Paper Implementation

GCN: SEMI-SUPERVISED CLASSIFICATION WITH GRAPH CONVOLUTIONAL NETWORKS

By Ahmed A. A. Elhag

How to define spectral graph convolution?

Main Idea

 Define layer-wise propagation rule for neural network models which operate directly on graphs.

 Use this form of of a graph-based neural network model for semi-supervised classification of nodes in a graph.

Graph Convolution Update Rule

$$H' = \sigma(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}HW)$$

$$\tilde{A} = A + I$$

$$\tilde{D}_{ii} = \sum_{j} \tilde{A}_{ij}$$

• Node-wise, this can be written as:

$$\overrightarrow{h}_i = \sigma(\sum_{i \in N_j} \frac{1}{\sqrt{|N_i||N_j|}} \overrightarrow{W} \overrightarrow{h}_j)$$

• Simple and Powerful: most commonly cited GNN paper!

Implementation approach

GCN paper

- Define one GCN layer: layer-wise propagation rule.
- Stack two GCN layers, use relu and dropout between them.
- Build the train function: (optimizer, loss...)
- Experiments

The Experiments

Results

Dataset	Туре	Nodes	Edges	Classes	Features	Test Accuracy
Cora	Citation network	2,708	5,429	7	1,433	81.5 ± 1
Citeseer	Citation network	3,327	4,732	6	3,703	69 ± 0.8

Comparison

Dataset	Our experiment	Paper's result
Cora	81.5 ± 1	81.5
Citeseer	69 ± 0.8	70.3

Improvement

A lot of architectures!

• MPNN (Gilmer et al., ICML 2017)

• GAT (Velickovic et al., ICLR 2018)

MPNN (Gilmer et al., ICML 2017)

• Let \overrightarrow{m}_{ij} be the message sent from node i to node j

• Compute \overrightarrow{m}_{ij} using a massage function:

$$\overrightarrow{m}_{ij} = f_e(\overrightarrow{h}_i, \overrightarrow{h}_j, \overrightarrow{e}_{ij})$$

• Aggregate all the messages entering a node:

$$\overrightarrow{h}_{i}' = f_{v}(\overrightarrow{h}_{i}, \sum_{j \in N_{i}} \overrightarrow{m}_{ji})$$

GAT (Velickovic et al., ICLR 2018)

• Let's consider the more general form of GCN:

$$\overrightarrow{h}_{i}' = \sigma(\sum_{j \in N_{i}} \alpha_{ij} W \overrightarrow{h}_{j})$$

$$\alpha_{ij} = a(\overrightarrow{h}_i, \overrightarrow{h}_j, \overrightarrow{e}_{ij})$$

$$\alpha_{ij} = \frac{exp(\alpha_{ij})}{\sum_{k \in N_i} exp(\alpha_{ik})}$$

• a is learnable!

Conclusion

• GCN: how to define spectral graph convolution.

• Simple and powerful, most commonly cited GNN paper.

• A lot of architectures came as improvement of GCN.

Thank you!