Self-Attention Graph Pooling

Paper ID:2233   Project page: github.com/inyeoplee77/SAGPool



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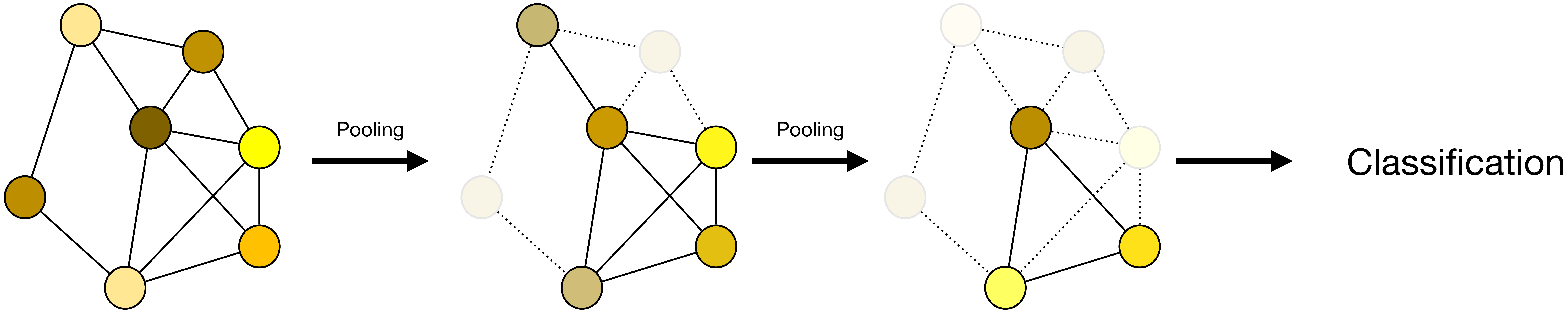
Research background & Motivation

- Advances in graph convolutional neural networks.
- Generalizing convolution operation to graphs.
- Growing interest in graph pooling methods.
- Graph pooling methods that can learn hierarchical representations of graphs.

Goal

- Task: Graph classification.
- Key Idea: Utilize GNNs as a graph pooling module.



Related Work

- Global pooling methods: use summation or neural networks to pool all the representations of nodes in each layer (Set2Set[1] and SortPool[2]).

- Hierarchical pooling methods: obtain intermediate graphs (adjacency, features) and pass them to the next layer (DiffPool[3] and gPool[4]).

[1]:Vinyals, O., Bengio, S., and Kudlur, M. Order mat- ters: Sequence to sequence for sets. *arXiv preprint arXiv:1511.06391*, 2015.
[2]:Zhang, M., Cui, Z., Neumann, M., and Chen, Y. An end-to- end deep learning architecture for graph classification. In Proceedings of AAAI Conference on Artificial Inteligence, 2018b.
[3]: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.
[4]:Gao, H. and Ji, S. Graph u-net. In Proceedings of the 36th International Conference on Machine Learning (ICML), 2019.

