Digraph Inception Convolutional Networks

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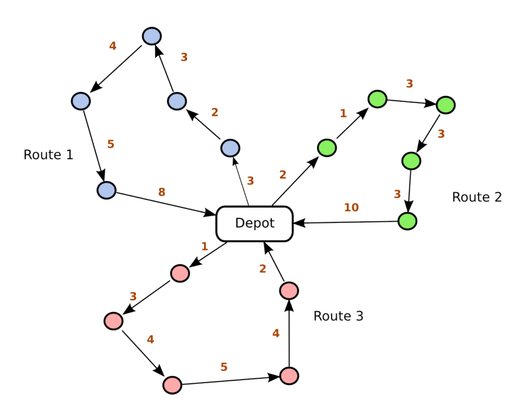
Summary

We make GCNs available in digraphs and propose an Inception network to learn multi-scale features in digraphs.

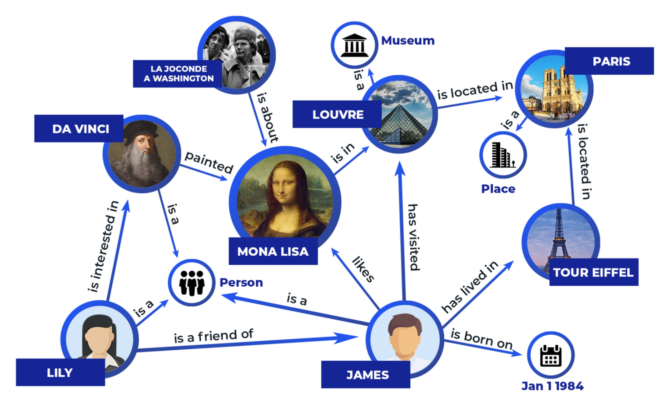
Why digraphs (directed graphs)?

Directed structures are everywhere:

- Recommender Systems
- Traffic Forecasting
- Biology (LGT)
- Neuroscience



Road network

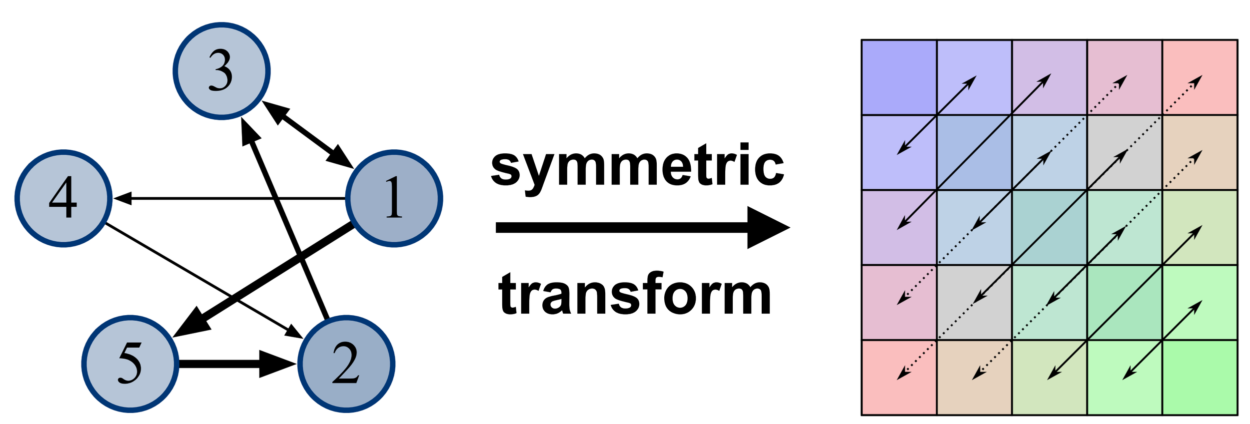


Knowledge graph

Directed graph structure is vital and undeveloped!

