Graph Representation Learning Network via Adaptive Sampling

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Abstract

Graph Attention Network (GAT) and GraphSAGE are neural network architectures that operate on graph-structured data and have been widely studied for link prediction and node classification. One challenge raised by GraphSAGE is how to smartly combine neighbour features based on graph structure. GAT handles this problem through attention, however the challenge with GAT is its scalability over large and dense graphs. In this work, we proposed a new architecture to address these issues that is more efficient and is capable of incorporating different edge type information. It generates node representations by attending to neighbours sampled from weighted multi-step transition probabilities. We conduct experiments on both transductive and inductive settings. Experiments achieved comparable or better results on several graph benchmarks, including the Cora, Citeseer, Pubmed, PPI, Twitter, and YouTube datasets.

1 Introduction

Graphs are a versatile and succinct way to describe entities through their relationships. The information contained in many knowledge graphs (KG) has been used in several machine learning tasks in natural language understanding [20], computer vision [16], and recommendation systems [29]. The same information can also be used to expand the graph itself via node classification [11], clustering [19], or link prediction tasks [14], in both transductive and inductive settings [15].

Recent graph models have focused on learning dense representations that capture the properties of a node and its neighbours. One class of methods generates spectral representation for nodes [3][7]. The rigidity of this approach may reduce the adaptability of a model to graphs with structural differences.

Model architectures that reduce the neighbourhood of a node have used pooling [13], convolutions [9], recurrent neural networks (RNN) [17], and attention [28]. These approaches often require many computationally-expensive message-passing iterations to generate representations for the neighbours of a target node. Sparse Graph Attention Networks (SGAT) [30] was proposed to address this inefficiency by producing an edge-sparsified graph. However, it may neglect the importance of local structure when graphs are large or have multiple edge types. Other methods have used objective functions to predict whether a node belongs to a neighbourhood [19][14], for example by using noise-contrastive estimation [12]. However, incorporating additional training objectives into a downstream task can be difficult to optimize, leading to a multi-step training process.

In this work, we present a graph network architecture (GATAS) that can be easily integrated into any model and supports general graph types, such as: cyclic, directed, and heterogeneous graphs. The method uses a self-attention mechanism over a multi-step neighbourhood sample, where the transition probability of a neighbour at a given step is parameterized.
We evaluate the proposed method in node classification tasks using the Cora, Citeseer and Pubmed citation networks in a transductive setting, and on a protein to protein interaction (PPI) dataset in an inductive setting. We also evaluate the method on a link prediction task using a Twitter and YouTube dataset. Results show that the proposed graph network can achieve better or comparable performance to state-of-the-art architectures.

2 Related Work

The proposed architecture is related to GraphSAGE [13], which also reduces neighbour representations from fixed-size samples. Instead of aggregating uniformly-sampled 1-hop neighbours at each depth, we propose a single reduction of multi-step neighbours sampled from parameterized transition probabilities. Such parameterization is akin to the Graph Attention Model [1], where trainable depth coefficients scale the transition probabilities from each step. Thus, the model can choose the depth of the neighbourhood samples. We further extend this approach to transition probabilities that account for paths with heterogeneous edge types.

We use an attention mechanism similar to the one in Graph Attention Networks (GAT) [28]. While GAT reduces immediate neighbours iteratively to explore the graph structure in a breadth-first approach that processes all nodes and edges at each step, our method uses multi-step neighbourhood samples to explore the graph structure. Our method also allows each neighbour to have a different representation for the target node, rather than using a single representation as in GAT.

MoNet [18] generalizes many graph convolutional networks (GCN) as attention mechanisms. More recently, the edge-enhanced graph neural network framework (EGNN) [10] consolidates GCNs and GAT. In MoNet, the attention coefficient function only uses the structure of the nodes. In addition, our model employs node representations to generate attention weights.

Other approaches use recurrent neural networks [22] [17] to reduce path information between neighbours and generate node representations. The propagation algorithm in Gated Graph Neural Networks (GG-NNs) [17] reduces neighbours one step at a time, in a breadth-first fashion. In contrast, we use a depth-first approach where a reduction operation is applied across edges of a path.

