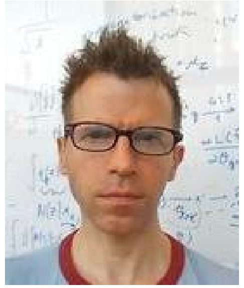
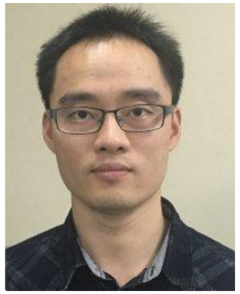
NodeFormer: A Scalable Graph Structure Learning Transformer for Node Classification



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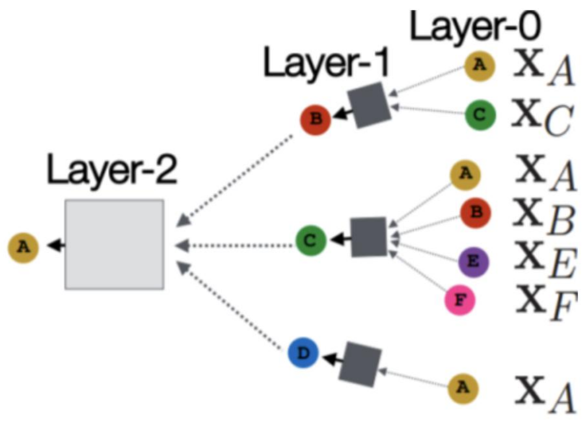
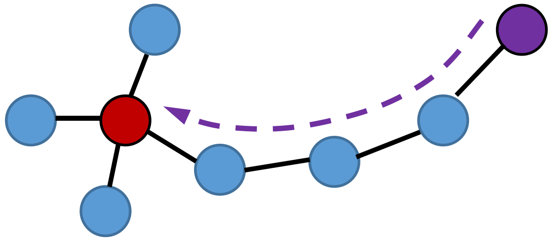
Pitfalls of Graph Neural Networks



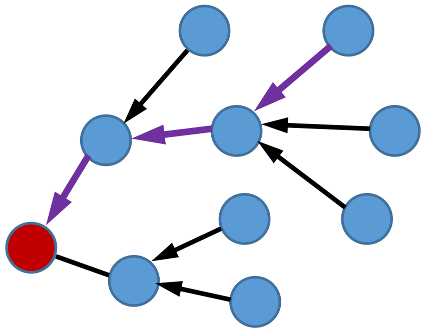
❑ The designs of GNN models:

- Locally aggregate neighbored nodes' features in each layer
- Use other nodes' information for prediction on the target node

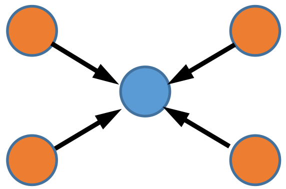
❑ Common scenarios GNNs show deficient power:



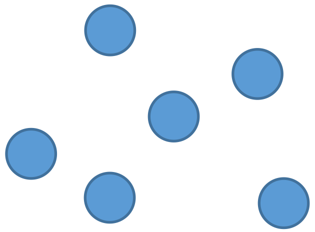
hard to capture long-range dependence [Dai et al., 2018]



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



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

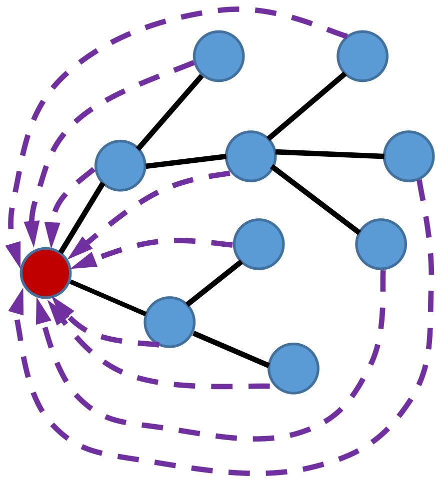


fail to work without input graphs

Message Passing Beyond Input Graphs

❑ Basic idea:

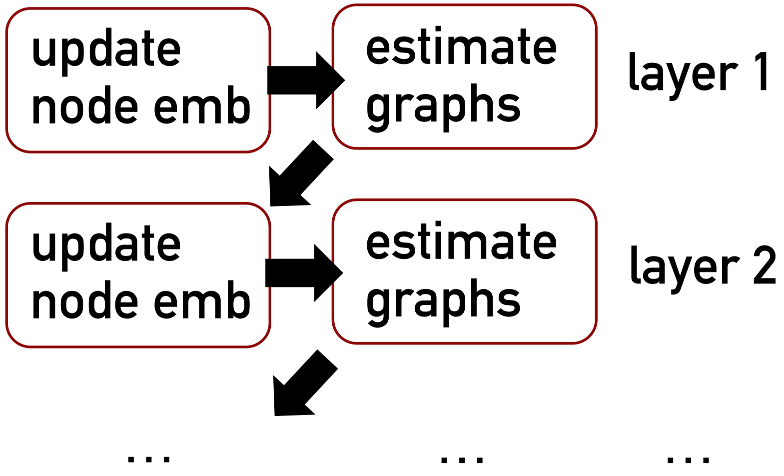
- Learn optimal graphs for message passing
- Use node embeddings to learn latent graphs, and use latent graphs for updating node embeddings



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

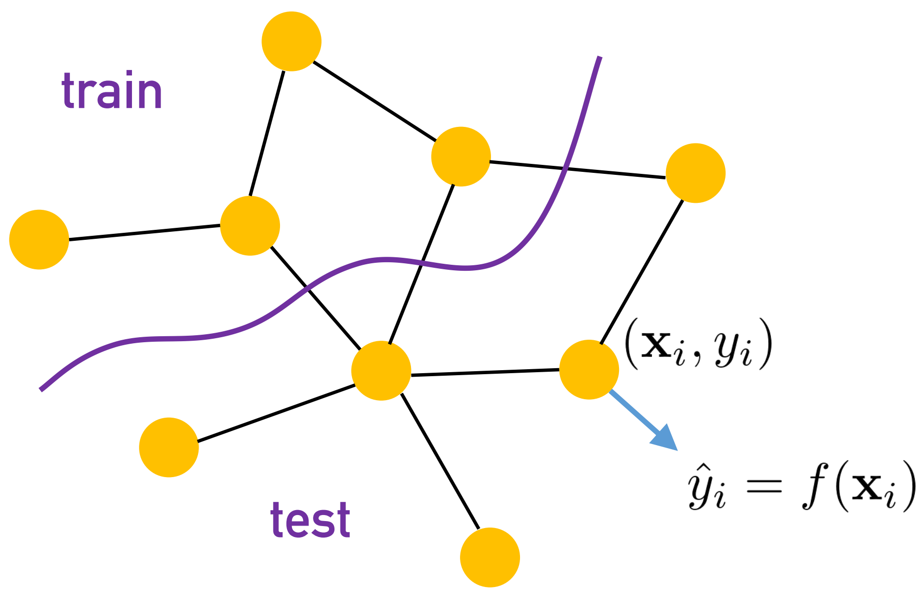
❑ Graph structure learning

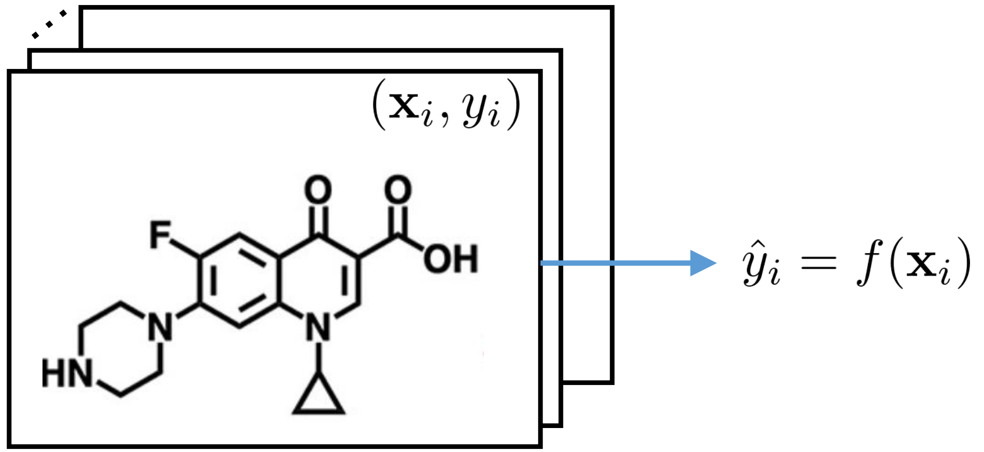
- Need quadratic complexity and hard to scale to large graphs (e.g.,10K)
  - ➡ *Our model has linear complexity with largest demonstration on 2M nodes*
- Only learn a single graph shared by all propagation layers
  - ➡ *Our model considers layer-wise graph learning for adaptive propagation*
- Use complicated 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)