Limitations of spectral-based GCNs

Definition Limit

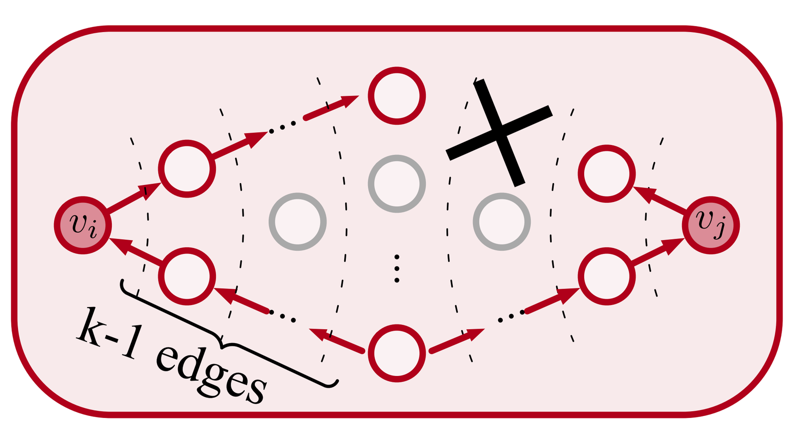


digraph — adjacency matrix

The adjacency matrix needs to be symmetric to use spectral graph convolutions.

Naive symmetric transform is not reasonable.

Structural Limit



long paths only exist between a few points and are often not bidirectional

The unique structure of the digraph makes it difficult to obtain long-range (global) features.

Receptive field would be unbalanced and limited.

Digraph Convolution

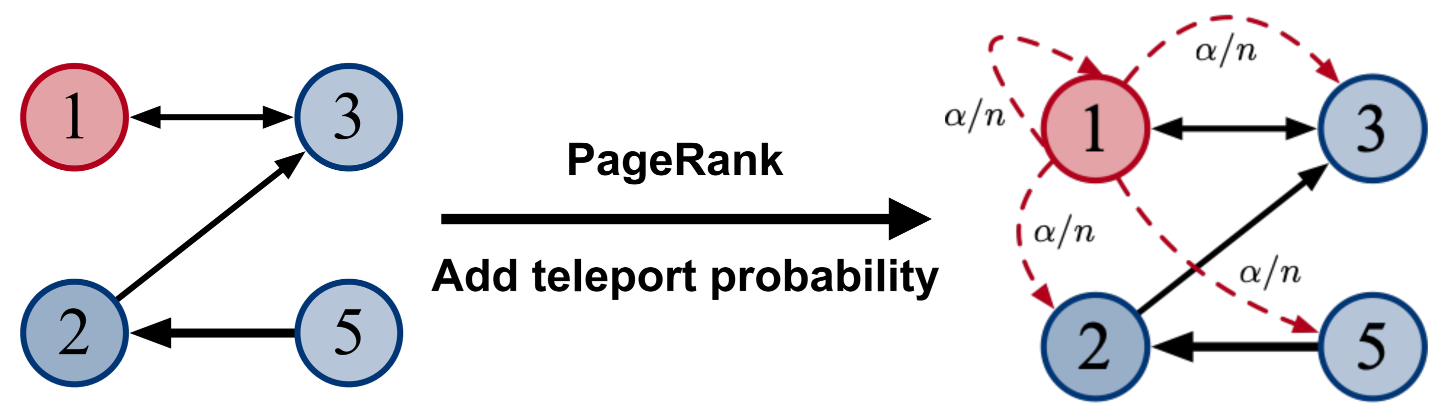
Theoretically define spectral digraph convolution.

Digraph Laplacian based on PageRank:

Given a digraph $\mathcal{G}$ and its adjacency matrix $\mathbf{A}$, $\mathbf{P}_{rw} = \mathbf{D}^{-1}\mathbf{A}$

Using PageRank to make $\mathcal{G}$ irreducible and aperiodic

$$\mathbf{P}_{pr} = (1-\alpha)\mathbf{P}_{rw} + \frac{\alpha}{n}\mathbf{1}^{n\times n} \quad \alpha \text{ is the teleport probability}$$

