

DIRECTION AWARE POSITIONAL AND STRUCTURAL ENCODING FOR DIRECTED GRAPH NEURAL NETWORKS

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Graph Representation Learning

- **Graph Neural Networks (GNNs)** are models that learn structural node representation via message passing between the nodes of graphs.

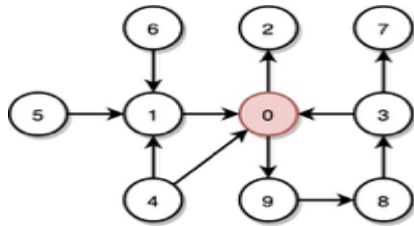
$$G = (V, E), \quad f(G) \rightarrow \mathbb{R}^d$$

Graph Representation Learning

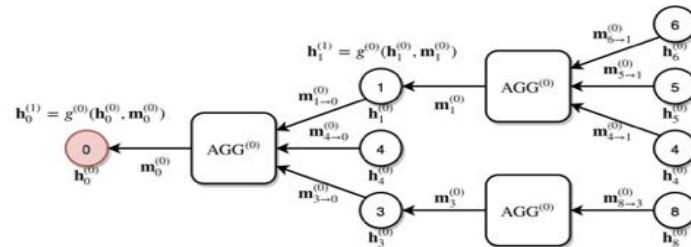
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- Graph Neural Networks(GNNs) are powerful at node classification because it learns node representations directly from k hop neighbors



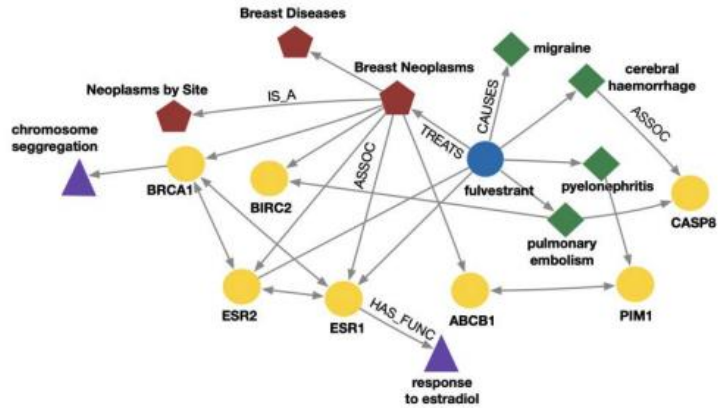
Original Graph



Node representation via MP-GNN

Application Of Directed Link Prediction

- Directed Link Prediction has many real world applications
- For example: Recommender Systems, Citation Networks, Biomedical knowledge graph



Biomedical knowledge graph



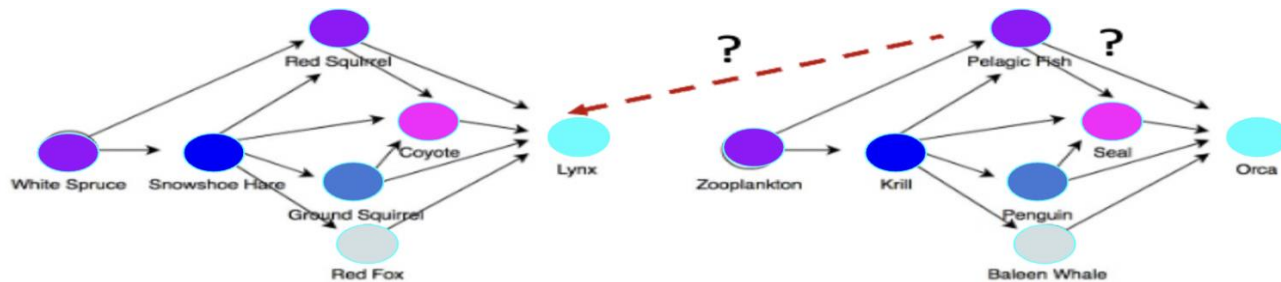
Citation network

Motivation

- Link prediction require a **joint representation learning** of the linked nodes

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- Graph Neural Networks(GNN), can not learn the latent link information between the linked nodes
- Nodes in Identical subgraphs get same representation(GIN, Xu et al. 2019)



Food web Network

[Srinivasan and Reibero, ICLR 2020]

Our Solution

Our Proposed Direction aware Positional Encoding

- For the nodes of the k hop subgraph around a directed link $u \mapsto v$, we computed **Truncated SVD** and **ranking score using HITS algorithm**.

