ADAPTIVE GRAPH DIFFUSION NETWORKS WITH HOP-WISE ATTENTION

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ABSTRACT

Graph Neural Networks (GNNs) have received much attention recent years and have achieved state-of-the-art performances in many fields. The deeper GNNs can theoretically capture deeper neighborhood information. However, they often suffer from problems of over-fitting and over-smoothing. In order to incorporate deeper information while preserving considerable complexity and generalization ability, we propose Adaptive Graph Diffusion Networks with Hop-wise Attention (AGDNs-HA). We stack multi-hop neighborhood aggregations of different orders into single layer. Then we integrate them with the help of hop-wise attention, which is learnable and adaptive for each node. Experimental results on the standard dataset with semi-supervised node classification task show that our proposed methods achieve significant improvements.

1 Introduction

Graph Neural Networks (GNNs) have achieved the state-of-the-art performances in many graph related tasks, especially node classification in citation networks [1, 2], social networks [2, 3], biology [4], etc.

Graph Convolution Network (GCN) [1] is a common and efficient GNN method. A GCN layer includes the neighborhood aggregation and the linear transformation. GCN acts as a first-order spectral low-pass-type filter, because of the re-normalization trick which adds self-loops before symmetric normalization [5]. The aggregation operation can be viewed as the matrix multiplication between the weighted adjacency matrix and the node feature matrix. The weighted adjacency matrix is the symmetrically normalized adjacency matrix in GCN.

Graph Attention Network (GAT) [6] is another popular GNN method. The attention mechanism [7] have been proven effective in the natural language processing (NLP) domain. GAT and its variants [6, 8] incorporate simplified attention mechanism into GNNs. In GAT, the weighted adjacency matrix is the attention matrix with attention scores as entries, which are calculated with representation vectors of directly connected nodes.

Including GCNs and GATs, the majority of GNNs can be classified as Message Passing Neural Networks (MPNNs) [9], which aggregate messages from 1-hop neighboring nodes in each layer. MPNNs are often considered as spatial methods, since they only use the first-hop neighborhood information.

Although MPNNs achieve state-of-the-art performances in many tasks, the best results are usually achieved with shallow network architectures (usually less than 5 layers). The deeper GNNs are often constructed with stacked GNN layers with non-linear activation functions except the output layer. Since the information from the high-order neighboring nodes are supposed to be potentially valuable for certain datasets, the deeper GNNs with larger receptive field should theoretically achieve better or comparable performances compared with shallow ones. However, many experiments show that stacking too many GNN layers results into significant performance degradation [10].

As each single GNN layer often contains one linear transformation, the parameters of linear transformations scale linearly with the number of layers. Empirically, the necessary complexity of machine learning algorithms is need-
Figure 1: **Multiple MPNN layers.** The dotted curves correspond to receptive field. The change of colors corresponds to a linear transformation. In MPNNs, the number of linear transformations is exactly the number of aggregations.

Figure 2: **Single layer with multi-hop aggregations.** With the same depth of receptive field in Figure 1, only one linear transformation is used. Moreover, multiple layers with multi-hop aggregations can be stacked in order to ensure higher model complexity.

