Navigating the *explainable* Molecular Graph:
Best Practices for Representation Learning in Bioinformatics

Supplementary Materials

I. Experiments

In this section, we detail the performance of the GNN models (`GCN`, `GIN`, and `GAT`) and graph embedding methods (`Node2Vec` + NN, `SDNE` + NN, and `HOPE` + NN) described in Section *Method* on the datasets `HIV`, `Bace`, `BBBP`, and `Clintox`. For each method and dataset, we provide the corresponding confusion matrix, offering a visual representation of the performance. In these 2×2 matrices, the rows represent the *actual* classes, and the columns represent the *predicted* classes. The value C_{ij} indicates the number of samples belonging to class i that were classified as class j. The confusion matrix evaluates model performance in binary classification, giving an overview of each class's accuracy. In our results, high values along the main diagonal indicate good classification ability.

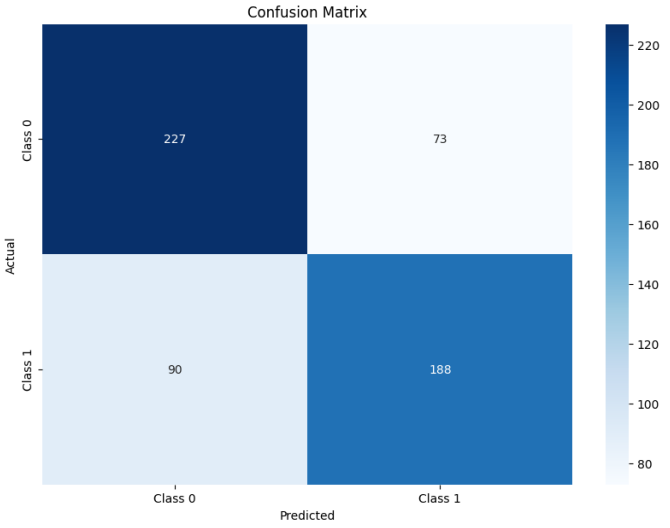

Fig. 1. Confusion Matrix of `GCN` model on the `HIV` dataset

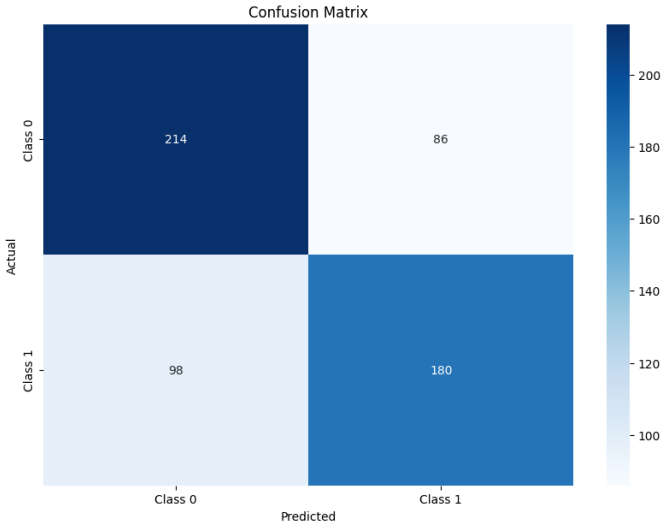

