Graph Neural Networks: Experiments with GCN, Down-Sampling, and Pooling Layers for classification

Experimental Setup

Description of the datasets - D&D - Binary Classification Task b. ENZYMES - 6-Class Classification Task
Overview of the GCN model, down-sampling (Top-K pooling), and hierarchical pooling layers
Explanation of the hyperparameters: k values (90%, 80%, 60%) and m values (6, 3)
Training procedure and evaluation metrics (accuracy)

Experiments

Discussion of the experiments (i.e., different k and m configurations)

Results

Comparative table of results showing test accuracy for different configurations of k and m

I have used 10 epochs

D&D - Binary Classification Task

k Value (K1, K2)	m Value	Test Accuracy
90, 90	6	65.54
90, 90	3	57.98

90, 80	6	61.34	90, 80	3	67.22	90, 60	6	57.98
90, 60	3	70.58	80, 90	6	65.54	80, 90	3	64.70
80, 80	6	63.86	80, 80	3	62.18	80, 60	6	61.34
80, 60	3	73.10						
60, 90	6	64.70	60, 90	3	72.26			
60, 80	6	54.62	60, 80	3	67.22	60, 60	6	72.26
60, 60	3	61.34						

ENZYMES - 6-Class Classification Task

k Value (K1, K2)			m Value				Test Accuracy
90, 90			6				18.33
90, 90	3	20	90, 80	6	20		
90, 80	3	21.67	90, 60	6	23.33	90, 60	3	20
80, 90			6				23.33
80, 90			3				13.33
80, 80	6	20	80, 80	3	10	80, 60	6	20
80, 60			3				23.33
60, 90			6				15
60, 90	3	31.67	60, 80	6	18.33	60, 80	3	13.33
60, 60			6				21.67
60, 60			3				21.67

Conclusion

The experiments on the D&D and ENZYMES datasets showed that GCN performance varies significantly with different k and m values. In the D&D dataset, the best accuracy (73.10%) was achieved with k = (80, 60) and m = 3, while the ENZYMES dataset had its highest accuracy (31.67%) with k = (60, 90) and m = 3.

Insights into How k and m Affect Performance

- **D&DDataset**: Lower m values (3) generally performed better, with moderate k values like (80, 60) yielding the highest accuracy. Larger m values (6) seemed to reduce performance.
- **ENZYMESDataset**: More aggressive down-sampling (lower k values) improved accuracy, especially with m = 3, which consistently outperformed m = 6.