3 Model

3.1 Preliminaries

An initial graph is defined as \( G = (V, R, Z) \), where \( V = \{v_1, ..., v_{|V|}\} \) is a set of nodes or vertices, \( R = \{r_1, ..., r_{|R|}\} \) is a set of edge types or relations, and \( Z = \{(v_i, r_k, v_j) \mid v_i, v_j \in V; r_k \in R\} \) is a set of triplets. Directed graphs are represented by having one edge type for each direction so that \( (v_i, r^+, v_j) \in Z \iff (v_j, r^-, v_i) \in Z \). To be able to incorporate information about the target node, the graph \( G \) is augmented with self-loops using a new edge type \( r_0 \). Thus, a new set of edge types \( \tilde{R} = \{r_0\} \cup R \) is created such that \( \tilde{r}_1 = r_0 \), and a new set of triplets \( \tilde{Z} = \{(v_i, r_0, v_i) \mid v_i \in V\} \cup \{(v_i, r_k+1, v_j) \mid (v_i, r_k, v_j) \in Z\} \) conforms a new graph \( \tilde{G} = (V, \tilde{R}, \tilde{Z}) \).

An edge type path between nodes \( v_i \) and \( v_j \) is defined as \( E^{(i,j)} = (a_1 | \tilde{r}_{n_i} \in \tilde{R}) \leq C \), where \( C \geq 1 \) is the maximum number of steps considered. The number of all possible edge type paths is given by \( M = \sum_{i=1}^{C} |\tilde{R}|^i \). The set of all possible edge type paths is defined as \( \mathcal{E} = \{E_1, ..., E_M\} \). The edge type sequences in the set are level-ordered so that \( \forall m \in \{1, ..., M - 1\}, |E_m| \leq |E_{m+1}| \), and so that \( \forall i \in \{1, ..., |E_m|\}, E_{m,i} \leq E_{n,i} \). As an example, if \( \tilde{R} = \{A, B\} \) and \( C = 2 \), then \( \mathcal{E} \) corresponds to: \( \{(A), (B), (A, A), (A, B), (B, A), (B, B)\} \). The subset of relation paths connecting nodes \( v_i \rightarrow v_j \) is defined as \( \mathcal{E}^{(i,j)} = \{E_{m,i} \mid E_m \in \mathcal{E}\} \), where \( \mathcal{E}^{(i,j)} = \{E_1\} \Rightarrow i = j \) represents the extraneous self-loops.

3.2 Neighbour Representations

Graph relations in \( \tilde{R} \) are represented by trainable vectors \( \vec{e} = \{\vec{e}_1, ..., \vec{e}_{|\tilde{R}|}\}, \vec{e} \in \mathbb{R}^D \). To reflect the position in a path, the edge representations can be infused with information that reflects its position in a path. Following [27], we assign a sinusoid of a different wavelength to each dimension, each
We represent nodes as a set of vectors \( \mathbf{h} \). An initial transition tensor \( \mathbf{A} \) is defined such that \( \sum_{t} A_{i,j,m} = 1 \) when applying the function \( \Psi \).

A set of shortest \( v \) cycles by disallowing transitions to nodes already visited in previous steps. This reduces to track the probability of an edge type path \( E \).

Given an edge type path \( E_{m} \in \mathcal{E}^{(i,j)} \) we generate a neighbour representation \( \tilde{n}_{i,j,m} \) using attention over transformed neighbour representations for each edge type in \( E_{m} \):

\[
\tilde{n}_{i,j,m} = \sum_{t=1}^{\mid E_{m} \mid} \beta_{i,m,t} z((\tilde{h}_{j} \| e_{Em,t} + \tilde{p}_{m})) \quad \beta_{i,m,t} = \frac{\exp(f(\|h_{i} \| e_{Em,t} + \tilde{p}_{m}))}{\sum_{x=1}^{\mid E_{m} \mid} \exp(f(\|h_{i} \| e_{Em,x} + \tilde{p}_{x})))}
\]

where \( z : \mathbb{R}^{F+R+D} \rightarrow \mathbb{R}^{F'} \) and \( f : \mathbb{R}^{F+R+D} \rightarrow \mathbb{R} \) are two different learnable transformations. The transformation given by \( z \) allows neighbour representations to be different according to the edge type in the path. For the self-loop edge type path \( E_{1} \), we set \( \tilde{n}_{i,j,1} = z(\|h_{i} \| e_{1} + \tilde{p}_{0}) \).

