NDGGNET-A Node Independent Gate based Graph Neural Networks

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Abstract
Graph Neural Networks (GNNs) is an architecture for structural data, and has been adopted in a mass of tasks and achieved fabulous results, such as link prediction, node classification, graph classification and so on. Generally, for a certain node in a given graph, a traditional GNN layer can be regarded as an aggregation from one-hop neighbors, thus a set of stacked layers are able to fetch and update node status within multi-hops. For nodes with sparse connectivity, it is difficult to obtain enough information through a single GNN layer as not only there are only few nodes directly connected to them but also can not propagate the high-order neighbor information. However, as the number of layer increases, the GNN model is prone to over-smooth for nodes with the dense connectivity, which resulting in the decrease of accuracy. To tackle this issue, in this thesis, we define a novel framework that allows the normal GNN model to accommodate more layers. Specifically, a node-degree based gate is employed to adjust weight of layers dynamically, that try to enhance the information aggregation ability and reduce the probability of over-smoothing. Experimental results show that our proposed model can effectively increase the model depth and perform well on several datasets.

1 INTRODUCTION
Graph neural network (GNN) is a powerful model that could transmit information along with connections within a given graph. Thus, for each node in a graph, the network collects information from neighbors and deduces its state after several stacked layers. On this mechanism, three famous fantastic improvements are proposed. GCN focus on aggregation and built a fundamental pipeline to combine node-wise state and neighbor-wise state[10]. GAT considered that one node should have various dependency levels with neighbors, then infer a set of scores by taking advantages of attention module for nodes updating[18]. GraphSage borrowed the idea of random walk[15] and unveil neighbor sampling instructively, that make GNN model suitable for inductive learning[5]. Inspired with these three ideas, tremendous related works have been published and adopted to tackle downstream task of all kinds of domains, including computer vision[6], nature language process[4], social network analysing[3], medical research[8], recommendation system[12] and so on. However, these models usually illuminate heterogeneous capability on graphs with various average number of edges[23].

Generally, in most graph based tasks, it is should be fully presented that each node has limited edge info, in meanwhile, the information of high connectivity node could help the lower one by the correlation between them. In graph neural network, the aggregation of high-order neighboring information in a graph is the key effective way to implement the between-node high correlation topology. When we deploy a deeper graph layer for the low connectivity node, in meanwhile, the active node which has abundant edges between nodes within lower order graph domain will be easily over-fitted as the most common structure of graph neural network is stacking-layer. Take Graph-Sage for instance, to overcome the probably over-fitting issue, for most state-of-the-art GNN implementation, the layer depth is generally not bigger than three. At the same time, the 3 layer depth is probably far away from the best performance because the imbalance connectivity distribution of different nodes is not take into consideration. However, the deeper GNN framework has been figured out by the inspiration of Res-Net, but the complexity of structure ignores the efficiency of forward propagation when it deepen the depth of the layer. How to deploy the dynamic multi layers of graph neural network by the different characteristic of nodes in a simple and efficient way is necessary.

On the other hand, a mass of thesis suggest that a GNN model would make all nodes tend to steady state eventually, and such so-called final state is detrimental to downstream tasks as nodes in graph may share similar vectorized expressions and make it indistinguishable[14, 24, 25]. Therefore, some studies have shown that, residual like architecture can slow the rate of convergence, that make it possible to build a network with numerous layers[2, 10, 24]. And some researchers lay emphasis on implicit relationship between features and graph structures, that spawn attention-wise methods[17, 22]. Parameter reduction is also an effective idea for over smooth dilution, and the ensuing framework are able to obtain modest computational complexity by wiping off some weak related parameters or make them shareable[13, 19].

In this thesis, we first analyze the factors affecting the increasing of network layers, then propose a node independent gate based graph neural network (NDGGNET) for the different connectivity topology node within a certain graph. The model should design an attention based gate structure which can establish the natural relation between over smooth issue and layer depth in propagation and achieve outperformed numerical results on several open datasets. The main contributions is summarized as follow:
- we analyse the factors that may related with over smoothing issue;
- a node independent gate is introduced to uniformize the operation process.