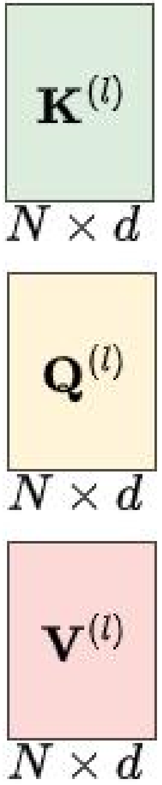
Algorithm 1: Scalable All-Pair Message Passing on Latent Graphs with Linear Complexity ($\mathcal{O}(N)$ or $\mathcal{O}(N+E)$)

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 $\hat{\mathbf{Y}} = \mathrm{MLP}(\{\mathbf{Z}^{(l)}\}_{l=0}^{L})$.



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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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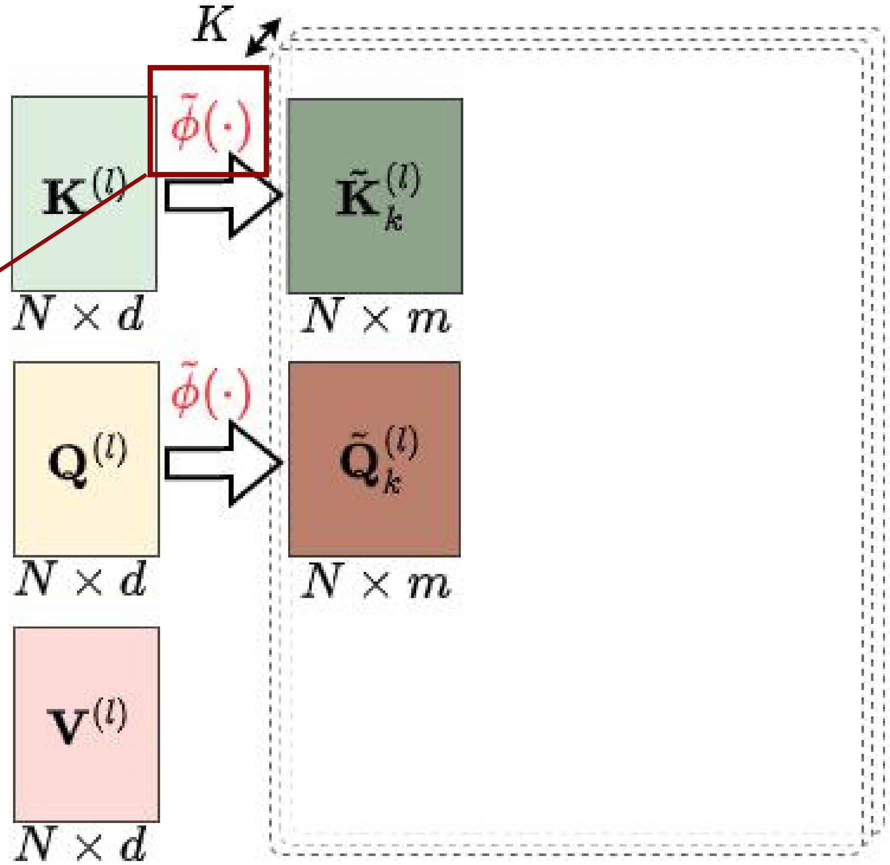

