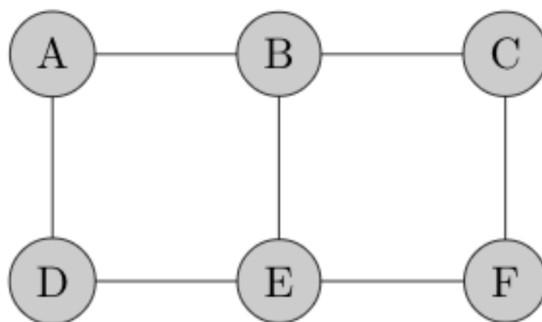


Furthermore, each node-level step is comprised of edge-level decisions, where the graph generation model decides whether to construct an edge between this new node and each of the pre-existing nodes. For example, S_4^π , the node-level step for node 4, is comprised of 3 decisions: $S_{4,1}^\pi = 0$ (do not connect nodes 4 and 1), $S_{4,2}^\pi = 1$ (connect nodes 4 and 2), $S_{4,3}^\pi = 1$ (connect nodes 4 and 3).

Q1.1 (12 points)

One important characteristic of GraphRNN is it uses breadth-first search (BFS) to come up with its node ordering. For this problem, we will focus on the following grid graph:



If we wanted GraphRNN to generate the graph above, what is the sequence of node and edge additions that the model would make? Recall that GraphRNN needs to predict, for each new node, which existing nodes it needs to wire an edge with. It outputs 1 when there should be an edge, and 0 when there should not. Nodes are added in BFS ordering starting from Node A. Assume that when exploring the neighbors of a node, they are explored in alphabetical order.

What to submit: We expect you to write the order of nodes, and then for each node, the edge-level predictions.

Q1.2 (8 points)

Explain 2 advantages of graph generation using a BFS ordering of nodes in the graph, as opposed to generating with a random ordering of nodes in the graph.

Hint: You are free to benefit from the claims made in the original GraphRNN paper.

Question 2: Subgraphs and Order Embeddings (35 points)

In the lecture, we demonstrate that subgraph matching can be effectively learned by embedding subgraphs into the order embedding space. The reason is that many properties associated with subgraphs are naturally reflected in the order embedding space.

For this question, we say "graph A is a subgraph of graph B " when there exists a subgraph of B that is graph-isomorphic to graph A . We additionally only consider the induced subgraph setting introduced in lecture with all order embeddings non-negative.

Recall that the order embedding constraint states that: A is a subgraph of B if and only if $z_A[i] \leq z_B[i]$ for all embedding dimension i . For simplicity, we do not consider anchor node in this question, and assume that the order embedding z_A is an embedding of the graph A .

Q2.1 Transitivity (8 points)

Show the transitivity property of the subgraph relation: if graph A is a subgraph of graph B , and graph B is a subgraph of C , then graph A is a subgraph of C .

The proof should make use of the subgraph isomorphism definition: if graph A is a subgraph of graph B , then there exists 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 .

Q2.2 Anti-symmetry (8 points)

Use the same subgraph isomorphism definition to show the anti-symmetry property of the subgraph relation: if graph A is a subgraph of graph B , and graph B is a subgraph of graph A , then A and B are graph-isomorphic.

Hint: What does the condition imply about the number of nodes in A and B , and why does this implication results in graph isomorphism?

Q2.3 Common subgraph (4 points)

Notation Clarification: The symbol " \preceq " means element-wise less than or equal to.

Consider a 2-dimensional order embedding space. Graph A is embedded into z_A , and graph B is embedded into z_B . Suppose that the order embedding constraint is perfectly preserved in the order embedding space. Prove that graph X is a common subgraph of A and B if and only if $z_X \preceq \min\{z_A, z_B\}$. Here \min denotes the element-wise minimum of the two embedding vectors.

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

Suppose that graphs A, B, C are non-isomorphic graphs that are not subgraphs of each other. We embed them into a 2-dimensional order embedding space. Without loss of generality, suppose that we compare the values of the embeddings in the first dimension (dimension 0), and have $z_A[0] > z_B[0] > z_C[0]$. What does this condition imply about the relation between $z_A[1], z_B[1], z_C[1]$, assuming that the order embedding constraint is perfectly satisfied?

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

Notation Clarification: The symbol " \preceq " means element-wise less than or equal to.

Here we show that 2-dimensional order embedding space is not sufficient to perfectly model subgraph relationships.

Suppose that graphs A, B, C are non-isomorphic graphs that are not subgraphs of each other. Construct an example of graphs X, Y, Z such that they are each subgraphs of one or more graphs

in $\{A, B, C\}$; for example, X could be a common subgraph of A and B , Y could be a common subgraph of A and C , and Z could be a subgraph of only C . Show how you would construct X , Y , Z such that the corresponding embeddings satisfy $z_X \preceq z_Y$ and $z_X \preceq z_Z$. You do not have to specify the embedding coordinates, but just the subgraph relationships between X, Y, Z and A, B, C . Please show why your example satisfies this condition.

(Note that this condition implies that X is a common subgraph of Y and Z . However, one can construct actual example graphs of A, B, C, X, Y, Z such that X is not a common subgraph of Y and Z . This proves that 2-dimensional order embedding space cannot perfectly model subgraph relations. Hence in practice we use high-dimensional order embedding space. For this question, you do not have to show such example graphs.)

Important Clarifications for Q2.5:

1. Without loss of generality, suppose $z_A[0] > z_B[0] > z_C[0]$.
2. The example graphs X, Y, Z can be constructed such that each of which is a common subgraph of exactly one, two or three graphs in $\{A, B, C\}$.
3. Your answer to construct X, Y, Z should ****guarantee**** that the condition $z_X \preceq z_Y$ and $z_X \preceq z_Z$ assuming order embedding constraint is satisfied and that we are using 2-dimensional order embedding.
4. You do not have to draw the actual graphs of X, Y, Z . Just specify X, Y, Z are subgraphs of which graphs in $\{A, B, C\}$, and provide the reasoning for why the condition has to be true for your construction.

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!******