CS224W Homework 3

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1 GraphRNN

1.1

Order of nodes

$$S^\pi = (S^\pi_A, S^\pi_B, S^\pi_D, S^\pi_C, S^\pi_E, S^\pi_F)$$

Note that node B and node D are both 2-hop neighbors of node A, so their order can be changed. Node C and node E are both 3-hop neighbors of node A, so their order can be changed as well. For the edge level predictions, we focus on the A-B-D-C-E-F order since the question specifies to visit neighbors in alphabetical order.

Edge Level Predictions: $S^\pi_B = \{S^\pi_{B,A} = 1\}, S^\pi_D = \{S^\pi_{D,A} = 1, S^\pi_{D,B} = 0\}, S^\pi_C = \{S^\pi_{C,A} = 0, S^\pi_{C,B} = 1, S^\pi_{C,D} = 0\}, S^\pi_E = \{S^\pi_{E,A} = 0, S^\pi_{E,B} = 1, S^\pi_{E,D} = 1, S^\pi_{E,C} = 0\}, S^\pi_F = \{S^\pi_{F,A} = 0, S^\pi_{F,B} = 0, S^\pi_{F,D} = 0, S^\pi_{F,C} = 1, S^\pi_{F,E} = 1\}$

1.2

First, training only on BFS ordering avoids computation on all possible permuations, and because multiple permutations map to the same BFS ordering, this trick reduces the sequences we have to compute. Secondly, BFS ordering reduces the number of edge predictions during each step in the RNN[You et al. 2018].

2 Subgraphs and Order Embeddings

2.1

Proof:
Since $A \subseteq B$, there exist a bijective mapping f that maps all nodes in V_A to a subset of nodes in V_B, such that the subgraph of B induced by $\{f(v)|v \in V_A\}$ is graph-isomorphic to A.
Since $B \subseteq C$, there exist a bijective mapping g that maps all nodes in V_B to a subset of nodes in V_C, such that the subgraph of C induced by $\{g(v)|v \in V_B\}$

is graph-isomorphic to B.
Now we consider such bijective mapping of $f \cdot g$, which maps all nodes in V_A to a subset of nodes in V_C. We have the subgraph of C induced by $\{f(g(v))|v \in V_A\}$ is graph-isomorphic to A. Therefore $A \subseteq C$, which completes the proof.

2.2

Proof:
Let $|\cdot|$ denote the number of nodes in a graph. Since $A \subseteq B$, we have $|A| \leq |B|$. Since $B \subseteq A$, we have $|B| \leq |A|$, therefore $|B| = |A|$. And since $B \subseteq A$ there exists a bijection from nodes in B to the subset of nodes in A. This subset contains all nodes in A because bijection implies the size of the entry is the same as the size of the outcome. Therefore there exists a bijection from all nodes in B to all nodes in A. Therefore A and B are graph-isomorphic.

2.3

Proof:
First we prove the forward direction. i.e. if X is a common subgraph of A and B, then $z_X \preceq \min\{z_a, z_b\}$.
Because $X \subseteq A$, and $X \subseteq B$. We have $z_X \preceq z_A$, $z_X \preceq z_B$. Therefore each element of z_X is smaller than the corresponding element of both z_A and z_B, certainly smaller than the minimum of z_A and z_B since it is smaller than both. Therefore we have $z_X \preceq \min\{z_A, z_B\}$.

Then we prove the backward direction i.e. if $z_X \preceq \min\{z_A, z_B\}$, then X is a common subgraph of A and B.
Because $\min\{z_A, z_B\} \preceq z_A$ and $\min\{z_A, z_B\} \preceq z_B$, we have $z_X \preceq \min\{z_A, z_B\} \preceq z_A$ and $z_X \preceq \min\{z_A, z_B\} \preceq z_B$, which completes the proof.

2.4

$z_A[1] < z_B[1] < z_C[1]$.

2.5

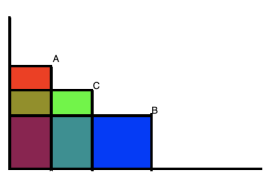

Figure 1: Embedding Space

As shown in the picture, A, B, C are represented in the embedding space. The red area corresponds to all the subgraphs of only A, the green area corresponds to the subgraphs of only C and the blue area of only B. The cross shaded region corresponds to the common subgraphs of two graphs: e.g. the cyan(darker blue) area corresponds to the common subgraphs of only B and C. As you can see, the common subgraphs of A and B(the purple area)are all embedded in the subgraph space of C.

References

You, Jiaxuan et al. (2018). "GraphRNN: Generating Realistic Graphs with Deep Auto-regressive Models." In: *ICML*. Ed. by Jennifer G. Dy and Andreas Krause. Vol. 80. Proceedings of Machine Learning Research. PMLR, pp. 5694–5703. URL: http://dblp.uni-trier.de/db/conf/icml/icml2018.html#YouYRHL18.