Developing

ID-GNN with Commonsense Reasoning

ID-GNN 이전의 $\boxed{\text{preliminaries}}$

$G = (V, E)$, $V = \{v_1, \cdots v_n\}$ (node set)

$E \subseteq V \times V$ (edge set)

$\times$ R 근추하기

Node feature $X = \{x_v \mid \forall v \in V\}$

edge feature $f = \{f_{uv} \mid \forall e_{uv} \in E\}$

k-th iteration (k-th layer)

$$m_u^{(k)} = MSG^{(k)}(h_u^{(k-1)})$$

$$h_v^{(k)} = AGG^{(k)}(\{m_u^{(k)}, u \in N(v)\}, h_v^{(k-1)})$$

h_v: node embedding

$h_v^{(0)} = x_v$

$m_v^{(k)}$ = message embedding

MSG(·), AGG(·) 은 다양하다

이제는 ID-GNN!!

ID-GNN is built with **two important components**

(1) inductive identity coloring where identity information is injected to each node

(2) heterogeneous message passing where the identity information is utilized in message passing

① Inductive identity coloring

- first extract the k-hop ego network $G_v^{(k)}$ of v (center node)
- Then assign a unique coloring to the central node of the ego network $G_v^{(k)}$
- coloring 노드와 non coloring 노드들가 각각 나뉜다

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② Heterogeneous message passing

k rounds of message passing are then applied to all the extracted ego networks.

$$m_s^{(k)} = MSG^{(k)}_{1[s=v]}\left(h_s^{(k-1)}\right)$$

$$h_u^{(k)} = AGG^{(k)}\left(\{m_s^{(k)}, s \in N(u)\}, h_u^{(k-1)}\right)$$

$MSG_1^{(k)}(\cdot)$: applied to nodes with Identity coloring.

$MSG_0^{(k)}(\cdot)$: 〃 〃 without coloring

$$1[s=v] \begin{cases} 1 & s=v \\ 0 & \text{otherwise} \end{cases}$$

This way, the inductive identity coloring's encoded into the ID-GNN computational graph

이 방법은 모든 MPGNN에 적용 가능!!

edge attributes f_{su}를 추가한다면??

$$m_{su}^{(k)} = MSG^{(k)}_{1[s=v]}\left(h_s^{(k-1)}, f_{su}\right)$$

$$h_u^{(k)} = AGG^{(k)}\left(\{m_{su}^{(k)}, s \in N(u)\}, h_u^{(k-1)}\right)$$

Algorithm: ID-GNN embedding computation

Input: Graph $G(V, E)$,

input node feature => $\{x_v, \forall v \in V\}$

Number of layers K

trainable functions => $MSG_1^{(k)}, MSG_0^{(k)}$

$EGO(v, k)$: extracts the k-hop ego network centered at node v

Output

Node embedding h_v for all $v \in V$

for $v \in V$ do

$G_v^{(K)} \leftarrow EGO(v, K)$, $h_u^{(0)} \leftarrow x_u, \forall u \in G_v^{(K)}$

for $k = 1, \cdots, K$ do

for $u \in G_v^{(K)}$ do

$h_u^{(k)} \leftarrow AGG^{(k)}\left(\{MSG^{(k)}_{1[s=v]}(h_s^{(k-1)}), s \in N(u)\}, h_u^{(k-1)}\right)$

$h_v \leftarrow h_v^{(K)}$

ID-GNNs Can Count Cycles.

$h_v^{(K)}[i]$ => equals the number of length i cycles starting and ending at node v, For $i = 1, \dots, k$

They prove this by showing that ID-GNNs can count paths from any node u to the identity node v

이 논문에서 Cycle count가 Node-level (predict clustering coefficient)에 도움이 된다고 한다 => Reasoning에 어떻게 사용할까

A_{uv}^{l} 은 # walks of length l between u and v

ID-GNN-Fast : Injecting Identity via Augmented Node features

$$x_v^{+}[k] = \mathrm{Diag}(A^k)[v]$$

$$x_v = \mathrm{Concat}(x_v, x_v^{+})$$

그렇다면 Commonsense Reasoning에서 도움이 될만한 것이 무엇일까? node-level?, edge-level? Graph-level?

Cycle specific한 Commonsense Reasoning

=> Cycle을 카운트 해서