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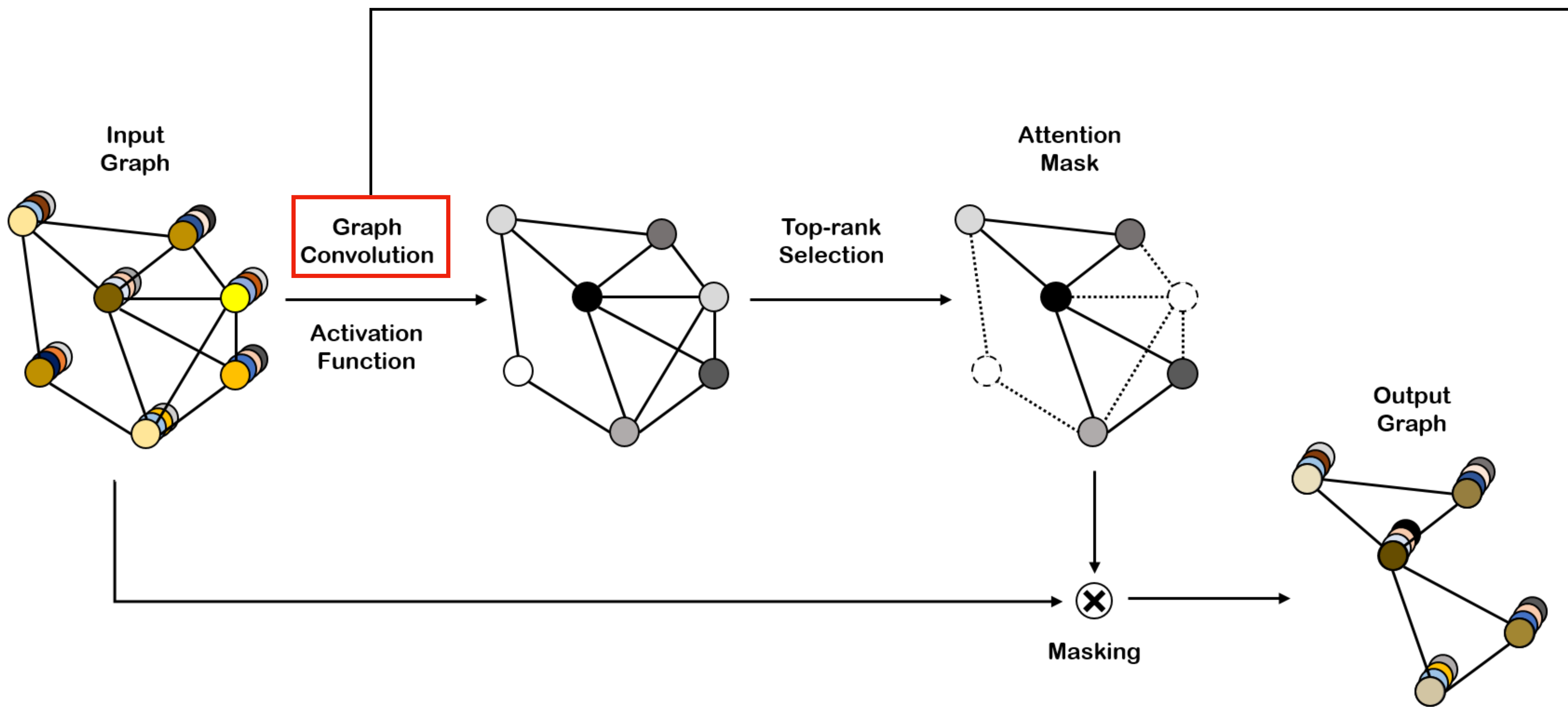


