NAGphormer: Neighborhood Aggregation Graph Transformer for Node Classification in Large Graphs

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Abstract

Graph Transformers have demonstrated superiority on various graph learning tasks in recent years. However, the complexity of existing Graph Transformers scales quadratically with the number of nodes, making it hard to scale to graphs with thousands of nodes. To this end, we propose a Neighborhood Aggregation Graph Transformer (NAGphormer) that is scalable to large graphs with millions of nodes. Before feeding the node features into the Transformer model, NAGphormer constructs tokens for each node by a neighborhood aggregation module called Hop2Token. For each node, Hop2Token aggregates neighborhood features from each hop into a representation, and thereby produces a sequence of token vectors. Subsequently, the resulting sequence of different hop information serves as input to the Transformer model. By considering each node as a sequence, NAGphormer could be trained in a mini-batch manner and thus could scale to large graphs. NAGphormer further develops an attention-based readout function so as to learn the importance of each hop adaptively. We conduct extensive experiments on various popular benchmarks, including six small datasets and three large datasets. The results demonstrate that NAGphormer consistently outperforms existing Graph Transformers and mainstream Graph Neural Networks.

1 Introduction

Graph Neural Networks (GNNs) [7, 22, 33], owing to the message passing mechanism [17], have been recognized as a type of powerful deep learning techniques for graph learning tasks [36, 13, 38, 40, 20] over the last decade. Though effective, however, message passing-based GNNs have a number of inherent limitations, including over-smoothing [4] and over-squashing [1] with the increment of the model depth, limiting their potential capability for graph representation learning.

Transformers [32], on the other hand, are well-known deep learning architectures that have shown superior performance in a variety of Euclidean data, such as natural languages [10, 25] and images [11, 26]. Due to their great modeling capability, researchers have increasingly focused on generalizing Transformers to non-Euclidean data, such as to graphs [12, 24, 37, 19]. In contrast, graph-structured data generally contains more complicated properties, including structural topology and edge features. These properties cannot be directly encoded into Transformers as the tokens.

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Existing Graph Transformers have developed three strategies to address this issue [28]. (I) To capture the structural feature of nodes, some researchers replace the positional encoding with Laplacian eigenvectors [12, 24] or degree-related feature vectors [37]. (II) In addition to the positional encoding, GNNs are used as auxiliary modules to enable the Transformer model to capture the structural information [19, 30]. (III) Another approach is to introduce graph information bias into the attention score of each node pair, e.g., the shortest-path distance [37].

Despite effectiveness, existing Graph Transformers are typically designed for graph-level tasks with a small number of nodes. However, as for node classification that is a node-level task, a graph would have millions of nodes. Existing Graph Transformers have high computational complexity that rises quadratically with the number of nodes, restricting them to be applied directly to large-scale networks for node classification. Gophormer [42] is a recent attempt that aims to reduce the training cost by sampling the ego-graphs of nodes. Nevertheless, such a sampling strategy is still time-consuming and limits the model to capture deeper structural information.

The construction of the pair-wise attention matrix for all the node pairs is the main drawback of current Graph Transformers. If no attention mask is implemented, such type of attention matrix can be regarded as the global information. But global information is not necessary for node classification. For instances, when there is a considerable distance between two nodes, the chance of them belonging to the same category is very small. Taking citation networks as an example, a paper in The Botanical Magazine is barely relevant to a paper analysing programming language. The distance between them could be considerable large in the network. As a result, information from a faraway node is rather useless, and even noisy with negative impact. Meanwhile, GNN-based studies [22, 33, 23] that aggregate neighborhood (or local) information, have shown superior performance on all kinds of node classification tasks. Consequently, neighborhood operation should be useful for Graph Transformers.

