free features are not strong enough to capture text semantics from the modern view of contextualized language models. For example, “transformer” in electrical engineering papers and “transformer” in machine learning papers should have different meanings given their context, but they are reflected in the same entry in bag-of-words and have the same context-free embedding.

To encode text semantics, transformer [37] is a powerful architecture featured by its fully connected attention mechanism. Taking transformer as the backbone, pretrained language models (PLMs) [4, 6, 21] learned from web-scale corpora can obtain contextualized semantics of words and documents. However, such models can hardly be adapted to encode network structure data due to their sequence architecture.

Because of the aforementioned limitations of GNNs and PLMs, it is imperative to explore a new model architecture that can collaborate their respective merits in representing network structures and text semantics, and can finally contribute to representation learning on heterogeneous text-rich networks. However, we identify three
challenges regarding the design of such an architecture, which are rarely considered in previous studies.

- **How to deeply couple GNNs and PLMs into a unified architecture?** Existing methods usually adopt a "cascaded architecture" [15, 20, 47, 52], where the text information of each node is first encoded via PLMs, then the node representations are aggregated via GNNs. (Figure 1(b) depicts this architecture.) In this way, text encoding and graph aggregation are operated consecutively, so network structures cannot provide hints to text understanding. However, according to network homophily [24], linked nodes have correlated semantics that can mutually clue each other. For example, given a paper on "LDA" and its authors who are experts in topic modeling. Based on the paper-author edges, "LDA" can be more likely interpreted as "Latent Dirichlet Allocation" rather than "Linear Discriminant Analysis". Thus, it is much needed to go beyond the "cascaded architecture" for better collaboration between GNNs and PLMs.

- **How to model network heterogeneity?** The recently proposed GraphFormers [43] introduces a GNN-nested transformer architecture. However, it focuses on homogeneous networks where all nodes/edges are of the same type. As mentioned at the beginning, a large number of real-world networks are heterogeneous. Different types of nodes/edges may naturally belong to different latent spaces and should be treated specifically. Moreover, it has been demonstrated that heterogeneous GNNs [12, 23, 40, 46] often outperform homogeneous GNNs [11, 19, 38] in various downstream tasks by capturing the diversity of node/edge types. Therefore, network heterogeneity should be considered in our unified architecture.

- **How to leverage textless nodes?** In heterogeneous networks, we cannot expect all types of nodes contain text information. Instead, in reality, there are both nodes associated with text (called text-rich, e.g., papers and tweets) and nodes without text information (called textless, e.g., users, authors, and venues). Most previous studies on homogeneous text-rich networks (e.g., GraphFormers [43]) are unaware of textless nodes. However, such textless nodes can be strong semantic indicators in the network. For example, given a venue node "KDD", its paper neighbors are likely related to "data mining". Moreover, textless nodes can indicate semantic relationships between text-rich nodes. For example, two papers sharing multiple authors should be of similar topics, so these authors can serve as bridges during information propagation. Thus, we should make full use of textless nodes in our model.

**Present Work.** Being aware of the three challenges above, we propose a heterogeneous GNN-nested transformer (Figure 1(e)), i.e., Heterformer, for node representation learning on text-rich networks. Specifically: (1) To deeply couple GNNs and PLMs into a unified model, we propose a graph-attention-based neighbor aggregation module and a transformer-based text and neighbor joint encoding module inside each Heterformer layer (Figure 1(c)). Different from the previous "cascaded architecture", our two modules are stacked alternately to form multiple GNN-nested transformer layers, where the parameters of each transformer layer are initialized by the corresponding layer in a PLM (e.g., BERT [6]). (2) To model network heterogeneity, we use type-specific transformation matrices to project different types of nodes into the same space. Also, for each text-rich node, our aggregation module collects information from its neighbors by characterizing node/edges types in graph attention. (3) To leverage textless nodes, we aggregate text-rich and textless neighbors into two embeddings respectively. Then, our joint encoding module employs a transformer encoder to fuse representations of each node’s text-rich neighbors, textless neighbors, and its own content via the fully connected attention mechanism. The overall model is optimized via an unsupervised link prediction objective [27]. We also demonstrate the importance of parameter initialization for Heterformer and propose methods to warm up the model before training.

The main contributions of our paper are summarized as follows:

- We formalize the problem of node representation learning on heterogeneous text-rich networks, which involves joint encoding of network structures and textual semantics.
- We propose a novel heterogeneous GNN-nested transformer architecture called Heterformer, which deeply couples GNNs and PLMs into a unified model while taking network heterogeneity and textless nodes into account.
- We conduct comprehensive experiments on three public text-rich networks from different domains and validate the superiority of Heterformer on various tasks, including link prediction, node classification, node clustering, and query-based retrieval.

## 2 PRELIMINARIES

In this section, we give an introduction to the concept of heterogeneous text-rich networks and define the problem of heterogeneous text-rich network node representation learning.

**Definition 2.1. Heterogeneous Networks** [33]. A heterogeneous network is defined as $G = (V, E, \mathcal{A}, \mathcal{R})$, where $V, E, \mathcal{A}, \mathcal{R}$ represent the sets of nodes, edges, node types, and edge types, respectively. $|\mathcal{A}| + |\mathcal{R}| > 2$. A heterogeneous network is also associated with a node type mapping function $\phi : V \rightarrow \mathcal{A}$ and an edge type mapping function $\psi : E \rightarrow \mathcal{R}$.

**Definition 2.2. Text-Rich Nodes and Textless Nodes.** In a heterogeneous network $G = (V, E, \mathcal{A}, \mathcal{R})$, $v \in V$ is text-rich if it is associated with text information. Otherwise, it is textless. We assume that nodes of the same type are either all text-rich or all textless. $a \in \mathcal{A}$ is a text-rich node type if for $\phi(v) = a$, $v$ is a text-rich node. Otherwise, $a$ is a textless node type.