### 3.3 Transition Tensors

We define transition probability distributions for neighbours and their possible edge type paths within \([1, C]\) steps. When there are multiple edge types connecting two nodes, their transition probabilities split. Thus, when computing transition probabilities for random walks starting at \( v_{i} \), it is necessary to track the probability of an edge type path \( E_{m} \in \mathcal{E}^{(i,j)} \) for each destination vertex \( v_{j} \), effectively computing \( P(v_{j}, \mathcal{E}|v_{i}) \). Also, when performing random walks from a starting node \( v_{i} \), we break cycles by disallowing transitions to nodes already visited in previous steps. This reduces \( \mathcal{E}^{(i,j)} \) to the set of shortest \( v_{i} \rightarrow v_{j} \) edge type paths possible.

Let \( \mathbf{A} \in \{0, 1\}^{\mathbb{V} \times \mathbb{V} \times M} \) be a sparse adjacency tensor for \( \mathcal{G} \), where:

\[
A_{i,j,m} = \begin{cases} 
1, & \text{if } (v_{i}, r_{m}, v_{j}) \in \tilde{E} \land 1 < m \leq \mid \tilde{R} \mid \\
0, & \text{otherwise}
\end{cases}
\]

An initial transition tensor \( \mathbf{T}^{(1)} \in \mathbb{R}^{\mathbb{V} \times \mathbb{V} \times M} \) can be computed by normalizing the \( \mathbf{A}_{v,v,*,*} \) matrices to sum to one, when applying the function \( \Psi : \mathbb{R}^{\mathbb{V} \times \mathbb{V} \times M} \rightarrow \mathbb{R}^{\mathbb{V} \times \mathbb{V} \times M} \):

\[
\Psi(Z)_{i,j,m} = \frac{Z_{i,j,m}}{\sum_{x=1}^{\mid \mathbb{V} \mid} \sum_{y=1}^{M} Z_{i,x,y}}
\]
3.4 Neighbourhood Sampling

When considering a neighbourhood $N_i = \{(j, m) \mid v_j \in V, E_m \in E^{(i,j)}\}$, it can be relevant to attend to nodes beyond the first degree neighbourhood. However, as the number of hops between nodes increases, their relationship weakens. It can also be prohibitive to attend to all nodes within $C$ hops, as the neighbourhood size $|N_i|$ grows proportionally with $C \times |E_{v \in V}| \{|\text{degree}(v)|\}^C$.

To overcome these complications, we create a fixed-size neighbourhood sample from an adjustable transition tensor $P \in \mathbb{R}^{|V| \times |V| \times M}$. Similar to the work in [1], we obtain neighbour probabilities by a linear combination of random walk transition tensors for each step $k$, with learnable coefficients $q$:

$$P = \sum_{k=0}^{C} q_k T^{(t)}$$

where $(q_0, ..., q_C) = \text{softmax}(\bar{q}_0, ..., \bar{q}_C)$ and $\bar{q} \in \mathbb{R}^{C+1}$ is a vector of unbounded parameters. $T^{(0)}$ corresponds to a transition tensor for the added self-loops:

$$T^{(0)}_{i,j,m} = \begin{cases} 1, & \text{if } (v_i, r_0, v_j) \in \tilde{E} \land m = 1 \\ 0, & \text{otherwise} \end{cases}$$

Depending on the task and graph, the model can control the scope of the neighbourhood by adjusting these coefficients through backpropagation.

To generate a neighbourhood $N_i$ for $v_i \in V$ we sample without replacement from $P$ so that $N_i = \{(j, m) \mid (j, m) \sim P_{i,*,*}\}^S$, where $S$ is the maximum size for a neighbourhood sample.

