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SDG: A Simplified and Dynamic Graph Neural Network

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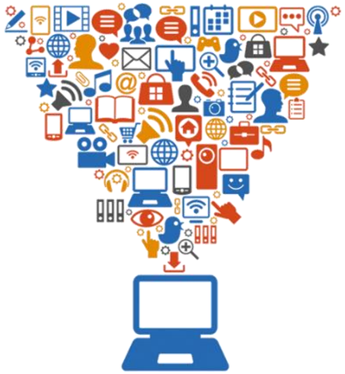
Roadmap

- Motivation
- Proposed SDG Framework
- Experiments
- Conclusion

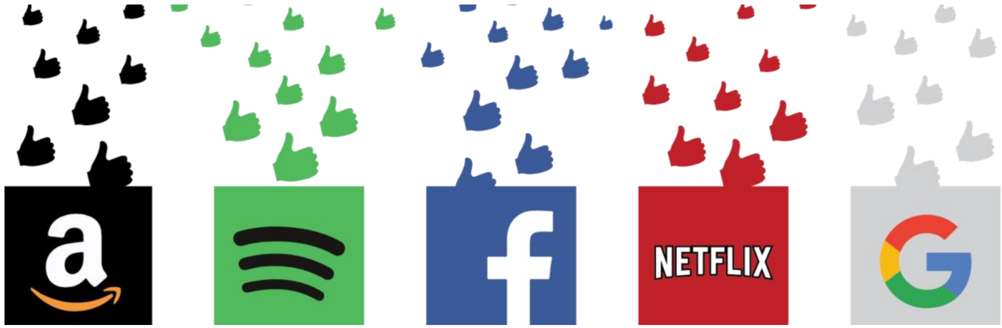
Graph Neural Networks

- Nowadays, GNNs have a wide range of applications, such like



Information Retrieval

Fraud Detection



Recommender Systems

Existing Work

- Goal of simplifying GNNs
  - To reduce computational complexity,
  - and maintain competitive performance in the meantime.

- Simplified GNNs from different perspectives
  - FastGCN [Chen et al., ICLR 2018]
  - SGC [Wu et al., ICML 2019]
  - APPNP [Klicpera et al., ICLR 2019]
  - LightGCN [He et al., SIGIR 2020]
  - ……

Challenges

- In complex real-world settings
  - In addition to scaling the GNNs structures,
  - evolving the structures of GNNs is overlooked.
- Compared with static models, dynamic neural networks have[1]:
  - Compatibility
  - Interpretability
- How can we synchronize simplification and dynamization of GNNs?

[1] Han et al., Dynamic Neural Networks: A Survey. CoRR 2021.

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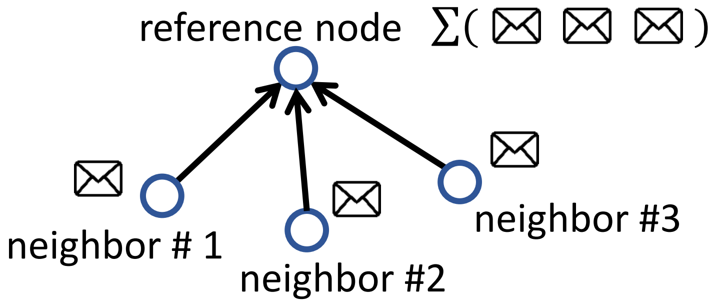
Preliminaries



- Information Aggregation in GNNs
  - A classic method: message-passing scheme to aggregate neighborhood information.

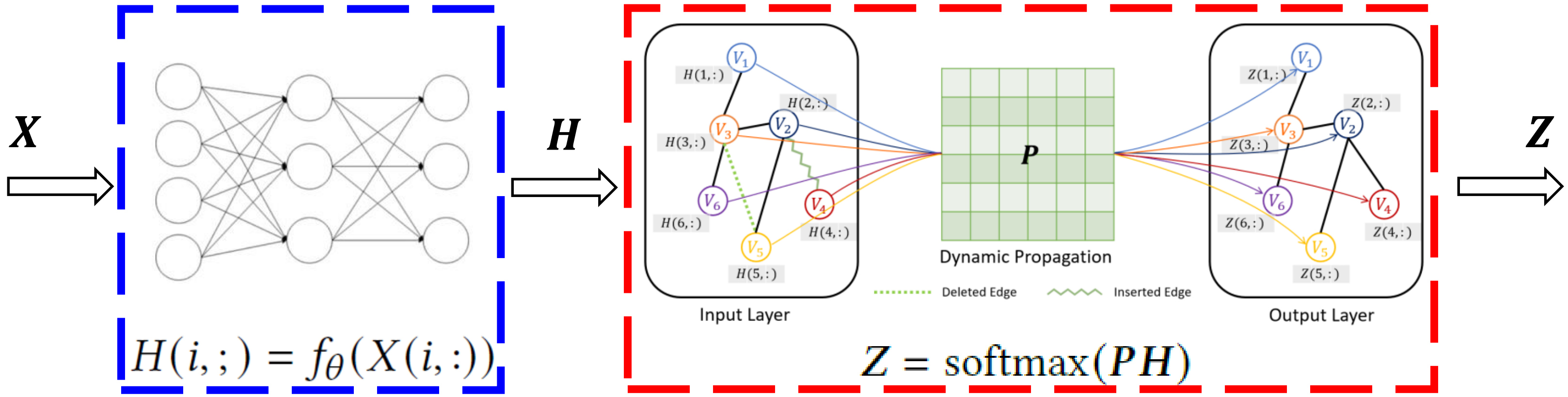
$$h_v^{(l)} = \sigma\left(W_l \cdot \text{AGGREGATE}\left(\{h_u^{(l-1)}, \forall u \in \widetilde{N}(v)\}\right)\right)$$