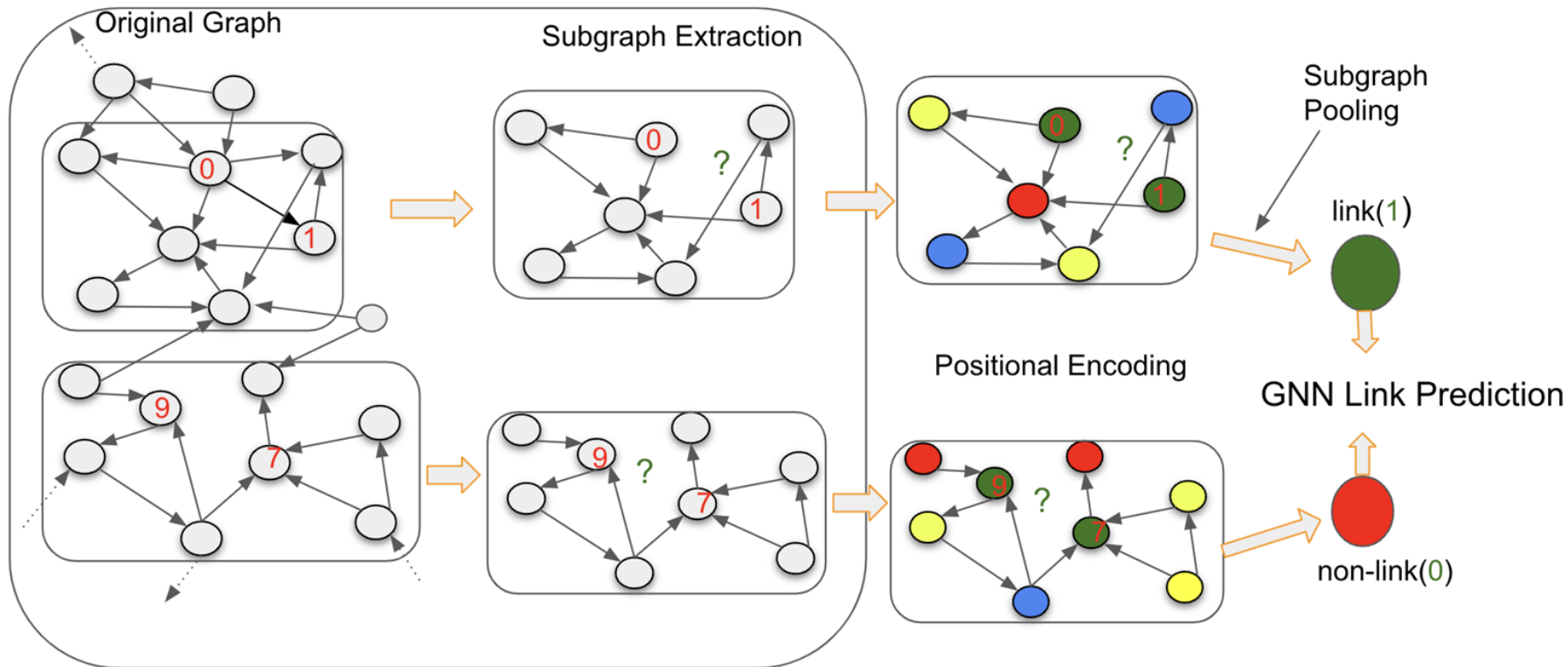
- **Truncated SVD** is an approximation of the $\mathbf{U}_d \in \mathbb{R}^{n \times d}$ of its left singular subspace corresponding to its top singular value
- **HITS algorithm** to compute ranking score using, the authority value \mathbf{a} and hub value \mathbf{h}

