What nodes vote to? Graph classification without readout phase

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ABSTRACT

In recent years, many researchers have started to construct Graph Neural Networks (GNNs) to deal with graph classification task. Those GNNs can fit into a framework named Message Passing Neural Networks (MPNNs), which consists of two phases: a Message Passing phase used for updating node embeddings and a Readout phase. In Readout phase, node embeddings are aggregated to extract graph feature used for classification. However, the above operation may obscure the effect of the node embedding of each node on graph classification. Therefore, a node voting based graph classification model is proposed in this paper, called Node Voting net (NVnet).Similar to the MPNNs, NVnet also contains the Message Passing phase. The main differences between NVnet and MPNNs are: 1, A decoder for graph reconstruction is added to NVnet to make node embeddings contain graph structure information as much as possible; 2, In NVnet, the Readout phase is replaced by a new phase called Node Voting phase. In this new phase, an attention layer based on the gate mechanism is constructed to help each node to observe the node embeddings of other nodes in the graph, and each node predicts the class of the graph from its own perspective. The above process is called node voting. After voting, the results of all nodes are aggregated to get the final graph classification result. In addition, considering that aggregation operation may also obscure the differences between node voting results, a regularization term is added to drive node voting results to reach group consensus. We evaluate the performance of NVnet on 4 benchmark datasets. The experimental results show that NVnet performs well on graph classification task.

INTUITION

When many models which can fit into MPNNs are used for graph classification, the graph features need to be extracted in the Readout phase. However, this process may obscure the effect of the node embedding of each node.

PRELIMINARY

A graph is denoted as $G = (V, E, A, X)$, where $V=\{v_i \mid i=1,\ldots,n_v\}$ is the set of nodes, $v_i \in V$ denotes a node, nv denotes the number of nodes. E is the set of edges. $e_{ij}=(v_i,v_j) \in E$ indicates that there is an edge between v_i and v_j. $A \in \mathbb{R}^{nv \times nv}$ denotes the adjacency matrix. Here we only consider the simple graph, that is A is a binary symmetric matrix with $A_{ij}=1$ if $e_{ij} \in E$ and $A_{ij}=0$ if $e_{ij} \notin E$. $X \in \mathbb{R}^{nv \times nv}$ denotes the input features of nodes, where d_x is the input feature dimension.

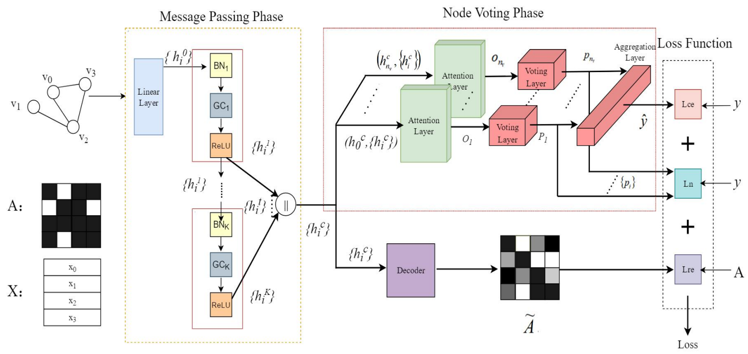
EXPERIMENT

TABLE I. AVERAGE CLASSIFICATION ACCURACY IN PERCENT, AND THE STANDARD DEVIATION (BEHIND ±)