We find that GCNs inherit complexity from their linear transformation components [5] and benefit from their global smoothing operations. In practice, the necessary depth of receptive fields does not always match the necessary complexity of linear transformations. Although they have a strong correlation in GNNs, since they are controlled with the same hyperparameter, as shown in Figure 1. We can increase the receptive field of each GNN layer besides stacking them [5][15][16][17][18][19]. By stacking multiple layers with multi-hop neighborhood aggregations, both of them can be controlled flexibly with more hyperparameters. As shown in Figure 2, in each layer, successive neighborhood aggregations with single linear transformation are performed, which enlarges the receptive field. While the number of linear transformations (or parameters) is under control, which effectively avoids the over-fitting problem. For example, SGC [5] simply uses the representation from the last aggregation in single layer. Moreover, enlarging receptive field of single layer brings the potential ability to avoid or alleviate the over-smoothing problem with suitable improvements or priors. DCNN, MixHop and TAGCN [16][20][15] concatenate representations from different aggregations, though MixHop uses aggregations in different layers. The combination of concatenation and linear transformation is actually weighted sum after separate linear transformations. Their outputs contain both shallow and deep information. An LSTM-attention mechanism is proposed in JKNet [21], which uses LSTM to embed distance information and adaptive attention scores to integrate different representations from different layers. DAGNN [22] also proposes adaptive weighting matrices to integrate representations from different aggregations. However, weighting matrices should be named more precisely as adjustment matrices, since they are not normalized. Moreover, weighting matrices are calculated solely based on each aggregation itself. In DAGNN, linear transformations and aggregations are separately stacked in forms of Multilayer Perceptrons (MLP) and single multi-hop convolution layer. DAGN [23] incorporates...
Additionally, GAT-HA can be further viewed as a graph neural network with two-step attention mechanism. In contrast to standard graph diffusion theory [19], the high-order diffusion matrices are computed implicitly with sparse transition matrix and weighting matrices are learnable. In contrast to approximated graph diffusion-based methods [18, 24], all of the intermediate representations can be directly used.

Suppose $G = (V, E)$ be a given graph with node set $V$ and edge set $E$. The number of nodes is denoted with $N = |V|$ and the number of edges is denoted with $M = |E|$. The adjacency matrix is denoted with $A \in \mathbb{R}^{N \times N}$. In general, a Graph neural Network (GNN) model learns continuous embedding vectors of nodes. We consider the initial node feature matrix $X \in \mathbb{R}^{N \times d^{(i)}}$ and the intermediate node representations $H^{(l)}, H^{(k,l)} \in \mathbb{R}^{N \times d^{(l)}}$, where $H^{(0)}$ represents the output representation at the $l$-th layer, $H^{(k,l)}$ represents the $k$-th intermediate representation at the $l$-th layer, $d$ represents the dimension of the input node feature, $d^{(l)}$ represents the dimension of representations at the $l$-th layer. For most of GNN models, the value of $k$ is restricted to 1.

### 2 Adaptive Graph Diffusion Networks with Hop-wise Attention

By defining generalized graph diffusion via the diffusion matrix, methods performing multi-hop aggregations in each layer can be concluded as graph diffusion-based models [18, 19, 24, 25]. More precisely, the generalized graph diffusion is defined with the transition matrix and weighting coefficients [19], which allows the spectral analysis with explicit eigendecomposition of associated laplacians. The transition matrix is exactly the weighted adjacency matrix mentioned above. GCN and GAT [1, 6] can be regarded as a special case in graph diffusion-based models using the first-order power of transition matrix. Many graph diffusion-based models including TAGCN [15], MixHop [20] and DAGNN [23] use symmetrically normalized adjacency matrix in GCN as transition matrix. DAGN [23] uses attention matrix as transition matrix. PAN [26] uses the transition matrix of maximal entropy random walks. Two popular weighting coefficients are personalized PageRank (PPR) [24, 18] and the heat kernel [25, 27], which both follow the prior that more distant neighboring nodes have less influences. PPNP [18] acts as a postprocessing method to propagate output probability generated by an arbitrary model in the graph with PPR. GDC [19] works as a preprocessing method to recover meaningful neighborhoods from noisy graphs. GraphHeat [27] uses the heat kernels as weighting coefficients. Attention walk [17] jointly optimizes the node embeddings and weighting coefficients $\theta^i$. However, without sparsification or approximation methods, graph diffusion-based models result in a dense matrix [19], which is computationally expensive. Moreover, the numeric form of weighting coefficients is invariant for each node, which is not flexible. Additionally, some of them are just preprocessing or postprocessing methods, which in somehow limits their usages.