Fig. 2. Confusion Matrix of `GIN` model on the `HIV` dataset

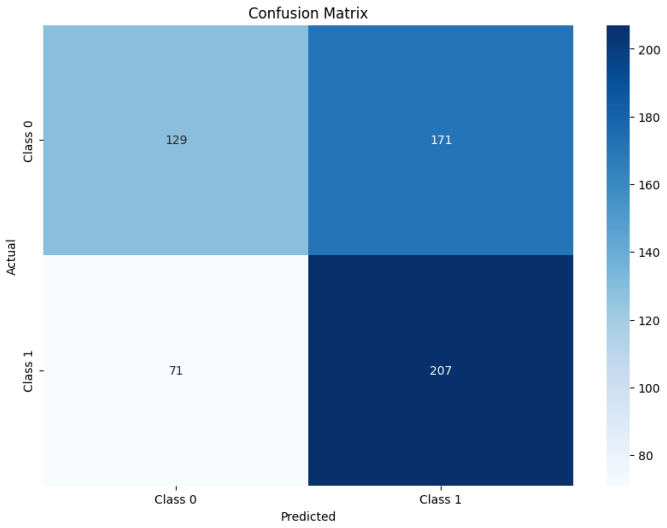

Fig. 3. Confusion Matrix of `GAT` model on the `HIV` dataset

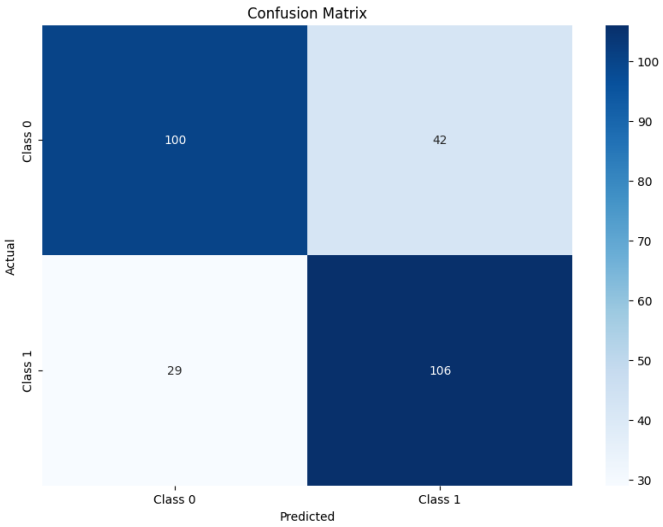

Fig. 4. Confusion Matrix of GCN model on the BACE dataset

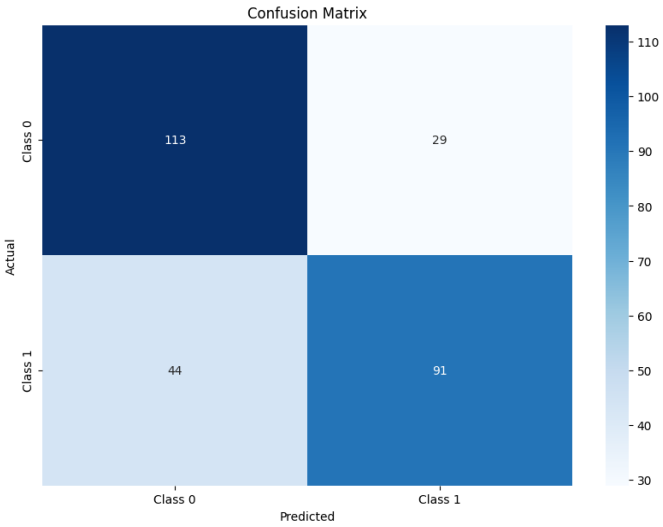

Fig. 5. Confusion Matrix of GIN model on the BACE dataset

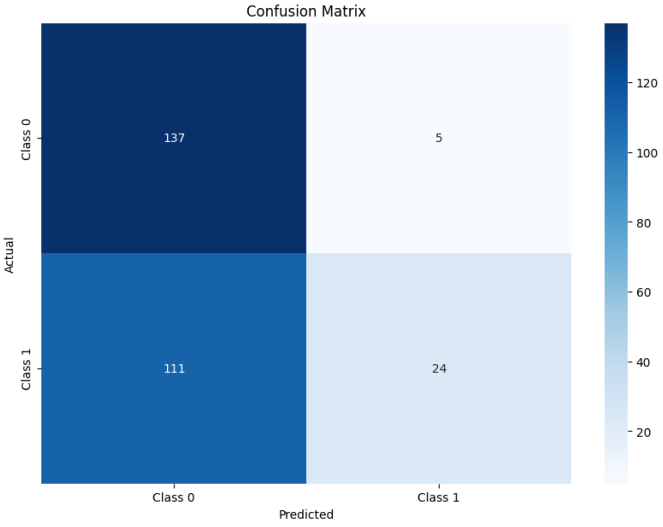

Fig. 6. Confusion Matrix of GAT model on the BACE dataset

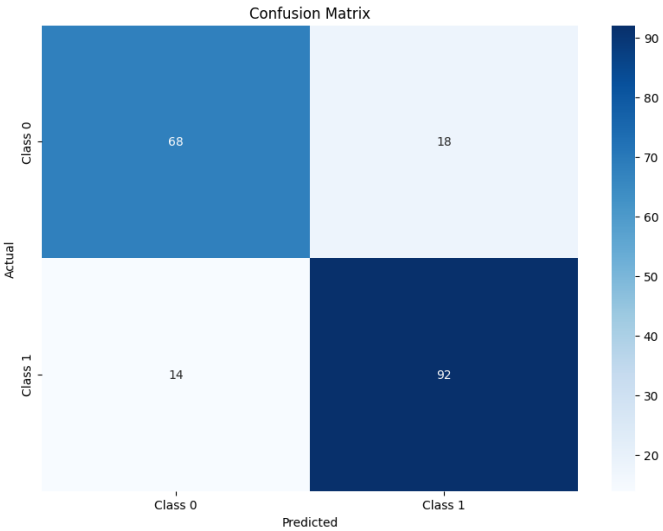