- Replacing message-passing with personalized PageRank[2]
  - The influence of other nodes on a selected node x through a k-layer GNN (e.g., GCN or GraphSAGE) is proportional to the k-step random walk distribution starting from that selected seed node x [3].

[2] Klicpera et al., Predict then Propagate: Graph Neural Networks meet Personalized PageRank. ICLR 2019.
[3] Xu et al., Representation Learning on Graphs with Jumping Knowledge Networks. ICML 2018.

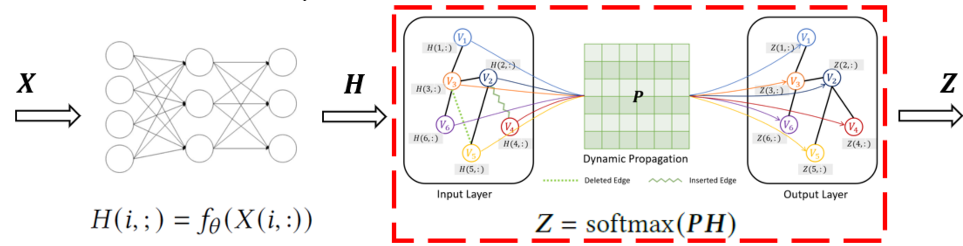
Overview of SDG

- SDG (A **S**implified and **D**ynamic **G**raph Neural Network)
  - Dynamic Propagation Scheme
    - Realized by tracking PageRank vectors.
    - Efficient fine-tuning for changed graphs.
    - Interpretable prediction by masking certain nodes and edges.
  - Model-Agnostic Neural Networks
    - To extract the qualified hidden node features $\boldsymbol{H}$.



loss function: $\mathcal{L}_{\mathrm{SDG}} = -\sum_{i}^{n}\sum_{j}^{c} Y(i,j)\ln Z(i,j)$

SDG Framework



- Dynamic Propagation Scheme
  - Realized by tracking the dynamic propagation matrix $\boldsymbol{P}$.
  - Each row $P(i,:)$ stores the stationary distribution starting from node i.

$$P(i,:)^\top = \alpha \boldsymbol{M} P(i,:)^\top + (1-\alpha)\boldsymbol{r}$$

$\boldsymbol{M} = \boldsymbol{A}\boldsymbol{D}^{-1} \in \mathbb{R}^{n\times n}$: column-stochastic transition matrix

α: teleport probability

  - When the input graph changes

$$P(i,:)_{pushout} = \alpha(\boldsymbol{M}' - \boldsymbol{M})P(i,:) \qquad P(i,:)' = P(i,:) + \sum_{k=0}^{\infty} (\alpha \boldsymbol{M}')^k \, P(i,:)_{pushout}$$

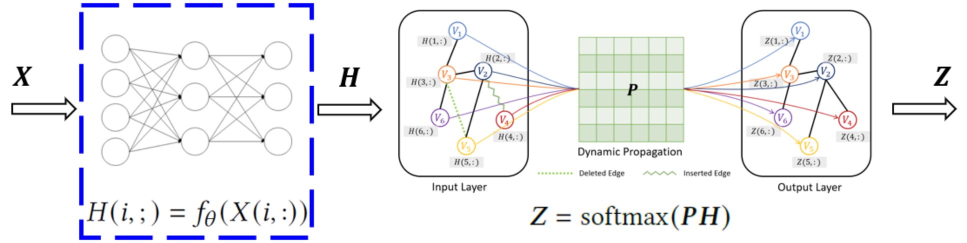
  - Time Complexity
    - $O(\frac{mn}{q}\log_\alpha(\frac{\epsilon}{2}))$ with error bound $\frac{n\epsilon}{1-\alpha}$

ϵ: stopping criterion

q: # of distributed machine

m: # of non-zero entries in $\boldsymbol{M}'$

SDG Framework



- Model-Agnostic Neural Networks
  - To capture hidden node features $\boldsymbol{H}$ from $\boldsymbol{X}$.
  - f_θ can take a variety of forms, like MLP, CNN, etc.
  - θ is the only parameter need to train in SDG.
  - When the input graph changes, f_θ only need to be fine-tuned with $\boldsymbol{M}'$ and/or $\boldsymbol{X}'$.
  - f_θ could also be paralleled.