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        $\mathbf{U}_k^{(l)} \leftarrow (\tilde{\mathbf{K}}_k^{(l)})^\top \mathbf{V}^{(l)}, \mathbf{O}_k^{(l)} \leftarrow (\tilde{\mathbf{K}}_k^{(l)})^\top \mathbf{1}_{N\times 1}$;

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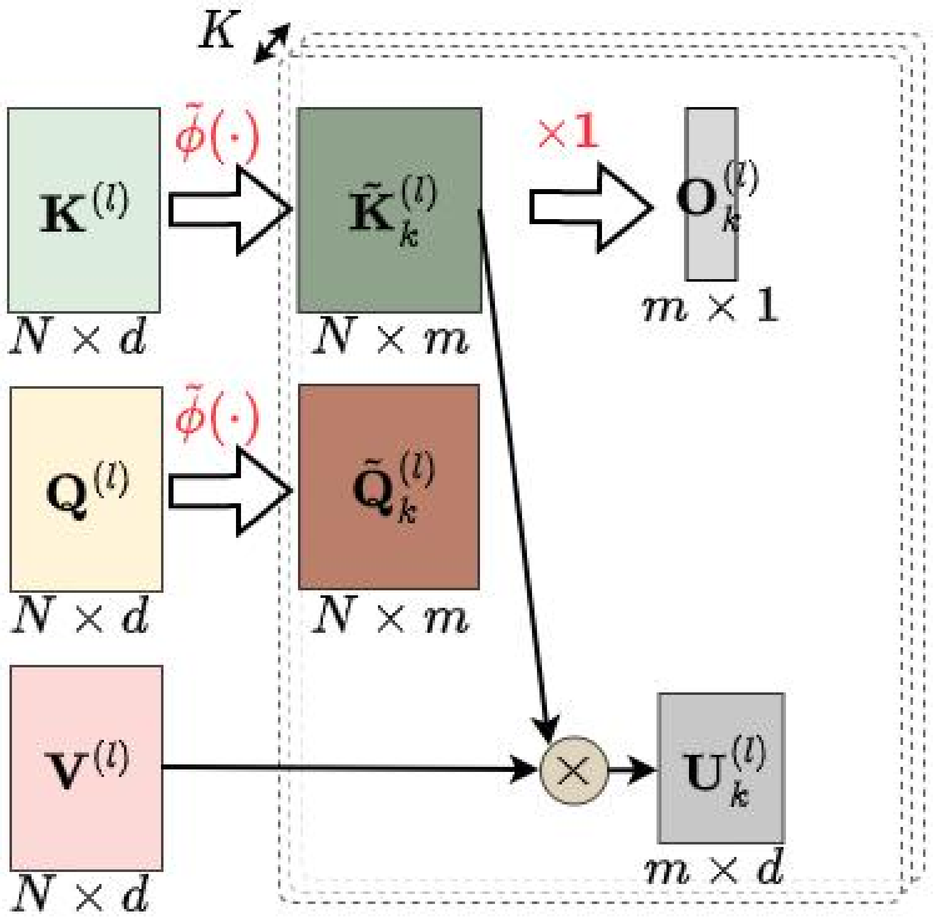

