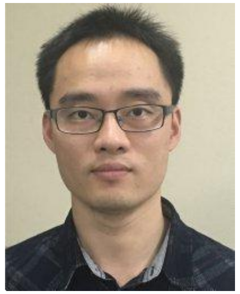
NodeFormer: A Scalable Graph Structure Learning Transformer for Node Classification







Qitian Wu, Wentao Zhao, Zenan Li, David Wipf, Junchi Yan

SHANGHAI JIAO TONG UNIVERSITY 1896

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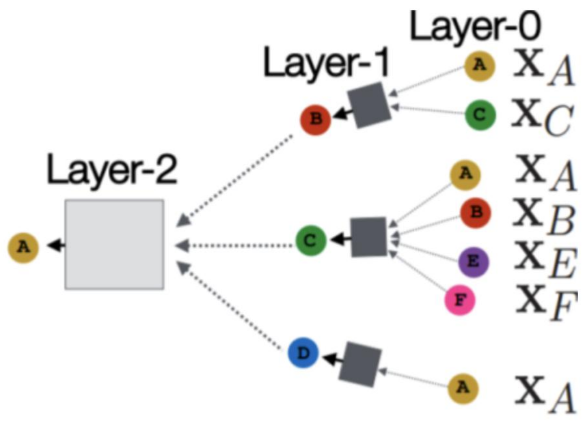
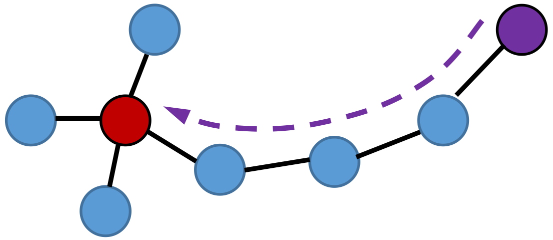
Pitfalls of Graph Neural Networks

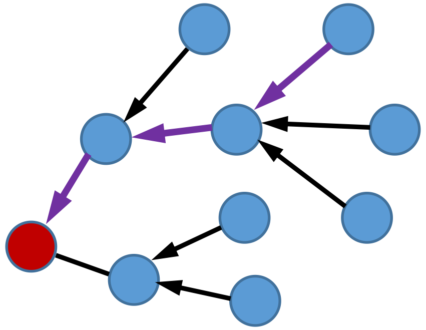
- **The designs of GNN models:**
  - Locally aggregate neighbored nodes' features in each layer
  - Use other nodes' information for prediction on the target node



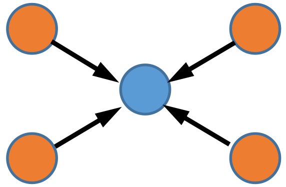
- **Common scenarios GNNs show deficient power:**



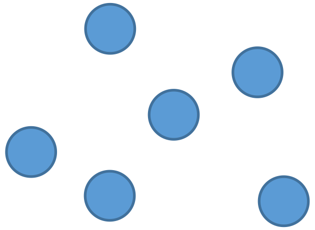
hard to capture long-range dependence [Dai et al., 2018]



distance signals are overly squashed [Alon et al., 2021]



dissimilar linked nodes propagate wrong signals [Zhu et al., 2020]

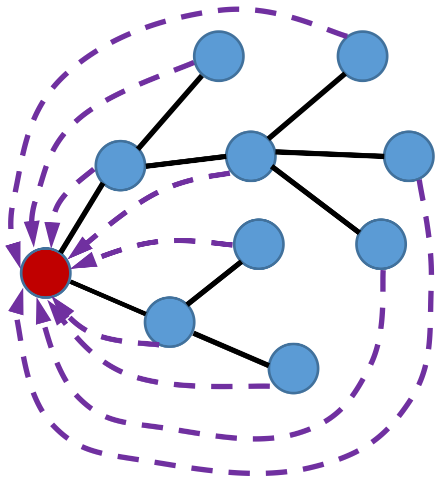


fail to work without input graphs

Message Passing Beyond Input Graphs

❑ **Basic idea:**

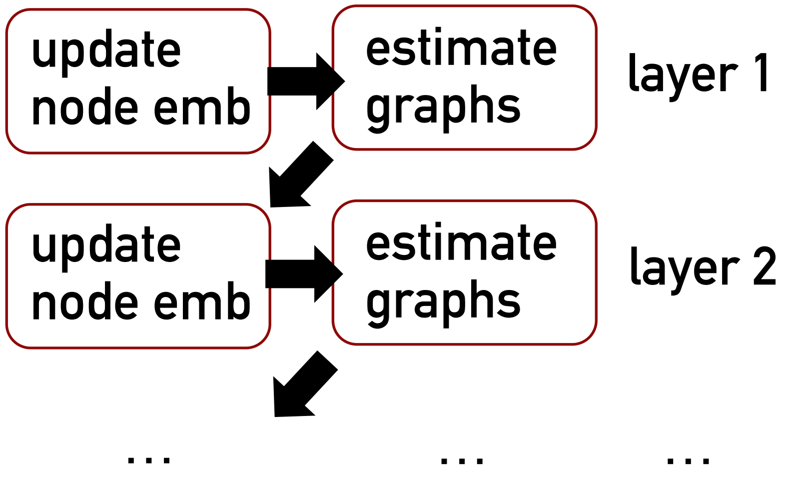
- Learn optimal graphs for message passing
- Use node embeddings to learn latent graphs, and use latent graphs for updating node embeddings



all-pair message passing on layer-specific latent graphs

❑ **Key challenges:**

- *Scalability:* quadratic complexity of all-pair message passing that requires $\mathcal{O}(N^2)$ complexity (N for #node)
- *Differentiability:* learning discrete structures introduces non-differentiability for gradient-based optimization



Comparison with Existing Works

❑ Graph structure learning

- Need quadratic complexity and hard to scale to large graphs (e.g.,10K)

