Self-Explainable Graph Neural Networks for Link PredictionI Network[1]

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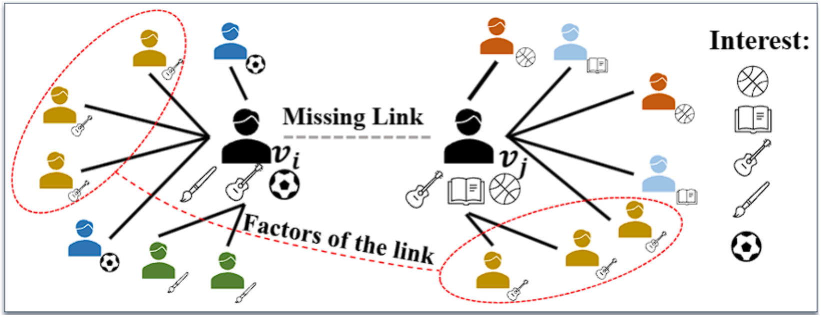
illustration



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Problems

1. for a pair of nodes (v_i, v_j), how we can identify K most important neighbors of v_j and v_i.
2.How to take both graph structure and node attributes into consideration when measuring node similarity for identifying important neighbors for link prediction?

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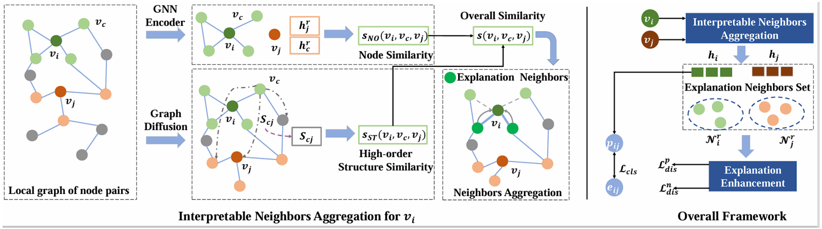
Overview



Local graph of node pairs
v_c
v_i
v_j
GNN Encoder
Graph Diffusion
h_j^r
h_c^r
$s_{NO}(v_i, v_c, v_j)$
Node Similarity
S_{cj}
$s_{ST}(v_i, v_c, v_j)$
High-order Structure Similarity
Overall Similarity
$s(v_i, v_c, v_j)$
Explanation Neighbors
Neighbors Aggregation
Interpretable Neighbors Aggregation for v_i
Interpretable Neighbors Aggregation
h_i
h_j
Explanation Neighbors Set
$\mathcal{N}_i^r$
$\mathcal{N}_j^r$
p_{ij}
e_{ij}
$\mathcal{L}_{cls}$
$\mathcal{L}_{dis}^p$
$\mathcal{L}_{dis}^n$
Explanation Enhancement
Overall Framework

High-order Structure Similarity

To measure this high-order similarity, we propose to use a Graph Diffusion matrix which calculates the closeness of nodes in the graph structure by repeatedly passing the weighting coefficients to the neighboring nodes and represents the high-order similarity between nodes based on graph structure:

$$\mathbf{S} = \sum_{k=0}^{\infty} \theta_k \mathbf{T}^k, \tag{1}$$

$\mathbf{T}$ represents the random walk transition matrix as $\mathbf{T} = \mathbf{A}\mathbf{D}^{-1}$
PPR chooses $\theta_k^{\mathrm{PPR}} = \gamma(1-\gamma)^k$ with teleport probability $\gamma \in (0,1)$. γ is set as 0.05 in the experiment.
$\tilde{\mathbf{S}} = \mathbf{D}_S^{-1/2}\mathbf{S}\mathbf{D}_S^{-1/2}$

$$s_{\mathrm{ST}}(v_i, v_c, v_j) = \tilde{S}_{cj}, \tag{2}$$

Node Similarity

$$\mathbf{H}^m = \mathrm{MLP}(\mathbf{X}), \quad \mathbf{H}^r = \sigma(\tilde{\mathbf{A}}[\mathbf{H}^m \| \mathbf{X}]\mathbf{W}) + \mathbf{H}^m, \tag{3}$$

$$s_{\mathrm{NO}}(v_i, v_c, v_j) = \mathrm{sigmoid}\big((\mathbf{h}_j^r)^T \mathbf{h}_c^r\big), \ \forall \ v_c \in \mathcal{N}_i \tag{4}$$

$$s(v_i, v_c, v_j) = \alpha \cdot s_{\mathrm{ST}}(v_i, v_c, v_j) + (1-\alpha) \cdot s_{\mathrm{NO}}(v_i, v_c, v_j), \tag{5}$$

$$b_{ic} = \frac{\exp\left(s\left(v_i, v_c, v_j\right)\right)}{\sum_{v_c \in \mathcal{N}_i^r} \exp\left(s\left(v_i, v_c, v_j\right)\right)}. \tag{6}$$

Finally, node v_i's representation vectors can be obtained as:

$$\mathbf{h}_i = \mathbf{h}_i^r + \beta \sum_{v_c \in \mathcal{N}_i^r} b_{ic} \mathbf{h}_c^r, \tag{7}$$

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$$p_{ij} = \text{sigmoid}(\mathbf{h}_i^T \mathbf{h}_j). \tag{8}$$

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$$\mathbf{h}_i^{\text{rand}} = \mathbf{h}_i^r + \beta \sum_{v_c \in \mathcal{N}_i^{\text{rand}}} b_{ic}^{\text{rand}} \mathbf{h}_c^r, \tag{9}$$

$$p_{ij}^{\text{rand}} = \text{sigmoid}((\mathbf{h}_i^{\text{rand}})^T \mathbf{h}_j^{\text{rand}}). \tag{10}$$

$$\mathcal{L}_{\text{dis}}^p = \sum_{e_{ij} \in \mathcal{E}_L, e_{ij}=1} \max(0, p_{ij}^{\text{rand}} + \delta - p_{ij}), \tag{11}$$