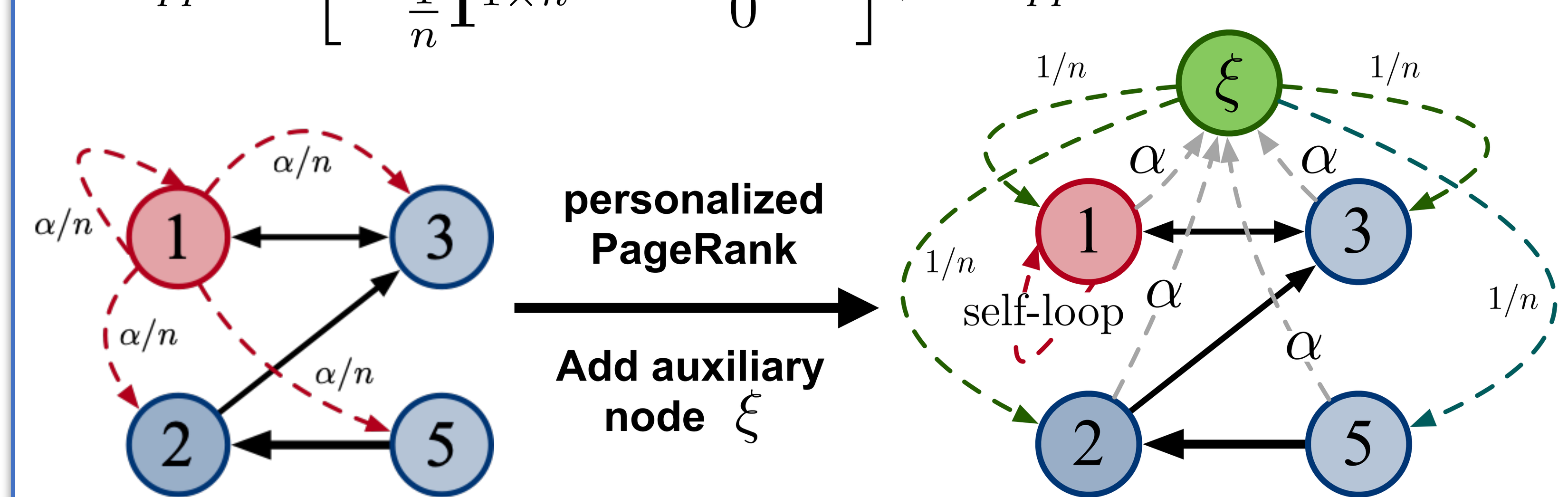


$$\mathcal{L}_{pr} = \mathbf{I} - \frac{1}{2}\left(\mathbf{\Pi}_{pr}^{\frac{1}{2}}\mathbf{P}_{pr}\mathbf{\Pi}_{pr}^{-\frac{1}{2}} + \mathbf{\Pi}_{pr}^{-\frac{1}{2}}\mathbf{P}_{pr}^{T}\mathbf{\Pi}_{pr}^{\frac{1}{2}}\right) \quad \textbf{(Dense)}$$

$\mathbf{\Pi}_{pr}$ is normalized diagonal Perron vector of $\mathbf{P}_{pr}$

Further simplify it using personalized PageRank:

$$\mathbf{P}_{ppr} = \begin{bmatrix} (1-\alpha)\tilde{\mathbf{P}} & \alpha\mathbf{1}^{n\times 1} \\ \frac{1}{n}\mathbf{1}^{1\times n} & 0 \end{bmatrix}, \quad \mathbf{P}_{ppr} \in \mathbb{R}^{(n+1)\times(n+1)}$$



$$\mathcal{L}_{appr} \approx \mathbf{I} - \frac{1}{2}\left(\mathbf{\Pi}_{appr}^{\frac{1}{2}}\tilde{\mathbf{P}}\Pi_{appr}^{-\frac{1}{2}} + \mathbf{\Pi}_{appr}^{-\frac{1}{2}}\tilde{\mathbf{P}}^{T}\mathbf{\Pi}_{appr}^{\frac{1}{2}}\right)$$

Generalize to other forms:

α is the degree of conversion from a directed form to undirected.

$\alpha \to 1$

$$\mathbf{I} - \tilde{\mathbf{D}}^{-1}\tilde{\mathbf{A}} \xleftarrow{\mathcal{G} \text{ is undirected}} \mathbf{I} - \frac{1}{2}\left(\tilde{\mathbf{P}} + \tilde{\mathbf{P}}^{T}\right)$$