  ➡ *Our model has linear complexity with largest demonstration on 2M nodes*

- Only learn a single graph shared by all propagation layers

  ➡ *Our model considers layer-wise graph learning for adaptive propagation*

- Use complicated optimization algorithms, e.g. bi-level optimization

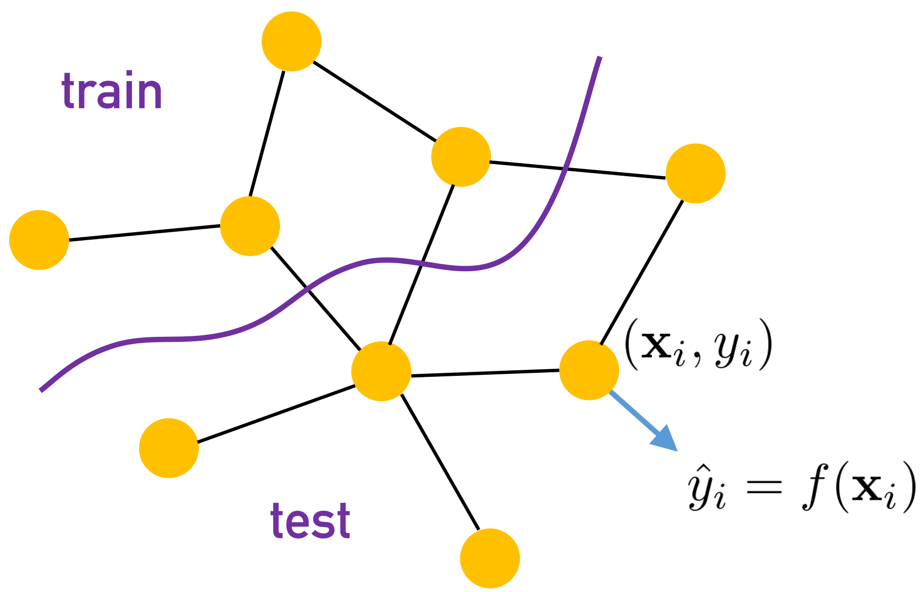
  ➡ *Our model enables efficient end-to-end training*

❑ Transformer models on Graphs

- Current methods focus on graph classification (a dataset of small graphs)

  ➡ *Our model aims at node classification (a dataset of inter-connected nodes)*

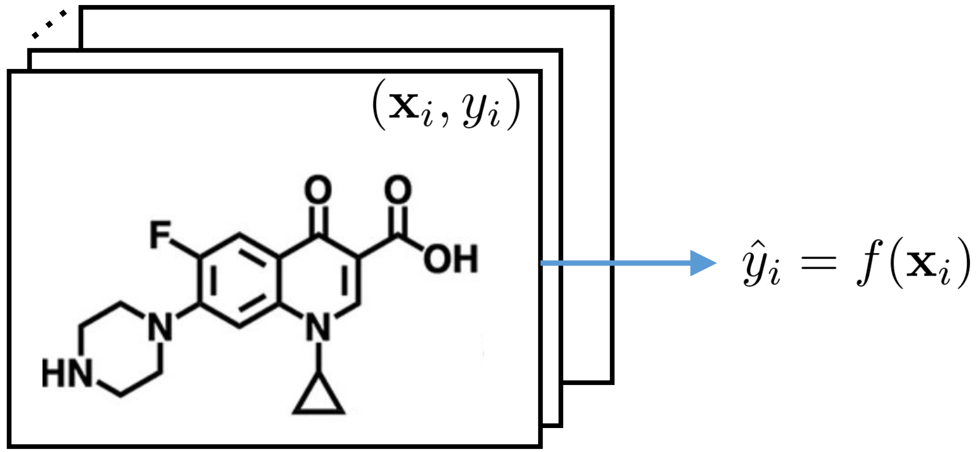
Two Problems on Graph Data



Node-Level Prediction/Classification (our focus)

- Each node is an instance with a label
- Train/test on a dataset of nodes in a graph
- The graph is often large (1K-100M nodes)

scalability issue



Graph-Level Prediction/Classification

- Each graph is an instance with a label
- Train/test on a dataset of graphs
- The graphs are often small (e.g., 10-100 nodes)

Scalable All-Pair Message Passing with O(N)

❑ Kernelized softmax message passing

$$\tilde{a}_{uv}^{(l)} = \frac{\boxed{\exp((W_Q^{(l)}\mathbf{z}_u^{(l)})^\top (W_K^{(l)}\mathbf{z}_v^{(l)}))}}{\sum_{w=1}^{N}\exp((W_Q^{(l)}\mathbf{z}_u^{(l)})^\top (W_K^{(l)}\mathbf{z}_w^{(l)}))}, \quad \mathbf{z}_u^{(l+1)} = \sum_{v=1}^{N} \tilde{a}_{uv}^{(l)} \cdot (W_V^{(l)}\mathbf{z}_v^{(l)})$$

$$\mathbf{z}_u^{(l+1)} = \sum_{v=1}^{N} \frac{\boxed{\kappa(W_Q^{(l)}\mathbf{z}_u^{(l)}, W_K^{(l)}\mathbf{z}_v^{(l)})}}{\sum_{w=1}^{N}\kappa(W_Q^{(l)}\mathbf{z}_u^{(l)}, W_K^{(l)}\mathbf{z}_w^{(l)})} \cdot (W_V^{(l)}\mathbf{z}_v^{(l)})$$

$\kappa(\cdot,\cdot) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a positive-definite kernel

[Mercer's theorem] $\kappa(\mathbf{a}, \mathbf{b}) = \langle \Phi(\mathbf{a}), \Phi(\mathbf{b}) \rangle_{\mathcal{V}} \approx \phi(\mathbf{a})^\top \phi(\mathbf{b})$