**Definition 2.3. Heterogeneous Text-Rich Networks** [32, 47]. A heterogeneous network $G = (V, E, \mathcal{A}, \mathcal{R})$ is a heterogeneous text-rich network if $\mathcal{A} = \mathcal{A}_{\text{TR}} \cup \mathcal{A}_{\text{TL}}, \mathcal{A}_{\text{TR}} \cap \mathcal{A}_{\text{TL}} = \emptyset$ and $\mathcal{R} \neq \emptyset$, where $\mathcal{A}_{\text{TR}}$ and $\mathcal{A}_{\text{TL}}$ denote the sets of text-rich node types and textless node types, respectively.

**Problem Definition.** (Heterogeneous Text-Rich Network Node Representation Learning.) Given a heterogeneous text-rich network $G = (V, E, \mathcal{A}, \mathcal{R})$, where $\mathcal{A} = \mathcal{A}_{\text{TR}} \cup \mathcal{A}_{\text{TL}}, \mathcal{A}_{\text{TR}} \cap \mathcal{A}_{\text{TL}} = \emptyset$ and $\mathcal{R} \neq \emptyset$, the task is to build a model $f_{\Theta} : V \rightarrow \mathbb{R}^d$ with parameters $\Theta$ to learn node embedding vectors for both text-rich and textless nodes, taking heterogeneous network structures and text semantics into consideration. The learned node embeddings can be further utilized in downstream tasks, such as link prediction, node classification, node clustering, and semantics-based retrieval.
3 METHODOLOGY

In this section, we present the details of Heterformer. We lay out its architecture in Figure 2. Heterformer consists of three main parts: (1) a textless node encoding module based on node type semantics; (2) a text-rich node encoding module based on GNN-nested transformers; and (3) an unsupervised training module.

3.1 Textless Node Encoding

In real-world heterogeneous networks, textless nodes are of a large population and a wide variety. For example, in academic graphs (e.g., DBLP [35]), there are millions of author nodes and thousands of venue nodes, which are not naturally associated with text; in social networks (e.g., Twitter [42]), there are millions of user nodes and hashtag nodes which are textless. Although lack of text, those nodes can be quite important as they may contribute significant signals to their neighbors. For example, in an academic network, two papers published in the same venue can be of similar topics. Moreover, textless nodes can also be target nodes for downstream tasks such as author classification.

To align with how we encode text-rich nodes using transformer-based architectures [37] (which will be introduced in Section 3.2), a straightforward idea of textless node encoding is to represent each textless node \( v \) with a high-dimensional learnable embedding vector \( h_v \) (e.g., \( h_v \in \mathbb{R}^{768} \) to be compatible with BERT-base [6] used in text-rich node encoding). Nevertheless, the large population of textless nodes will then introduce a large number of parameters to our framework, which may finally lead to model underfitting. To overcome this challenge, we calculate \( h_v \) as follows,

\[
 h_v = W_{\phi_i} z_v, \quad \text{where} \; \phi(v) = \phi_i, \; \phi_i \in \mathcal{A}_{TL}. \tag{1}
\]

We set \( z_v \) up as a low-dimensional embedding vector of \( v \) (e.g., \( z_v \in \mathbb{R}^{64} \)) and project it into a more flexible high-dimensional space with a projection matrix \( W \). Due to node heterogeneity, different types of nodes can naturally belong to different latent semantic spaces. Therefore, for each kind of textless node type \( \phi_i \in \mathcal{A}_{TL} \), we design a type-specific projection matrix \( W_{\phi_i} \) for the transformation. It is worth noting that the column vectors of \( W_{\phi_i} \) can be viewed as "semantic topic embedding vectors" [5] for nodes in type \( \phi_i \), and each entry of \( z_v \) represents \( v \)'s weight towards one particular topic. In experiments, we find that good initialization of \( z_v \) and \( W_{\phi_i} \) is essential for model performance, and we will introduce our initialization strategy in Section 3.3.2.

3.2 Text-Rich Node Encoding

Given a text-rich node \( x \), its text information is denoted as \( T_x \); its text-rich and textless neighbors are denoted as \( \bar{N}_x = \{ t \mid (t, x) \in E, \phi(t) \in \mathcal{A}_{TR} \} \) and \( \bar{N}_x = \{ u \mid (u, x) \in E, \phi(u) \in \mathcal{A}_{TL} \} \), respectively. The two groups of neighbors make up \( x \)'s whole neighbor set \( N_x = \bar{N}_x \cup \bar{N}_x \). The text-rich node encoding module aims to learn the representation vector of node \( x \) by jointly considering \( T_x \), \( \bar{N}_x \), and \( \bar{N}_x \).

The text feature \( T_x \) is a sequence of tokens, with the [CLS] token inserted in the front, the hidden state of which is used for node representation. Following common practice of transformer [37], \( T_x \) is mapped into an initial sequence of embeddings \( H^{(0)}_x \) based on the summation of word embeddings and position embeddings. The embedding sequence is then encoded by Heterformer which is made up of multiple layers of GNN-nested transformers. In each Heterformer layer, there is a graph-attention-based neighbor information aggregation step and a transformer-based text and neighbor information joint encoding step.

