

# Homework3

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## 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.

### 1 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.

#### Solution

We have a bijective map  $f_1$  such that  $\{f_1(v)|v \in V_A\}$  is a subgraph of B and graph-isomorphic to A. We also have a bijective map  $f_2$  such that  $\{f_2(v)|v \in V_B\}$  is a subgraph of C and graph-isomorphic to B. So  $f_2 \circ f_1$  is a bijective map and  $\{(f_2 \circ f_1)(v)|v \in V_A\}$  is a subgraph of C and graph-isomorphic to A.



## 2 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?

### Solution

For A to be a subgraph of B we must have  $|A| \leq |B|$ . Simultaneously for B to be a subgraph of A we must have  $|B| \leq |A|$ , therefore  $|A| = |B|$ . by using the subgraph isomorphism definition from above we have that there exist a bijective map  $f$  such that  $\{f(v)|v \in V_A\}$  is isomorphic to A and a subgraph of B, with the same number of nodes as B, i.e.  $\{f(v)|v \in V_B\}$  is B.



## 3 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.

### Solution

For X to be a subgraph of A we must have  $z_X \preceq z_A$  and for X to be a subgraph of B we must have  $z_X \preceq z_B$ . For X to be a common subgraph we must have  $z_X \preceq z_A$  and  $z_X \preceq z_B$ , i.e  $z_X \preceq \min\{z_A, z_B\}$ .



## 4 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?

### Solution

In order to have a subgraph we must have that  $z_X[i] \preceq_Y[i] \forall i$ . We know that they are not subgraphs of each other so relation between  $z_A[1]$ ,  $z_B[1]$ ,  $z_C[1]$  must



contradict this, hence  $z_A[0] < z_B[0] < z_C[0]$



## 5 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.

### Solution

A, B and C are not subgraphs of each other and  $z_A[0] > z_B[0] > z_C[0]$  and  $z_A[1] < z_B[1] < z_C[1]$ . If we construct X, Y and Z such that Y and Z are subgraphs of B and X is a subgraph of A, B and C. Then  $z_B[0] > z_Y[0] > z_C[0]$ ,  $z_B[0] > z_Z[0] > z_C[0]$ ,  $z_A[1] < z_Y[1] < z_B[1]$  and  $z_A[1] < z_Z[1] < z_B[1]$ . For X,  $z_X[0] < z_C[0]$  and  $z_X[1] < z_A[1]$ . That guarantee that  $z_X[0] < z_Y[0]$ ,  $z_X[0] < z_Z[0]$ ,  $z_X[1] < z_Y[1]$  and  $z_X[1] < z_Z[1]$ . So  $z_X \preceq z_Y$  and  $z_X \preceq z_Z$ .