undirected random-walk form — trivial-symmetric form

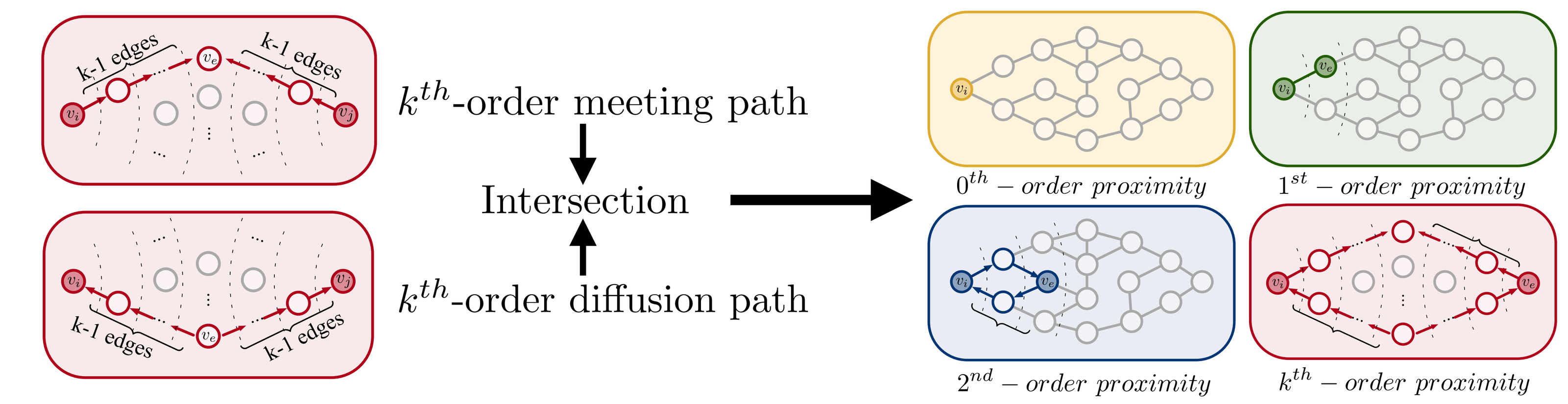
Spectral Digraph Convolution:

$$\mathbf{Z} = \frac{1}{2}\left(\mathbf{\Pi}_{appr}^{\frac{1}{2}}\tilde{\mathbf{P}}\Pi_{appr}^{-\frac{1}{2}} + \mathbf{\Pi}_{appr}^{-\frac{1}{2}}\tilde{\mathbf{P}}^{T}\mathbf{\Pi}_{appr}^{\frac{1}{2}}\right)\mathbf{X}\Theta$$

Digraph Inception Networks

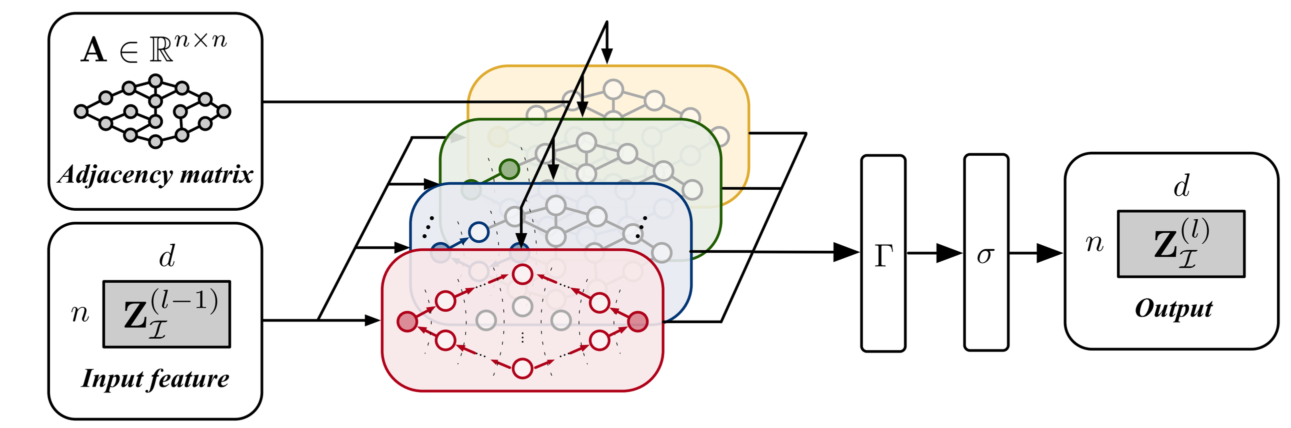
Key idea: friends' friends tend to be mine friends.