Motivated by the above observation, We propose a novel model, termed Neighborhood Aggregation Graph Transformer (NAGphormer), for node classification. Unlike existing Graph Transformers that regard all nodes as fully-connected, NAGphormer first constructs tokens for each node by a novel neighborhood aggregation module called Hop2Token. The key idea behind Hop2Token is to aggregate neighborhood features from multiple hops and transform them into a representation, which can be thought as a token. To preserve the local information of nodes, Hop2Token constructs a sequence for each node based on the tokens of neighbors in different hops. The sequences are then fed into a Transformer-based module for learning the node representations. By treating each node as a sequence, NAGphormer can be trained in a mini-batch manner and hence can handle large graphs. Given the fact that the contributions of neighbors in different hops to the final node representation differ, NAGphormer provides an attention-based readout function so as to adaptively learn the importance of each hop.

Figure 1: Model framework of NAGphormer. NAGphormer first uses a novel neighborhood aggregation module, Hop2Token, to construct a sequence for each node based on the tokens of different hops of neighbors. Then NAGphormer learns the node representation using the standard Transformer backbone. An attention-based readout function is developed to aggregate neighborhood information of different hops adaptively. In the end, an MLP-based module is adopted for label prediction.
The main contributions of this work are as follows:

- We propose Hop2Token, a novel neighborhood aggregation method that aggregates the neighborhood features from each hop into a node representation, resulting in a sequence of token vectors that preserves the neighborhood information for different hops.
- We propose a new Graph Transformer method, NAGphormer, for node classification. NAGphormer can be trained in a mini-batch manner depending on the output of Hop2Token, and therefore enable the Graph Transformers to handle large graphs.
- We further develop an attention-based readout function to adaptively learn the importance of different hops to continue to boost the model performance.
- Extensive experiments on popular datasets from small to large demonstrate the superiority of the proposed methodology over existing Graph Transformers and mainstream Graph Neural Networks.

2 Preliminaries

2.1 Problem Formulation

Let \( G = (V, E) \) denote an unweighted and undirected attributed network (graph), where \( V = \{v_1, v_2, \ldots, v_n\} \), \( n = |V| \) is the number of nodes. Each node \( v \in V \) has a feature vector \( x_v \in X \), where \( X \in \mathbb{R}^{n \times d} \) is the feature matrix describing the attribute information of nodes and \( d \) is the dimension of the feature vector. \( A \in \mathbb{R}^{n \times n} \) represents the adjacency matrix and we can obtain the normalized adjacency matrix \( \hat{A} \) with the diagonal degree matrix \( D \). Typical normalization for the adjacency matrix includes: \( \hat{A} = D^{-1/2}AD^{-1/2} \) [3] or \( \hat{A} = D^{-1}A \) [41].

In this work, we focus on the node classification task in attributed networks. Concretely, the node classification task provides a labeled node set \( V_l \) and an unlabeled node set \( V_u \). Let \( Y \in \mathbb{R}^{n \times c} \) denote the label matrix where \( c \) is the number of classes. Given the labels \( Y_{V_l} \), the goal is to predict the labels \( Y_{V_u} \) for unlabeled nodes.

2.2 Transformer

The Transformer encoder [32] contains a sequence of Transformer layers, where each layer is comprised with a multi-head self-attention (MSA) and a position-wise feed-forward network. The MSA module is the critical component that aims to capture the semantic correlation between the input items (tokens). For simplicity, we use the single-head self-attention module for description. Suppose we have an input \( H \in \mathbb{R}^{n \times d} \) for the self-attention module where \( n \) is the number of items and \( d \) is the hidden dimension. The self-attention module first projects \( H \) into three subspaces, named \( Q, K \) and \( V \):

\[
Q = HW^Q, \quad K = HW^K, \quad V = HW^V,
\]

where \( W^Q \in \mathbb{R}^{d \times d_Q}, W^K \in \mathbb{R}^{d \times d_K} \) and \( W^V \in \mathbb{R}^{d \times d_V} \) are the projection matrices. And the output matrix is calculated as:

\[
H' = \text{softmax} \left( \frac{QQ^T}{\sqrt{d_K}} \right) V.
\]

The attention matrix \( QQ^T \) captures the pair-wise similarity of the input tokens in the sequence. Specifically, it calculates the dot product between each token pair after projection. The softmax is applied row-wise.