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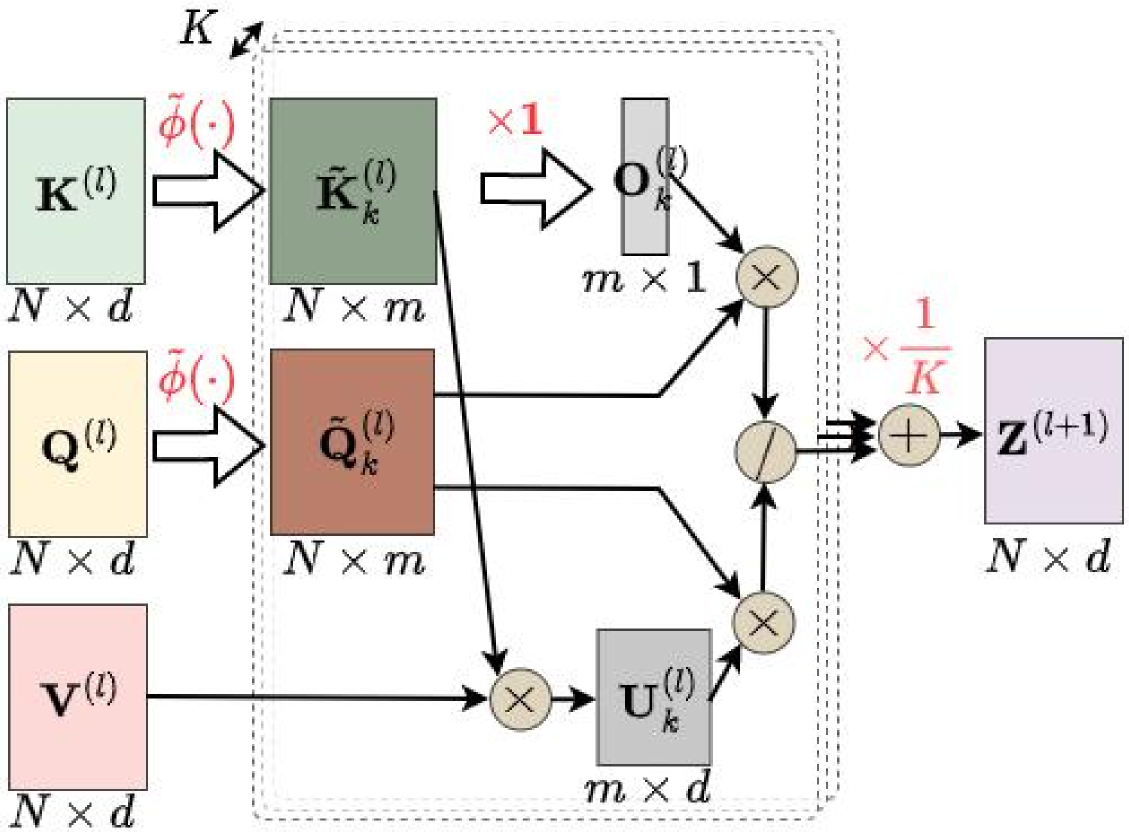
  $\mathbf{Z}^{(l+1)} \leftarrow \frac{1}{K} \sum_{k=1}^{K} \frac{\tilde{\mathbf{Q}}_k^{(l)} \mathbf{U}_k^{(l)}}{\tilde{\mathbf{Q}}_k^{(l)} \mathbf{O}_k^{(l)}}$; % average K samples

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



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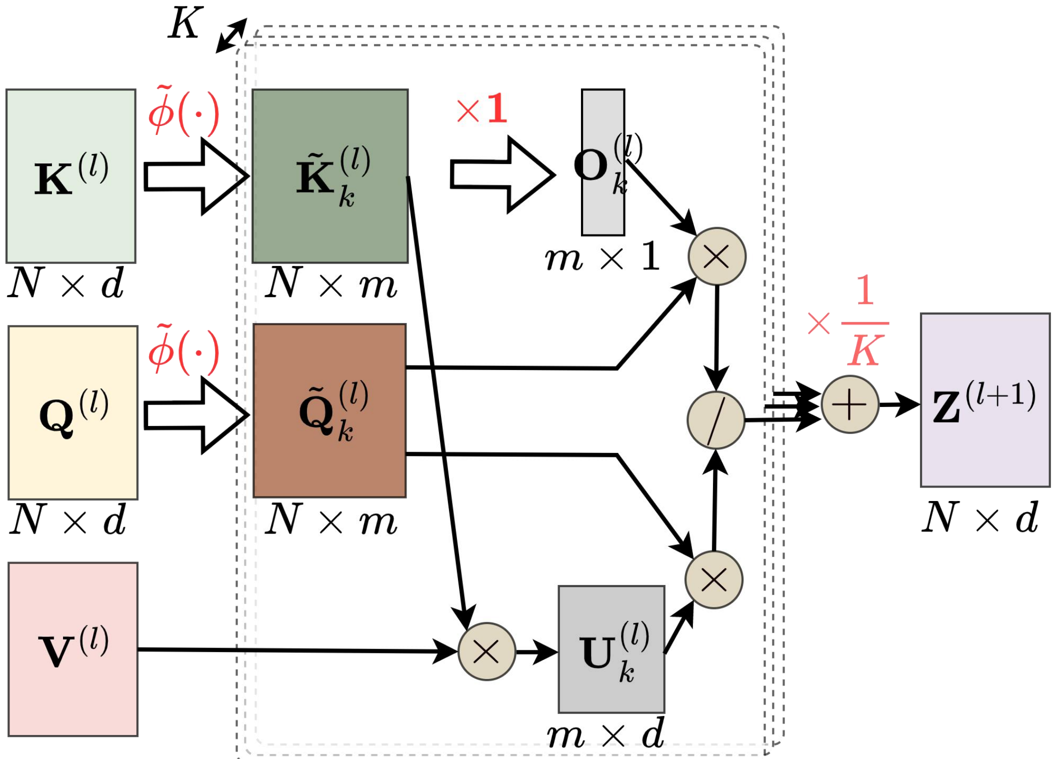
  $\boxed{\mathbf{Z}^{(l+1)} \leftarrow \mathbf{Z}^{(l+1)} + \sigma(b^{(l)}) \cdot \mathbf{A}\mathbf{Z}^{(l+1)};\ \text{\% add relational bias}}$