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Experimental Setup

- Comparison methods
  - PPNP: Simplified GNN with PageRank.
  - APPNP: Simplified GNN with approximated PageRank.
  - SDG-S: Ablated SDG without Dynamic Propagation Scheme.
  - SDG
- Task: text classification (i.e., node classification)
- Dataset

Table 1: Dataset Statistics

Dataset	Classes	Nodes	Edges	Label Rate
Citeseer	6	2,110	3,668	0.036
Cora-ML	7	2,810	7,981	0.047
PubMed	3	19,717	44,324	0.003

[2] Klicpera et al., Predict then Propagate: Graph Neural Networks meet Personalized PageRank. ICLR 2019.

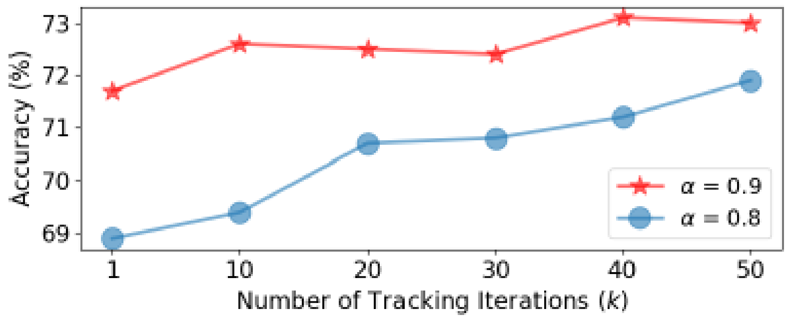
Experimental Results

- Effectiveness and Efficiency

Table 2: Effectiveness and Efficiency Comparison

Methods	Citeseer		Cora-ML		PubMed	
	Accuracy (%)	Time Consumption (s)	Accuracy (%)	Time Consumption (s)	Accuracy (%)	Time Consumption (s)
PPNP	74.07±0.53	10.89±0.91	84.40±0.18	19.81±1.65	84.03±0.32	109.75±7.68
APPNP	73.93±0.30	22.80±1.69	84.63±0.34	49.70±6.18	83.73±0.21	39.91±4.29
SDG-S	74.10±0.30	6.65±0.69	84.60±0.28	8.51±3.26	84.10±0.28	12.74±5.05
SDG	74.17±0.39	7.11±0.93	84.87±0.68	5.89±3.22	84.70±0.59	16.06±6.45

- Parameter Analysis



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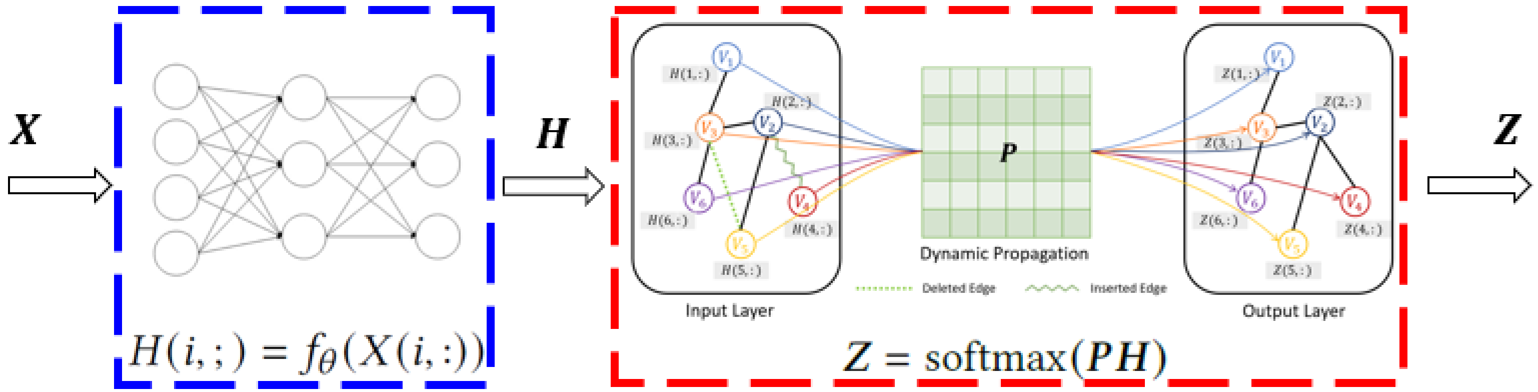
Conclusion

- SDG: A Simplified and Dynamic Graph Neural Network
  - Dynamic Propagation Scheme.
  - Model-Agnostic Neural Networks.

- Results
  - Extensive experiments demonstrate the effectiveness, scalability, and interpretability of SDG.



Structure of SDG

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Thanks！

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Please refer to our paper and code at
https://github.com/DongqiFu/SDG

NSF

Homeland Security

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