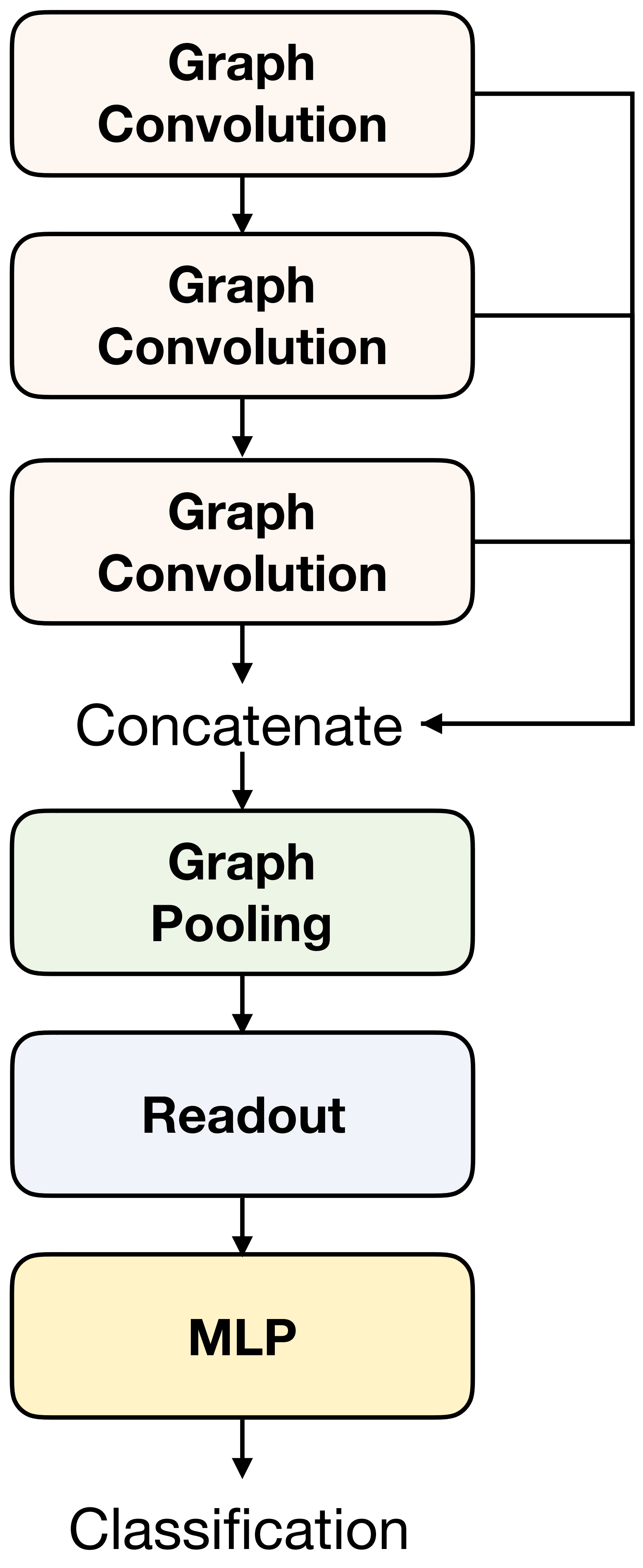
Graph Convolution
SAGPool_h
$\text{SAGPool}_{h,\text{Cheb}}$ $\text{SAGPool}_{h,\text{SAGE}}$ $\text{SAGPool}_{h,\text{GAT}}$
$\text{SAGPool}_{h,\text{augmentation}}$ $\text{SAGPool}_{h,\text{serial,2layers}}$
$\text{SAGPool}_{h,\text{parallel},M=2}$ $\text{SAGPool}_{h,\text{parallel},M=4}$

$$Z = \sigma(\mathbf{GNN}(X, A)) \qquad \mathbf{idx} = \mathbf{top\text{-}rank}(Z, \lceil kN \rceil), \quad Z_{mask} = Z_{\mathbf{idx}}$$