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 $q(\tilde{\mathbf{A}}|\mathbf{X}, \mathbf{A})$

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

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

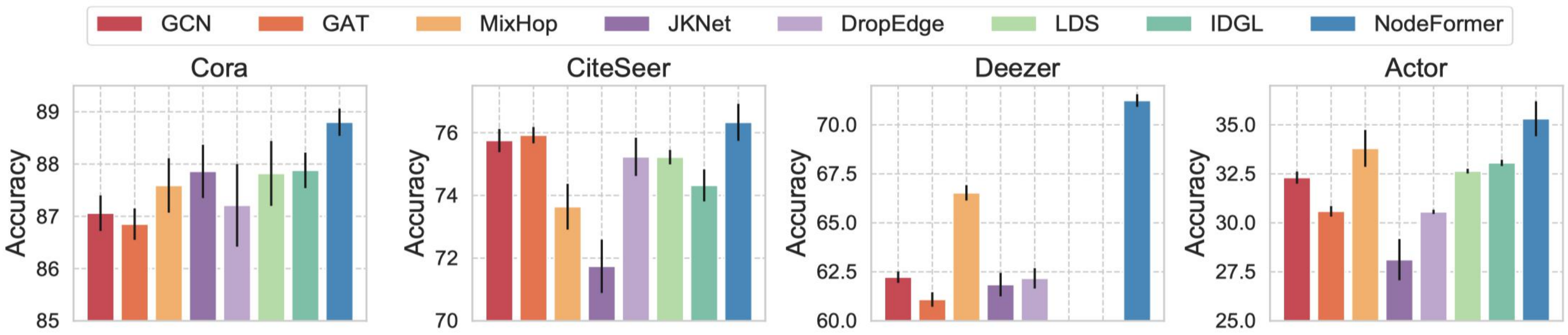
$$p^*, q^* = \arg\min_{p,q} \underbrace{-\mathbb{E}_q[\log p(\mathbf{Y}|\tilde{\mathbf{A}}, \mathbf{X}, \mathbf{A})]}_{\mathcal{L}_s} + \underbrace{\mathcal{D}(q(\tilde{\mathbf{A}}|\mathbf{X}, \mathbf{A})\|p_0(\tilde{\mathbf{A}}|\mathbf{X}, \mathbf{A}))}_{\mathcal{L}_e}$$