3.2.1 Graph-Attention-based Neighbor Information Aggregation

Heterogeneous networks provide not only adjacency information between nodes but also type information of nodes/edges. To capture network homophily [24] indicated by node adjacency, we utilize neighbor embedding propagation and aggregation; to capture node/edge type information, we make such propagation and aggregation type-aware. In addition, text-rich neighbors \( \bar{N}_x \) and textless neighbors \( \bar{N}_x \) are distinguished during the aggregation process by being considered separately.
Text-Rich Neighbor Aggregation. Consider a text-rich neighbor $t \in \mathcal{N}_x$. The first token embedding (corresponding to [CLS]) is taken as its node representation for the $l$-th layer: $h_x^{(l)} = H_y^{(l)}[0]$. Inspired by the multi-head attention (MHA) mechanism in transformer architectures [37, 43], the text-rich neighbor aggregation vector $\tilde{h}_x^{(l)}$ of the $l$-th layer for $x$ is calculated as follows:

$$
\tilde{h}_x^{(l)} = \{ \text{head}^{(l)}(h_{x,i}^{(l)}, h_{x_{-x,i}}^{(l)} | \{ t \in \mathcal{N}_x \}) \},
$$

$$
\text{head}^{(l)}(h_{x,i}^{(l)}, h_{x_{-x,i}}^{(l)} | \{ t \in \mathcal{N}_x \}) = \sum_{t \in \mathcal{N}_x \cup \{ x \}} \alpha_{x,i}^{(l)} W_V^i h_{x_{-x,i}}^{(l)},
$$

$$
\alpha_{x,i}^{(l)} = \text{softmax}(e_{x,i}^{(l)}) = \frac{\exp(e_{x,i}^{(l)})}{\sum_{u \in \mathcal{N}_x \cup \{ x \}} \exp(e_{u,i}^{(l)})},
$$

where $\alpha_{x,i}^{(l)}$ denotes the relative importance of a neighbor $i$ to center node $x$. $h_{x,i}^{(l)}$ and $h_{x_{-x,i}}^{(l)}$ denote $i$-th token embedding (corresponding to [CLS]) and the edge between $x$ and $i$, respectively.

Textless Neighbor Aggregation. For a textless neighbor $u \in \mathcal{N}_x$, we follow the way in Sec. 3.1 to obtain its embedding vector for the $l$-th layer: $h_u^{(l)} = W_{\phi_i} z_u$, where $\phi(u) = \phi_i$. Based on the MHA mechanism in transformers, the textless neighbor aggregation vector $\tilde{h}_u^{(l)}$ of the $l$-th layer for $u$ is calculated as follows:

$$
\tilde{h}_u^{(l)} = \{ \text{head}^{(l)}(h_{u,i}^{(l)}, h_{u_{-x,i}}^{(l)} | \{ t \in \mathcal{N}_x \}) \},
$$

$$
\text{head}^{(l)}(h_{u,i}^{(l)}, h_{u_{-x,i}}^{(l)} | \{ t \in \mathcal{N}_x \}) = \sum_{u \in \mathcal{N}_x \cup \{ x \}} \alpha_{x,i}^{(l)} W_V^i h_{u_{-x,i}}^{(l)},
$$

$$
\alpha_{x,i}^{(l)} = \text{softmax}(e_{x,i}^{(l)}) = \frac{\exp(e_{x,i}^{(l)})}{\sum_{u \in \mathcal{N}_x \cup \{ x \}} \exp(e_{u,i}^{(l)})},
$$

where $\alpha_{x,i}^{(l)}$ denotes the relative importance of a neighbor $i$ to center node $x$. $h_{u,i}^{(l)}$ and $h_{u_{-x,i}}^{(l)}$ denote $i$-th token embedding (corresponding to [CLS]) and the edge between $u$ and $i$, respectively.

Neighborhood Embedding Dispatch. Both text-rich and textless neighbor aggregation vectors are then concatenated to $H_x^{(l)}$, the text embedding sequence of $x$ in layer $l$, as follows:

$$
\tilde{H}_x^{(l)} = \tilde{h}_x^{(l)} \| \tilde{H}_y^{(l)} \| \tilde{h}_y^{(l)}.
$$

Here, the graph-augmented token embedding sequence $\tilde{H}_x^{(l)}$ contains not only $x$’s text semantics but also information from both its text-rich and textless neighbors.

3.2.2 Transformer-based Text and Neighbor Information Joint Encoding. After obtaining $\tilde{H}_x^{(l)}$ in layer $l$, we utilize a transformer layer [37] to encode the original text semantics and neighbor information jointly and obtain token embeddings as input to the next layer. The encoding process is as follows:

$$
\tilde{H}_x^{(l+1)} = \text{Normalize}(H_x^{(l)} + \text{MHA}_y(\tilde{H}_x^{(l)})),
$$

$$
H_y^{(l+1)} = \text{Normalize}(H_y^{(l)} + \text{MLP}(\tilde{H}_y^{(l)})).
$$

In the equation, Normalize(·) and MLP(·) are layer normalization [1] and multi-layer perceptron, respectively. MHA_y(·) denotes asymmetric multi-head self-attention. Formally, let $\tilde{H}_x \in \mathbb{R}^{d \times (s+2)}$ be the graph-augmented token embedding sequence.

$$
\text{MHA}_y(\tilde{H}_x) = \{ \text{head}^{(l)}(\tilde{H}_x,i),
$$

$$
\text{head}^{(l)}(\tilde{H}_x,i) = V_{x,i} \cdot \text{softmax}(K_{x,i}^T Q_{x,i}) \sqrt{d/k},
$$

where $H_x \in \mathbb{R}^{d \times s}$ and $\tilde{H}_x \in \mathbb{R}^{d \times (s+2)}$ represent the $i$-th chunk of $H_x$ and $\tilde{H}_x$ respectively; $s$ is the length of $T_x$; $W_Q, W_K, W_V$ are query, key, and value projection matrices, respectively. The transformer layer here encodes both token embeddings in the previous layer and neighbor aggregation embeddings. As a result, the output will contain signals from both text semantics and neighbor information of $x$. $H_x^{(l+1)}$ has the same size as $H_x^{(l)}$ and will be utilized as the input token embedding sequence to the next layer.