In this paper, we propose Adaptive Graph Diffusion Networks with Hop-wise Attention (AGDNs-HA). Firstly, we define the Adaptive Graph Diffusion (AGD) with weighting matrices and limited multi-hop neighborhood aggregations. Secondly, we incorporate hop-wise attention (HA) mechanism, which computes attention scores as weighting matrices to integrate representations from different aggregations. The attention score for each aggregation are based on the initial representation and associated intermediate representation. "Hop-wise" means that these weighting matrices are normalized over hops. With different transition matrices, there are two variants proposed: Graph Convolution Network with Hop-wise Attention (GCN-HA) and Graph Attention Network with Hop-wise Attention (GAT-HA).

Moreover, AGD extends the definition of weighting coefficients from numeric to diagonal matrix. In spatial domain, the weighting matrices act as scaling matrices and vary with different aggregations, which implies that they differently disturbs the distribution of representations over nodes for each aggregation. Then the eigenvectors of final diffusion matrix are usually implicit. Thus AGDN-HA is hard to analyse in spectral domain. If the graph pooling operation is employed before attention computation, it becomes non-adaptive graph diffusion networks with hop-wise attention (GDNs-HA). We leave this discuss in future researches.

Our proposed method has two main advantages: 1. Single AGDN-HA layer has larger receptive field compared with GCN, which implies that the long-range interactions between distant nodes can be captured in each layer. Furthermore, the computational complexity of AGDNs-HA is lower than GNNs with the same transition matrix and receptive field. 2. The incorporation of adaptive hop-wise attention makes the graph diffusion convolution more flexible and learnable with stronger generalization capability. In contrast to standard graph diffusion theory [19], the high-order diffusion matrices are computed implicitly with sparse transition matrix and weighting matrices are learnable. In contrast to approximated graph diffusion-based methods [18, 24], all of the intermediate representations can be directly used. Additionally, GAT-HA can be further viewed as a graph neural network with two-step attention mechanism.

Experimental results on standard dataset for semi-supervised node classification [28] show that GCN-HA and GAT-HA respectively outperform GCN and GAT. GAT-HA without using labels outperforms most of models using labels. GAT-HA with using labels achieves the best result. We respectively compare results from models with or without using labels for more fair comparison.
Generalized Graph Diffusion (GGD). The multi-hop neighborhood aggregations in single layer can be regarded as generalized graph diffusion, which is defined via the diffusion matrix \( \Theta \):

\[
S = \sum_{k=0}^{\infty} \theta_k T^k,
\]

with the weighting coefficients \( \theta_k \) and the generalized transition matrix \( T \). Eq. [1] is guaranteed to converge, with associated constraints that \( \sum_{k=0}^{\infty} \theta_k = 1, \theta_k \in [0, 1] \) and that the eigenvalues of \( T \) are bounded by \( \lambda_i \in [0, 1] \).

Adaptive Graph Diffusion (AGD). In this paper, we further generalize graph diffusion:

\[
S = \sum_{k=0}^{K} \Theta^{(k)} T^k,
\]

where \( \Theta^{(k)} \) is a generalized weighting matrix and \( K \) is the maximum order. \( \Theta^k \) meets two constraints: diagonal (\( \Theta^{(k)} = \text{diag}(\theta_1^{(k)}, \theta_2^{(k)}, ..., \theta_N^{(k)}) \)) and normalized along hops (\( \sum_{k=0}^{K} \theta_i^{(k)} = 1, \forall i \in [0, 1, 2, ..., N], \theta_i^{(k)} \in [0, 1] \)). We remove the constraint of the convergence via cutting off the diffusion and use weighting coefficients varying among nodes.

In this paper, we propose AGDNs-HA, based on the further generalized graph diffusion (AGD) with the hop-wise attention (HA). Some popular graph diffusion-based methods use the prior that the influences of neighbors decrease with the distance, while we remove this prior and incorporate attention mechanism.