3 The Proposed NAGphormer

In this section, we present the proposed NAGphormer in detail. To handle networks at scale, we first introduce a novel neighborhood aggregation module called Hop2Token, then we build NAGphormer together with structural encoding and attention-based readout function.
Aggregating information from neighboring nodes into a node representation is a crucial strategy in reasonably powerful Graph Neural Network (GNN) architectures. It addresses the issue that each node has a variable number of neighbors. To inherit the desirable properties, we design Hop2Token considering different hops of the neighborhood information.

Let $N^k(v) = \{ v \in V | d(v, u) \leq k \}$ be the $k$-hop neighborhood of a node $v$, where $d(v, u)$ represents the distance of the shortest path between $v$ and $u$. We define $N^0(v) = \{ v \}$, i.e., the 0-hop neighborhood of a node is the node itself. In Hop2Token, we transform the $k$-hop neighborhood $N^k(v)$ into a neighborhood embedding $x_v^k$ with an aggregation operator $\phi$. In this way, the $k$-hop representation of a node $v$ can be expressed as:

$$ x_v^k = \phi(N^k(v)). $$

By this equation, we can calculate the neighborhood embeddings for variable hops of a node and further construct a sequence to represent its neighborhood information. The sequence length of $K$ is fixed as a hyperparameter. Assume $x_v^k$ is a $d$-dimensional vector. The sequences of all nodes on graph $G$ will construct a tensor $X_G \in \mathbb{R}^{n \times (K+1) \times d}$. To better illustrate the implementation of Hop2Token, we decompose $X_G$ to a sequence $S = (X_0, X_1, \ldots, X_K)$, where $X_k \in \mathbb{R}^{n \times d}$ can be seen as the $k$-hop neighborhood matrix for the entire graph. Here we define $X_0$ as the original feature matrix $X$.

In practice, we apply a propagation process similar to the method in Chien et al. [9] to obtain the sequence of $K$-hop neighborhood matrices. Given the normalized adjacency matrix $\hat{A}$ (also known as transition matrix [16]) and $X$, multiplying $\hat{A}$ with $X$ aggregates immediate neighborhood information. Applying this multiplication consecutively allows us to propagate information at larger distances. For example, we can access 2-hop neighborhood information by $\hat{A}(\hat{A}X)$. Simply put, the $k$-hop neighborhood matrix can be described as:

$$ X_k = \hat{A}^k X. $$

For the normalization strategy, we choose $\hat{A} = D^{-1/2}AD^{-1/2}$ due to its popularity [9, 22, 23]. The detailed implementation is drawn in Algorithm 1.

The advantages of Hop2Token are two-fold: 1) Hop2Token is a non-parametric method. It can be conducted offline before the model training. And the output of Hop2Token supports minibatch training, the model can handle graphs of arbitrary sizes, thus allowing the generalization of Graph Transformers to large-scale graphs. 2) Encoding $k$-hop neighborhood of a node into one representation is helpful for capturing the hop-wise semantic relevance, which is ignored in most GNNs [23, 22, 9, 33].

### 3.2 NAGphormer for Node Classification

Figure 1 depicts the architecture of NAGphormer. Given an attributed graph, we first reconstruct the feature matrix into a structure-aware matrix. To this end, an additional matrix constructed from eigendecomposition is concatenated to the original feature matrix. Accordingly, the effective feature vector for node $v$ is extended as $x_v \in \mathbb{R}^d$. The detailed construction is described in Section 3.3.
Next, we assemble an aggregated neighborhood sequence as $S_v$ by applying Hop2Token. Each element of $S_v$ is a token and can be expanded as $(x_{0v}^u, x_{1v}^u, ..., x_{Kv}^u)$, where $x_{kv}^u$ is calculated from $x_{u}^{(k-1)} (u \in N^k(v))$ and $x_{0v}^u = x_u$. $K$ is the predefined sequence length. Then we map to the hidden dimension $d_m$ of the Transformer with a learnable linear projection:

$$Z^{(0)} = [x_{0v}^u E; x_{1v}^u E; \cdots; x_{Kv}^u E],$$

where $E \in \mathbb{R}^{d' \times d_m}$ and $Z^{(0)} \in \mathbb{R}^{(K+1) \times d_m}$.

Then, we feed the projected sequence into the Transformer encoder. The building blocks of the Transformer is described in Section 2.2, i.e., multi-head self-attention (MSA) and position-wise feed-forward network (FFN). We follow the implementation of the vanilla Transformer encoder described in [32], while LayerNorm (LN) is applied before each block [35]. And the FFN consists of two layers with a GELU non-linearity.

$$Z^{(\ell)} = \text{MSA} \left( \text{LN} \left( Z^{(\ell-1)} \right) \right) + Z^{(\ell-1)},$$

$$Z^{(\ell)} = \text{FFN} \left( \text{LN} \left( Z^{(\ell)} \right) \right) + Z^{(\ell)},$$

where $\ell = 1, \ldots, L$ implies the $\ell$-th layer of the Transformer.

Finally, a novel readout function is applied to the output of the Transformer encoder. Through several Transformer layers, the corresponding output $Z^{(L)}$ contains the embeddings for all neighborhoods. It requires a readout function to aggregate the information of different neighborhoods into one embedding. Common readout functions include summation and mean [18]. However, these methods ignore the importance of different neighborhoods. Inspired by GAT [33], we propose an attention-based readout function to learn such importance by computing the attention coefficients between 0-hop neighborhood (i.e., the node itself) and every other neighborhood. Details are described as follows.

### 3.3 Implementation details

#### Structural encoding.

Besides the attribute information of nodes, the structural information of nodes is also a crucial feature for graph learning tasks. We adopt the eigenvectors of the Laplacian matrix of the graph which have been widely used in spectral clustering [34] for capturing the structural information of nodes. Specifically, we select the eigenvectors corresponding to the $s$ smallest non-trivial eigenvalues to construct the structure matrix $U \in \mathbb{R}^{n \times s}$ [12, 24]. Then we combine the original feature matrix $X$ with the structure matrix $U$ to preserve both attribute and structural information:

$$X' = X \| U,$$

where $\|$ indicates the concatenation operator and $X' \in \mathbb{R}^{n \times (d+s)}$ denotes the fused feature matrix.

#### Attention-based readout function.

For the output matrix $Z \in \mathbb{R}^{(K+1) \times d_m}$ of a node, $Z_0$ is the token representation of the node itself and $Z_k$ is its $k$-hop representation. We calculate the normalized attention coefficients for its $k$-hop neighborhood:

$$\alpha_k = \frac{\exp((Z_0 \| Z_i) W^T_a)}{\sum_{i=1}^{K} \exp((Z_0 \| Z_i) W^T_a)},$$

where $W_a \in \mathbb{R}^{1 \times 2d_m}$ denotes the learnable projection and $i = 1, \ldots, K$. Therefore, the readout function takes the correlation between each neighborhood and the node representation into account. The node representation is finally aggregated as follows:

$$Z_{out} = Z_0 + \sum_{k=1}^{K} \alpha_k Z_k.$$

### 4 Experiments

#### 4.1 Experimental Setup

**Datasets.** We conduct experiments on nine widely used datasets of different scales, including six small-scale datasets and three relatively large-scale datasets. For small-scale datasets, we adopt
Table 1: Statistics on datasets.