3.2.3 Discussion. It is worth noting that, the graph-attention-based neighbor aggregation step and the transformer-based joint encoding step are stacked alternately, while the initial token embedding sequence is encoded by the first transformer layer. Our proposed Heterformer is essentially a GNN-nested transformer structure (Figure 1(c)) rather than a GNN-cascaded transformer structure (Figure 1(b)) proposed in previous studies [15, 20, 22, 51, 52]. In addition, given a center node with $M$ text-rich neighbors (each of which has $P$ tokens) and $N$ textless neighbors, the time complexity of each Heterformer layer’s encoding step is $O(P^2 (M + 1) + M + N)$, which is on par with the complexity $O(P^2 (M + 1))$ of per GNN-cascaded transformers layer since $M, N \ll P^2 M$. Another straightforward idea of fusing center node text information with its neighbor representations is to directly concatenate token embeddings of the center node, its text-rich neighbors, and its textless neighbors together and feed them into a PLM. However, in this way, the time complexity of one such layer becomes $O((P(M + 1) + N)^2)$, which is significantly larger than that of our method. Further Discussion of time complexity can be found in Section A.2.
3.3 Model Training

3.3.1 Training Objective. To train our model, we define the following likelihood objective with parameters $\Theta$:

$$\max_{\Theta} O = \prod_{u \in V} \prod_{v \in N_u} p(u|v; \Theta),$$

(7)

Here, the conditional probability $p(u|v; \Theta)$ is calculated as follows:

$$p(u|v; \Theta) = \frac{\exp(h_u^v h_v)}{\sum_{u' \in V, \phi(u') \in \mathcal{A}_{TR}} \exp(h_{u'}^v h_v) + \sum_u \exp(h_u^v h_v)},$$

(8)

where $h_u = h_u^{(L+1)}$ is the output node embedding generated by Heterformer with parameters $\Theta$. $L$ is the number of layers in Heterformer. However, calculating Eq. (7) requires enumerating all $(u, v)$ pairs, which is costly on big graphs. To make the calculation more efficient, we leverage the negative sampling technique [14, 25] to simplify the objective and obtain our loss function below.

$$\min_{\Theta} L = \sum_{u \in V} \sum_{v \in N_u} -\log \frac{\exp(h_u^v h_v)}{\exp(h_u^v h_v) + \sum_u \exp(h_u^v h_v)},$$

(9)

In the equation above, $u'$ stands for a random negative sample. In our implementation, we use “in-batch negative samples” [17, 43] to reduce the encoding cost.

3.3.2 Parameter Initialization. It is shown in [10] that good parameter initialization before downstream task fine-tuning is essential for deep learning models. Recently, significant improvements achieved by PLMs [4, 6, 21] in various NLP tasks have also demonstrated this finding. In this section, we discuss ways to make good initialization for parameters in Heterformer.

Token Embeddings & Transformer Layers. A large proportion of parameters in Heterformer are token embeddings and parameters in transformer layers. Fortunately, these parameters are well-pre-trained in many PLMs [2, 4, 6, 21, 29, 44]. As a result, Heterformer can directly load this part of initial parameters from a PLM.

Textless Node Embeddings. Another main proportion of parameters appear in textless node embeddings $z_u$ and projection matrices $W_{\phi}$. To distill information from semantic-rich PLMs into textless node embeddings, we conduct warm-up training as shown below:

$$\min_{h_u} L_u = \sum_{u \in V} \sum_{v \in N_u} \sum_{\phi(u) \in \mathcal{PLM}, \phi(v) \in \mathcal{TR}} -\log \frac{\exp(h_u^v h_v)}{\exp(h_u^v h_v) + \sum_u \exp(h_u^v h_v)},$$

(10)

where $u'$ is a text-rich node as negative sample; $h_u$ is the encoding vector of the textless node $u$ in Section 3.1; $h_v$ is the output vector of a PLM after encoding the text-rich node $v$. Note that parameters in the PLM are fixed here to make this warm-up process efficient. The PLM utilized here should be the same with that loaded for transformer layers. After the warm-up, semantic information from the PLM will be transferred to textless node embeddings. We will demonstrate the effectiveness of this process in Section 4.6.2.

4 EXPERIMENT

4.1 Experimental Settings

4.1.1 Datasets. We conduct experiments on three datasets (i.e., DBLP [35], Twitter [48], and Goodreads [39]) from three different domains (i.e., academic papers, social media posts, and books). For DBLP, we extract papers published from 1990 to 2020 with their author and venue information. For Twitter, we merge the original LA and NY datasets to form a larger dataset. For Goodreads, we remove books without any similar books, and the remaining books with their meta-data fields form the dataset. The main statistics of the three datasets are summarized in Table 1, and the detailed information can be found in Section A.4.

| Dataset  | Node | Edge |
|----------|------|------|
| DBLP     | # paper*: 5,597,191 | # paper-paper: 36,787,329 |
|          | # venue: 28,638 | # venue-paper: 3,633,613 |
|          | # author: 2,717,797 | # author-paper: 10,212,497 |
| Twitter  | # tweet*: 279,694 | # tweet-POI: 279,694 |
|          | # POI: 36,895 | # user-tweet: 195,785 |
|          | # hashtag: 72,297 | # hashtag-tweet: 194,939 |
|          | # user: 76,398 | # mention: 24,089 |
|          | # mention: 24,089 | # mention: 24,089 |
| Goodreads| # book*: 1,097,438 | # book-book: 11,745,415 |
|          | # shelves: 6,632 | # shelves-book: 27,599,160 |
|          | # author: 205,891 | # author-book: 1,089,145 |
|          | # format: 768 | # format-book: 588,677 |
|          | # publisher: 62,934 | # publisher-book: 59,456 |
|          | # language code: 139 | # language code-book: 485,733 |

4.1.2 Baselines. We compare Heterformer with two groups of baselines: GNN-cascaded transformers and GNN-boosted transformers. The former group can be further classified into homogeneous GNN-cascaded transformers, including BERT+MeanSAGE [11], BERT+MaxSAGE [11] and BERT+GAT [38], and heterogeneous GNN-cascaded transformers, including BERT+RGCN [30], BERT+HAN [40], BERT+HGT [12] and BERT+SHGN [23]. The latter group includes the recent GraphFormers [43] model. However, GraphFormers can only deal with homogeneous textual networks. To apply it to heterogeneous text-rich networks, we add heterogeneous graph propagation and aggregation in its final layer. This generalized model is named GraphFormers++. To verify the importance of both text and network information in text-rich networks, we also include vanilla GraphSAGE [11] and vanilla BERT [6] in comparison. The details of all baselines can be found in Appendix A.3.