The main challenges are computation complexity and memory costs. We need to design a flexible and scalable hop-wise attention, with possibly less additional parameters. The way to proceed aggregations is also important and variable.

In practice, we do not need to explicitly calculate the high-order powers of the initial transition matrix, which results in dense matrix \( S \). Instead, applying successive neighborhood aggregations with the initial transition matrix is more computationally efficient. Some graph diffusion methods \([18, 25, 27]\) have efficient and accurate approximations in linear time and space, with maintaining only one matrix.

2.1 Transition matrix

The transition matrix is variable and not restricted to be symmetric. There are several common matrices: column-stochastic random walk transition matrix \( T_{rw,\text{col}} = AD^{-1} \), row-stochastic random walk transition matrix \( T_{rw,\text{row}} = D^{-1}A \) and the symmetric transition matrix \( T_{\text{sym}} = D^{-\frac{1}{2}}AD^{-\frac{1}{2}} \), where \( D \) is the degree matrix (\( D_{ii} = \sum_{j=1}^{N} A_{ij} \)).

In this paper, we consider following transition matrices:

- Symmetrically normalized transition matrix with adding self-loops in GCN [1]:

\[
T_{\text{gcn}} = (I_N + D)^{-\frac{1}{2}}(I_N + A)(I_N + D)^{-\frac{1}{2}}.
\]

- Attention transition matrix in GAT [6] with adding self-loops:

\[
T_{\text{att}} = D_{\text{att},r}(s)^{-1}A_{\text{att}}(s),
\]

\[
\left[A_{\text{att}}(s)\right]_{ij} = \begin{cases} 
\exp(\text{LeakyRelu}([H_i][H_j] \cdot a) - s), & j \in N_i \cup \{i\} \\
0, & j \notin N_i \cup \{i\}
\end{cases},
\]

\[
\left[D_{\text{att},r}(s)\right]_{ii} = \sum_{j \in N_i} \exp(\text{LeakyRelu}([H_i][H_j] \cdot a) - s)
\]

where \( \cdot \) denotes the inner product, \( \| \) denotes the operation of concatenation, \( i \) denotes the \( i \)-th node, \( j \) denotes the \( j \)-th node, \( N_i \) denotes the first-order neighboring nodes of the \( i \)-th node, \( H_i \) denotes the representation vector of the \( i \)-th node, and \( a \) represents the attention vector. \( T_{\text{att}} \) can be viewed as a row-stochastic matrix. \( A_{\text{att}}(s) \) is the equivalent adjacency matrix and \( D_{\text{att}}(s) \) is the equivalent degree matrix with row sum of \( A_{\text{att}}(s) \) as entries. \( s \) is a scale factor.
• Attention transition matrix with adjacency normalization \(29\):

\[
T_{\text{att, gc}n} = (I_N + D)^{\frac{1}{2}} \text{att}(I_N + D)^{-\frac{1}{2}}
\]

\[
= (I_N + D)^{\frac{1}{2}} (D^{-1}_{\text{att}, r} A_{\text{att}}) (I_N + D)^{-\frac{1}{2}}
\]

\[
= \left((I_N + D)^{\frac{1}{2}} D^{-1}_{\text{att}, r}\right) A_{\text{att}} (I_N + D)^{-\frac{1}{2}}.
\]

The first type of transition matrix in Eq. [3] is based on symmetric transition matrix with adding self-loops, depending solely on the original adjacency matrix \(A\). It can be viewed as a low-pass filter in the spectral domain [5].

The second type of transition matrix in Eq. [4] depends on the distribution of neighboring node features (including the node itself). Its normalization operation in the edge softmax component is only calculated from the viewpoint of the destination nodes, which means that this transition matrix is a row stochastic matrix.