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

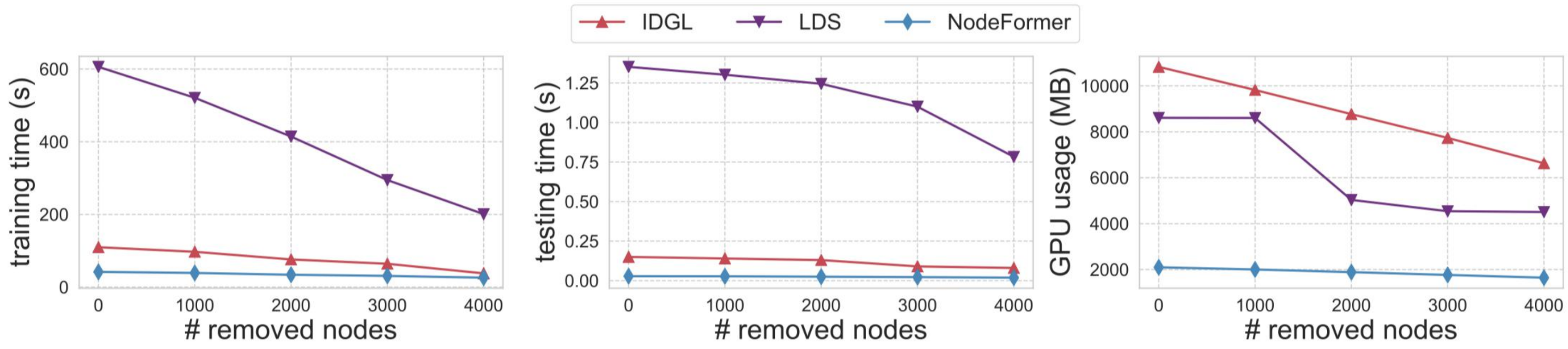
Comparative Experiments

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

Method	Mini-ImageNet $k=5$	$k=10$	$k=15$	$k=20$	20News-Group $k=5$	$k=10$	$k=15$	$k=20$
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				**65.79** ± 0.62			

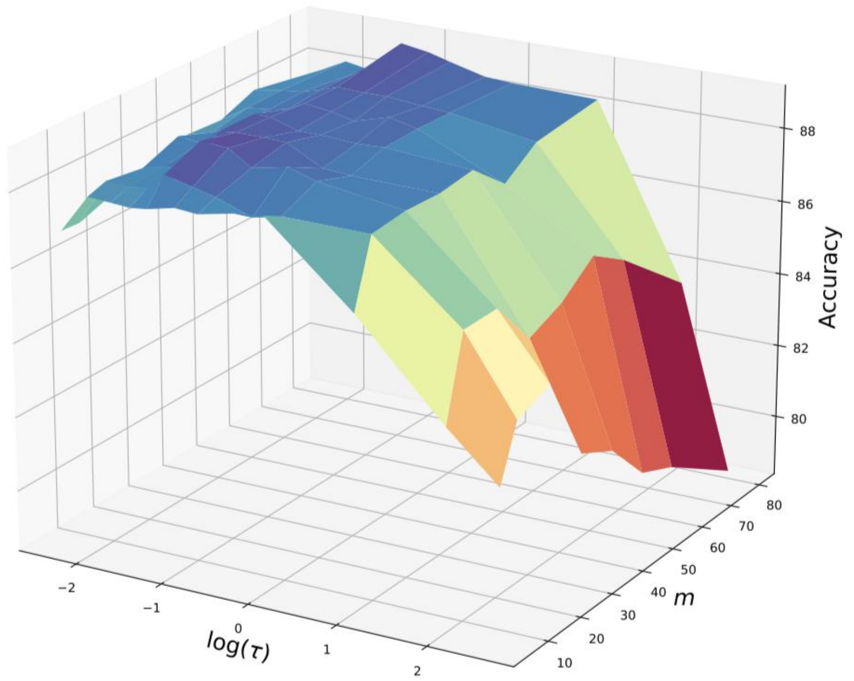
NodeFormer also works with no input graph