$$\mathbf{a}, \mathbf{h} \in \mathbb{R}^n$$

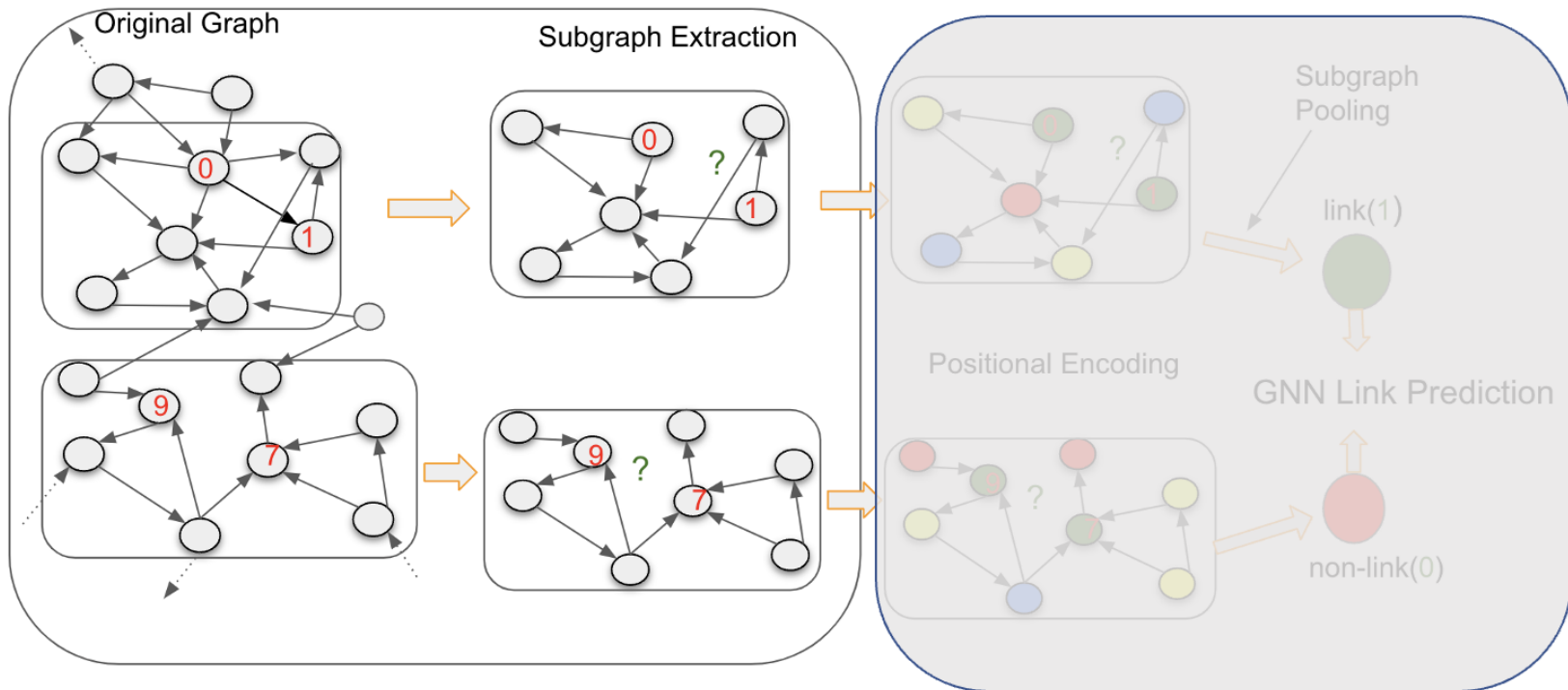
- Get the Positional encoding of node [i] around $u \mapsto v$ by concatenating Truncated SVD and HITS value and use it as initial feature during GNN training