The third type of transition matrix in Eq. [7] from DGL’s GAT implementation [29] combines two types of transition matrices above. Since attention matrix is already row-stochastic, the mean power of adjacency normalization terms should be equal to 0. In Eq. [7] we further obtain the final equivalent standard form with attention adjacency matrix and two normalization terms. For a graph without node attributes (or with invariant node attributes), this transition matrix becomes symmetrically normalized transition matrix in GCN.

Obviously, attention transition matrices are usually non-symmetric. An essential condition for obtaining symmetric transition matrix without iterative computation is that \(A_{\text{att}}\) is symmetric. Furthermore, \(A_{\text{att}}(s)\) is symmetric if and only if \([H_i]_j = [H_j]_i\) · \(a\), \(\forall(i, j) \in E\).

In this paper, GCN-HA uses the first type of transition matrix in Eq. [3] and GAT-HA uses the third type of transition matrix in Eq. [7]. Actually the choice of the transition matrix is very free. The matrices mentioned above are just representative examples.

2.2 Hop-wise attention

In original graph diffusion-based models, the weighting coefficients have many choices. The coefficients defined in PPR and the heat kernel satisfying the convergence are found to be efficient. The weighting coefficients can also be analogously trainable parameters, with using label propagation [30, 31] and node embedding models [17]. AGD uses more flexible weighting matrices, which is normalized over hops. Motivated by attention mechanism in GAT, we further propose hop-wise attention to integrate different representations. Noticeably, weighting matrices are not restricted to satisfy the convergence.

The original self-attention mechanism in Transformer includes separated \(Q, K, V\) matrices as query, key and value matrix, while the attention mechanism in GAT is simplified with only one transformation matrix and one attention vector. The hop-wise attention continues to use this simplification, with matrix \(W^{(l)}\) and hop-wise attention vector \(a_{hw}^{(l)}\).

An AGDN-HA layer is defined as below:

\[
H^{(l)} = \text{AGDN-HA} \left(G, H^{(l-1)}, W^{(l)}, a_{hw}^{(l)}\right).
\]

(8)

The input node feature matrix is encoded into given dimension \(d^{(l)}\) as below:

\[
H^{(0,l)} = H^{(l-1)} W^{(l)}.
\]

(9)

The intermediate representations in the \(l\)-th layer are updated as below:

\[
H^{(k,l)} = T^{(l)} H^{(k-1,l)},
\]

(10)

\(T^{(l)}\) represents the transition matrix in the \((l)\)-th layer.

The output representation in the \(l\)-th layer is updated with a residual term as below:

\[
H^{(l)} = \sum_{k=0}^{K} \Theta^{(k,l)} H^{(k,l)} + H^{(l-1)} W^{(l)}r,
\]

(11)

where \(\Theta^{(k,l)} = \text{diag}(\theta_1^{(k,l)}, \theta_2^{(k,l)}, ..., \theta_N^{(k,l)})\) represents the hop-wise attention weighting matrix for the \(k\)-th aggregation in the \(l\)-th layer.
The hop-wise attention (HA) weighting matrix is calculated as below:

\[
\Theta^{(k,l)} = HA\left( \{ H^{(k,l)} \}_{k=0}^{K}, a^{(l)}_{hw} \right),
\]

where \( \cdot \) represents inner product, \( || \) represents the concatenation operation, \( \hat{H}^{(k,l)} \) represents the representation vector of the \( i \)-th node in the \( k \)-hop aggregation at the \( l \)-th layer, \( a^{(l)}_{hw} \) represents the hop-wise attention vector at the \( l \)-th layer. Obviously, the attention weighting vector \( \theta^{(0,l)}_i, \theta^{(1,l)}_i, ..., \theta^{(K,l)}_i \) varies on different nodes, which implies that hop-wise attention scores are adaptive.

The diagram of an AGDN-HA layer is shown in Figure 3. With hop-wise attention, the AGDN-HA layer is able to adaptively integrate features from different hops, which is more flexible than previous graph diffusion-based methods.