$\phi(\cdot) : \mathbb{R}^d \to \mathbb{R}^m$ is a random feature map

$$\mathbf{z}_u^{(l+1)} = \sum_{v=1}^{N} \frac{\boxed{\phi(\mathbf{q}_u)^\top \phi(\mathbf{k}_v)}}{\sum_{w=1}^{N}\phi(\mathbf{q}_u)^\top \phi(\mathbf{k}_w)} \cdot \mathbf{v}_v = \boxed{\frac{\phi(\mathbf{q}_u)^\top \sum_{v=1}^{N}\phi(\mathbf{k}_v)\cdot \mathbf{v}_v}{\phi(\mathbf{q}_u)^\top \sum_{w=1}^{N}\phi(\mathbf{k}_w)}}$$

only require O(N)
compute the sum at once

❑ Kernelized Gumbel-Softmax

$$\mathbf{z}_u^{(l+1)} = \sum_{v=1}^{N} \frac{\boxed{\exp((\mathbf{q}_u^\top \mathbf{k}_u + g_v)/\tau)}}{\sum_{w=1}^{N}\exp((\mathbf{q}_u^\top \mathbf{k}_w + g_w)/\tau)} \cdot \mathbf{v}_u$$

$$= \sum_{v=1}^{N} \frac{\boxed{\kappa(\mathbf{q}_u/\sqrt{\tau}, \mathbf{k}_v/\sqrt{\tau})e^{g_v/\tau}}}{\sum_{w=1}^{N}\kappa(\mathbf{q}_u/\sqrt{\tau}, \mathbf{k}_w/\sqrt{\tau})e^{g_w/\tau}} \cdot \mathbf{v}_v$$

$$\approx \sum_{v=1}^{N} \frac{\boxed{\phi(\mathbf{q}_u/\sqrt{\tau})^\top \phi(\mathbf{k}_v/\sqrt{\tau})e^{g_v/\tau}}}{\sum_{w=1}^{N}\phi(\mathbf{q}_u/\sqrt{\tau})^\top \phi(\mathbf{k}_w/\sqrt{\tau})e^{g_w/\tau}} \cdot \mathbf{v}_v$$

$$= \boxed{\frac{\phi(\mathbf{q}_u/\sqrt{\tau})^\top \sum_{v=1}^{N} e^{g_v/\tau}\phi(\mathbf{k}_v/\sqrt{\tau}) \cdot \mathbf{v}_v}{\phi(\mathbf{q}_u/\sqrt{\tau})^\top \sum_{w=1}^{N} e^{g_w/\tau}\phi(\mathbf{k}_w/\sqrt{\tau})}}$$

*approximate sampling discrete edges from a potential, large graph that connects **all nodes***

Approximation Error and Concentration

Theorem 1 (Approximation Error for Softmax-Kernel)

Assume $\|\mathbf{q}_u\|_2$ and $\|\mathbf{k}_v\|_2$ are bounded by r, and ϕ the Positive Random Features, then with probability at least $1-\epsilon$, the approximation error gap will be bounded by

$$\Delta = \left|\phi(\mathbf{q}_u/\sqrt{\tau})^\top \phi(\mathbf{k}_v/\sqrt{\tau}) - \kappa(\mathbf{q}_u/\sqrt{\tau}, \mathbf{k}_v/\sqrt{\tau})\right| \leq \boxed{\mathcal{O}\left(\sqrt{\frac{\exp(6r/\tau)}{m\epsilon}}\right)}$$

m for random feature dimension, τ for temperature
the error is independent of node number N

Theorem 2 (Concentration of Kernelized Gumbel-Softmax Random Variables)

Suppose the random feature dimension m is sufficiently large, we have the convergence property for the kernelized Gumbel-Softmax operator

$$\lim_{\tau \to 0} \mathbb{P}(c_{uv} > c_{uv'}, \forall v' \neq v) = \frac{\exp(\mathbf{q}_u^\top \mathbf{k}_v)}{\sum_{w=1}^N \exp(\mathbf{q}_u^\top \mathbf{k}_w)}, \quad \lim_{\tau \to 0} \mathbb{P}(c_{uv} = 1) = \frac{\exp(\mathbf{q}_u^\top \mathbf{k}_v)}{\sum_{w=1}^N \exp(\mathbf{q}_u^\top \mathbf{k}_w)}$$

The sampled results converge to the ones induced by the Softmax categorical distribution

Scalable All-Pair Message Passing with O(N)

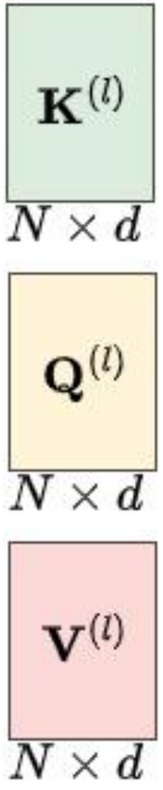
Algorithm 1: Scalable All-Pair Message Passing on Latent Graphs with Linear Complexity ($\mathcal{O}(N)$ or $\mathcal{O}(N+E)$)

Input: Node features $\mathbf{Z}^{(0)} = \mathbf{X}$, input adjacency $\mathbf{A}$.

for $l = 0 \ldots, L-1$ **do**

$\quad \mathbf{Q}^{(l)} \leftarrow W_Q^{(l)} \mathbf{Z}^{(l)}, \mathbf{K}^{(l)} \leftarrow W_K^{(l)} \mathbf{Z}^{(l)}, \mathbf{V}^{(l)} \leftarrow W_V^{(l)} \mathbf{Z}^{(l)};$

Output: Predict node labels $\hat{\mathbf{Y}} = \text{MLP}(\{\mathbf{Z}^{(l)}\}_{l=0}^{L})$.