4.1.3 Reproducibility. For all compared models, we adopt the same training objective and the 12-layer BERT-base-uncased [6] as the backbone PLM. The Adam optimizer [18] with a learning rate 1e-5 and in-batch negative samples with training batch size 30 are used to fine-tune the model. In-batch testing is used for efficiency and the test batch size is 100, 300, 100 for DBLP, Twitter, and Goodreads, respectively. The maximum length of the PLM is set to be 32, 12,
and 64 on the three datasets according to their average document length. For heterogeneous GNN approaches, the embedding size of textless nodes is 64. We run experiments on one NVIDIA RTX A6000 GPU. Detailed information on experimental settings can be found in Section A.4 and Section A.5.

Following previous studies on network representation learning, we consider three fundamental tasks for quantitative evaluation: link prediction, node classification, and node clustering.

### 4.2 Link Prediction

**Settings.** Link prediction aims to predict missing edges in a network. In order to evaluate the models’ ability to encode both text semantics and network structure, we focus on link prediction between two text-rich nodes. Specifically, on DBLP, Twitter, and Goodreads, the prediction is between paper-paper, tweet-tweet, and book-book, respectively. The model is trained and tested with in-batch negative sampling and we adopt 70-10-20 train-dev-test split. Precision@1 (PREC), Mean Reciprocal Rank (MRR), and Normalized Discounted Cumulative Gain (NDCG) are used as evaluation metrics. Given a query node \(u\), PREC measures whether the key node \(v\) linked with \(u\) is ranked the highest in the batch; MRR calculates the average of the reciprocal ranks of \(v\); NDCG further takes the order and relative importance of \(v\) into account and here we calculate on the full candidate list, the length of which equals to test batch size.

**Results.** Table 2 shows the performance of all compared methods. From Table 2, we can observe that: (a) Heteroformer outperforms all the baseline methods consistently; (b) Transformer+GNN models perform better than both vanilla GNN and vanilla BERT, which demonstrates the importance of encoding both text and network signals in text-rich networks; (c) GNN-nested transformers including Heteroformer, GraphFormers, and GraphFormers++ are more powerful than GNN-cascaded transformers; (d) By considering heterogeneity, Heteroformer can have better performance than GraphFormers in heterogeneous text-rich networks, but the improvement depends on how heterogeneity is utilized; (e) Heteroformer yields a large performance improvement when network is more dense and heterogeneous (i.e., DBLP, Goodreads vs. Twitter).

### 4.3 Node Classification

**Settings.** In node classification, we train a 2-layer MLP classifier to classify nodes based on the output node representation embeddings of each method. The experiment is conducted on DBLP and Goodreads (because node labels are available in these two datasets) for both text-rich and textless nodes. For text-rich node classification, we focus on paper nodes and book nodes in DBLP and Goodreads, respectively. We select the most frequent 30 classes in DBLP and keep the original 10 classes in Goodreads. Also, we study both transductive and inductive node classification to understand the capability of our model comprehensively. For transductive node classification, the model has seen the classified nodes during representation learning (using the link prediction objective), while for inductive node classification, we focus on author nodes in both DBLP and Goodreads. The label of each author is obtained by aggregating the labels of his/her publications. We separate the whole dataset into train set, validation set, and test set in 7:1:2 in all cases and each experiment is repeated 5 times in this section with the average performance reported.

**Results.** Tables 3 and 4 demonstrate the results of different methods in transductive and inductive text-rich node classification. We observe that: (a) our Heteroformer outperforms all the baseline methods significantly on both tasks, showing that Heteroformer can learn more effective node representations for these tasks; (b) Heterogeneous GNN-based methods generally achieve better results than homogeneous GNN-based methods, which demonstrates the necessity of encoding heterogeneity in heterogeneous text-rich networks; (c) Heteroformer generalizes quite well on unseen nodes as its performance on inductive node classification is quite close to that on transductive node classification. Moreover, Heteroformer even achieves higher performance in inductive settings than the baselines do in transductive settings. Table 5 reports the result on textless node classification, where we have the following findings: (a) Heteroformer outperforms all heterogeneous GNN-based methods significantly; (b) Compared with text-rich node classification, the improvement of Heteroformer on textless node classification over baselines is more significant, indicating that Heteroformer better captures neighbors’ text semantics in textless node representations.
Table 3: Transductive text-rich node classification.

| Method          | DBLP               | Goodreads          |
|-----------------|--------------------|--------------------|
|                 | PREC | NDCG  | PREC | NDCG  |
| BERT            | 0.73098 | 0.84403 | 0.97510 | 0.93349 |
| BERT+MaxSAGE    | 0.73737 | 0.84706 | 0.97985 | 0.94029 |
| BERT+MeanSAGE   | 0.73845 | 0.84756 | 0.97950 | 0.93902 |
| BERT+GAT        | 0.72164 | 0.83734 | 0.97660 | 0.93418 |
| GraphFormers    | 0.74169 | 0.85111 | 0.97919 | 0.93861 |
| BERT+HAN        | 0.72303 | 0.83834 | 0.97692 | 0.93493 |
| BERT+HGT        | 0.76753 | 0.86559 | 0.98169 | 0.94265 |
| BERT+SHGN       | 0.72316 | 0.83835 | 0.97708 | 0.93451 |
| GraphFormers++  | 0.75955 | 0.86058 | 0.98187 | 0.94370 |
| Heterformer     | 0.77572* | 0.87062* | 0.98140* | 0.94794* |