❑ Scalability analysis on time/space costs



NodeFormer reduces training time by 93.1%

Ablation Study and Hyper-parameters



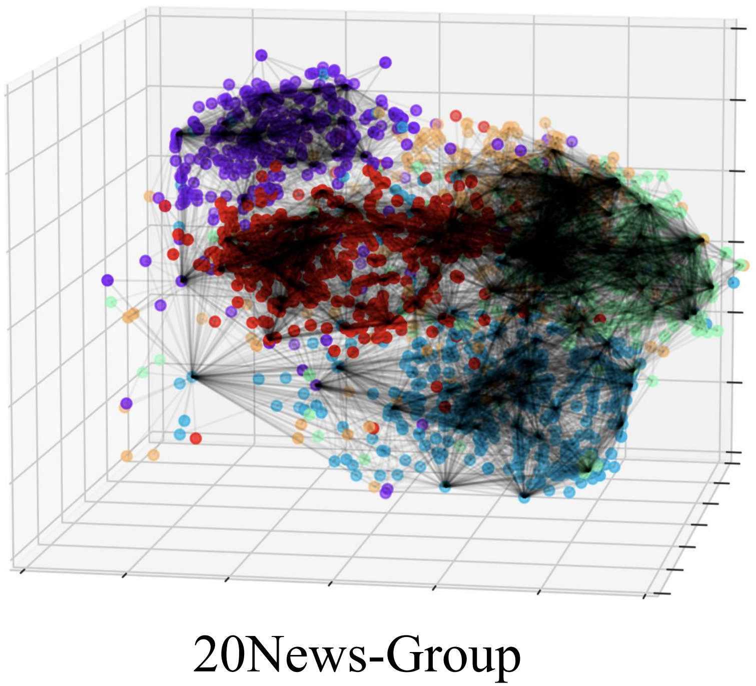
Larger random feature dimension m allows better approximation

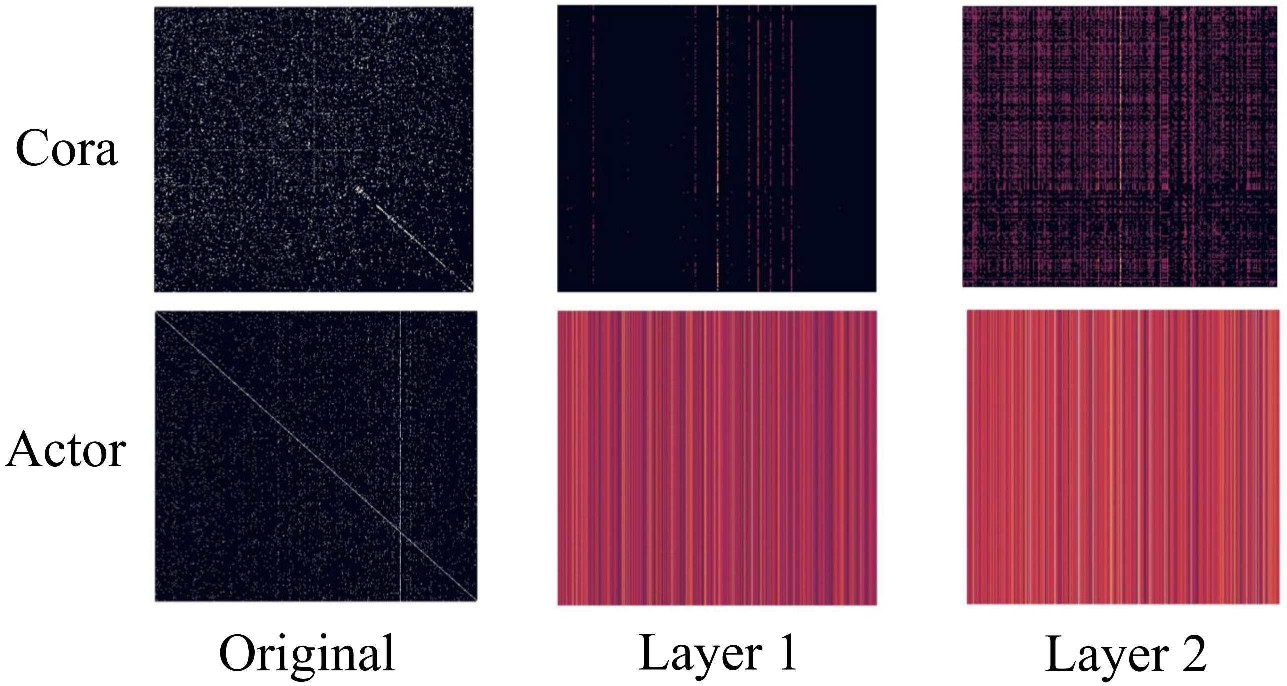
Moderate temperature (tau=0.25) yields stably good performance

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





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

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