| Dataset    | #Nodes  | #Edges  | #Features | #Classes |
|------------|---------|---------|-----------|----------|
| Pubmed     | 19,717  | 44,324  | 500       | 3        |
| CoraFull   | 19,793  | 126,842 | 8,710     | 70       |
| Computer   | 13,752  | 491,722 | 767       | 10       |
| Photo      | 7,650   | 238,163 | 745       | 8        |
| CS         | 18,333  | 163,782 | 6,805     | 15       |
| Physics    | 34,493  | 495,924 | 8,415     | 5        |
| AMiner-CS  | 593,486 | 6,217,004 | 100      | 18       |
| Reddit     | 232,965 | 11,606,919 | 602     | 41       |
| Amazon2M   | 2,449,029 | 61,859,140 | 100     | 47       |

Table 2: Comparison of all models in terms of mean accuracy ± stdev (%) on small-scale datasets. The best results appear in bold. OOM indicates the out-of-memory error.

| Method | Pubmed | CoraFull | Computer | Photo | CS | Physics |
|--------|--------|----------|----------|-------|----|---------|
| GCN    | 84.65 ± 0.10 61.76 ± 0.14 | 89.65 ± 0.52 92.70 ± 0.20 | 92.92 ± 0.12 96.18 ± 0.07 |
| GAT    | 85.77 ± 0.15 64.47 ± 0.18 | 90.78 ± 0.13 93.87 ± 0.11 | 93.61 ± 0.14 96.17 ± 0.08 |
| APPNP  | 86.80 ± 0.11 65.16 ± 0.28 | 90.18 ± 0.17 94.32 ± 0.14 | 94.49 ± 0.07 96.54 ± 0.07 |
| GraphSAINT | 88.96 ± 0.16 67.85 ± 0.21 | 90.22 ± 0.15 91.72 ± 0.13 | 94.41 ± 0.09 96.43 ± 0.05 |
| PPRGo  | 87.38 ± 0.11 63.54 ± 0.25 | 88.69 ± 0.21 93.61 ± 0.12 | 92.52 ± 0.15 95.51 ± 0.08 |
| GRAND+ | 88.64 ± 0.09 71.37 ± 0.11 | 88.74 ± 0.11 94.75 ± 0.12 | 93.92 ± 0.08 96.47 ± 0.04 |
| GT     | 88.79 ± 0.12 61.05 ± 0.38 | 91.18 ± 0.17 94.74 ± 0.13 | 94.64 ± 0.13 97.05 ± 0.05 |
| Graphformer | OOM | OOM | 92.74 ± 0.14 OOM | OOM | OOM |
| SAN    | 88.22 ± 0.15 59.01 ± 0.34 | 89.83 ± 0.16 94.86 ± 0.10 | 94.51 ± 0.15 OOM |

NAGphormer 89.17 ± 0.13 71.51 ± 0.13 91.22 ± 0.14 95.49 ± 0.11 95.75 ± 0.09 97.34 ± 0.03

Pubmed [29], CoraFull [31], Computer [31], Photo [31], CS [31] and Physics [31] from the Deep Graph Library (DGL) 3. Since DGL does not provide identical data splits for these datasets, we apply 60%/20%/20% train/val/test splits for experiments. For large-scale datasets, we adopt AMiner-CS [15], Reddit [18] and Amazon2M [8] from [14]. The data splits of these datasets follow the settings as Grand+ [14]. The statistics on datasets are reported in Table 1.

Baselines. To evaluate the effectiveness of NAGphormer on the node classification task, we compare NAGphormer with nine representative baselines, including (I) three full-batch GNNs: GCN [22], GAT [33] and APPNP [23]; (II) three scalable GNNs: GraphSAINT [39], PPRGo [2] and GRAND+ [14]; (III) three Graph Transformers: GT [12], SAN [24] and Graphformer [37].