2 PRELIMINARIES

2.1 Graph Neural Network

Give a graph \(G(\nu,\epsilon, X)\), where \(\nu\) is node set, \(\epsilon\) is edge set, and \(X\) is initial feature of nodes, graph convolution operator can be illuminated by two steps, i.e. propagating and mapping. Seeing in Eq.1, GNN aggregate intensities of nodes in kth layer, \(H^k\), by
following the normalized adjacency matrix \( \hat{A} \), then extend these features with weight matrix of this layer, \( W^k \), and a non-linear activation function \( \sigma(\cdot) \)

\[
H^k = \sigma(\hat{A}H^{k-1}W^k) \\
H^0 = X
\]  

(1)

2.2 Over Smoothing
Following equation in Eq. 1, a graph neural network can transmit message among nodes continuously, and update feature of each node according with its neighbor nodes, thus makes every nodes are able to sense information in the graph. However, suggesting by massive of existing papers [2, 25], such framework with sufficient number of layers will force each node to achieve stable and reduce diversity. This phenomenon is called over smoothing.

To simplify the analysis, we assume activation function in Eq. 1 as RELU[1], so it can be ignored if input feature values are all non negative, then the calculation formula of each node, \( v \), in GNN can be written as expansion in Eq.2, where \( W^l \) is weight matrix in \( l \)-th layer, \( W^0 = \prod_{l=0}^n W^l \), \( N(v) \) is set nodes of graph, \( G \), \( \hat{A} = A + I \) is normalized adjacent matrix and \( D \) is degree matrix with self loop.

\[
\lim_{k \to \infty} H^k = \hat{A}^kX^0W^* \\
\quad = (\hat{D}^{-\frac{1}{2}}\hat{A}\hat{D}^{-\frac{1}{2}})^k X^0W^* \\
\quad = \sum_{u \in N(G)} \sqrt{(d_u + 1)(d_u + 1)} x_u^0W^*
\]  

(2)

Based on this assumption, the final state of one node only related with its own degree, input features and transformation matrices, that means over smoothing issue could be mitigated if these factors are well processed.

2.3 Influence of Smoothing

The above analysis shows that the node features converge with infinity layers. In other words, the distance between nodes becomes very small to result in weak feature classification. In Eq.3, we define a mean distance of connected nodes (MDCN) to show the variation of distance, where \( x_i \) is feature vector of \( i \)-th node and \( \| \cdot \|_2^2 \) is L2-norm distance.

\[
MDCN = \frac{1}{n} \sum_{i=1}^{N} \sum_{j \in N(i)} \| x_i - x_j \|_2^2
\]  

(3)

In Figure 1 shows for the MDCN of different number layer in cora dataset[21], the distance among connected nodes drops dramatically within few layers, and that is a hard evidence to decipher strong correlation between number of layers and over smoothing issue.

![Figure 1: MDCN with different layers in cora dataset.](image)

3 METHODOLOGY

In this section, we first give a description of degree based gate and dynamic degree based gate. The model is shown in figure 2.

3.1 Intuition

In order to reveal the relationship between expression decay and node degree, we will conduct the stationary state for each node-i in graph, we now hypothesis the stationary state for any node reaching is \( K(i, \epsilon) \) (\( \epsilon \) is a very small constant express the node will be effected quite limited by other nodes with the increasing iteration), in Eq.4, we found that the \( K \) is vary by the different nodes in graph and related to the connectivity of the node itself.

\[
K(i, \epsilon) <= \log \lambda_2 \left( \sqrt{\frac{\hat{d}_i}{2m+n}} \right)
\]  

(4)

where \( \lambda_2 \) is the second largest eigenvalue of \( \hat{A} \), \( \hat{d}_i \) denotes the degree of node \( v_i \), and \( m \) denote the number of edges and \( n \) denotes the number of nodes separately. It is obviously that the lower connectivity node \( i \) pretend to be company with the smaller \( K(i, \epsilon) \) and the higher node j company with a bigger \( K(j, \epsilon) \).

3.2 Fundamental Framework

Inspiring by solid work in computer vision[7], we adopt a residual wise framework to slow the variation between layers. Specially, seeing in Eq.5, for \( k_{1h} \) layer in GNN model, the output feature of previous layer can be regarded as a momentum term, and a weighted summation is deployed to combine the current term, \( \hat{A}X^{k-1}W^k \) and history term, \( X^{k-1} \).

\[
H^k = (1 - \alpha^k)\sigma(\hat{A}H^{k-1}) + \alpha^kH^{k-1} \\
H^0 = \sigma(\hat{A}X^0)
\]  

(5)

Figure.2 shows basic architecture of our model, that we set a node-wise gate, \( \alpha^i \), to balance terms in \( i_{th} \) layer.

