Appendix

This document complements the article entitled "Embedding Knowledge Graphs Attentive to Positional and Centrality Qualities". In particular, it provides the reader with proof of Proposition 1 and the hyperparameters settings.

A Proof of the proposition from Section 3.1 about the non-existence of g

Reminder of the proposition:

For position attentive networks, we know (You *et al.* [1]) that there exists a mapping g that maps structure-based embeddings $f_sq(v_i)$, $\forall v_i \in V$ to position attentive embeddings $f_p(v_i)$, $\forall v_i \in V$, if and only if no pair of nodes have isomorphic local q-hop neighbourhood graphs.

This proposition <u>does not hold</u> for centrality attentive embeddings.

Proof. If no pair of nodes have isomorphic local q-hop neighborhood graphs, it is still possible for them to have the same centrally attentive embeddings. To show that, it is enough that two nodes have the same centrally value in the graph: for example, for degree centrality, when the two nodes have the same number of neighbors, that are consisting of different nodes, their neighborhoods are non-isometric; however, they have the same degree centrality.

Therefore $f_p(v_i)$ can not be a function of $f_{st}(v_i)$, and the two pairs of nodes would have different structure-aware node embeddings while their centrally attentive embeddings are equal.

References

 You, J., Ying, R., Leskovec, J.: Position-aware graph neural networks. In: ICML. (2019) 7134–7143

B Hyperparameters Settings

We list the best hyperparameters setting of GPA-NN on the benchmark datasets in Table 1. The learning rate in all the experiments is fixed to 0.0005, adversarial temperature for negative sampling is fixed to 2.5, and ψ , the dividend for the score aggregation in $f_{1\times 1}$ is fixed to 14.

Dataset	Dimension	Batch size	# neg	#iterations
WN18RR	400	300	800	100000
FB15K-237	1000	1000	200	200000
OGBL-BIOKG	400	600	850	700000
WN18RR- v_3 -IND	300	1000	200	30000
WN18RR- v_4 -IND	200	1400	10	30000
NELL-995- v_1 -ind	200	300	600	20000
NELL-995- v_4 -ind	200	1000	700	20000

Table 1. Best hyperparameters setting of GPA-NN on the benchmark datasets.