

ASSIGNMENT SET XII

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02/11/2020

Assignment 12 of
Deep Learning Course Given by
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written in L^AT_EX

Exploring GNNs on Different Tasks

In this assignment I have developed two models each for a different task (node classification and graph classification). In both models we generate a hidden representation h_u for each node u and we use these node embeddings in downstream tasks e.g. node classification.

0.1 GNNs Applied to The Cora Dataset

For Cora dataset, I have adopted the straightforward method of classification. Performance of the GNNs monitored as a function of the GNN depth. Figure 1 shows how the Cora dataset looks like and Figure 2 shows the performance of a GNN with given depth. As a counter-intuitive result, we see fluctuations at higher depths.

0.2 GNNs Applied to The Enzymes Dataset

Enzymes dataset turned out to be much more complex as a graph classification problem. I used the following formula as the bridge between graph embedding and node embedding methods:

$$z_G = \frac{\sum_{u \in G} z_u}{|V_G|}$$

I gradually increased the model complexity to perform better on this task but I did not find satisfying results. However the final model deserves a quick review. The final architecture is shown in Figure 3.

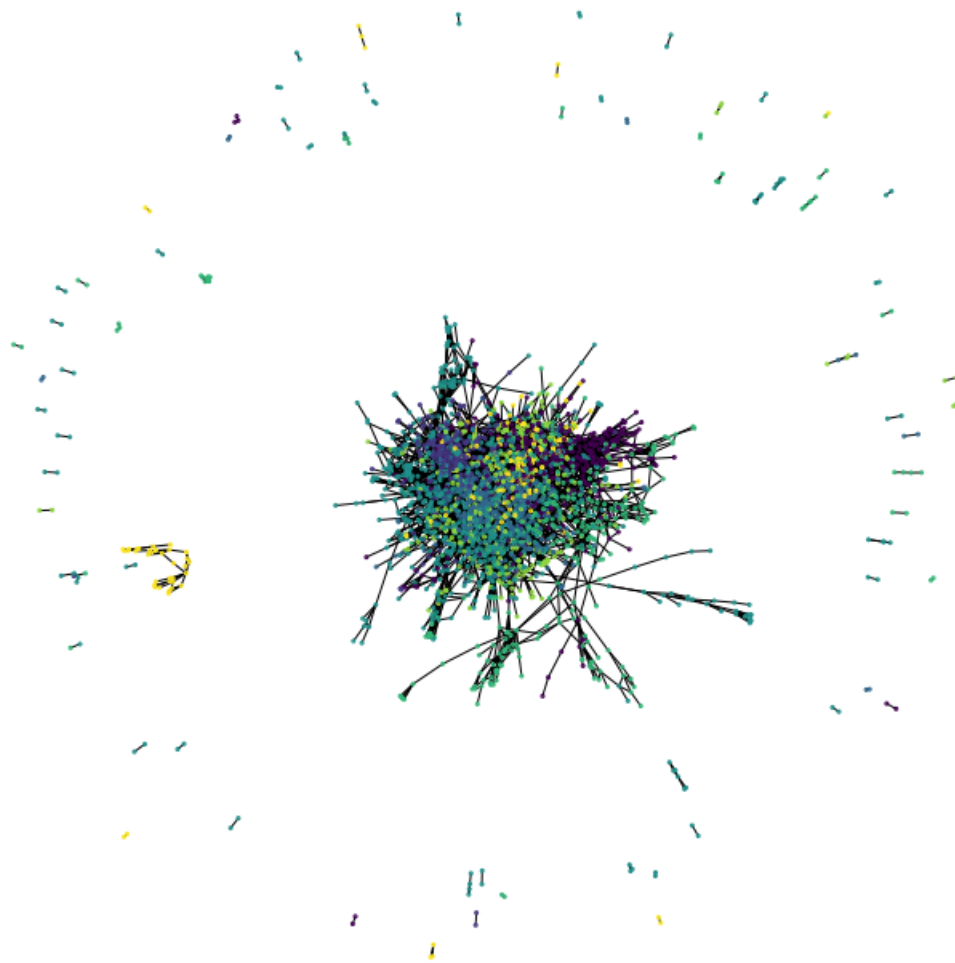


Figure 1: Cora dataset visualized using Networkx package. Colors shows the class to which a given node belongs.

