CS224W-Homework 2 Solutions

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February 2022

1 GCN

1.1

The following two graphs are isomorphic, which we demonstrate by showing a 1-to-1 correspondence between the nodes.
1 - A, 2 - D, 3 - H, 4 - E, 5 - B, 6 - C, 7 - G, 8 - F

1.2

Assume that the two graphs both have three nodes of labelled v_1, v_2 and v_3. In both graphs, edges exist between v_1, v_2 and v_1, v_3. Each node has feature of 1. If we use the sum and mean aggregator on both v_1 nodes, the result would be the same since $aggregate_{mean}(1,1) = 1 = aggregate_{max}(1,1)$. However $aggregate_{sum}(1,1) = 1 + 1 = 2$

1.3

Proof:
Assume that the WL test cannot decide whether G_1 and G_2 are isomorphic at the end of K'th iteration. Let $G_1 = (V_1, E_1) and G_2 = (V_2, E_2)$. According to our assumption, we have:

$$\{l_v^{(K)}, \forall v \in V_1\} = \{l_v^{(K)}, \forall v \in V_2\}$$

Therefore,

$$HASH(l_v^{(k-1)}, \{l_u^{(k-1)}, \forall u \in N(v)\}), \forall v \in V_1 = HASH(l_v^{(k-1)}, \{l_u^{(k-1)}, \forall u \in N(v)\}), \forall v \in V_2$$

The hash function is an injective function on a set, so we have

$$l_v^{(K-1)}, \forall v \in V_1 = l_v^{(K-1)}, \forall v \in V_2$$

and

$$\{l_u^{(k-1)}, \forall u \in N(v), v \in V_1\} = \{l_u^{(k-1)}, \forall u \in N(v), \forall v \in V_2\}$$

This means that

$$combine(l_v^{(K-1)}, aggregate(\{l_u^{(k-1)}, \forall u \in N(v), v \in V_1\}))$$

is equal to

$$combine(l_v^{(K-1)}, aggregate(\{l_u^{(k-1)}, \forall u \in N(v), v \in V_2\}))$$

Therefore

$$readout(\{h_v^{(K)}, \forall v \in V_1\}) = readout(\{h_v^{(K)}, \forall v \in V_2\})$$

Contradiction! Therefore the assumption is false, meaning that the *Weisfeiler-Lehman* test also decides that the two graphs are different.

2 Node Embeddings with TransE

2.1

Assume there are 3 nodes of A, B and C. A is connected to B and C with the same relationship vector of $l = (0, 0)$. The embedding vector learned by TransE for A, B, C would all be the same, minimizing the loss function to zero.

$$\mathcal{L} = d(v_a + l, v_b) + d(v_a + l, v_c) = 0$$

However, $d(v_b + l, v_c) = 0$. B and C does not have the l relationship in between. Therefore the embeddings would be useless.

2.2

The example for the previous question also works here because

$$\mathcal{L} = d(v_a + l, v_b) + d(v_a + l, v_c) - d(v_b + l, v_c) = 0$$

B and C would also have the l relationship according to the embeddings but in fact they do not have the l relationship.

2.3

The algorithm would artificially increase the entity norms of the negative(corrupted samples) to minimize the loss function, resulting in the embedddings of the corrupted nodes much larger than others.

2.4

The type of relations that TransE cannot model are symmetric but not reflexive. Wang et al. 2019 mentions that since

$$d(i,l,j) + d(j,l,i) \leq -||e_i + 0 - e_j|| + ||e_j + 0 - e_I||$$

the TransE algorithm would push the embeddings e_i, e_j to be similar and the relation l to be zero. However$d(i,l,i)$ would also be small that we would consider the relation to be reflexive.

3 Expressive Power of Knowledge Graph Embeddings

3.1

TransE cannot model symmetric relations because if $a + l = b$, we cannot make $b + l = a$ unless $l = 0$.
TransE can model inverse relations since $a + l = b$ we can make the inverse to be $-l$ and $b + (-l) = a$.
TransE cannot model composition because if we make $l_{aunt} = l_{father} + l_{sister}$, we also have $l_{aunt} = l_{sister} + l_{father}$. Father's sister and sister's father would both be recognized as aunt.

3.2

RotateE can model symmetric relations, we can make the rotate angle $l = \frac{\pi}{2}$, therefore if $A \circ l = B$, we have $B \circ l = A$
RotateE can model inverse relations with any arbitary angle besides π RotateE cannot model composition because if we make $l_{aunt} = l_{father} + l_{sister}$, we also have $l_{aunt} = l_{sister} + l_{father}$. Father's sister and sister's father would both again be recognized as aunt.

3.3

RotateE cannot model inreflexive relations because if A and A itself have some kind of relation, so does any node with any node itself, therefore the relation would be reflexive. TransE also fails in this case.

References

Wang, Yanjie et al. (Aug. 2019). "On Evaluating Embedding Models for Knowledge Base Completion". In: *Proceedings of the 4th Workshop on Representation Learning for NLP (RepL4NLP-2019)*. Florence, Italy: Association for Computational Linguistics, pp. 104–112. DOI: 10.18653/v1/W19-4313. URL: https://aclanthology.org/W19-4313.