2.3 Multi-head hop-wise attention

Multi-head attention allows the model to gather information from representations at different sub-spaces. The hop-wise attention for each head \( i \) is processed separately and then aggregated:

\[
H^{(0,l+1)} = MultiHead(G, H^{(l)}) = \frac{\sum_{i=1}^{M} \text{heads}^{(l)}_i}{M},
\]

\[
\text{heads}^{(l)}_i = AGDN_{HA}\left( G, H^{(l-1)}, W^{i,(l)}, a^{i,(l)}_{hw} \right),
\]

where \( i \) denotes the \( i \)-th head and \( M \) denotes the number of heads. For computational efficiency, we use average values of multi-heads instead of concatenating them. In addition, for GAT-HA, the number of heads in hop-wise attention is set by default the same as GAT aggregations.

2.4 Overall model

As shown in Algorithm 1 we present the overall architecture of a model for node classification task with multiple AGDN-HA layers. We denote the number of layers with \( L \), the depth of each layer with \( K \), the number of heads with...
$M$, the input dimension with $d^{(0)}$, the output dimension of the $l$-th layer with $d^{(l)}$, the linear transformation matrix of the $l$-th layer in the $i$-th head with $W^{i,(l)}$ and the hop-wise attention vector of the $l$-th layer in the $i$-th head with $a_{hw}^{i,(l)}$.

---

**Algorithm 1: Adaptive Graph Diffusion Networks with Hop-wise Attention**

**Data:** Adjacency matrix $A$, node feature matrix $X$  
**Result:** Node classification probabilities

\[
\begin{align*}
H^{(0)} & \leftarrow X; \\
l & \leftarrow 1; \\
\text{while } l \leq L \text{ do} & \\
\quad i & \leftarrow 1; \\
\quad \text{while } i \leq n_h \text{ do} & \\
\quad \quad k & \leftarrow 1; \\
\quad \quad \hat{H}^{i,(0,l)} & \leftarrow H^{(l-1)} W^{i,(l)}; \\
\quad \quad \text{calculate transition matrix } T^{i,(l)}; \\
\quad \quad \text{while } k \leq K \text{ do} & \\
\quad \quad \quad \hat{H}^{i,(k,l)} & \leftarrow T^{i,(l)} \hat{H}^{i,(k-1,l)}; \\
\quad \quad \quad k & \leftarrow k + 1; \\
\quad \quad \{ \Theta^{i,(k,l)} \}_{k \in [0,1,2,...,K]} & \leftarrow \text{HA} \left( \{ \hat{H}^{i,(k,l)} \}_{k \in [0,1,2,...,K]}, a_{hw}^{i,(l)} \right); \\
\quad \quad i & \leftarrow i + 1; \\
\quad \text{end} & \\
\text{end} & \\
H^{(l)} & \leftarrow \frac{1}{\sum_{i=1}^{M} \left( \sum_{k=0}^{K} \Theta^{i,(k,l)} \hat{H}^{i,(k,l)} \right) / M + H^{(l-1)} W^{(l)}}; \\
\text{if } l < L \text{ then} & \\
\quad H^{(l)} & \leftarrow \text{ReLU} \left( \text{BatchNorm} \left( H^{(l)} \right) \right); \\
\text{end} & \\
l & \leftarrow l + 1; \\
\text{end} & \\
\text{return } \text{softmax} \left( H^{(L)} \right)
\end{align*}
\]

3 Analysis

In this section, we discuss the characteristics of AGDNs-HA from the spectral view. We demonstrate that, only in special case, AGDNs-HA can be analysed as a polynomial graph filter in the spectral domain with explicit eigenvalues. Moreover, we view GAT-HA as a extended GAT model with two-step attention mechanism.