Design k^{th}-order Proximity in digraphs



$$\mathbf{P}^{(k)} = \begin{cases} \mathbf{I} & k=0 \\ \tilde{\mathbf{D}}^{-1}\tilde{\mathbf{A}} & k=1 \\ \text{Intersect}\left((\mathbf{P}^{(1)})^{k-1}(\mathbf{P}^{(1)^T})^{k-1}, (\mathbf{P}^{(1)^T})^{k-1}(\mathbf{P}^{(1)})^{k-1}\right)/2 & k \geqslant 2 \end{cases}$$

Multi-scale Conv



Inception block of l^{th} layer

Brief Experimental Results

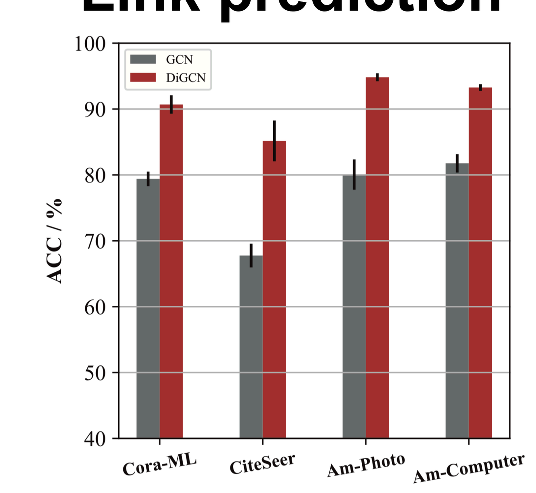
Semi-supervised node classification in digraphs

Table 1: Overall accuracy and training time. "w/ pr" means using $\mathcal{L}_{pr}$; "w/ appr" means using $\mathcal{L}_{appr}$; "w/o IB" means using digraph convolution only; "w/ IB" means using Inception block. The best results are highlighted with **bold** and the second are highlighted with underline.

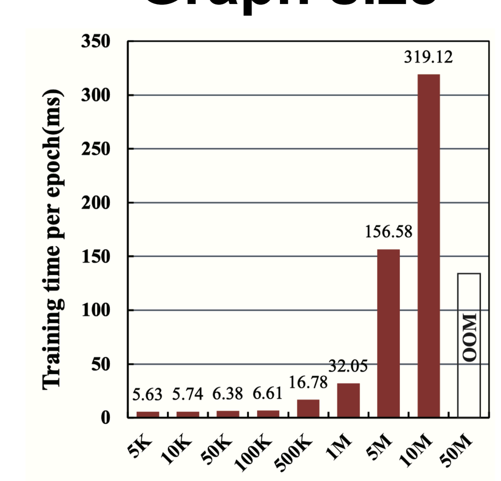
Model	Cora-ML		CiteSeer		Am-Photo		Am-Computer	
	acc	time	acc	time	acc	time	acc	time
ChebNet	64.02 ± 1.5	7.23	56.46 ± 1.4	7.45	80.91 ± 1.0	10.52	73.25 ± 0.8	16.96
GCN	53.11 ± 0.8	4.48	54.36 ± 0.5	4.80	53.20 ± 0.4	4.86	60.50 ± 1.6	5.04
SGC	51.14 ± 0.6	1.92	44.07 ± 3.5	3.58	71.25 ± 1.3	2.31	76.17 ± 0.1	3.68
APPNP	70.07 ± 1.1	6.84	65.39 ± 0.9	6.94	79.37 ± 0.9	6.72	63.16 ± 1.4	6.47
InfoMax	58.00 ± 2.4	4.11	60.51 ± 1.7	4.85	74.40 ± 1.2	31.80	47.32 ± 0.7	41.96
GraphSage	72.06 ± 0.9	6.22	63.19 ± 0.7	6.21	87.57 ± 0.9	8.52	79.29 ± 1.3	14.49
GAT	71.91 ± 0.9	6.02	63.03 ± 0.6	6.12	<u>89.10 ± 0.7</u>	8.83	79.45 ± 1.5	14.66
DGCN	75.02 ± 0.5	6.53	<u>66.00 ± 0.4</u>	6.84	83.66 ± 0.8	36.29	OOM	-
SIGN	66.47 ± 0.9	2.81	60.69 ± 0.4	2.96	74.13 ± 1.0	5.33	69.40 ± 4.8	4.97
Ours								
w/ pr w/o IB	<u>77.11 ± 0.5</u>	39.13	64.77 ± 0.6	47.19	OOM*	-	OOM	-
w/ appr w/o IB	77.01 ± 0.4	2.71	64.92 ± 0.3	2.69	88.72 ± 0.3	2.95	<u>85.55 ± 0.4</u>	4.23
w/ appr w/ IB	**80.28 ± 0.5**	6.38	**66.11 ± 0.7**	6.42	**90.02 ± 0.5**	11.77	**85.94 ± 0.5**	26.63

* OOM stands for out of memory

Link prediction



Graph size



More info