CS224W: Machine Learning with Graphs | Fall 2021

Homework 3

Due 11:59pm PT Thursday November 11 2021

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Question 1: GraphRNN (20 points)

Q1.1 (12 points)

★ **Solution** ★ The sequence of node and edge additions using BFS ordering starting from Node A (with neighbors explored in alphabetical order) is:

$$\{S^{\pi}_{A} : [],\ S^{\pi}_{B} : [S^{\pi}_{B,A} = 1],\ S^{\pi}_{D} : [S^{\pi}_{D,A} = 1, S^{\pi}_{D,B} = 0],\ S^{\pi}_{C} : [S^{\pi}_{C,A} = 0, S^{\pi}_{C,B} = 1, S^{\pi}_{C,D} = 0],$$

$$S^{\pi}_{E} : [S^{\pi}_{E,A} = 0, S^{\pi}_{E,B} = 1, S^{\pi}_{E,C} = 0, S^{\pi}_{E,D} = 1],\ S^{\pi}_{F} : [S^{\pi}_{F,A} = 0, S^{\pi}_{F,B} = 0, S^{\pi}_{F,C} = 1,$$

$$S^{\pi}_{F,D} = 0, S^{\pi}_{F,E} = 1]\}$$

Note: The sequence follows BFS ordering from Node A, with neighbors explored in alphabetical order at each step.

Q1.2 (8 points)

★ **Solution** ★ Two advantages of using BFS ordering over random ordering in graph generation:

1. **Reduces long-range dependencies**: BFS ordering tends to connect new nodes to recently added nodes, making the sequence more local and easier for RNNs to learn.

2. **Automatic sparsity pattern**: In BFS ordering, edges are only predicted between the new node and existing nodes in the current BFS frontier, reducing the number of required predictions and enforcing a natural sparsity pattern that matches real-world graphs.

Question 2: Subgraphs and Order Embeddings (35 points)

Q2.1 Transitivity (8 points)

★ Solution ★ We prove that if graph A is a subgraph of graph B, and graph B is a subgraph of graph C, then graph A is a subgraph of graph C.

Proof:

Let: - $f : V_A \to V'_B \subseteq V_B$ be the subgraph isomorphism from A to B - $g : V_B \to V'_C \subseteq V_C$ be the subgraph isomorphism from B to C

Construct composite mapping $h : V_A \to V_C$ defined as $h(v) = g(f(v))$ for all $v \in V_A$.

Verification:

- **Bijectivity**: Since f and g are bijective, h is bijective.
- **Edge preservation**: For any $(u, v) \in E_A$, $(f(u), f(v)) \in E_B$ and thus $(g(f(u)), g(f(v))) = (h(u), h(v)) \in E_C$.
- **Non-edge preservation**: For any $(u, v) \notin E_A$, $(f(u), f(v)) \notin E_B$ and thus $(h(u), h(v)) \notin E_C$.

Therefore, h is a valid subgraph isomorphism mapping from A to C.

Q2.2 Anti-symmetry (8 points)

★ Solution ★ Proof: Let $f : V_A \to V'_B \subseteq V_B$ and $g : V_B \to V'_A \subseteq V_A$ be the subgraph isomorphisms.

Since f and g are bijections: $|V_A| = |V'_B| \leq |V_B|$ and $|V_B| = |V'_A| \leq |V_A|$, so $|V_A| = |V_B|$, hence $V'_B = V_B$ and $V'_A = V_A$.

Now $f : V_A \to V_B$ and $g : V_B \to V_A$ are bijections between equal-sized sets. For any $(u, v) \in E_A$, $(f(u), f(v)) \in E_B$, and for any $(x, y) \in E_B$, $(g(x), g(y)) \in E_A$. Since $g = f^{-1}$, f preserves both edges and non-edges bidirectionally.

Thus f is a graph isomorphism between A and B.

Q2.3 Common subgraph (4 points)

★ Solution ★ Proof:

($\Rightarrow$) If X is a common subgraph of A and B:

$$X \subseteq A \Rightarrow z_X \preccurlyeq z_A, \quad X \subseteq B \Rightarrow z_X \preccurlyeq z_B$$

$$\Rightarrow z_X \preccurlyeq \min\{z_A, z_B\}$$

($\Leftarrow$) If $z_X \preccurlyeq \min\{z_A, z_B\}$:

$$z_X \preccurlyeq z_A \Rightarrow X \subseteq A, \quad z_X \preccurlyeq z_B \Rightarrow X \subseteq B$$

$$\Rightarrow X \text{ is a common subgraph of } A \text{ and } B.$$

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

★ Solution ★ Given: A, B, C are non-isomorphic and not subgraphs of each other, with $z_A[0] > z_B[0] > z_C[0]$ in a 2D order embedding space.

Since B is not a subgraph of A and $z_B[0] < z_A[0]$, we must have $z_B[1] > z_A[1]$ to violate $z_B \preccurlyeq z_A$.

Since C is not a subgraph of B and $z_C[0] < z_B[0]$, we must have $z_C[1] > z_B[1]$ to violate $z_C \preccurlyeq z_B$.

Since C is not a subgraph of A and $z_C[0] < z_A[0]$, we must have $z_C[1] > z_A[1]$ to violate $z_C \preccurlyeq z_A$.

Combining these: $z_C[1] > z_B[1] > z_A[1]$.

Thus the second dimension must satisfy:

$$z_C[1] > z_B[1] > z_A[1]$$

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

★ Solution ★ Construct X, Y, Z as follows:

- X is a common subgraph of A, B, and C
- Y is a common subgraph of A and B only
- Z is a common subgraph of A and C only

Reasoning:

From Q2.3 and the coordinate ordering $z_A[0] > z_B[0] > z_C[0]$, $z_C[1] > z_B[1] > z_A[1]$:

- $z_X \preccurlyeq \min(z_A, z_B, z_C) = (z_C[0], z_A[1])$
- $z_Y \preccurlyeq \min(z_A, z_B) = (z_B[0], z_A[1])$
- $z_Z \preccurlyeq \min(z_A, z_C) = (z_C[0], z_A[1])$

Thus:

- $z_X \preccurlyeq (z_C[0], z_A[1]) \preccurlyeq (z_B[0], z_A[1]) = z_Y \Rightarrow z_X \preccurlyeq z_Y$
- $z_X \preccurlyeq (z_C[0], z_A[1]) = z_Z \Rightarrow z_X \preccurlyeq z_Z$

However, X may not actually be a common subgraph of Y and Z, demonstrating the limitation of 2D order embedding space.

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).
None
Note: Read our website on our policy about collaboration!