3.5 Node Representations

Given a neighbourhood $N_i$ for node $v_i \in V$ and a transition tensor $P$, we apply an attention mechanism with attention coefficients given by:

$$\alpha_{i,j,m}^{(k)} = \frac{\exp[g^{(k)}(\|\bar{h}_i \|\|\bar{n}_{i,j,m}\|) + \ln(P_{i,j,m})]}{\sum_{(x,y) \in N_i} \exp[g^{(k)}(\|\bar{h}_i \|\|\bar{n}_{i,x,y}\|) + \ln(P_{i,x,y})]}$$

where $g^{(k)} : \mathbb{R}^{F'} \rightarrow \mathbb{R}$ is a learnable transformation. The logits produced by $g^{(k)}$ are scaled by the transition probabilities, exerting the importance of the neighbour, and allowing the coefficients $q$ to be trained. We concatenate multi-head attention layers to create a new node representation $\bar{h}_i'$:

$$\bar{h}_i' = \left[ \sum_{k=1}^{K} \sigma \left( \sum_{(j,m) \in N_i} \alpha_{i,j,m}^{(k)} d^{(k)}(\|\bar{n}_{i,j,m}\|) \right) \right]$$

where $d^{(k)} : \mathbb{R}^{F'} \rightarrow \mathbb{R}^{F''}$ is another learnable transformation, and $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ is a non-linear activation function, such as the ELU function. The transformation allows relevant information for the node to be selected.
3.6 Algorithmic Complexity

The complexity of generating node representations with the proposed algorithm (GATAS) is governed by $O(C \times S \times B \times F_{max})$, where $B$ is the batch size and $F_{max} = \max(F + R + D, F', F'')$. GraphSAGE [13] has a similar complexity of $O(S^C \times B \times F)$. GAT [28], on the other hand, has a complexity that is independent of the batch size but processes all nodes and edges. It is given by $O(C \times (|V| \times F + |Z|))$, where $C$ is the number of layers that controls depth. For downstream tasks where only a small subset of nodes are actually used, the overhead complexity of GAT can be overwhelming. Generalizing, our model is more efficient when $|V| + |Z| > B \times S$.

4 Evaluation

We evaluate the performance of GATAS using node classification tasks in transductive and inductive settings. To evaluate the performance of the proposed attention mechanism over heterogeneous multi-step neighbours, we rely on a multi-class link prediction task.

For the transductive learning experiments we compare against GAT [28] and some of the approaches specified in [15], including a CNN approach that uses Chebyshev approximations of the graph eigendecomposition [7], the Graph Convolutional Network (GCN) [15], MoNet [18], and the Sparse Graph Attention Network (SGAT) [30]. We also benchmark against a multi-layer perceptron (MLP) that classifies nodes only using its features without any graph structure.

For the inductive experiments we compare once again against GAT [28] and SGAT [30]. We also compare against GraphSAGE [13], a method that aggregates node representations from fixed-size neighbourhood samples, using different methods such as LSTMs and max-pooling.

GATAS is capable of utilizing edge information, which we consider to be an important advantage. Hence we also conducted link prediction experiments on multiplex heterogeneous network datasets against some of the state-of-the-art models, namely GATNE [4], MNE [31], and MVE [21]. GATNE creates multiple representations for a node under different edge type graphs, aggregates these individual views using reduction operations similar to GraphSAGE, and combines these node representations using attention.

4.1 Datasets

For the transductive node classification tasks we use three standard citation network datasets: Cora, Citeseer, and Pubmed [23]. In these datasets, each node corresponds to a publication and undirected edges represent citations. Training sets contain 20 nodes per class. The validation and test sets have 500 and 1000 unseen nodes respectively.

For the inductive node classification experiments, we use the protein interaction dataset (PPI) in [13]. The dataset has multiple graphs, where each node is a protein, and undirected edges represent an interaction between them. Each graph corresponds to a different type of interaction between proteins. 20 graphs are used for training, 2 for validation and another 2 for testing.

For the link prediction task, we use the heterogeneous Higgs Twitter Dataset [6]. It is made up of four directional relationships between more than 450,000 Twitter users. We also use a multiplex bidirectional network dataset that consists of five types of interactions between 15,088 YouTube users [25, 26]. Using the dataset splits provided by the authors of GATNE [4], we work with subsets of 10,000 and 2,000 nodes for Twitter and YouTube respectively, reserving 5% and 10% of the edges for validation and testing. Each split is augmented with the same amount of non-existing edges, that are used as negative samples.