3.1 AGDN-HA in spectral domain

The transition matrices can be viewed as weighted adjacency matrices. We define the laplacian as $L = I - T$. The laplacian can be decomposed as $L = U \Lambda U^{-1}$, with real-valued $U$ and $\Lambda$. The columns of $U$ are eigenvectors of $L$. $\Lambda$ is diagonal $\Lambda = \text{diag}(\lambda_i)$, where $\lambda_i$ is the $i$-th eigenvalue of $L$. The Fourier transform of a graph signal $x$ is performed as $\hat{x} = U^{-1} x$ with inverse Fourier transform as $x = U \hat{x}$. 

7
GDC has shown the close relationship between polynomial filters and generalized graph diffusion [19]:

$$
\sum_{k=0}^{K} \theta_k T^k = \sum_{k=0}^{K} \theta_k U (I_N - \Lambda)^k U^{-1}
$$

$$
= U \left( \sum_{j=0}^{K} \left( \sum_{k=j}^{K} \binom{j}{k} (-1)^j \theta_k \right) \Lambda^j \right) U^{-1}
$$

$$
= U \left( \sum_{j=0}^{K} \xi_j \Lambda^j \right) U^{-1}
$$

$$
= \sum_{j=0}^{K} \xi_j L^j,
$$

where $$\xi_j$$ is the coefficient of the $$j$$-th order term in the polynomial filter.

In our further generalized graph diffusion, the output representation is updated as below:

$$
SH = \sum_{k=0}^{K} \Theta^{(k)} T^k H
$$

$$
= \sum_{k=0}^{K} (I_N - L^{(k)}) H
$$

$$
= \sum_{k=0}^{K} U^{(k)} (I_N - \Lambda^{(k)}) U^{(k)-1} H.
$$

Since the left multiplication with the scaling matrix $$\Theta^{(k)}$$ can change directions of column vectors in $$U$$, the basis matrix $$U^{(k)}$$ does not vary with $$k$$ if and only if $$\Theta^{(k)}$$ has identical diagonal entries, when AGD degrades into original graph diffusion. In most cases, we cannot directly merge different representations with the same set of eigenvectors. In another word, AGDN-HA cannot be directly considered as a polynomial graph filter. The decomposition of merged diffusion matrix can be defined as below:

$$
SH = \sum_{k=0}^{K} \Theta^{(k)} T^k H
$$

$$
= (I_N - L_S) H
$$

$$
= U_S (I_N - \Lambda_S) U_S^T H
$$

where $$L_S = I_N - \sum_{k=0}^{K} \Theta^{(k)} T^k$$ is the laplacian associated with $$S$$, and $$L_S = U_S \Lambda_S U_S^T$$ is the eigendecomposition of $$L_S$$ with real-valued $$U_S$$ and $$\Lambda_S$$. Unfortunately, $$\Theta^{(k)}$$ is non-negative, hop-wise normalized and learnable attention score matrix without extra constraints, which implies that eigenvalues of $$L_S$$ are implicit and hard to analyse in the spectral domain.

We can still analyse from other aspects. The number of parameters is still limited, due to the simplified attention mechanism. The adaptive hop-wise attention weighting matrix integrates multi-hop neighborhood aggregations in different ways for different nodes. We also remove the prior that high-order terms should have smaller weighting coefficients, which is expected to be automatically learned in certain configurations.

### 3.2 Attention mechanism in GAT-HA

GAT-HA is a variant of AGDN-HA with weighted attention matrix as transition matrix. Meanwhile, GAT-HA can also be viewed as an extended GAT model with two-step attention mechanism. The sentences fed into Transformer can be viewed as fully connected graphs with much less nodes than common graph datasets. For graph data, if the high-order neighboring nodes without direct edges are defined as to be reached with multi-hop walks, then we may obtain a nearly fully connected graph. This graph is considered to contain richer information than raw graph. However, the number of nodes is often much larger than the length of a sentence. The attention scores from all other nodes can not be explicitly
Table 1: Experimental results on ogbn-arxiv dataset.

