GNN report

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1 Data and features

We use the denominator graph edges $7, 8, 9, 10, 11$ loops as well as their corresponding coefficients to train a GNN on binary classification. The coefficient is either 1 or 0, depending on whether there is a numerator completion of the graph that contributes to the correlator. We input various features (as node features) into the model and see which lead to the best performance. The whole list of features considered follows

1. Columns of the adjacency matrix
2. Columns of identity matrix
3. Laplacian eigenvectors with the 3 biggest eigenvalues
4. degree
5. betweenness
6. clustering
7. pagerank
8. closeness
9. face count

Eventually features $3 - 9$ were the most expressive for the GNN.

2 Runs and results

2.1 GIN

In terms of the architecture, we almost exclusively work with a simple GINN (Graph Isomorphism Neural Network). This ensures that the model will treat equally graphs that are isomoprhic. However it might still fail to distinguish between non-isomorphic graphs that cannot be distinguished by the 1-WL graph isomorphism test. This makes it as expressible as the 1-WL test. The architecture is expected to be ideal for graph level tasks with few nodes.

Based on features 3-9 we trained and tested the model for graphs of various loop orders. Since we deal with binary classification, the choice of a threshold affects heavily whether a graph will be identified with 0 or 1. Therefore, we present the ROC AUC and PR AUC metrics which are threshold independent. ROC AUC is the area under the curve of true positive rates (TPR) and false positive (FPR) rates, for different thresholds. These are defined as:

$$\mathrm{TPR} = \frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FN}}, \qquad \mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{FP}+\mathrm{TN}} \tag{1}$$

The value ROC AUC can be interpreted as follows: It gives the probability of a classifier to rank a randomly chosen denominator graph that contributes (coefficient=1) higher than one that does not contribute (coefficient=0).

With the increase in the number of loops however, most of the graphs at hand do not contribute. For instance at 11-loop just 10 % of the graphs have coefficient 1. In this case FPR becomes very small, since there are many TN resulting in an artificially large FPR. To overcome this problem we use PR AUC. This computes the area under the precision-recall curve for different thresholds. These are defined as[1]

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}, \qquad \text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} \tag{2}$$

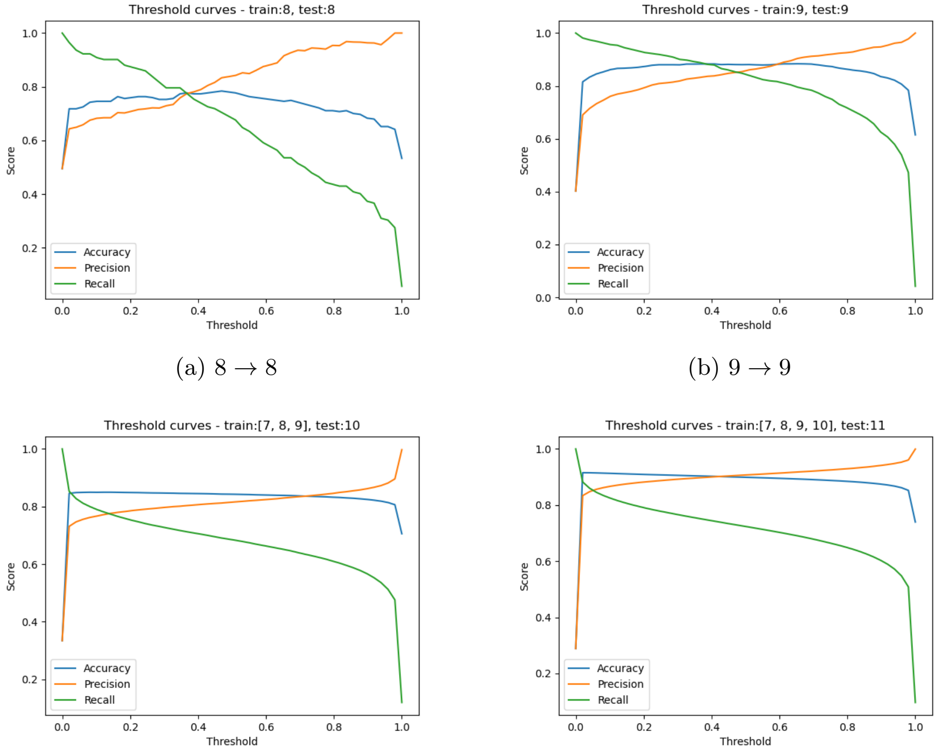
Note that since we are mostly interested in minimizing FN while FP are not a problem, the performance of the model on an unbalanced set (negatives dominate) is better described by PR AUC. The reason is that these metrics focus on the minority class (TP,FN,FP) only.

Next follows a table with our findings. We use a 80-20 split for training and testing and run over 100 epochs. Moreover, the single loop runs are performed with 3 layers of 64 hidden channels. Then for testing on 10 loops we used 256 hidden channels and finally for testing on 11 loops we chose 512 hidden channels. Finally, the following choices have been made: learning rate: 0.0003, weight decay: 0.00003, dropout: 0.3.

Table 1: Experimental Results GIN

ROC/PR AUC (%)	8 → 8	9 → 9	7,8,9 → 10	7,8,9,10 → 11
train	96.0/96.2	98.4/97.7	99.0/98.9	99.9/ 99.7
test	85.8/86.2	95.8/93.9	92.6/86.4	97.2/ 93.2

Additionally we present the behaviour of accuracy, precision and recall for different thresholds and for different experiments below.



(a) $8 \to 8$

(b) $9 \to 9$

(c) $7, 8, 9 \to 10$

(d) $7, 8, 9, 10 \to 11$

Figure 1: Accuracy, Precision and Recall as functions of the threshold for the GIN experiments.

[1] In our application we are interested in reducing the ansatz for the correlator, therefore including extra graphs in the ansatz that eventually do not contribute (recall on 0) is not as bad removing graphs that eventually contribute to the ansatz (recall on 1). Thus, instead of using ROC AUC and PR AUC we can optimize the threshold to maximize the recall on 1's.

As a reminder the accuracy is defined by,

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{P} + \text{N}}. \tag{3}$$

As expected, Accuracy is not affected at all while Recall and Precision swap roles.

2.2 PlanE

Additionally we studied the performance of the model described in `https://arxiv.org/abs/2307.01180` on our dataset. This is representation learning model on planar graphs. It takes as input the graph structure and possible node or edge features. Based on these, it determines a representation through certain decompositions on the planar graph (BLOCKCUT, SPQR). The authros claim that any pair of graphs with V_1, V_2 number of vertices can be distinguished by a variant of their model with at most $\log_2(\max\{|V_1|, |V_2|\}) + 1$ layers.

Training for 50 epochs on a 80/10/10 split for training test and validation using 4 layers of 64 dimensions produced [2]:

Table 2: Experimental Results PlanE

ROC AUC (%)	7 → 7	8 → 8	9 → 9
train	96.0	94.0	99.0
test	87.3	78.8	85.5
valid	87.3	79.4	85.3

It turns out that for our dataset PlanE does not perform significantly better at least for single loop cases. Given the much higher training time required for this model compared to our GIN we did not test on further cases.

[2] These are lower loop cases where PR AUC and ROC AUC are not expected to differ much.