

Graph U-Nets

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Introduction

- ▶ Convolutional neural networks (CNNs) have been very successful in image-related tasks.
- ▶ Images can be considered as special cases of graphs, in which nodes lie on regular 2D lattices.
- ▶ An important part of CNNs is the pooling (down-sampling) operation, which enables high-level feature encoding and receptive field enlargement.

Related works

- ▶ Topology based pooling: $O(|V|^3)$ for eigendecomposition; result is not very good.
- ▶ DiffPool*: $O(k|V|^2)$

*Ying, R., You, J., Morris, C., Ren, X., Hamilton, W. L., and Leskovec, J. Hierarchical graph representation learning with differentiable pooling. CoRR, abs/1806.08804, 2018.

Graph U-Nets

- ▶ Proposed gPool and gUnpool operation that are counterparts of the pooling and up-sampling of CNNs respectively.
- ▶ A encoder-decoder structure based on the two operations. Similar to the U-Net for images.
- ▶ Experiments show it outperforms the GNNs without gPool and gUnpool operations in both inductive and transductive tasks.

gPool operation

$$X_{l+1} = \sigma(\hat{D}^{-\frac{1}{2}} \hat{A} \hat{D}^{-\frac{1}{2}} X_l W_l)$$

$$\Downarrow$$

$$y = X^l p^l / \|p^l\|,$$

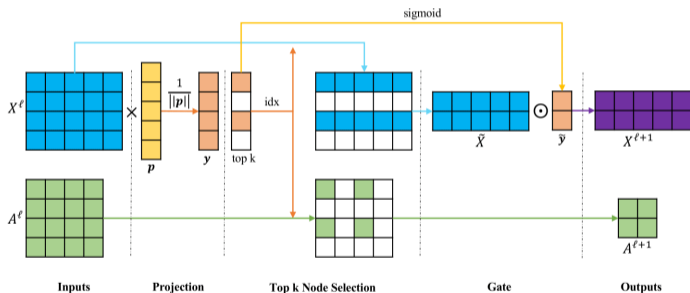
$$\text{idx} = \text{rank}(y, k),$$

$$\tilde{y} = \text{sigmoid}(y(\text{idx})),$$

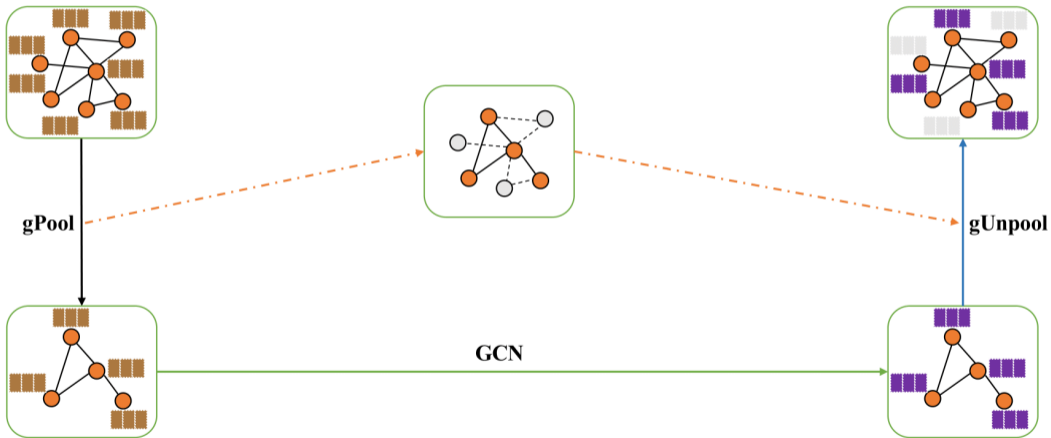
$$\tilde{X}^l = X(\text{idx}, :),$$

$$A^{l+1} = A^l(\text{idx}, \text{idx}),$$

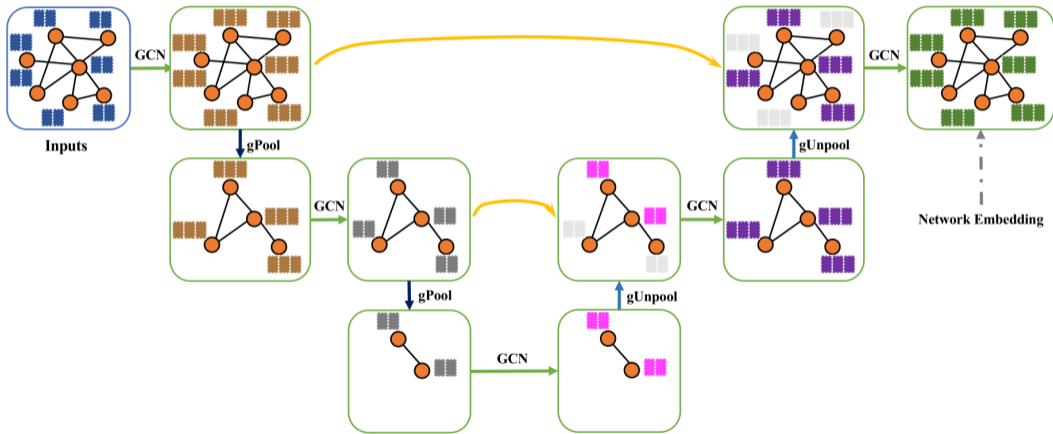
$$X^{l+1} = \tilde{X}^l \odot (\tilde{y} \mathbf{1}_C^T)$$