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  for $k = 1, 2, \ldots, K$ **do**

    $G_k = \{e^{g_{ku}/\tau}\}_{u=1}^{N}, \; g_{ku} \sim Gumbel(0,1);$

    $\tilde{G}_k = G_k.unsqueeze(1).repeat(1, m);$

    $\tilde{\mathbf{K}}_k^{(l)} = \tilde{G}_k \odot \phi(\mathbf{K}^{(l)}/\sqrt{\tau}), \tilde{\mathbf{Q}}_k^{(l)} = \tilde{G}_k \odot \phi(\mathbf{Q}^{(l)}/\sqrt{\tau});$

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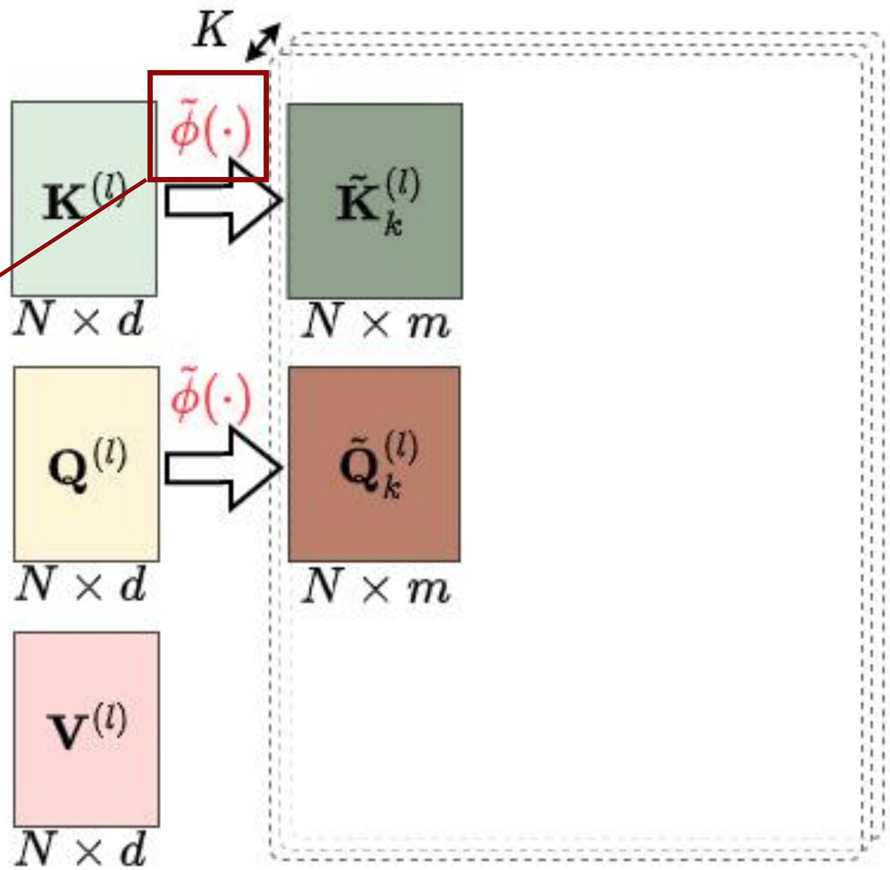

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    $\mathbf{U}_k^{(l)} \leftarrow (\tilde{\mathbf{K}}_k^{(l)})^\top \mathbf{V}^{(l)}, \mathbf{O}_k^{(l)} \leftarrow (\tilde{\mathbf{K}}_k^{(l)})^\top \mathbf{1}_{N\times 1}$;

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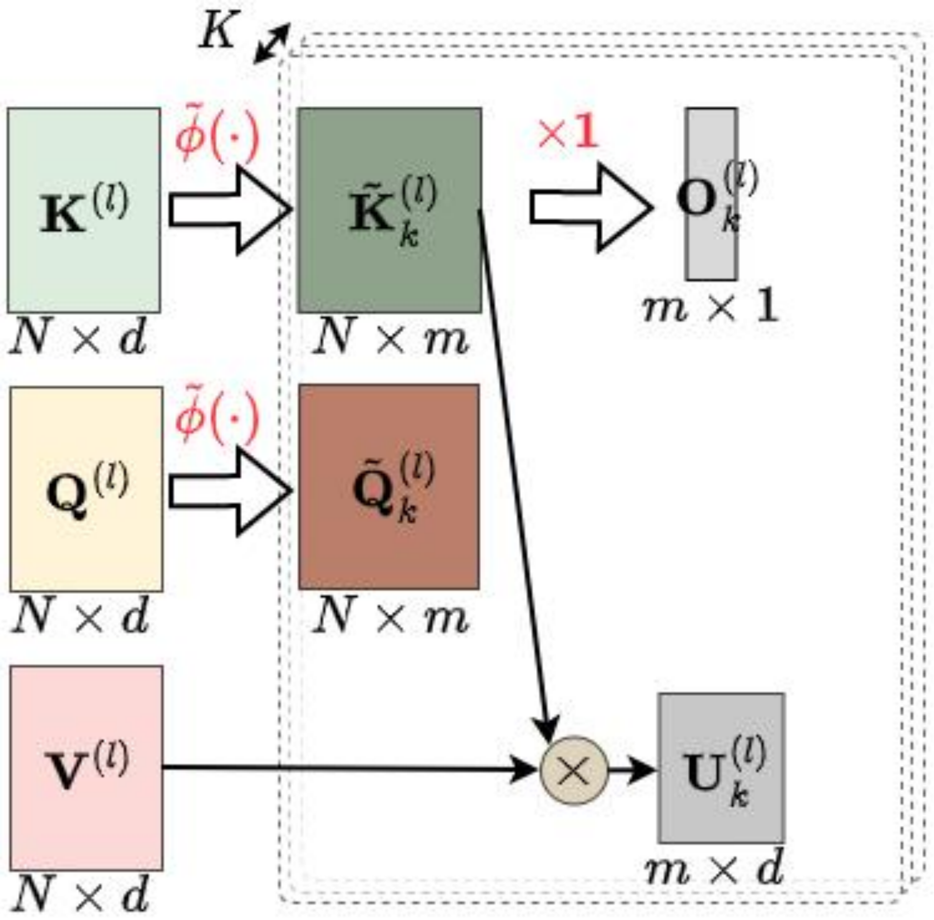