| Settings          | Models                  | Test accuracy | Notes                          |
|-------------------|-------------------------|---------------|--------------------------------|
| Not use labels    | GCN                     | 71.74 ± 0.29  | pytorch_geometric implementation |
|                   | DeeperGCN               | 72.14 ± 0.19  |                                |
|                   | GCNII                   | 72.74 ± 0.16  |                                |
|                   | GAT                     | 73.48 ± 0.17  | dgl implementation with 3 heads |
|                   | GCN-HA                  | 73.24 ± 0.20  |                                |
|                   | GAT-HA                  | 73.49 ± 0.15  | 1 head                         |
|                   | GAT-HA                  | 73.75 ± 0.21  | 3 heads                         |
| Use labels        | GCN+linear+labels       | 73.06 ± 0.24  | dgl implementation              |
|                   | GAT+adj.norm+labels     | 73.65 ± 0.11  | dgl implementation with 3 heads |
|                   | UniMP                   | 73.11 ± 0.20  |                                |
|                   | UniMP_large             | 73.79 ± 0.14  | label embedding                 |
|                   | GCN-HA+labels           | 73.39 ± 0.12  |                                |
|                   | GAT-HA+labels           | 73.81 ± 0.13  | 1 head                         |
|                   | GAT-HA+labels           | 73.98 ± 0.09  | 3 heads                         |

calculated at one step. GAT-HA performs hierarchical two-step attention computation. The first step is to calculate the direct neighborhood attention scores as entries of the transition matrix to calculate high-order neighborhood attention scores implicitly. The second step is to calculate hop-wise attention scores to incorporate distance (or hop) information. As we mentioned, GAT-HA does not rely on the prior that distant neighbors have less influences.

4 Experiments

We evaluate GCN-HA and GAT-HA on the ogbn-arxiv dataset from Open Graph Benchmark [28] with standard splits, which contains 170k nodes and 1.2m edges. Our proposed models are implemented with Deep Graph Library (DGL) [29]. The experiments are done on Nvidia Tesla V100 with 16 Gb GPU memory. Several representative and state-of-the-art models are compared with our proposed methods: GCN [1], DeeperGCN [13], GCNII [14], GAT [6, 29] and UniMP [8].

Incorporating labels information in transductive node classification task is recently a popular trend. Following most of baselines, we randomly mask node labels in train set and concatenate node feature matrix with one-hot encoded label matrix. In Table 1 GCN-HA and GAT-HA share the most of hyperparameters: learning_rate = 0.002, L = 3, K = 3, hidden_dim = 256, dropout = 0.5, epochs = 2000, input_drop = 0.1, attn_drop = 0.05. For GAT-HA model with 3 heads, dropout is set to 0.75 and input_drop is set to 0.25. Both of GCN-HA and GAT-HA are trained with stochastic gradient descend (SGD) optimizer. We use the framework of training and evaluating provided by DGL [29].

As shown in Table 1 we can conclude that GCN-HA outperforms GCN-based models with/without using labels, and GAT-HA with 3 heads outperforms other models with both settings. In Table 1 “linear” means using residual linear layers and "adj.norm" means using attention matrix in Eq. 7 [29].

5 Conclusions

We first discuss the ways of enlarging the receptive field of GNNs and two main problems followed (over-fitting and over-smoothing). By incorporating multi-hop aggregations in single layer, the correlation between complexity and depth of receptive field can be removed. The model using layers with multi-hop aggregations can be generalized as graph diffusion-based models. Motivated by graph diffusion theory, we propose AGDN-HA that generalizes weighting coefficients into matrices and incorporates hop-wise attention mechanism. Although the spectral analysis is hard to perform because of adaptive weighting matrices, the adaptive graph diffusion with learnable weighting matrices brings more flexibility and generalization capability to avoid over-smoothing. In addition, GAT-HA shows a feasible two-step attention mechanism in a high-order neighborhood graph. Experimental results on standard dataset in semi-supervised node property prediction task demonstrate that our proposed methods achieve significant improvements.
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