Paper Implementation

GCN: SEMI-SUPERVISED CLASSIFICATION WITH GRAPH CONVOLUTIONAL NETWORKS

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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:

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

- 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 funcion: (optimizer, loss...)
- Experiments

The Experiments

Results

Dataset	Type	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	68.9 ± 0.5
Pubmed	Citation network	19,717	44,338	3	500	

Comparison

Dataset	Our experiment	Paper’s result
Cora	81.5 ± 1	81.5
Citeseer	68.9 ± 0.5	70.3
Pubmed		79

Improvement

A lot of architectures!

- MPNN (Gilmer et al., ICML 2017)
- GAT (Velickovic et al., ICLR 2018)

MPNN (Gilmer et al., ICML 2017)

- Let $\vec{m}_{ij}$ be the message sent from node i to node j

- Compute $\vec{m}_{ij}$ using a massage function:

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

- Aggregate all the messages entering a node:

$$\vec{h}'_i = f_v(\vec{h}_i, \sum_{j \in N_i} \vec{m}_{ji})$$

GAT (Velickovic et al., ICLR 2018)

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

$$\vec{h}'_i = \sigma(\sum_{j \varepsilon N_i} \alpha_{ij} W \vec{h}_j)$$

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

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

- 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!