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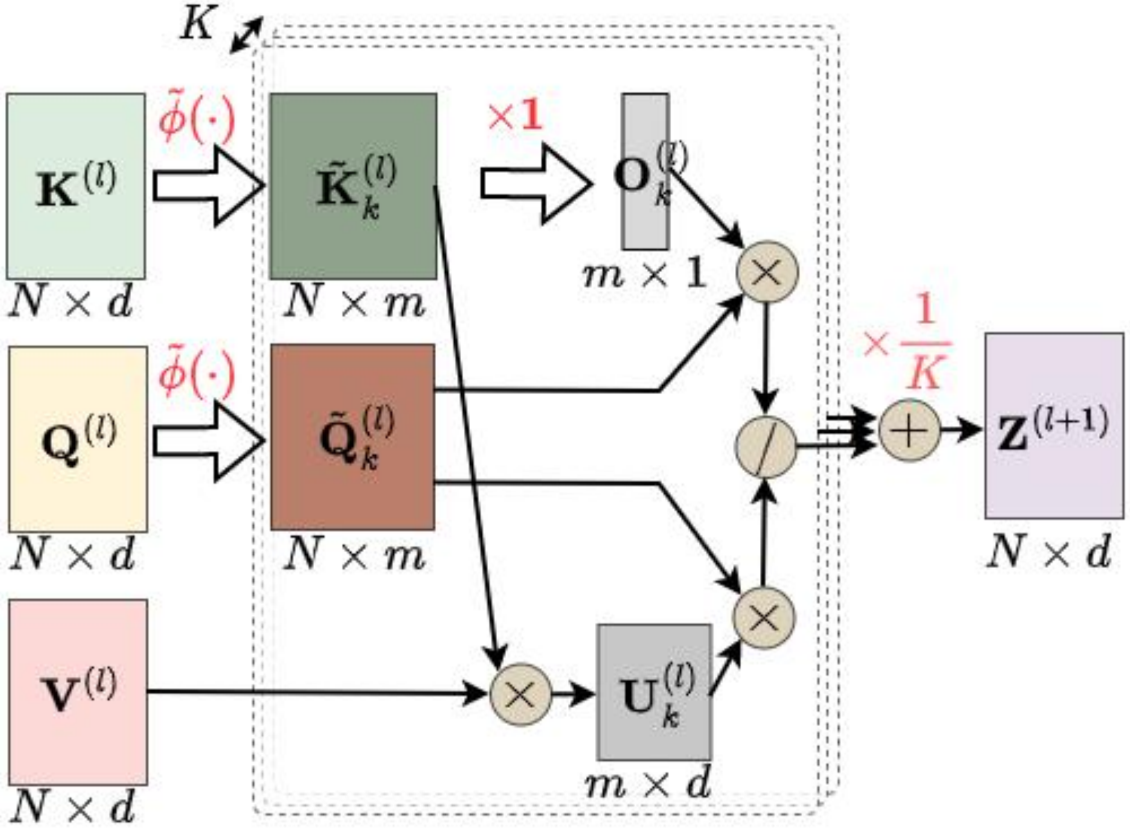
  $\mathbf{Z}^{(l+1)} \leftarrow \frac{1}{K}\sum_{k=1}^{K} \frac{\tilde{\mathbf{Q}}_k^{(l)}\mathbf{U}_k^{(l)}}{\tilde{\mathbf{Q}}_k^{(l)}\mathbf{O}_k^{(l)}}$; % average K samples

Output: Predict node labels $\hat{\mathbf{Y}} = \mathrm{MLP}(\{\mathbf{Z}^{(l)}\}_{l=0}^{L})$.



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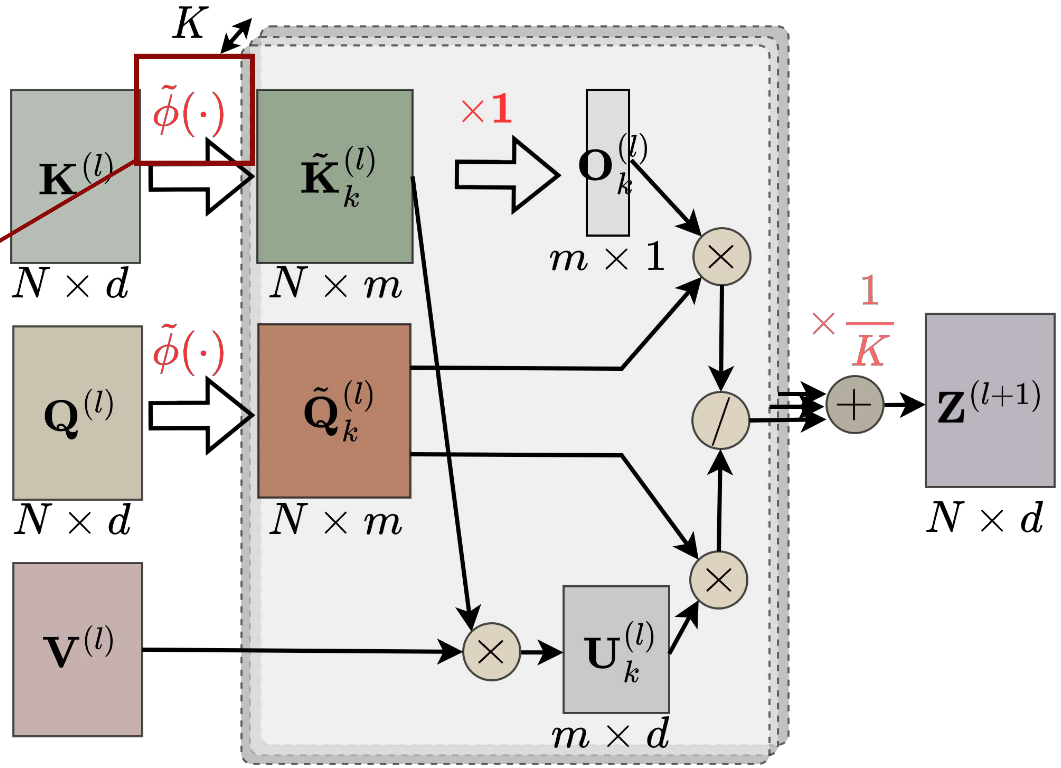
- $\mathbf{Z}^{(l+1)} \leftarrow \mathbf{Z}^{(l+1)} + \sigma(b^{(l)}) \cdot \mathbf{A}\mathbf{Z}^{(l+1)}$; % add relational bias