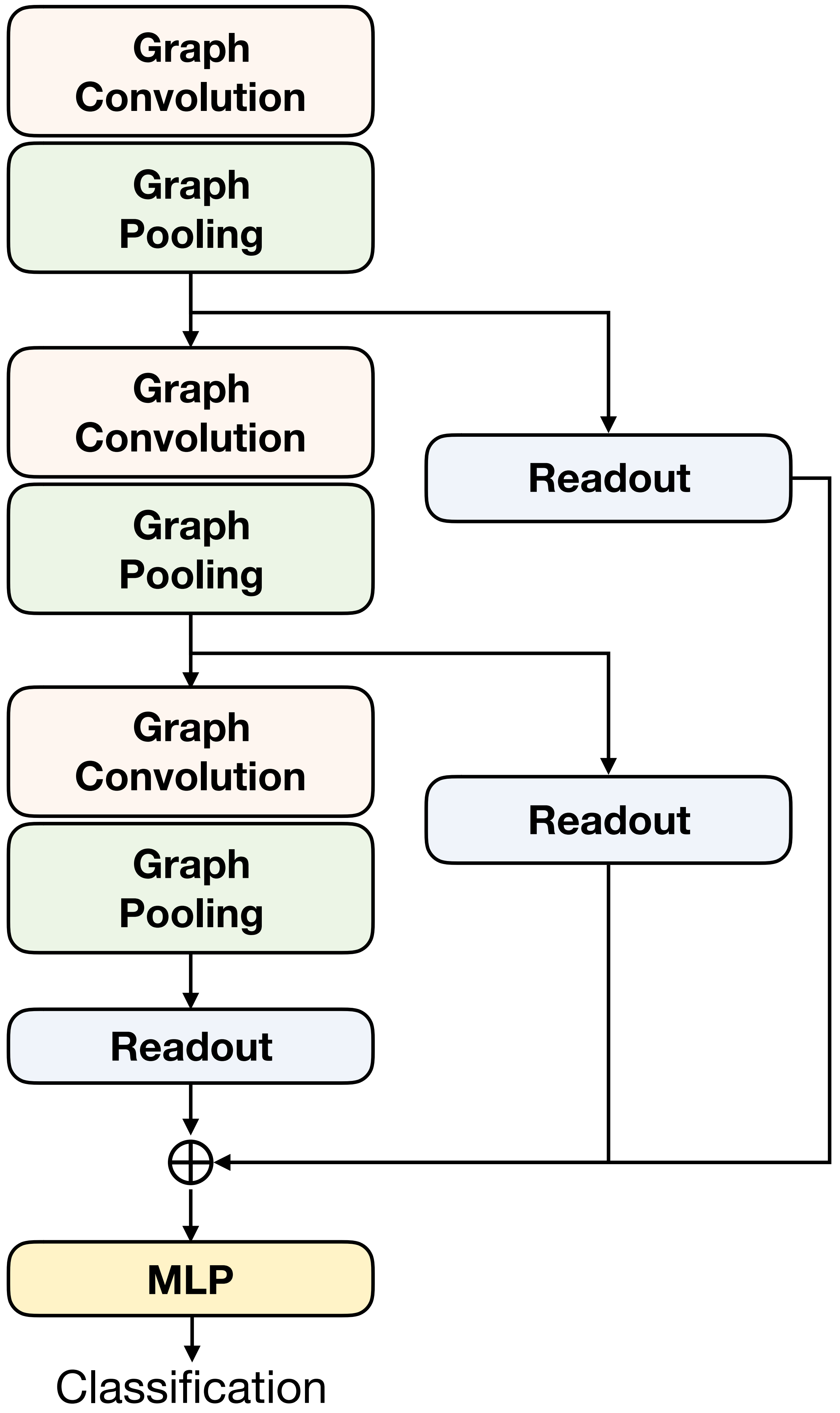
$$X' = X_{\mathbf{idx},:}, \; X_{out} = X' \odot Z_{mask}, \; A_{out} = A_{\mathbf{idx},\mathbf{idx}}$$

Evaluation

Global pooling methods



Hierarchical pooling methods



Evaluation

- Graph benchmark datasets.
- the same early stopping criterion and hyper-parameter selection strategy for a fair comparison
- 20 random seeds to split each dataset.
- 10-fold cross validation for evaluations (a total of 200 testing results for each evaluation).
- pytorch_geometric[1] for implementation.

[1]: Fey, M. and Lenssen, J. E. Fast graph representation learning with PyTorch Geometric. In *ICLR Workshop on Repre- sentation Learning on Graphs and Manifolds*, 2019.

Results

	D&D	PROTEINS	NCI1	NCI109	FRANKENSTEIN
Set2Set	71.27±0.84	66.06±1.66	68.55±1.92	69.78±1.16	61.92±0.73
SortPool	72.53±1.19	66.72±3.56	73.82±0.96	74.02±1.18	60.61±0.77
SAGPool	**76.19**±0.944	**70.04**±1.47	**74.18**±1.20	**74.06**±0.78	**62.57**±0.60
DiffPool	66.95±2.41	68.20±2.02	62.32±1.90	61.98±1.98	60.60±1.62
gPool	75.01±0.86	71.10±0.90	67.02±2.25	66.12±1.60	61.46±0.84
SAGPool	**76.45**±0.97	**71.86**±0.97	**67.45**±1.11	**67.86**±1.41	**61.73**±0.76

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- Additional details and discussion at the poster (Pacific Ballroom #8).