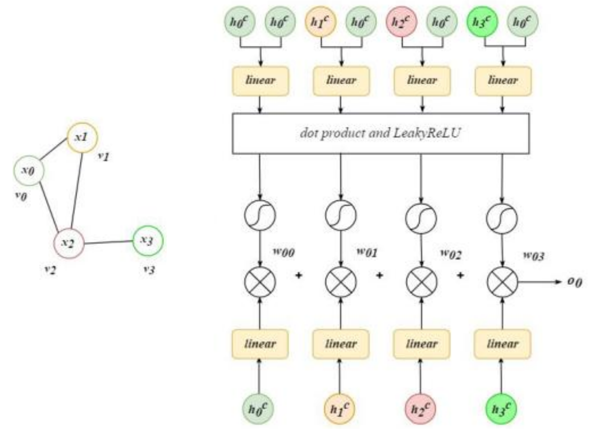
Method	Dataset MUTAG	PROTEINS	COLLAB	IMDB-B
GCN[14]	74.6±7.7	73.1±3.8	***80.6±2.1***	72.6±4.5
GraphSAGE[14]	74.9±8.7	73.8±3.6	79.7±1.7	72.4±3.6
GIN-0[14]	***85.7±7.7***	72.1±5.1	79.3±2.7	***72.8±4.5***
GIN-ε[14]	83.4±7.5	72.6±4.9	79.8±2.4	72.1±5.1
Graclus[14]	77.1±7.2	73.0±4.1	79.6±2.0	72.2±4.2
top$_k$ pooling[14]	76.3±7.5	72.7±4.1	79.7±2.2	72.5±4.6
DiffPool[14]	85.0±10.3	***75.1±3.5***	78.9±2.3	72.6±3.9
Global Attention[14]	74.6±8.0	72.5±4.5	79.6±2.2	72.3±3.8
Set2Set[14]	73.3±6.9	73.6±3.7	79.6±2.3	72.2±4.2
SortPool[14]	77.3±8.9	72.4±4.1	77.7±3.1	72.4±3.8
NVnet(GCNconv)	80.2±9.7	74.8±3.7	***81.8±1.0***	73.7±5.7
NVnet(SAGEconv)	79.8±6.2	75.7±3.5	81.3±2.3	74.0±5.5
NVnet(GIN-0conv)	85.4±9.6	76.1±3.1	80.6±1.0	73.4±5.3
NVnet(GIN-εconv)	***87.3±6.1***	***76.3±3.0***	80.5±1.8	***74.0±3.7***

- ***NVnet(GIN-εconv) achieves the highest average accuracy on MUTAG, PROTEINS and IMDB-BINARY. Meanwhile, NVnet(GCNconv) achieves the highest average accuracy on COLLAB.***

PROPOSED METHOD



- ***Fig. 1. The left part is the input sample. The middle part is the NVnet framework, which consists of three components: a Message Passing phase for node embeddings updating, a decoder block for graph reconstruction and a Node Voting phase for graph classification. The calculation diagram of the loss function is shown on the right.***



- ***Fig. 2. A toy example to show the calculation process of the attention mechanism in NVnet.***

The calculation process of $\{o_i \mid i=1,\ldots,n_v\}$,$\{p_i \mid i=1,\ldots,n_v\}$ and predict result will be introduced below.

$$w_{ij}^{h\_m} = \mathrm{sigmoid}(\mathrm{LeakyReLU}(\mathrm{concat}(\{h_i^c \Phi_m, h_j^c \Phi_m\})\theta_m^T))$$

$$a_i^m = \sum_{j=1,\ldots n_v} w_{ij}^{h\_m}(h_j^c \Phi_m)$$

$$o_i = \mathrm{concat}(\{a_i^m \mid m=1,\ldots M\})$$

Loss function

The Loss function consists of three parts. λ_{re} and λ_n are hyper-parameters. Lce represents the cross entropy loss between the targets $\{y^s\}$ and predictions $\{\hat{y}^S\}$.

$$Loss = L_{ce} + \lambda_{re} L_{re} + \lambda_n L_n$$

CONTRIBUTIONS

1. ***We propose a new phase named Node Voting phase based on the attention mechanism. In this phase, each node predicts the class of the graph by observing the node embeddings of other nodes.***

2. ***A new model called NVneta is proposed for graph classification task. The new model includes a Message Passing phase, a Node Voting phase and a decoder. Unlike MPNNs, the new model no longer needs to extract graph feature.***

CONCLUSION

- ***A node voting based graph classification model named NVnet is proposed.***