3.3 Node Independent Gate

Generally, weights in moving strategy is high related with model performance, and it is sensitive and uneasy to assign an optimal value artificially. As it is mentioned in front pages, final state of GNN is strongly related with degree of vertex and initial features, it controls convergence rate. Thus, we build a attention gate, seeing in Eq.6, which takes a concatenation of d-dim degree embedding, \( E(D) \in R^{nd} \), initial feature, \( X_0 \), output of last layer, \( H_{k-1} \), and output of this layer, \( H_k \), then a value between 0 and 1 is derived by

\[
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Figure 2: flowchart of the proposed model.

making use of MLP mapping with softmax, \( g(\bullet) \), that balances the residual link between input and output of one GNN layer.

\[
\alpha^k = g(E(D)||X_0||H_k||H_{k-1})
\]

Additionally, if Figure 3, we treat elements in gate value of one node separately and independently, that means the output of gate function should be a vector, \( \alpha^k = \{\alpha_1^k, \alpha_2^k, ..., \alpha_c^k\} \), where \( c \) is dim size of node feature. Details can be found in section 4.

Figure 3: framework of node independent gate.

4 EXPERIMENTS

In this section, we will demonstrate the results of our proposed architecture in contrast with popular GNN methods on open datasets.

4.1 Implementation Details

In experiment, NDGGNET based models are well trained by Adam optimizer[9] with exponential learning rate decay(LR decay), and other parameters, including weight decay, drop rate, max epochs, are depicted in table 1. And for clarity of definition, notation NDGGNET(*) in all tables means our standard proposed method and NDGGNET(*) is a degraded version that the attention scores of both terms in Eq.5 is set with 1.

Moveover, we evaluated proposed method and its variants in contrast with other widely applied GNN methods, i.e. GCN and its decoupled version[10], GAT[18], SGC[19], SIGN[16], APPNP[11] and JK-NET[20] on three datasets, i.e. cora, citeseer and pubmed[21], and accuracy. To be fair, accuracy is employed to measure the effects respectively, details of datasets are shown in table 2.

| dataset | nodes | edges | features | classes |
|---------|-------|-------|----------|---------|
| cora    | 2708  | 5429  | 1433     | 7       |
| citeseer| 3327  | 4732  | 3707     | 6       |
| pubmed  | 19717 | 44338 | 500      | 3       |

Table 2: Details of open datasets.

4.2 Numerical Results

In table 3, the accuracy of our method is significantly improved in compare with both coupled methods and decoupled methods. That proves the effectiveness of the functionality of node independent gating function.

Table 3: Experimental results of graph learning. Take accuracy as metrics.

| method     | cora  | citeseer | pubmed |
|------------|-------|----------|--------|
| GCN        | 81.5  | 73.4     | 79.0   |
| GCN-decoupled | 83.0 | 70.8     | 78.8   |
| GAT        | 83.0  | 72.5     | 78.8   |
| APPNP      | 83.3  | 71.8     | 80.1   |
| SGC        | 81.0  | 71.3     | 79.8   |
| SIGN       | 82.1  | 72.4     | 79.5   |
| JK-Net     | 81.8  | 70.7     | 78.8   |
| NDGGNET    | 84.3  | 73.8     | 79.0   |
| NDGGNET(*) | 81.3  | 69.0     | 78.1   |

Table 3: Experimental results of graph learning. Take accuracy as metrics.

Further, we adopt traditional GCN model and NDGGNET, and divide each dataset into three barrels according node degree, i.e. \( deg \in [2, 4) \), \( deg \in [4, 8) \), \( deg \in [8, \infty) \). Therefore, in Figure 4, the relationships between number of layers, connectivity of nodes and test accuracy are exhibited clearly, each subfigure contains six plots and each plot stands for one GNN method and one barrel. Accuracy of GCN network will drop apace after few layers, but in NDGGNET the accuracy could increase along with layer’s number. Specifically, for nodes with sparse connected edges, the NDGGNET model could help them to achieve higher accuracy value by adding more layers, and for nodes with dense connected edges, the accuracy could maintain high values.
with different node degree and number of layers.

REFERENCES

In this thesis, we first analyze the nature of over smooth, show the cause of the issue, and deduce the relevant factors, then propose a node independent gate function to control the rate of transmission of the GNN network, that make it possible to dilute over smooth and expend the number of layers. The experimental results illuminate the designed gate could regulate the increment in updating and deduce the relevant factors, then propose a node dependent local smoothing for scalable graph neural networks.

5 CONCLUSION

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