A Flexible, Equivariant Framework for Subgraph GNNs via Graph Products and Graph Coarsening

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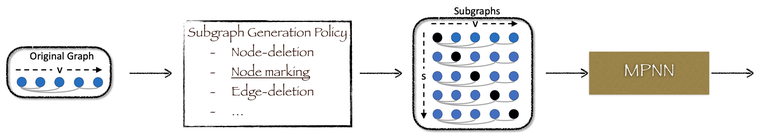
Subgraph GNNs

Provably expressive Graph Neural Networks (GNNs) that represent graphs as a collection of subgraphs.



Main drawback: High computational complexity. For node-based policies, the complexity increases significantly— from n nodes up to n^2 nodes.

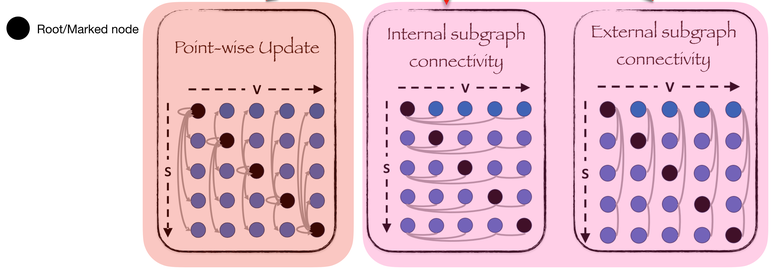
Our Goals

Devise a Subgraph GNN architecture that can flexibly generate and process variable-sized collection of subgraphs, and deliver strong experimental results.

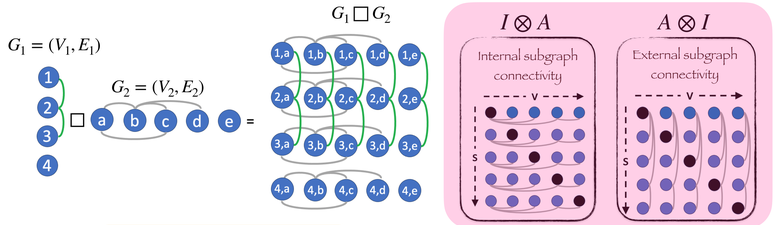
Subgraph GNNs and Graph Products

Maximally expressive node-based Subgraph GNN [1].

$$\mathcal{X}(s,v)^{t+1} = f^t\Big(\mathcal{X}(s,v)^t, \mathcal{X}(v,v)^t, \{\mathcal{X}(s,v')^t\}_{v'\sim_G v}, \{\mathcal{X}(s',v)^t\}_{s'\sim_G s},\Big)$$



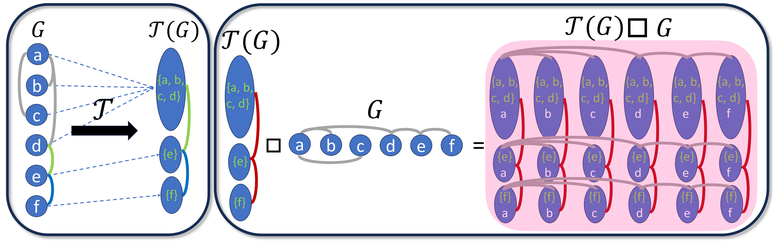
Connection to Graph Products [2]. Taking $G \square G$ gives the internal and external connectivities of the maximally expressive node-based Subgraph GNN.



CS-GNN Main Idea

How can we devise a more efficient Subgraph GNN?

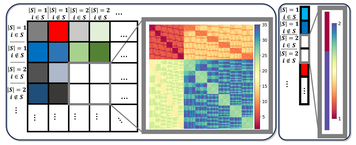
- Use a coarsening function $\mathcal{T}$.
- Apply $\mathcal{T}(G)\square G$ instead of $G\square G$ to get the internal and external connectivities.

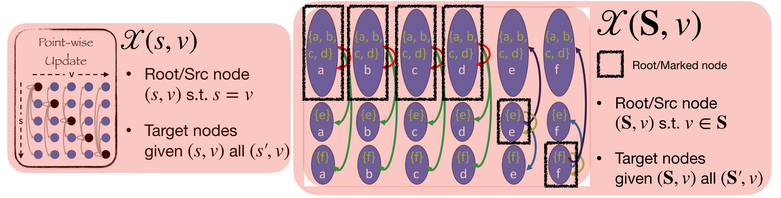


- Study the symmetries of the new node feature tensor, $\mathcal{X}(\mathbf{S}, v)$ to come up with symmetry-based updates, which are analogous to the point-wise updates.

CS-GNN Symmetry-Based Updates

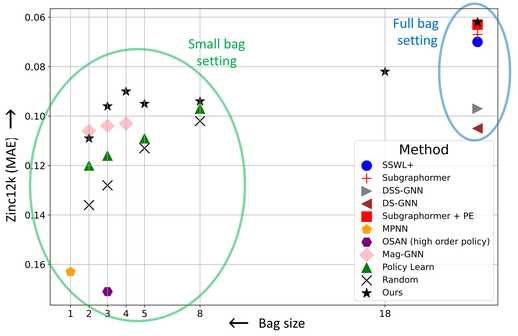
We characterize all equivariant linear maps $\mathbf{L} : \mathbb{R}^{\mathcal{P}([n])\times[n]} \to \mathbb{R}^{\mathcal{P}([n])\times[n]}$, where n is the number of nodes in the graph. We use a subset of the basis vectors, which correspond to the following updates:





Experiments

- Our method outperforms baseline models in the small bag setting.
- Our method matches state-of-the-art Subgraph GNNs in the full bag setting.



References

[1] Bohang Zhang, Guhao Feng, Yiheng Du, Di He, Liwei Wang.
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