Implementation details. Referring to the recommended settings in the official implementations, we perform hyperparameter tuning for each of the baselines. For model configuration of NAGphormer, we try the number of Transformer layers in {1,2,...,5}, the hidden dimension in {128, 512}, and the propagation steps in {2,3,...,12}. Parameters are optimized with AdamW [27] optimizer, with the learning rate of 1e-4 and weight decay of 1e-3. The batch size is set to 2000. The training process is early stopped within 50 epochs. All experiments are conducted on a Linux server with 1 I9-9900k CPU, 1 RTX 2080TI GPU and 64G RAM.

4.2 Performance of Node Classification on Small-scale Datasets

For small-scale datasets, we conduct ten trials with random seeds for each model and take the mean accuracy and standard deviation for comparison. Table 2 reports the results. Overall, NAGphormer outperforms the baselines consistently on all the small-scale datasets, demonstrating the superiority of our proposed model. For the superiority over GNN-based methods, it is because NAGphormer utilizes our proposed Hop2Token and the Transformer model to capture the semantic relevance of different hop neighbors that is overlooked in most GNNs. Besides, the performance of NAGphormer also surpasses Graph Transformer-based methods, indicating that leveraging the local information is beneficial for node classification. Moreover, we observe that Transformer-based models show

3https://docs.dgl.ai/
Table 3: Comparison of all models in terms of mean accuracy ± stdev (%) on large-scale datasets. The best results appear in bold.

| Method       | AMiner-CS     | Reddit         | Amazon2M       |
|--------------|---------------|----------------|----------------|
| PPRGo        | 49.07 ± 0.19  | 90.38 ± 0.11   | 66.12 ± 0.59   |
| GraphSAINT   | 51.86 ± 0.21  | 92.35 ± 0.08   | 75.21 ± 0.15   |
| GRAND+       | 54.67 ± 0.25  | 92.81 ± 0.03   | 75.49 ± 0.11   |
| NAGphormer   | **55.61 ± 0.22** | **93.52 ± 0.02** | **76.72 ± 0.27** |

Table 4: Ablation study results on Aminer-CS dataset.

| Structural encoding | Readout function | Accuracy (%) | Gain  |
|---------------------|------------------|--------------|-------|
| -                   | Sum              | 50.21        | + 5.40|
| ✓                   | Single           | 52.53        | + 3.08|
| ✓                   | ✓                | 54.23        | + 1.38|
| ✓                   | ✓                | 55.61        |       |

competitive performance among the six datasets, demonstrating that the Transformer architecture is competent for node classification task by introducing structural information. We also observe that Graphormer and SAN suffer from the out-of-memory error even in some small graphs, further demonstrating the necessity of designing an scalable Graph Transformer for node-level tasks.

4.3 Performance of Node Classification on Large-scale Datasets

To verify the scalability of NAGphormer, we continue to compare NAGphormer with three scalable GNNs on three large-scale datasets. Due to the huge computational cost, existing Graph Transformers can not work on such large-scale datasets. We also run each model ten times with different random seeds and report the mean accuracy. The results are summarized in Table 3. We can observe that NAGphormer consistently outperform the scalable GNNs on all datasets, indicating that NAGphormer can better preserve the local information of nodes.

4.4 Ablation Study

To analyze the importance of structural encoding and attention-based readout function, we perform a series of ablation studies on the Aminer-CS dataset. The results are summarized in Table 4.

**Structural encoding.** In order to investigate the effectiveness of structural encoding, we compare our proposed NAGphormer to its variant without the structural encoding module. The experimental results show that the structural encoding can significantly improve the performance of NAGphormer, demonstrating the necessity of structural encoding for node-level task.

**Attention-based readout function.** We conduct a comparative experiment between the proposed attention-based readout function \( \text{Att.} \) (Equation 9) with previous readout functions: Single and Sum. Similar to [19], the function of Single utilizes the corresponding representation of the node itself as the final output to predict labels. And Sum can be regarded as aggregating all information of the neighbors equally. From Table 4, we observe that \( \text{Att.} \) outperforms other readout functions, indicating the effectiveness of aggregating the information of neighbors in different hops adaptively.