Output: Predict node labels $\hat{\mathbf{Y}} = \mathrm{MLP}(\{\mathbf{Z}^{(l)}\}_{l=0}^{L})$.



leverage the input graph as relational bias (reinforce the weights for observed edges)

Training Objective

❑ Supervised classification loss

$$\mathcal{L}_s(\mathbf{Y}, \hat{\mathbf{Y}}) = -\frac{1}{N}\sum_{v=1}^{N}\sum_{c=1}^{C}\mathbb{I}[y_u = c]\log \hat{y}_{u,c}$$

Key observation:

labeled nodes < N << N^2 = # node pairs

❑ Edge-level regularization loss

$$\mathcal{L}_e(\mathbf{A}, \tilde{\mathbf{A}}) = -\frac{1}{NL}\sum_{l=1}^{L}\boxed{\sum_{(u,v)\in\mathcal{E}}\frac{1}{d_u}\log \pi_{uv}^{(l)}}$$

$$\pi_{uv}^{(l)} = \frac{\phi(W_Q^{(l)}\mathbf{z}_u^{(l)})^\top \phi(W_K^{(l)}\mathbf{z}_v^{(l)})}{\phi(W_Q^{(l)}\mathbf{z}_u^{(l)})^\top \sum_{w=1}^{N}\phi(W_K^{(l)}\mathbf{z}_w^{(l)})}$$

The log-likelihood of observed edges, if assuming data distribution as

$$p_0(v|u) = \begin{cases} \frac{1}{d_u}, & a_{uv} = 1 \\ 0, & otherwise. \end{cases}$$

only require O(E)

Since we only need to query the probability for each observed edges, where the complexity of each query is $\mathcal{O}(1)$

❑ Final loss function

$$\mathcal{L} = \mathcal{L}_s + \lambda\mathcal{L}_e$$

Dissecting the Rationale of New Objective

A variational perspective look at the training objective

Key insights:

Treat the latent structure estimation as a variational distribution $p(\mathbf{Y}|\tilde{\mathbf{A}}, \mathbf{X}, \mathbf{A})$

The all-pair message passing module induces a predictive distribution $q(\tilde{\mathbf{A}}|\mathbf{X}, \mathbf{A})$

$$\mathcal{L}_e(\mathbf{A}, \tilde{\mathbf{A}}) = -\frac{1}{NL}\sum_{l=1}^{L}\sum_{(u,v)\in\mathcal{E}}\frac{1}{d_u}\log \pi_{uv}^{(l)}$$

$$\mathcal{L}_s(\mathbf{Y}, \hat{\mathbf{Y}}) = -\frac{1}{N}\sum_{v=1}^{N}\sum_{c=1}^{C}\mathbb{I}[y_u = c]\log \hat{y}_{u,c}$$

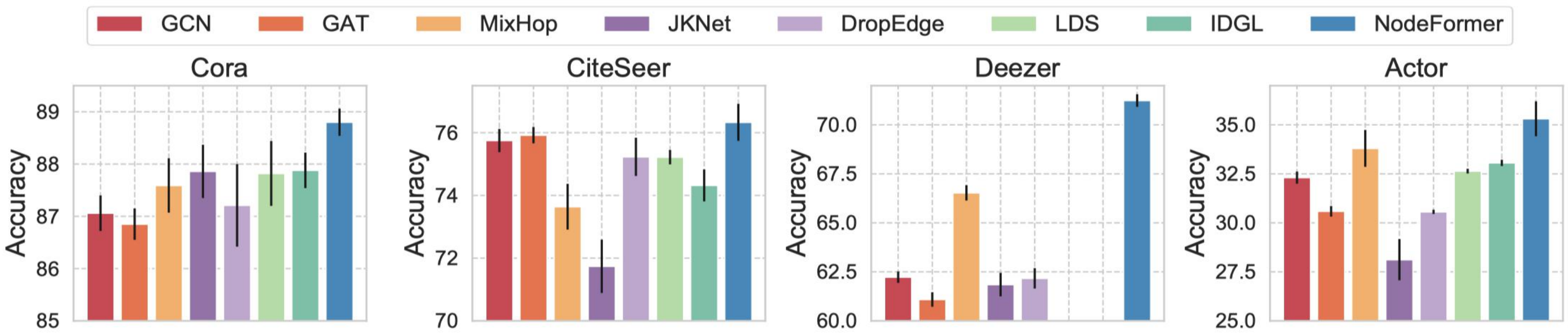
$$p^*, q^* = \arg\min_{p,q} \underbrace{-\mathbb{E}_q[\log p(\mathbf{Y}|\tilde{\mathbf{A}}, \mathbf{X}, \mathbf{A})]}_{\mathcal{L}_s} + \underbrace{\mathcal{D}(q(\tilde{\mathbf{A}}|\mathbf{X}, \mathbf{A})\|p_0(\tilde{\mathbf{A}}|\mathbf{X}, \mathbf{A}))}_{\mathcal{L}_e}$$

Proposition (Underlying Effect for Learning Optimal Structures)

Assume q can exploit arbitrary distributions over $\tilde{\mathbf{A}}$. When the objective achieves the optimum, we have 1) $\mathcal{D}(q(\tilde{\mathbf{A}}|\mathbf{X}, \mathbf{A})\|p(\tilde{\mathbf{A}}|\mathbf{Y}, \mathbf{X}, \mathbf{A})) = 0$, and 2) $\log p(\mathbf{Y}|\mathbf{X}, \mathbf{A})$ is maximized.