gUnpool operation



Graph U-Net



Graph Augmentation

After the removal of some nodes, the graph may be broken into disconnected parts. To handle this, Graph U-Net augments the graph with:

$$A^2 = A^l A^l, \quad A^{l+1} = A^2(\text{idx}, \text{idx})$$

Also they empirically found that adding higher weights to self-loops can increase the performance:

$$\hat{A} = A + 2I$$

Datasets

Table 1. Summary of datasets used in our node classification experiments (Yang et al., 2016; Zitnik & Leskovec, 2017). The Cora, Citeseer, and Pubmed datasets are used for transductive learning experiments.

Dataset	Nodes	Features	Classes	Training	Validation	Testing	Degree
Cora	2708	1433	7	140	500	1000	4
Citeseer	3327	3703	6	120	500	1000	5
Pubmed	19717	500	3	60	500	1000	6

Table 2. Summary of datasets used in our inductive learning experiments. The D&D (Dobson & Doig, 2003), PROTEINS (Borgwardt et al., 2005), and COLLAB (Yanardag & Vishwanathan, 2015) datasets are used for inductive learning experiments.

Dataset	Graphs	Nodes (max)	Nodes (avg)	Classes
D&D	1178	5748	284.32	2
PROTEINS	1113	620	39.06	2
COLLAB	5000	492	74.49	3

Transductive task (node classification)

Table 3. Results of transductive learning experiments in terms of node classification accuracies on Cora, Citeseer, and Pubmed datasets. g-U-Nets denotes our proposed graph U-Nets model.

Models	Cora	Citeseer	Pubmed
DeepWalk (Perozzi et al., 2014)	67.2%	43.2%	65.3%
Planetoid (Yang et al., 2016)	75.7%	64.7%	77.2%
Chebyshev (Defferrard et al., 2016)	81.2%	69.8%	74.4%
GCN (Kipf & Welling, 2017)	81.5%	70.3%	79.0%
GAT (Veličković et al., 2017)	83.0 ± 0.7%	72.5 ± 0.7%	79.0 ± 0.3%
g-U-Nets (Ours)	84.4 ± 0.6%	73.2 ± 0.5%	79.6 ± 0.2%

Inductive task (graph classification)

Table 4. Results of inductive learning experiments in terms of graph classification accuracies on D&D, PROTEINS, and COLLAB datasets. g-U-Nets denotes our proposed graph U-Nets model.

Models	D&D	PROTEINS	COLLAB
PSCN (Niepert et al., 2016)	76.27%	75.00%	72.60%
DGCNN (Zhang et al., 2018)	79.37%	76.26%	73.76%
DiffPool-DET (Ying et al., 2018)	75.47%	75.62%	82.13%
DiffPool-NOLP (Ying et al., 2018)	79.98%	76.22%	75.58%
DiffPool (Ying et al., 2018)	80.64%	76.25%	75.48%
g-U-Nets (Ours)	82.43%	77.68%	77.56%

Ablation study

Table 5. Comparison of g-U-Nets with and without gPool or gUnpool layers in terms of node classification accuracy on Cora, Citeseer, and Pubmed datasets.

Models	Cora	Citeseer	Pubmed
g-U-Nets without gPool or gUnpool	82.1 \pm 0.6%	71.6 \pm 0.5%	79.1 \pm 0.2%
g-U-Nets (Ours)	84.4 \pm 0.6%	73.2 \pm 0.5%	79.6 \pm 0.2%

Table 6. Comparison of g-U-Nets with and without graph connectivity augmentation in terms of node classification accuracy on Cora, Citeseer, and Pubmed datasets.

Models	Cora	Citeseer	Pubmed
g-U-Nets without augmentation	83.7 \pm 0.7%	72.5 \pm 0.6%	79.0 \pm 0.3%
g-U-Nets (Ours)	84.4 \pm 0.6%	73.2 \pm 0.5%	79.6 \pm 0.2%

Parameter size

Table 8. Comparison of the g-U-Nets with and without gPool or gUnpool layers in terms of the node classification accuracy and the number of parameters on Cora dataset.

Models	Accuracy	#Params	Ratio of increase
g-U-Nets without gPool or gUnpool	$82.1 \pm 0.6\%$	75,643	0.00%
g-U-Nets (Ours)	$84.4 \pm 0.6\%$	75,737	0.12%

This suggests that the improvement is not a result of more parameters, and adding gPool and gUnpool will not increase the risk of over-fitting.

What I learnt

- ▶ We can find inspirations from CNN techniques when dealing with GNN.
- ▶ The adjacency matrix can be augmented to impose different weights for links.

Thank you!