$$pe[i] = (\text{hits}[i] || \text{svd}[i]) \in \mathbb{R}^{d+2}$$

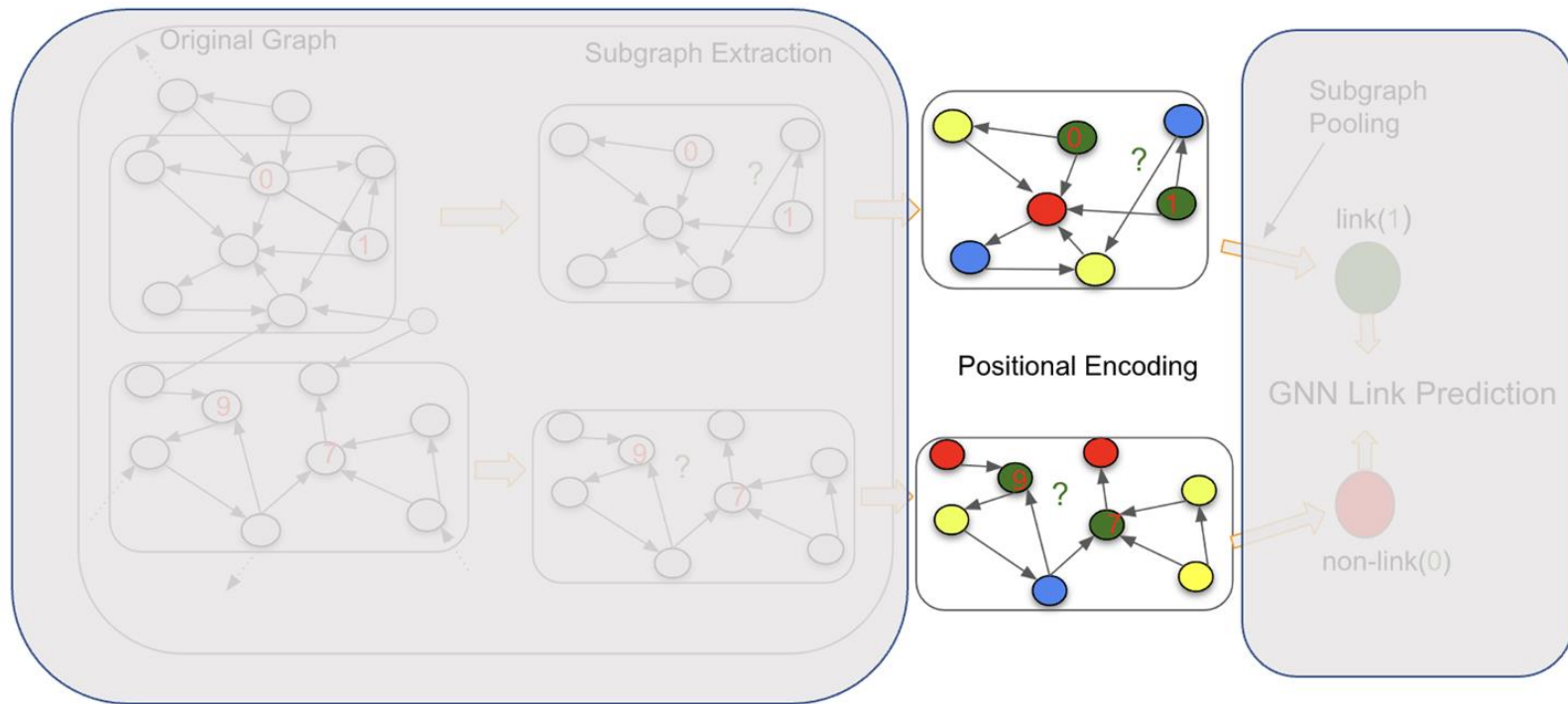
Proposed Framework



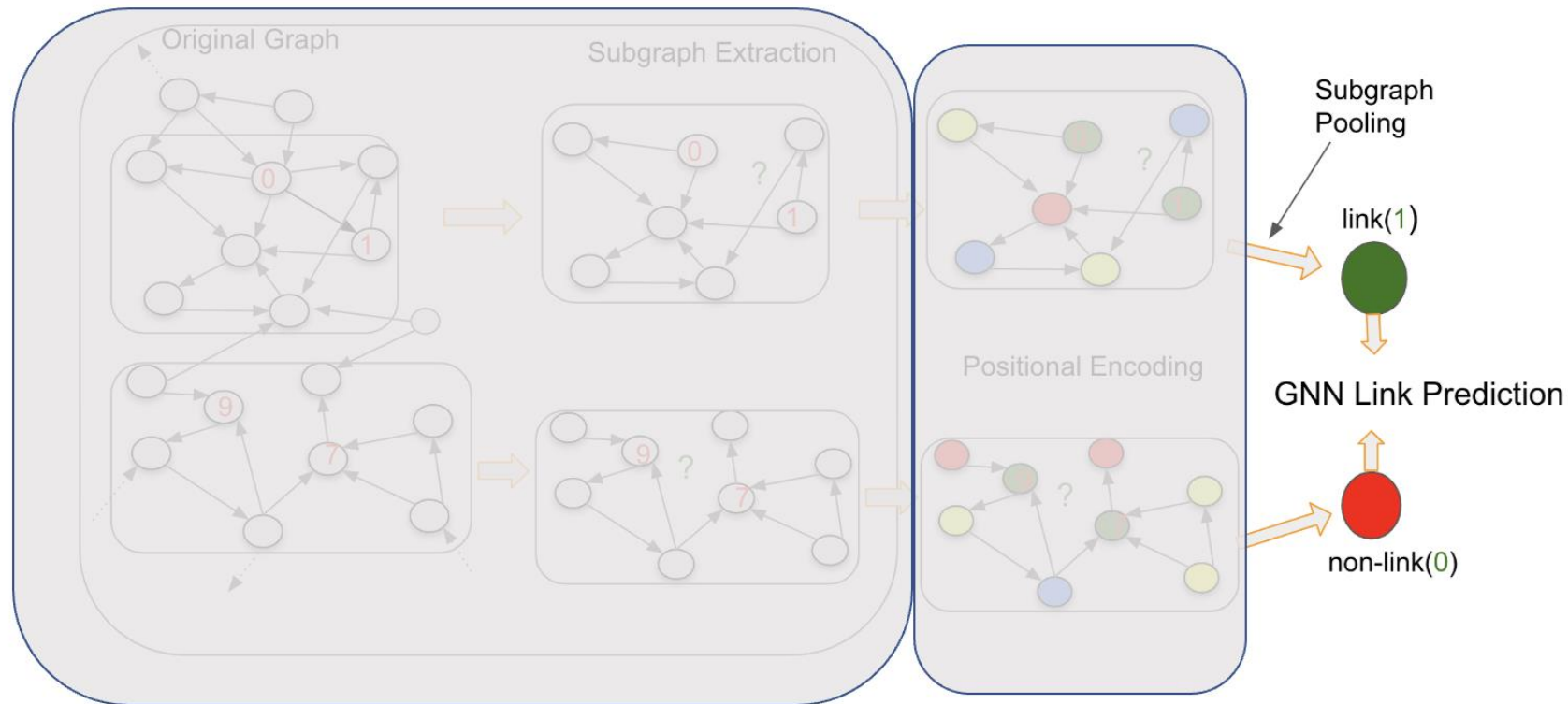
Proposed Framework



Proposed Framework



Proposed Framework



Experimental Results on directed link prediction

: AUC performance for Directed Link Prediction, when both truncated SVD and Rank positional encodings are used.

Model	Cornel	Texas	Wisconsin	Citeseer	CoraML
GCN(SVD + Rank)	86.16 \pm 1.52	87.27 \pm 2.77	82.13 \pm 2.26	87.97 \pm 0.57	88.15 \pm 0.73
GIN(SVD + Rank)	88.01 \pm 2.75	90.72 \pm 2.24	90.72 \pm 1.68	89.12 \pm 0.57	88.28 \pm 0.25
SAGE(SVD + Rank)	88.24 \pm 3.2	88.88 \pm 2.72	89.13 \pm 2.27	87.47 \pm 1.97	87.92 \pm 0.23
DGCN	82.24 \pm 3.47	84.01 \pm 1.67	82.89 \pm 1.74	82.02 \pm 0.8	82.92 \pm 0.37
DiGraphIB	81.93 \pm 1.65	82.72 \pm 1.58	81.67 \pm 1.74	84.89 \pm 0.76	85.27 \pm 0.62
Magnet	83.32 \pm 2.71	83.01 \pm 1.72	84.7 \pm 1.92	86.72 \pm 1.42	85.77 \pm 0.42
DGCN(SVD + Rank)	89.24 \pm 2.47	87.04 \pm 1.92	87.21 \pm 1.74	88.75 \pm 0.66	90.21 \pm 1.37
DiGraphIB(SVD + Rank)	87.58 \pm 2.17	87.01 \pm 2.87	88.11 \pm 2.74	89.82 \pm 0.68	89.2 \pm 0.58
Magnet(SVD + Rank)	91.98 \pm 1.62	89.98 \pm 2.91	90.82 \pm 1.08	91.66 \pm 0.81	93.85 \pm 1.27

Conclusion

- Adding **direction aware positional encoding** can help GNNs to predict directed link
- Both **Truncated SVD** and **ranking score using HITS algorithm** can make GNNs more powerful for directed link prediction

Thank You for Listening!