Detailed statistics for these datasets are summarized in Table 4 in Supplementary Materials.

4.2 Experiment Setup

Node features are normalized using layer normalization [2]. These features are then passed through a single dense layer to obtain the input features $\mathbf{b}$. The Twitter dataset does not provide node features.

\footnotesize

[1] http://snap.stanford.edu/data/higgs-twitter.html
[2] http://github.com/thudm/gatne
We define $f$ with 0.9 probability, and apply Dropout [24] with 0.5 probability to the attention coefficients and

Table 1 summarizes our results on the node classification tasks. For the transductive tasks, we report

The optimization objective is the multi-class or multi-label cross-entropy, depending on the task. It is

so $\mathbf{h} = \mathbf{b}$. The inductive node classification task does not use learnable node embeddings so $\mathbf{h} = \mathbf{b}$.

We define $f(\cdot)$ as a linear transformation, $g(k)(\cdot)$ as a two-layer neural network with a non-linear hidden layer and a linear output layer, and $z(\cdot)$ and $d(k)(\cdot)$ as one-layer non-linear neural networks. Non-linear layers use ELU [5] activation functions.

For all models we set $F, F', F'' = 50$. We experimented with learnable node embeddings and edge type embedding sizes of 10 and 50 for the transductive node classification and link prediction tasks respectively. We use an edge type embedding size of 5 for the inductive tasks. The transductive tasks have 8 attention heads, while the other tasks have 10 heads.

For the transductive node classification tasks, the output layer is directly connected to the concatenated attention heads. For the inductive task, the concatenated attention heads are passed through 2 non-linear layers before going through the output layer. In the link prediction task, the concatenated attention heads are passed through a non-linear layer and a pair of corresponding node representations are concatenated before they pass through 2 non-linear layers and an output layer. All these hidden layers have a size of 256.

The optimization objective is the multi-class or multi-label cross-entropy, depending on the task. It is minimized by the Nadam SGD optimizer [8]. The validation set is used for early stopping and hyper-parameter tuning. Since the training sets for the transductive node classification tasks are very small, it is crucial to add noise to the model inputs to prevent overfitting. We mask out input features with 0.9 probability, and apply Dropout [24] with 0.5 probability to the attention coefficients and resulting representations. We also add $L_2$ regularization with $\lambda = 0.05$.

In the node classification and link prediction tasks, neighbourhood candidates can be at most 3 and 2 steps $C$ away from the target node respectively. The unnormalized transition coefficients are initialized with a non-linear decay given by $\tilde{q}_t = -t / \ln(C + 1)$. To accommodate for an inductive setting, edges across graphs in the protein interaction dataset are treated as the same type and use the same edge type representations. In the link prediction task we reuse the node representations during test time and rely on the neighbours given by the edges in the training set.

The experiment parameters are summarized in Table 5 in Supplementary Materials. In the transductive node classification experiments, the architecture hyper-parameters were optimized on the Cora dataset and are reused for Citeseer and Pubmed. A single experiment can be run on a V100 GPU under 12 hours. Implementation code is available on GitHub

4.3 Results

Table 1 summarizes our results on the node classification tasks. For the transductive tasks, we report

http://github.com/wattpad/gatas

Table 1: Node Classification Results

| Model       | Transductive (Accuracy %) | Inductive (Micro-F1) |
|-------------|---------------------------|----------------------|
|             | Cora                      | Citeseer             | Pubmed   | PPI      |
| MLP         | 55.1%                     | 46.5%                | 71.4%    | 0.422    |
| Chebyshev   | 81.2%                     | 69.8%                | 74.4%    | —        |
| GCN         | 81.5%                     | 70.3%                | 79.0%    | —        |
| MoNet       | 81.7% ± 0.5%              | —                    | 78.8% ± 0.3% | —        |
| GraphSAGE   | —                         | —                    | —        | 0.768    |
| GAT         | 83.0% ± 0.7%              | 72.5% ± 0.7%         | 79.0% ± 0.3% | 0.973 ± 0.002 |
| SGAT*       | 84.2%                     | 68.2%                | 77.6%    | 0.966    |

| GATAS_{10}  | 80.2% ± 1.1%              | 69.4% ± 1.3%         | 76.1% ± 0.8% | 0.818 ± 0.015 |
| GATAS_{100} | 82.3% ± 0.9%              | 69.6% ± 1.1%         | 78.4% ± 0.6% | 0.981 ± 0.002 |
| GATAS_{500} | 82.1% ± 0.8%              | 69.7% ± 1.4%         | 78.7% ± 0.6% | 0.985 ± 0.001 |