Loss

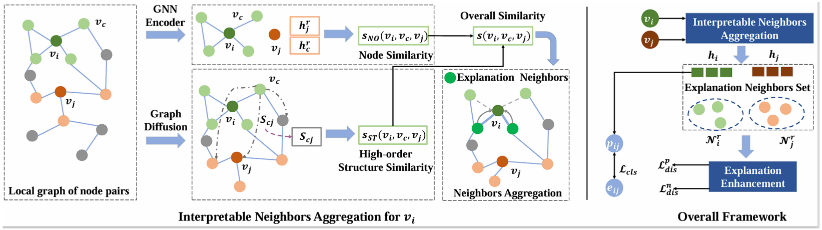
If nodes v_i and v_j have lower similarity scores with nodes in $\mathcal{N}_j^r$ and $\mathcal{N}_j^r$ respectively, the similarity of $\mathbf{h}_i$ and $\mathbf{h}_j$ will be small and the model will give a lower probability for the link of (v_i, v_j). To achieve this purpose, we randomly sample unlinked pairs $e_{ij} = 0$ which have the same number as the number of linked pairs $e_{ij} = 1$ in $\mathcal{E}_L$. The set of randomly selected unlinked pairs can be denoted as $\mathcal{E}_N$. The similarity scores can be minimized through the following loss function:

$$\mathcal{L}_{\text{dis}}^{n} = \sum_{e_{ij} \in \mathcal{E}_N} \Bigg(\sum_{v_c \in \mathcal{N}_i^r} s(v_i, v_c, v_j)^2 + \sum_{v_c \in \mathcal{N}_j^r} s(v_j, v_c, v_i)^2 \Bigg). \tag{12}$$

Overall Objective Function

$$\mathcal{L}_{\text{cls}} = \sum_{e_{ij} \in \mathcal{E}_L} -\log p_{ij} + \sum_{e_{ij} \in \mathcal{E}_N} -\log\left(1 - p_{ij}\right), \tag{13}$$

$$\min_{\Theta} \mathcal{L} = \mathcal{L}_{\text{cls}} + \lambda(\mathcal{L}_{\text{dis}}^{p} + \mathcal{L}_{\text{dis}}^{n}), \tag{14}$$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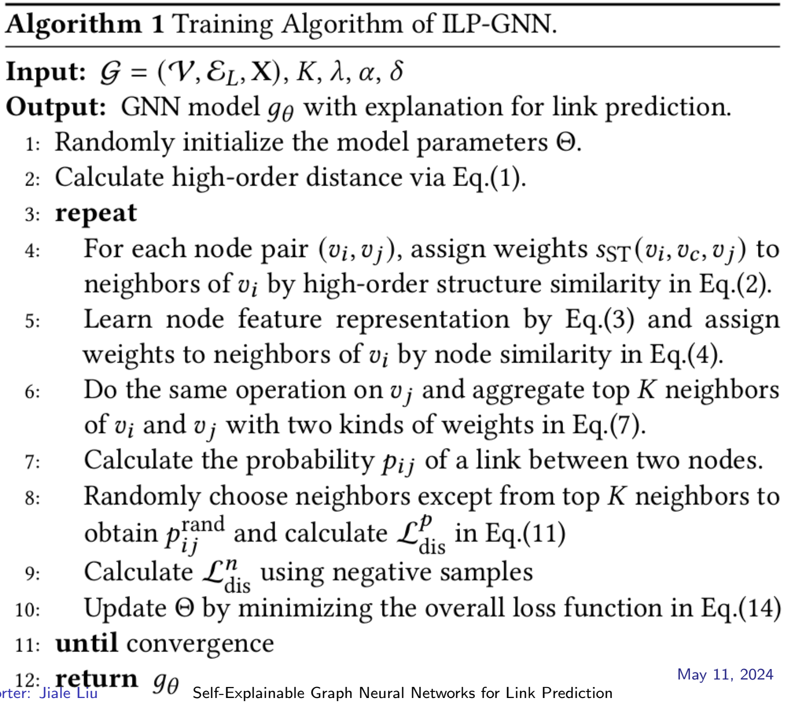

Algorithm 1 Training Algorithm of ILP-GNN.

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Input: $\mathcal{G} = (\mathcal{V}, \mathcal{E}_L, \mathbf{X})$, $K$, $\lambda$, $\alpha$, $\delta$
Output: GNN model $g_\theta$ with explanation for link prediction.
 1: Randomly initialize the model parameters $\Theta$.
 2: Calculate high-order distance via Eq.(1).
 3: repeat
 4:     For each node pair $(v_i, v_j)$, assign weights $s_{\mathrm{ST}}(v_i, v_c, v_j)$ to
        neighbors of $v_i$ by high-order structure similarity in Eq.(2).
 5:     Learn node feature representation by Eq.(3) and assign
        weights to neighbors of $v_i$ by node similarity in Eq.(4).
 6:     Do the same operation on $v_j$ and aggregate top $K$ neighbors
        of $v_i$ and $v_j$ with two kinds of weights in Eq.(7).
 7:     Calculate the probability $p_{ij}$ of a link between two nodes.
 8:     Randomly choose neighbors except from top $K$ neighbors to
        obtain $p_{ij}^{\mathrm{rand}}$ and calculate $\mathcal{L}_{\mathrm{dis}}^{p}$ in Eq.(11)
 9:     Calculate $\mathcal{L}_{\mathrm{dis}}^{n}$ using negative samples
10:     Update $\Theta$ by minimizing the overall loss function in Eq.(14)
11: until convergence
12: return $g_\theta$
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