Comparative Experiments

❑ Experiment on small node classification benchmarks



LDS [Franceschi et al., 2020]
IDGL [Chen et al., 2021]

❑ Experiment on large-scale datasets OGB-Proteins and Amazon2M

Method	Accuracy (%)	Train Mem
MLP	63.46 ± 0.10	1.4 GB
GCN	83.90 ± 0.10	5.7 GB
SGC	81.21 ± 0.12	1.7 GB
GraphSAINT-GCN	83.84 ± 0.42	2.1 GB
GraphSAINT-GAT	85.17 ± 0.32	2.2 GB
NodeFormer	**87.85** ± 0.24	4.0 GB
NodeFormer-dt	87.02 ± 0.75	2.9 GB
NodeFormer-tp	87.55 ± 0.11	4.0 GB

NodeFormer successfully scales to graphs with 2M nodes

NodeFormer using batch size 0.1M only requires 4GB memory and hours for training on a single GPU

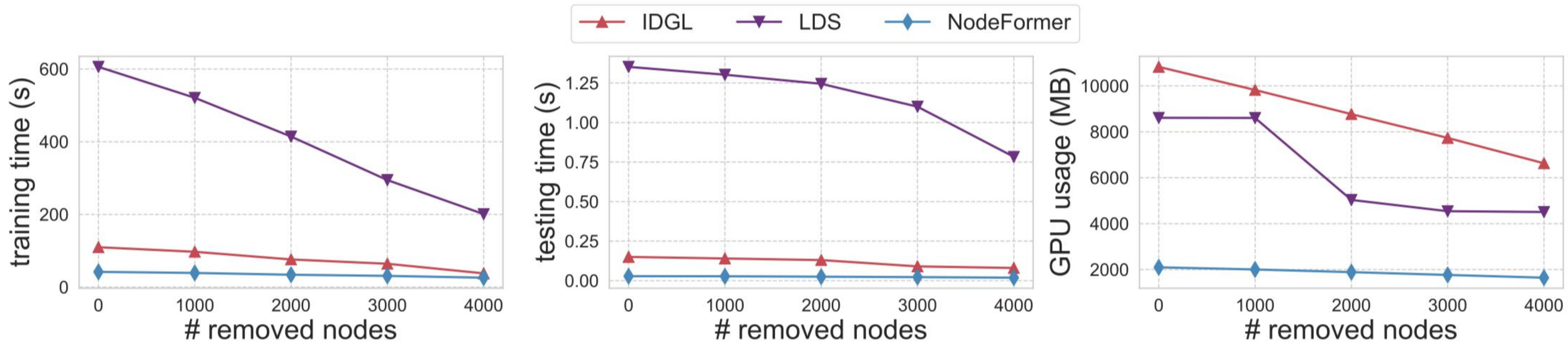
Comparative Experiments

❑ Experiment on image/text classification (no input graph)

Method	Mini-ImageNet k = 5	Mini-ImageNet k = 10	Mini-ImageNet k = 15	Mini-ImageNet k = 20	20News-Group k = 5	20News-Group k = 10	20News-Group k = 15	20News-Group k = 20
GCN	84.86 ± 0.42	85.61 ± 0.40	85.93 ± 0.59	85.96 ± 0.66	65.98 ± 0.68	64.13 ± 0.88	62.95 ± 0.70	62.59 ± 0.62
GAT	84.70 ± 0.48	85.24 ± 0.42	85.41 ± 0.43	85.37 ± 0.51	64.06 ± 0.44	62.51 ± 0.71	61.38 ± 0.88	60.80 ± 0.59
DropEdge	83.91 ± 0.24	85.35 ± 0.44	85.25 ± 0.63	85.81 ± 0.65	64.46 ± 0.43	64.01 ± 0.42	62.46 ± 0.51	62.68 ± 0.71
IDGL	83.63 ± 0.32	84.41 ± 0.35	85.50 ± 0.24	85.66 ± 0.42	65.09 ± 1.23	63.41 ± 1.26	61.57 ± 0.52	62.21 ± 0.79
LDS	OOM	OOM	OOM	OOM	**66.15** ± 0.36	64.70 ± 1.07	63.51 ± 0.64	63.51 ± 1.75
NodeFormer	**86.77** ± 0.45	**86.74** ± 0.23	**86.87** ± 0.41	**86.64** ± 0.42	66.01 ± 1.18	**65.21** ± 1.14	**64.69** ± 1.31	**64.55** ± 0.97
NodeFormer w/o graph	**87.46** ± 0.36				**64.71** ± 1.33			

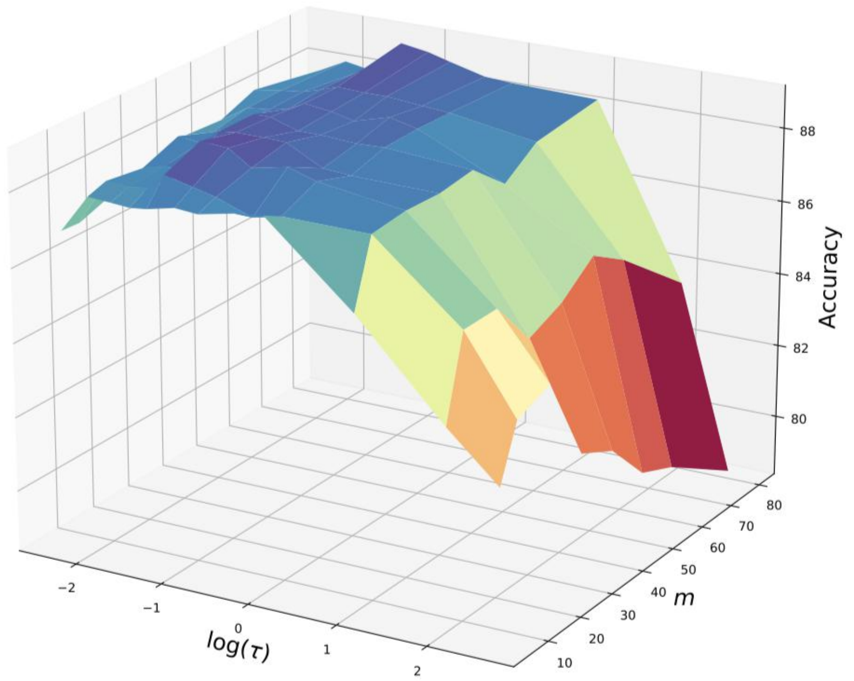
NodeFormer also works with no input graph