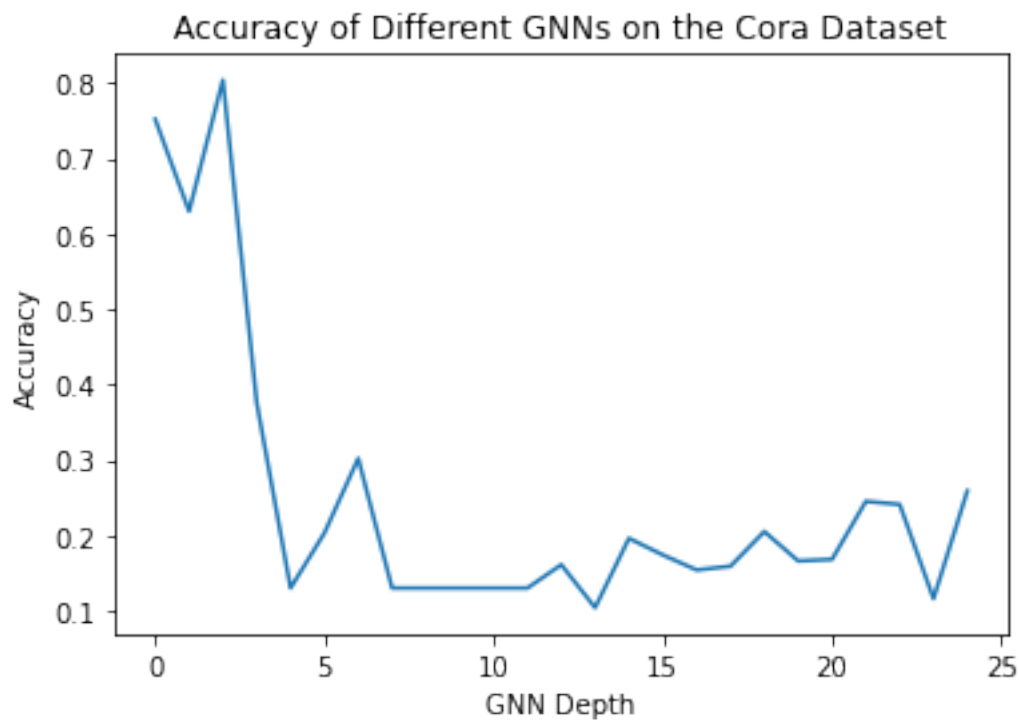


Figure 2: A three layer GNN performs better than all depths on Cora dataset. The performance drops dramatically for GNNs having more than three layers (which indicates the over-smoothing behaviour) and fluctuates for very deep versions.

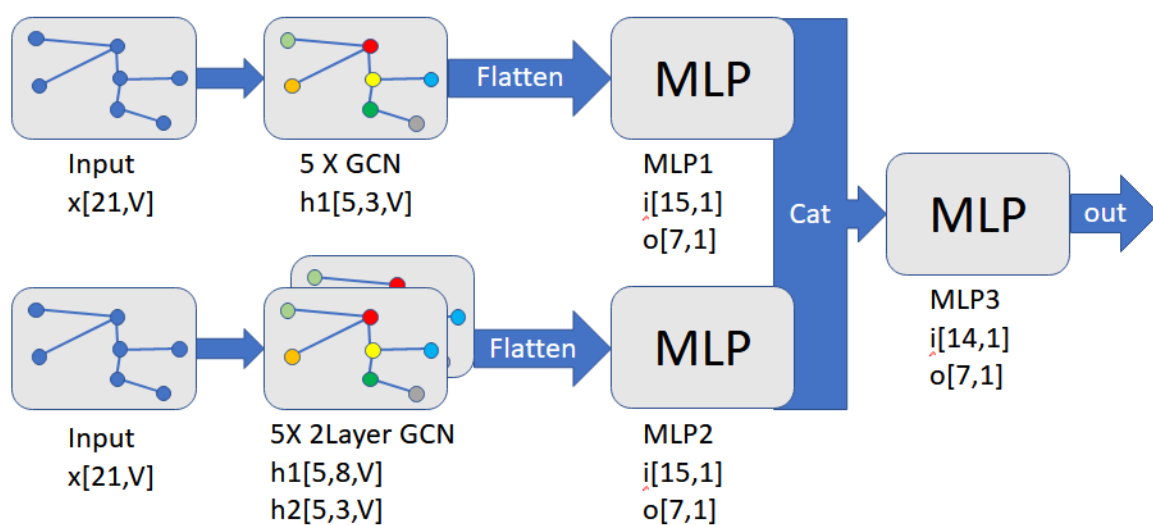


Figure 3: Final architecture of EnzymeNet model that is not powerful enough to capture the complexity of enzyme classification.