Graph pooling and unpooling in Graph Neural Network with its applications in graph classification

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Introduction

$$X^{(l+1)} = S^{(l)^T} Z^{(l)} \in \mathbb{R}^{n_{l+1} \times d},$$

$$A^{(l+1)} = S^{(l)^T} A^{(l)} S^{(l)} \in \mathbb{R}^{n_{l+1} \times n_{l+1}}.$$

$$S^{(l)} = \text{softmax}\left(\text{GNN}_{l,\text{pool}}(A^{(l)}, X^{(l)})\right),$$

$$Z^{(l)} = \text{GNN}_{l,\text{embed}}(A^{(l)}, X^{(l)}),$$

The DIFFPOOL structure is a neural network layer that performs pooling operations in the graph. It can be combined with any GNN structure to learn network information. The GNN model of each layer takes the graph feature X and the adjacency matrix A as input, and finally outputs each The embedding of a node, then use these embeddings to cluster similar nodes to obtain the coarsening input of the next layer, and then run another GNN layer on these coarsened graphs. Finally, use the final output to represent the graph classification task.

Visualization
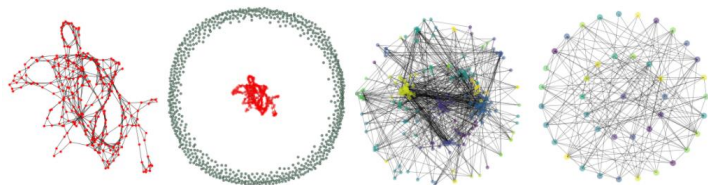
Results

Data sets	Baseline (3-layer diff-pool network)	6-layer U-Net (3 pooling and 3 unpooling)
...		
D&D	79.49%	85.47%
ENZYMES	55.00%	58.33%
Peking_1	77.6%	87.5%
Proteins	77.78%	88.89%
...		

Traditional Unpool

-initialize empty feature matrice for the new graph

-place nodes back to their original positions in the graph

-inherit original adjacency matrix

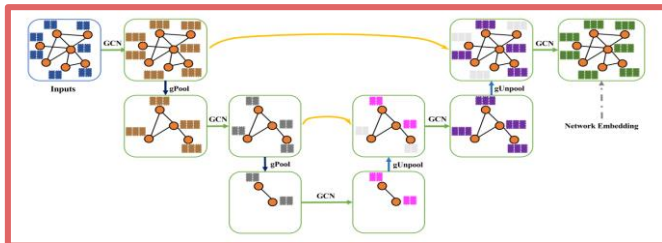### Our Model

$$A_{l,up} = MLP(S_{l,up}^T A_{l-1} S_{l,up})$$

$$S_{l,up} = MLP(S_{l,p}^T)$$

$$Z_{l,up} = Attention(GCN(A_{l-1}, X_{l-1}))$$

$$X_{l,up} = S_{l,up} Z_{l,up}$$

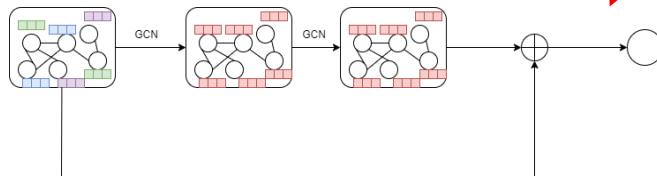$$Attention(k) = Softmax(k) \cdot k$$

Related Model

Model
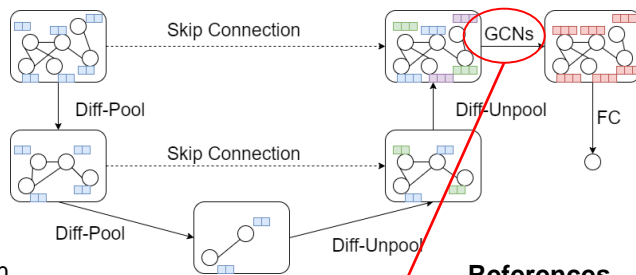
Global Feature Extraction

References

[1] Ying, Z., You, J., Morris, C., Ren, X., Hamilton, W. and Leskovec, J., 2018. Hierarchical graph representation learning with differentiable pooling. In Advances in neural information processing systems (pp. 4800-4810)
[2] Gao, Hongyang, and Shuiwang Ji. "Graph u-nets." arXiv preprint arXiv:1905.05178 (2019).