Table 4: Inductive text-rich node classification.

| Method          | DBLP               | Goodreads          |
|-----------------|--------------------|--------------------|
|                 | PREC | NDCG  | PREC | NDCG  |
| BERT            | 0.71782 | 0.83493 | 0.96373 | 0.91734 |
| BERT+MaxSAGE    | 0.72987 | 0.84266 | 0.97746 | 0.93670 |
| BERT+MeanSAGE   | 0.73058 | 0.84285 | 0.97697 | 0.93552 |
| BERT+GAT        | 0.71328 | 0.83205 | 0.97345 | 0.93035 |
| GraphFormers    | 0.73634 | 0.84652 | 0.97667 | 0.93512 |
| BERT+HAN        | 0.71233 | 0.83371 | 0.97365 | 0.93057 |
| BERT+HGT        | 0.75917 | 0.86049 | 0.97890 | 0.93869 |
| BERT+SHGN       | 0.71512 | 0.83306 | 0.97365 | 0.93099 |
| GraphFormers++  | 0.75906 | 0.85534 | 0.97984 | 0.94027 |
| Heterformer     | 0.76700* | 0.86526* | 0.98243* | 0.94513* |

Table 5: Textless node classification.

| Method          | DBLP               | Goodreads          |
|-----------------|--------------------|--------------------|
|                 | PREC | NDCG  | PREC | NDCG  |
| BERT+HAN        | 0.37760 | 0.56270 | 0.71567 | 0.82017 |
| BERT+HGT        | 0.38450 | 0.56980 | 0.71544 | 0.81726 |
| BERT+SHGN       | 0.37791 | 0.56348 | 0.71514 | 0.82048 |
| BERT+RGCN       | 0.42891 | 0.61775 | 0.77566 | 0.85823 |
| GraphFormers++  | 0.38306 | 0.57133 | 0.72831 | 0.82692 |
| Heterformer     | 0.52369* | 0.68410* | 0.82459* | 0.88109* |

4.5 Query-based Retrieval: Case Study

To further demonstrate the capability of Heterformer in encoding text semantics, we now present a case study of query-based paper retrieval on DBLP.

**Settings.** The models are asked to retrieve relevant papers for a user-given query based on the inner product of the encoded query embedding and the paper embedding, where the query embedding is obtained by encoding query text only with each model.

**Results.** Table 7 lists the top-7 papers for the query “news recommendation with personalization” retrieved by BERT, GraphFormers, and Heterformer. It is shown that our model can have more accurate retrieved results than both baselines. In fact, according to network homophily [24], papers on the same topics (e.g., personalization/news recommendation) are likely to have connections (i.e., become text-rich neighbors) or share similar meta-data (i.e., share similar textless neighbors). While BERT can consider text information only and GraphFormers enrich text information with text-rich neighbors only, our Heterformer is capable of utilizing both text-rich neighbors and textless neighbors to complement text signals via graph-attention-based aggregation and transformer-based joint encoding (Section 3.2), which finally contributes to higher retrieval accuracy.

4.6 Ablation and Parameter Studies

4.6.1 Ablation Study on Graph Neighbor Aggregation.

used here again, but nodes with more than one ground-truth label are filtered. The number of clusters $K$ is set as the number of classes. For DBLP, since the dataset is quite large, we pick the 10 most frequent classes and randomly select 20,000 nodes for efficient evaluation. NMI and ARI [13] are used as evaluation metrics. Since the performance of KMeans can be affected by the initial centroids, we run each experiment 10 times and report the average performance.

In addition to quantitative evaluation, we conduct visualization to depict the distribution of Heterformer embeddings, where t-SNE [36] is utilized to project node embeddings into a 2-dimensional space and the nodes are colored based on their ground-truth label.

**Results.** The quantitative result can be found in Table 6, where Heterformer is the best on DBLP and outperforms most baselines on Goodreads. The embedding visualization result of Heterformer is presented in Figure 3. In both datasets, the clustering structure is quite evident, indicating that node representations learned by Heterformer are class-discriminative, even though the training process is based on link prediction only.
Table 7: Case study of query-based retrieval on DBLP. Top-7 retrieved papers are shown for each method.

| Query: News recommendation with personalization | Retrieved Paper Title |
|------------------------------------------------|------------------------|
| (a) DBLP Validation PREC | (b) Goodreads Validation PREC |

Figure 4: Ablation study on neighbor aggregation.

Figure 5: Performance of Heterformer during training process with and without textless node warm-up.

Figure 6: Effect of textless node embedding dimension.

5 RELATED WORK

5.1 Heterogeneous Graph Neural Networks

Graph neural networks (GNNs) such as GCN [19], GraphSAGE [11], and GAT [38] have been widely adopted in representation learning on graphs. Since real-world objects and interactions are often multi-typed, recent studies have considered extending GNNs to heterogeneous graphs [33]. The basic idea of heterogeneous graph neural networks (HGNNs) is to leverage node types, edge types, and meta-path semantics [34] in projection and aggregation. For example, RGCN [30] uses a weighted sum of graph convolution with different edge types; HAN [40] proposes a hierarchical attention mechanism to capture both node and meta-path importance; HetGNN [46] uses random walks with restart to sample neighbors and then performs aggregation within each node type and among different node types; GATNE [3] aggregates information from neighbors according to edge types and applies to both transductive and inductive settings; GTN [45] automatically learns meaningful meta-paths and then performs graph convolution over meta-path neighbors; HGT [12] proposes an architecture similar to transformer [37] to carry out attention on edge types. For more HGNN models, one can refer to recent surveys [9, 41]. Lv et al. [23] further perform a benchmark study of 12 HGNNs and propose a simple HGNN model based on GAT. Despite the success of these models, when some types of nodes carry text information, they lack the power of handling textual signals in a contextualized way.
In contrast, Heterformer jointly models text and node semantics in each transformer layer.