* We selected the best results reported by SGAT.
Table 2: Link Prediction Results

| Dataset   | ROC-AUC | F1  | ROC-AUC | F1  | ROC-AUC | F1  | ROC-AUC | F1  |
|-----------|---------|-----|---------|-----|---------|-----|---------|-----|
| Twitter*  | 72.62   | 67.40 | 91.37   | 84.32 | 92.30   | 84.96 | 95.44   | 87.13 |
| YouTube*  | 70.39   | 65.10 | 82.30   | 75.03 | 84.61   | 76.83 | 96.63   | 83.59 |

* Results reported for GATNE, MNE and MVE are from the original GATNE paper [4].

report the mean micro-F1 score and standard deviation over 10 runs. We compare against the metrics already reported in [28, 15], and use the same dataset splits provided. For GraphSAGE, we report the better results obtained in [28].

Using the settings described in the previous section, we provide variations of our method using different neighbourhood sample sizes: 10, 100, and 500. We notice that the model can achieve comparable performance, and that we have achieved a new state-of-the-art performance on the PPI dataset in an inductive setting, by a 1.2% margin.

Performance increases with the neighbourhood sample size, as it expands the graph structure covered. However, we do not see substantial improvements for a sample size of 500. Given the average number of neighbours per node for each dataset, as shown in Table 1, we can see that an increased neighbourhood sample size of 500 might not add additional neighbours to the models in the transductive experiments. However, for the PPI dataset, 500 is still significantly below an estimated average neighbourhood size of 28.3^C, where C = 3 is the number of steps considered.

We note that in the PPI dataset, a small neighbourhood sample size of 10 impacts performance considerably more than in the transductive setting. This could be because there is no support from the learnable node representations. As the amount of information provided by neighbours decreases, the model might become more dependent on these parameters. The proposed neighbourhood sampling technique trades in a small amount of accuracy to gain efficiency. As a result, the model can easily be used with large datasets and downstream tasks.

Table 2 summarizes our results on the link prediction task. We report the macro area under the ROC curve and the macro F1 score for a single run. When comparing against GATNE, we use the transductive version of the model since we do not precompute raw features for the nodes and rely on the learned representations during test time.

The results suggest the produced node representations are able to capture path attributes as part of the neighbourhood information. GATAS outperforms GATNE-T, with a lift of 3.14% and 12.02% in ROC-AUC, as well as 3.17% and 6.76% in the F1 score, on the Twitter and YouTube datasets respectively. The results achieved new state-of-the-art performances, to the best of our knowledge.

4.4 Ablation Study

The proposed architecture has three independent components that have not been considered in previous work: (1) the neighbour sampling technique using transition probabilities with learnable step coefficients that affect the attention weights; (2) the learnable node representations  that augment node features with neighbourhood information; and (3) the attention network that allows neighbour representations to adapt to the target node given itself and the path information.

In this section we measure the impact of each component on the Cora and Pubmed datasets for the transductive setting and the PPI dataset for the inductive setting. We consider five model variations that test the importance of each component. All variations of the inductive models do not use learnable node representations because of the nature of its setting. We would like to test the importance of edge type information but the link prediction datasets do not provide node features that would allow us to run all variations. We define the following variations:

- **Base** only samples immediate neighbours with uniform probability and the transition probabilities are not part of the attention weights. The model does not adapt neighbour represen-
Table 3: Ablation Study Results

| Model          | Transductive (Accuracy %) | Inductive (Micro-F1) |
|----------------|---------------------------|----------------------|
|                | Cora                      | Pubmed               | PPI                  |
| Base           | 79.3% ± 0.7%              | 76.2% ± 0.7%         | 0.974 ± 0.001        |
| GATAS w/o trans| 76.7% ± 0.8%              | 77.8% ± 0.5%         | 0.982 ± 0.001        |
| GATAS w/o embed| 82.2% ± 0.7%              | 78.3% ± 0.8%         | —                    |
| GATAS w/o paths| 82.3% ± 0.7%              | 78.4% ± 0.7%         | 0.983 ± 0.001        |
| GATAS          | 82.3% ± 0.9%              | 78.4% ± 0.6%         | 0.985 ± 0.001        |

