CS224W: Machine Learning with Graphs **Fall 2021**

Homework 3

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Question 1: GraphRNN (20 points)

Q1.1 (12 points)

★ **Solution** ★ BFS would return the following ordering

$$S^\pi = (A, B, D, C, E, F).$$

The edge level predictions are given by

$$\begin{aligned}
&S^\pi_{B,A} = 1 \\
&S^\pi_{D,A} = 1 \quad S^\pi_{D,B} = 0 \\
&S^\pi_{C,A} = 0 \quad S^\pi_{C,B} = 1 \quad S^\pi_{C,D} = 0 \\
&S^\pi_{E,A} = 0 \quad S^\pi_{E,B} = 1 \quad S^\pi_{E,D} = 1 \quad S^\pi_{E,C} = 0 \\
&S^\pi_{F,A} = 0 \quad S^\pi_{F,B} = 0 \quad S^\pi_{F,D} = 0 \quad S^\pi_{F,C} = 1 \quad S^\pi_{F,E} = 1.
\end{aligned}$$

Q1.2 (8 points)

★ **Solution** ★ One benefit is that during training only the possible BFS orderings need to be considered instead of considering all the possible permutations of the nodes of the graph. Another benefit is that the number of predictions for edges between nodes that need to made are reduced by only considering edges to nodes that a prior to the current node w.r.t. the BFS ordering.

Question 2: Subgraphs and Order Embeddings (35 points)

Q2.1 Transitivity (8 points)

★ **Solution** ★ Since A is a subgraph of B there exist an injective map $\varphi\colon V_A \to V_B$ such that $\varphi\colon V_A \to \varphi(V_B)$ is a graph isomorphism of the subgraph of B induced by $\varphi(B)$. Similarly, there exists an injective map $\psi\colon V_B \to V_C$ such that $\varphi\colon V_B \to \varphi(V_C)$ is a graph isomorphism of the subgraph of C induced by $\varphi(C)$. The function $\mu := \psi \circ \varphi$ is injective because the composition of injective functions is injective. We show that the subgraph of C induced by $\{\mu(v); v \in V_A\}$ is graph isomorphic to A. Let

$u, v \in V_A$. Since φ and ψ induce graph isomorphisms, we have (u, v) is an edge of A iff $(\varphi(u), \varphi(v))$ is an edge of B which is the case iff $(\psi(\varphi(u)), \psi(\varphi(v))) = (\mu(u), \mu(v))$ is an edge of C. Thus, A is also a subgraph of C.

Q2.2 Anti-symmetry (8 points)

★ **Solution** ★ Again, we have injective maps $\varphi\colon V_A \to V_B$ and $\psi\colon V_B \to V_A$ such that the induced subgraphs of the images are graph isomorphimic to A and B, respectively. Due to injectivity of the functions we have $|V_A| \leq |V_B| \leq |V_A|$, so that A and B have the same number of nodes. This implies that φ and ψ are bijections. Therefore $\{\varphi(V); v \in V_A\} = V_B$ and since the subgraph of B induced by B is V_B itself, it is isomorphic to A.

Q2.3 Common subgraph (4 points)

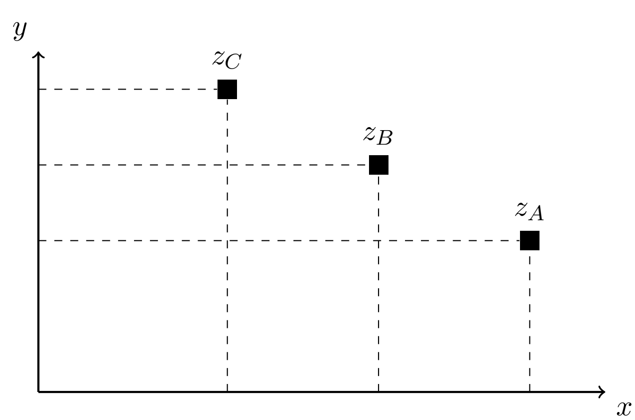
★ **Solution** ★ The graph X is a subgraph of A and B if and only if $z_X \preceq z_A$ and $z_X \preceq z_B$ which holds iff $z_X[i] \preceq z_A[i]$ and $z_X[i] \preceq z_B[i]$ is true for all components i. This is the case iff $z_X[i] \preceq \min\{z_A[i], z_B[i]\}$ for each possible i which by definition is $z_X \preceq \min\{z_A, z_B\}$.

Q2.4 Order embeddings for graphs that are not subgraphs of each other (5 points)

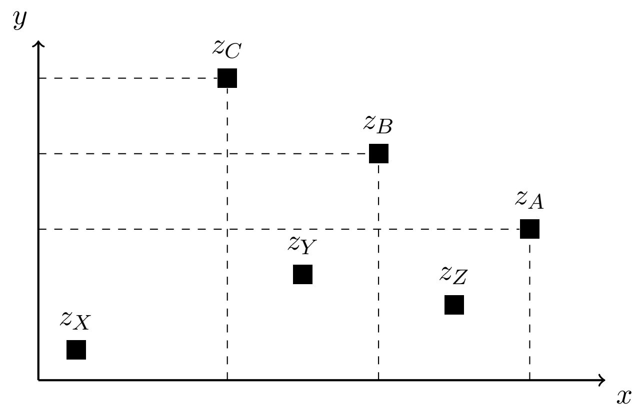
★ **Solution** ★ Suppose we would have $z_C[1] \leq z_B[1]$, then C would be a subgraph of B, which is not the case. So we must have $z_C[1] > z_B[1]$. With the same argumentation for A and B we obtain $z_B[1] > z_A[1]$.

Q2.5 Limitation of 2-dimensional order embedding space (10 points)

★ **Solution** ★ If we suppose $z_A[0] > z_B[0] > z_C[0]$, then the graphs A, B and C satisfy the relation of Q2.4, so that we must be in a situation like



To obtain $z_X \preceq z_Y$ and $z_X \preceq z_Z$ the embeddings should be distrubuted on the xy plane as described in the following figure.



(Note that we could just pick $z_X \preceq z_Y \preceq z_Z$ so that $z_X \preceq z_Y$ and $z_X \preceq z_Z$ would be satisfied by transitivity.)

Let X be a subgraph of A, B, C that is largest in size (with respect to number nodes). Such a graph exists since a single node is a graph. Pick a node u in B that is not part of A and pick a node v in C that is not in B. Such nodes must exist since the graphs A, B, C are not subgraphs of each other. Let Y be the induced subgraph given by the nodes in X together with u and let Z be induced by the nodes in X together with v. Under the assumption that the order embedding constraint is satisfied we must have $z_X \preceq z_Y$ and $z_X \preceq z_Z$.

Honor Code (0 points)

(X) I have read and understood Stanford Honor Code before I submitted my work.
Collaboration: Write down the names & SUNetIDs of students you collaborated with on Homework 3 (None if you didn't).
Note: Read our website on our policy about collaboration!