5.2 Pretrained Language Models

Pretrained language models (PLMs) aim to learn general language representations from large-scale corpora, which can be used to perform downstream text-related tasks. Early studies on PLMs mainly focus on context-free text embeddings such as word2vec [25] and GloVe [26]. Recently, motivated by the fact that the same word can have different meanings conditioned on different contexts, deep language models such as ELMo [28], BERT [6], RoBERTa [21], XLNet [44], ELECTRA [4], and GPT [2, 29] are proposed to learn contextualized word representations. These models employ the transformer architecture [37] to capture long-range and high-order semantic dependency and achieve significant improvement on many downstream NLP tasks. However, these models only utilize text information in the corpora. In contrast, Heterformer leverages both text and network signals when the latter is available.

5.3 Text-Rich Networks

Most previous studies on homogeneous text-rich networks adopt a “cascaded architecture” [15, 20, 22, 51, 52], where the text information of each node is first encoded via transformers, then the node representations are aggregated via GNNs. One drawback of such models is that text and network signals are processed consecutively, so the network information cannot benefit text encoding. To overcome this drawback, GraphFormers [43] introduces GNN-nested transformers so that text and node features can be encoded jointly. However, GraphFormers assumes that the network is homogeneous and all nodes have text information. These assumptions do not hold in real-world text-rich networks. Most previous studies on heterogeneous text-rich networks focus on specific text-related tasks. For example, HyperMine [32] and NetTaxo [31] study how network structures can benefit taxonomy construction from text corpora; LTRN [49] and MATCH [50] leverage document metadata for network structures can benefit taxonomy construction from text corpora. In contrast, Heterformer leverages the joint text-graph encoding framework of GraphFormers to heterogeneous text-rich networks.

6 CONCLUSIONS

In this paper, we introduce the problem of node representation learning on heterogeneous text-rich networks and propose Heterformer, a heterogeneous GNN-nested transformer architecture to address the problem. Different from previous “cascaded architectures”, Heterformer alternately stacks a graph-attention-based aggregation module and a transformer-based text and neighbor joint encoding module. Experimental results on various graph mining tasks, including link prediction, node classification, node clustering, and query-based retrieval, demonstrate the superiority of Heterformer. Moreover, the proposed framework can serve as a building block with different task-specific inductive biases. It would be interesting to see its future applications on real-world text-rich networks such as recommendation, abuse detection, tweet-based network analysis, and text-rich social network analysis.

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A SUPPLEMENTARY MATERIAL

A.1 Summary of Heterformer’s Encoding Procedure

Algorithm 1: Encoding Procedure of Heterformer

Input: The center node x, its text-rich neighbors N_t and textless neighbors N_x. Initial token sequence encoding H^{(0)}_t for t ∈ N_x ∪ {x}.

Output: The embedding h_x of the center node x.

begin
// obtain text-rich nodes’ first layer encoded token embeddings
for t ∈ N_x ∪ {x} do
    H^{(1)}_t ← Normalizer(H^{(0)}_t + MHA^{(0)}(H^{(0)}_t));
end
// textless initial embedding
for u ∈ N_x do
    z_u ← WarmUp(u);
end
for l = 1,...,L do
    // text-rich neighbor aggregation
    for t ∈ N_x ∪ {x} do
        h^{(l)}_t ← h^{(l)}_t[CLS];
    end
    // GNN
    h^{(l)}_x ← GNN([h^{(l)}_t | t ∈ N_x ∪ {x}]);
    // textless neighbor aggregation
    for u ∈ N_x do
        h^{(l)}_u ← W^{(l)}_φ z_u, where φ(u) = φ;
    end
    // obtain the center node’s token embedding for next layer
    h^{(l)}_x ← h^{(l)}_x + MHA^{(l)}(h^{(l)}_x);
    h^{(l+1)}_x ← Normalizer(h^{(l)}_x + MLP^{(l)}(h^{(l)}_x));
end
// update text-rich neighbors’ token embeddings
for t ∈ N_x do
    H^{(l)}_t ← Normalizer(H^{(l)}_t + MHA^{(l)}(H^{(l)}_t));
end
return h_x ← H^{(L+1)}_x[CLS];

A.2 Complexity Analysis

Given a center node with M text-rich neighbors (each of which has P tokens) and N textless neighbors, the time complexity of each Heterformer layer’s encoding step is O(P^2(M + 1) + M + N), which is on par with the complexity O(P^2(M + 1)) of per GNN-cascaded transformer layer since M, N ≪ P^2M. The time complexity of our warm-up process is O(MN) ≪ O(P^2(M + 1)). An empirical efficiency comparison among BERT+MeanSAGE, GraphFormers, and Heterformer is shown in Table 8. We run each model for one mini-batch and report the average running time.

Table 8: Time cost per mini-batch for BERT+MeanSAGE, GraphFormers and Heterformer.

| Model              | DBLP | Goodreads |
|--------------------|------|-----------|
| BERT+MeanSAGE      | 256.18ms | 440.18ms |
| GraphFormers       | 289.04ms | 490.27ms |
| Heterformer        | 313.87ms | 508.27ms |

A.3 Details of Baselines

We have 11 baselines including vanilla text/graph encoding models, GNN-cascaded transformers, and GNN-nested transformers.