The table shows our results. The largest jump in performance corresponds to the use of the neighbourhood sampling technique and incorporation of the transition probabilities. The use of learnable embeddings as part of node representations does not seem to cause a big impact on performance but this could be a consequence of a large neighbourhood size $S$, which might reduce the need to utilize these parameters. Finally, the use of adaptable neighbour representations does not seem to affect performance for these tasks. We hypothesize that the nature of the tasks might not require such neighbour transformations but note that edge direction and different edge types are not present in these datasets.

5 Conclusion

In this paper, we proposed a new neural network architecture for graphs. The algorithm represents nodes by reducing their neighbour representations with attention. Multi-step neighbour representations incorporate different path properties. Neighbours are sampled using learnable depth coefficients. Our model achieves comparable results across different tasks and various baselines, on the benchmark datasets: Cora, Citeseer, Pubmed, PPI, Twitter and YouTube. We successfully retained performance while increasing efficiency on large graphs, achieving state-of-the-art performance on multiple datasets from different tasks. We conducted an ablation study in transductive and inductive settings. The experiments show that sampling neighbourhoods according to weighted transition probabilities achieves the largest performance gain, especially in the inductive setting.

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A Supplementary Materials

A.1 Dataset Statistics

Table 4: Dataset Statistics

|                  | Cora | Citeseer | PubMed | PPI  | Twitter† | YouTube† |
|------------------|------|----------|--------|------|----------|----------|
| Node Classes     | 7    | 6        | 3      | 121  | 1        | 1        |
| Edge Types       | 1    | 1        | 1      | 1    | 4        | 5        |
| Node Features    | 1,433| 3,703    | 500    | 50   | 0        | 0        |
| Nodes            | 2,708| 3,327    | 19,717 | 56,944| 456,626  | 15,088   |
| Edges            | 5,429| 4,732    | 44,338 | 818,716| 15,367,315| 13,628,895|
| Training Nodes   | 140  | 120      | 60     | 44,906| 9,990    | 2,000    |
| Training Edges   | —    | —        | —      | 1,246,382| 282,115 | 1,114,025|
| Validation Nodes | 500  | 500      | 500    | 6,514 | 9,891    | 2,000    |
| Validation Edges | —    | —        | —      | 201,647| 16,463   | 65,512   |
| Testing Nodes    | 1,000| 1,000    | 1,000  | 5,524 | 9,985    | 2,000    |
| Testing Edges    | —    | —        | —      | 164,319| 32,919   | 131,007  |
| Neighbours per Node | 3.9 | 2.7     | 4.4    | 28.3 | 28.2     | 557.0    |

† Shared nodes across dataset types with access to training set edges only.
* Access to all edges.

A.2 Experiment Settings

Table 5: Experiment Settings

| Parameter                              | Node Classification | Link Prediction |
|----------------------------------------|---------------------|-----------------|
| Parameter                              | Transductive        | Inductive       | Transductive |
| Maximum number of steps (C)            | 3                   | 3               | 2             |
| Neighbourhood sample size (S)          | 10/100/500          | 10/100/500      | 100           |
| Layer size (F, F', F'')                | 50                  | 50              | —             |
| Node embedding size (R)                | 10                  | —               | 50            |
| Edge type embedding size (D)           | 10                  | 5               | 50            |
| Number of attention heads              | 8                   | 10              | 10            |
| Input noise rate                       | 0.9                 | 0               | 0             |
| Dropout probability                    | 0.5                 | 0               | 0             |
| $L_2$ regularization coefficient (λ)   | 0.05                | 0               | 0             |
| Learning rate                          | 0.001               | 0.001           | 0.001         |
| Maximum number of epochs               | 1000                | 1000            | 1000          |
| Early stopping patience                | 100                 | 10              | 5             |
| Batch size ($B$)                       | 5000                | 100             | 200           |