❑ Scalability analysis on time/space costs



NodeFormer reduces training time by 93.1%

Ablation Study and Hyper-parameters



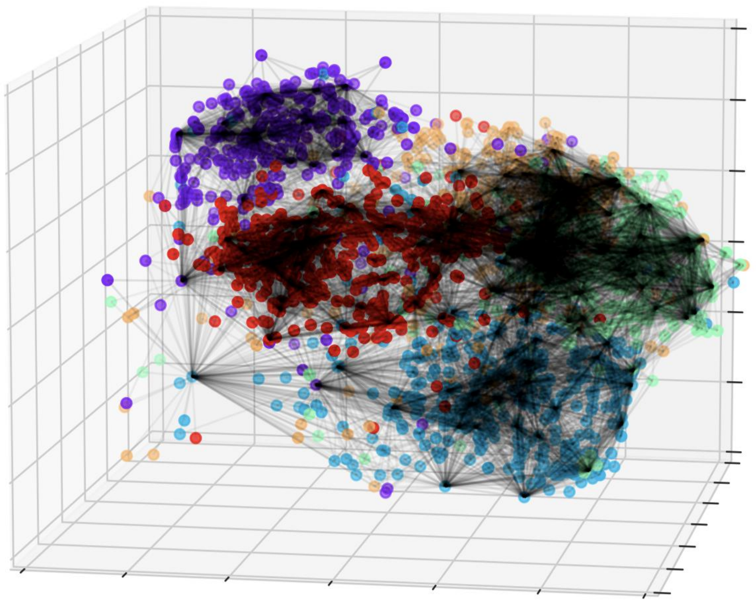
Larger random feature dimension m allows better approximation

Moderate temperature (tau=0.25) yields stably good performance

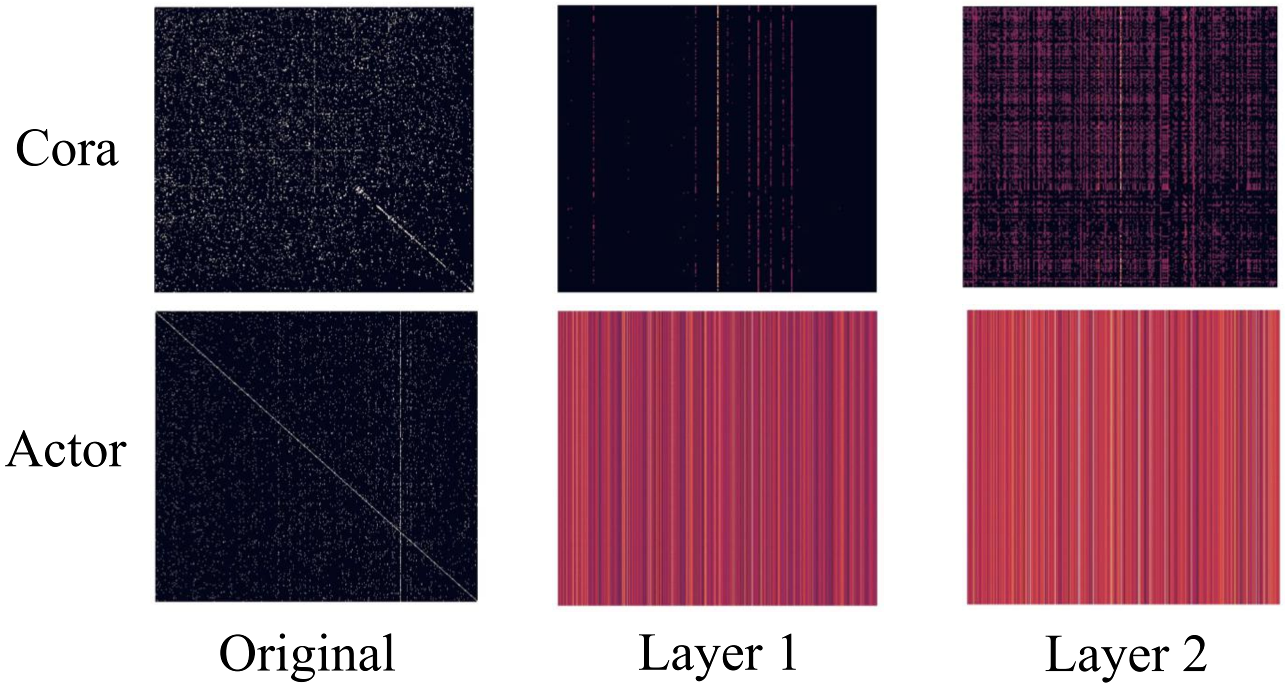
Dataset	NodeFormer	NodeFormer w/o reg	NodeFormer w/o rb
Cora	**88.69** ± 0.46	81.98 ± 0.46	88.06 ± 0.59
Citeseer	**76.33** ± 0.59	70.60 ± 1.20	74.12 ± 0.64
Deezer	**71.24** ± 0.32	71.22 ± 0.32	71.10 ± 0.36
Actor	**35.31** ± 1.29	35.15 ± 1.32	34.60 ± 1.32

Ablation study on edge regularization loss and relational bias

Visualization of Learned Structures



20News-Group



The latent structures produced by NodeFormer tend to connect nodes within the same class and increase the overall connectivity of the whole graph

Conclusion

❑ Contributions of this work:

- Propose a kernelized Gumbel-Softmax operator that achieves all-pair message passing with linear complexity.
- Introduce NodeFormer as a new class of graph networks with layer-wise message passing as operated over latent graphs potentially connecting all nodes.
- Verify the efficacy of NodeFormer for handling long-range dependence, heterophily, large graphs, graph incompleteness and the absence of graphs.

Code will be available at: https://github.com/qitianwu/NodeFormer

Email: echo740@sjtu.edu.cn
Wechat: myronwqt228