Vanilla text/graph models:
- MeanSAGE [11]: This is a GNN method utilizing the mean function to aggregate information from neighbors for center node embedding learning. The initial node feature vector is bag-of-words weighted by TF-IDF. The number of entries in each attribute vector is the vocabulary size of the corresponding dataset, where we keep the most representative 10000, 2000, and 5000 words for DBLP, Twitter, and Goodreads, respectively, according to the corpus size.
- BERT [6]: This is a benchmark PLM pretrained on two tasks: next sentence prediction and mask token prediction. For each text-rich node, we use BERT to encode its text and take the output of the [CLS] token as node representation.

Homogeneous GNN-cascaded transformers:
- BERT+MeanSAGE [11]: We stack BERT with MeanSAGE (i.e., using the output text representation of BERT as the input node attribute vector of MeanSAGE). The BERT+MeanSAGE model is trained in an end-to-end way. Other BERT+GNN baselines below have the same cascaded architecture.
- BERT+MaxSAGE [11]: MaxSAGE is a GNN method utilizing the max function during neighbor aggregation for center node representation learning.
- BERT+GAT [38]: GAT is a GNN method with attention-based neighbor importance calculation, and the weight of each neighbor during aggregation is based on its importance score.

Homogeneous GNN-nested transformers:
- GraphFormers [43]: This is the state-of-the-art GNN-nested transformer model, which has graph-based propagation and aggregation in each transformer layer. Since homogeneous baselines assume all nodes are associated with text information, when applying them to our datasets, we remove all textless nodes. Therefore, homogeneous baselines cannot be used for textless node classification (i.e., Table 5).

Heterogeneous GNN-cascaded transformers:
- BERT+RGCN [30]: RGCN is a heterogeneous GNN model. It projects neighbor representations into the same latent space according to the edge types. The initial embeddings for textless nodes are initialized using RGCN’s heterogeneous propagation.
nodes are learnable vectors for baselines in this section which is the same to Heterformer.

- **BERT+HAN** [40]: HAN is a heterogeneous GNN model. It proposes a heterogeneous attention-based method to aggregate neighbor information.

- **BERT-HGT** [12]: HGT is a heterogeneous GNN model. Inspired by the transformer architecture, it utilizes multi-head attention to aggregate neighbor information obtained by heterogeneous message passing.

- **BERT-SHGN** [23]: SHGN is a heterogeneous GNN model. Motivated by the observation that GAT is more powerful than many heterogeneous GNNs [23], it adopts GAT as the backbone with enhancements from learnable edge-type embeddings, residual connections, and normalization on the output embeddings.

**Heterogeneous GNN-nested transformers:**

- **GraphFormers++** [43]: To apply GraphFormers to heterogeneous text-rich networks, we add heterogeneous graph propagation and aggregation in its final layer. The generalized model is named GraphFormers++.

### A.4 Dataset Description

**A.4.1 Training.** We train our model in an unsupervised way via link prediction. For each paper in DBLP, we select one neighbor paper for it and construct a positive node pair. For each POI in Twitter, we select one neighbor tweet for it to become a positive node pair. For each book in Goodreads, one neighbor book is selected where we build a positive node pair. All these node pairs are used as positive training samples. The model is then trained via in-batch negative sampling.

**A.4.2 Link Prediction.** The training, validation, and testing sets in this section are the same as those in Section A.4.1.

**A.4.3 Node classification.** The 30 classes of DBLP papers are: "Artificial intelligence", "Mathematics", "Machine learning", "Computer vision", "Computer network", "Mathematical optimization", "Pattern recognition", "Distributed computing", "Data mining", "Real-time computing", "Algorithm", "Control theory", "Discrete mathematics", "Engineering", "Electronic engineering", "Theoretical computer science", "Combinatorics", "Knowledge management", "Multimedia", "Computer security", "World Wide Web", "Human-computer interaction", "Control engineering", "Parallel computing", "Information retrieval", "Software", "Artificial neural network", "Communication channel", "Simulation", and "Natural language processing".

The 10 classes of Goodreads books are: "children", "fiction", "poetry", "young-adult", "history", "historical fiction", "biography", "fantasy", "paranormal", "non-fiction", "mystery", "thriller", "crime", "comics", "graphic", and "romance".

**A.4.4 Node Clustering.** For DBLP, since the dataset is quite large, we pick the most frequent 10 classes and randomly select 20,000 nodes for efficient evaluation. The 10 selected classes are: "Artificial intelligence", "Mathematics", "Machine learning", "Computer vision", "Computer network", "Mathematical optimization", "Pattern recognition", "Distributed computing", "Data mining", and "Real-time computing". For Goodreads, we use all the 10 classes in the original dataset for clustering.

### A.4.5 Embedding Visualization

In this section, we use t-SNE [36] to project node embeddings into low-dimensional spaces. Nodes are colored based on their ground-truth labels. To make the visualization clearer, we select 4 naturally separated classes for DBLP and 5 for Goodreads. The 4 selected classes in DBLP are "Mathematics", "Computer network", "Information retrieval", and "Electronic engineering". The 5 selected classes in Goodreads are "fiction", "romance", "mystery, thriller, crime", "non-fiction", and "children".

Besides 2D embedding visualization already shown in Figure 3, we also show 3D embedding visualization in Figure 7.

**Figure 7: 3D embedding visualization.**

### A.5 Reproducibility Settings

**A.5.1 Hyper-parameters.** For a fair comparison, the training objective for all compared methods including Heterformer and baselines are the same. The hyper-parameter configuration for the node representation learning process can be found in Table 9, where "neighbor sampling" means the number of each type of neighbors sampled for the center node during learning.

In Section 4.3, we adopt a multi-layer perceptron (MLP) with 3 layers and hidden dimension 200 to be our classifier. We employ Adam optimizer [18] and early stop 10 to train the classifier. For text-rich node classification, the learning rate is set as 0.001. While for textless node classification, the learning rate is 0.01.

**Table 9: Hyper-parameter configuration.**