4.5 Parameter Study

To further evaluate the performance of NAGphormer, this subsection studies the influence of two key parameters: the number of propagation steps \( K \) and the number of Transformer layers \( L \). Specifically, we perform the experiments on AMiner-CS, Reddit and Amazon2M by setting different values of \( K \) and \( L \).

**The influence of \( K \).** We select the number of propagation steps \( K \) from \{4, 6, ..., 12\} and fix \( L = 1 \). Figure 2(a) reports the model performance. The results demonstrate that with the increment of \( K \), the performance increases significantly in the beginning, since a larger \( K \) means a broader scope
5 Related Work

In this section, we first review the progress of Graph Transformer based models with an emphasis on their strategies for structural information extraction, then briefly present the most recent works that generalize GNN to large-scale graphs.

5.1 Graph Transformers

There are several works that make efforts to generalize transformer neural networks [32] to graph-structured data. Similar to the positional encoding in the original Transformer, some notable works compress the graph structure into positional encoding to capture the topological information. Dwivedi et al. [12] utilize Laplacian eigenvectors to represent positional encodings and fuse them with the raw attribute of nodes as the input of Transformer. Derived from [12], Devin et al. [24] leverage the full spectrum of Laplacian matrix to learn the positional encodings. In addition to representing structural information by the eigenvectors, Ying et al. [37] propose a spatial encoding method that model the structural similarity of node pairs based on their shortest path lengths. Wu et al. [19] regard GNNs as an auxiliary module to extract local structural information of nodes and further feed them into the Transformer to learn long-range pairwise relationships. Besides, by modeling edge features in chemical and molecular graphs, Dwivedi et al. [12] extend Graph Transformer to edge feature representation by injecting them into the self-attention module of Transformer.

Nevertheless, like the original Transformer, these aforementioned methods adopt the fully-connected attention mechanism upon all node pairs, in which the spatial complexity is quadratic with the number of nodes. Such high cost makes these methods hard to handle graph mining task on large-scale networks with millions of nodes.

![Figure 2: Performance under different parameters.](image-url)
5.2 Scalable Graph Neural Networks

Graph Neural Networks (GNNs) have become a powerful technique to model graph-structured data. Based on the message passing framework, typical GNNs [7, 21, 22, 33] require the entire adjacency matrix as the input during training. In this way, when applying to large-scale graphs, the cost of training will be too high to afford. To generalize GNNs to large-scale networks and meanwhile reduce the training cost, a general approach is to design a sampling strategy. Existing strategies can be divided into two categories: node sampling-based methods [18, 5, 43] that aim at reducing the number of neighborhood nodes, and graph sampling-based methods [8, 39] that dedicate to decrease the size of the input graph.

Besides the sampling strategy, recent studies have developed a variety of approximate propagation methods to accelerate the message passing process, such as Approximate Personalized PageRank [2], Localized Bidirectional Propagation [6] and Generalized Forward Push [14].

However, by designing various sampling-based or approximation-based methods to reduce the training cost, these models will inevitably lead to information loss, and somehow restrict their performance on large-scale networks.

6 Conclusion

In this work, we propose a powerful and scalable Graph Transformer, called NAGphormer, for the node classification task in attributed graphs. NAGphormer first utilizes Hop2Token to aggregate neighborhoods into a series of representations. Hop2Token can be seen as a preprocessing step before the model training. In this way, NAGphormer can be trained in a mini-batch manner since necessary local information is acquired in advance for each node. Benefited from batch training, NAGphormer can easily handle large-scale networks with millions of nodes. Then NAGphormer subsequently learns the node representations by a standard Transformer encoder. And an attention-based readout function is developed to aggregate the neighborhood information of different hops adaptively. Experiments on various datasets from small to large demonstrate the effectiveness of NAGphormer, outperforming representative Graph Transformers and Graph Neural Networks.

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