Fig. 7. Confusion Matrix of GCN model on the BBBP dataset

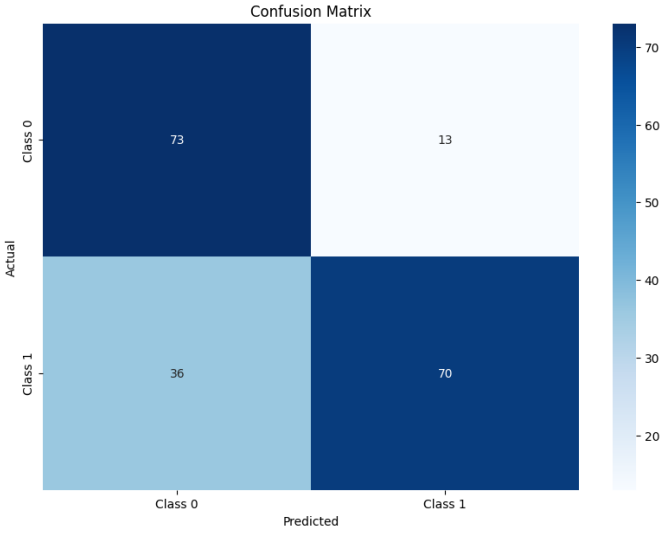

Fig. 8. Confusion Matrix of GIN model on the BBBP dataset

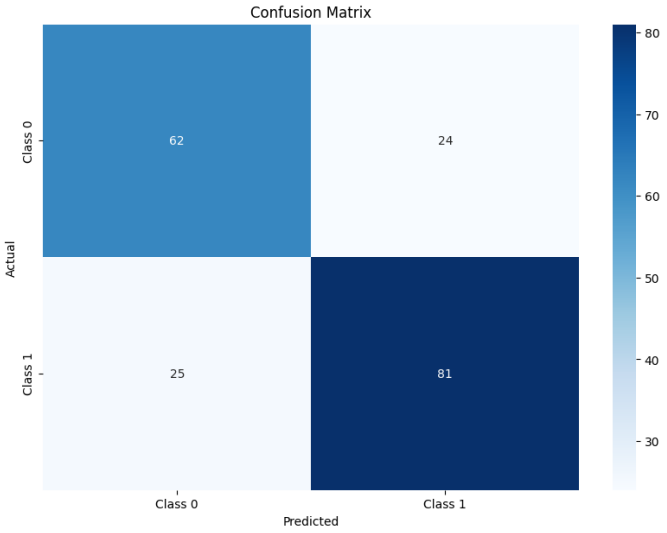

Fig. 9. Confusion Matrix of GAT model on the BBBP dataset

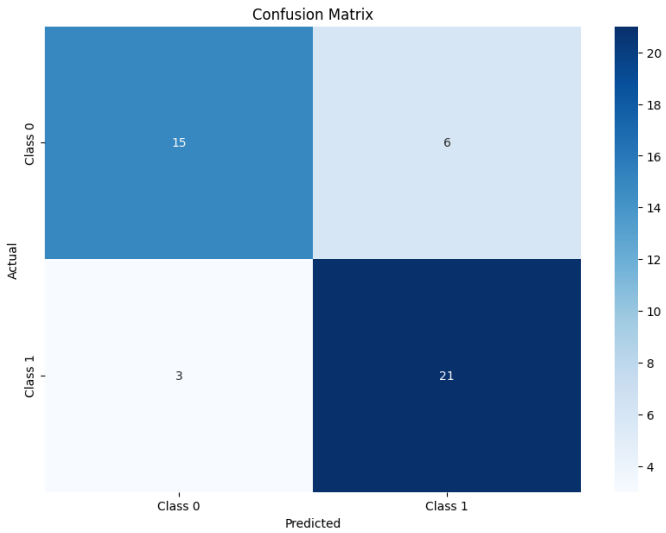

Fig. 10. Confusion Matrix of GCN model on the Clintox dataset

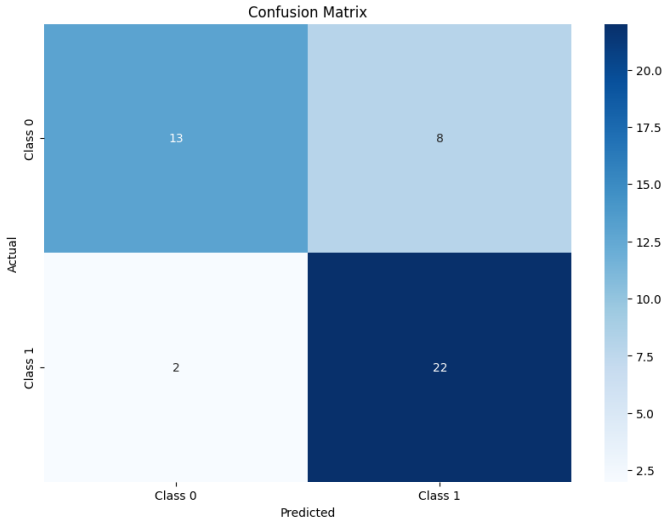

Fig. 11. Confusion Matrix of GIN model on the Clintox dataset

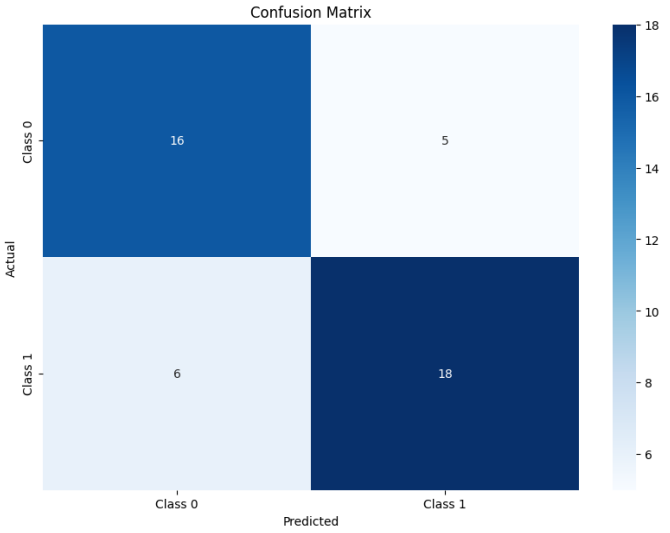

Fig. 12. Confusion Matrix of GAT model on the Clintox dataset

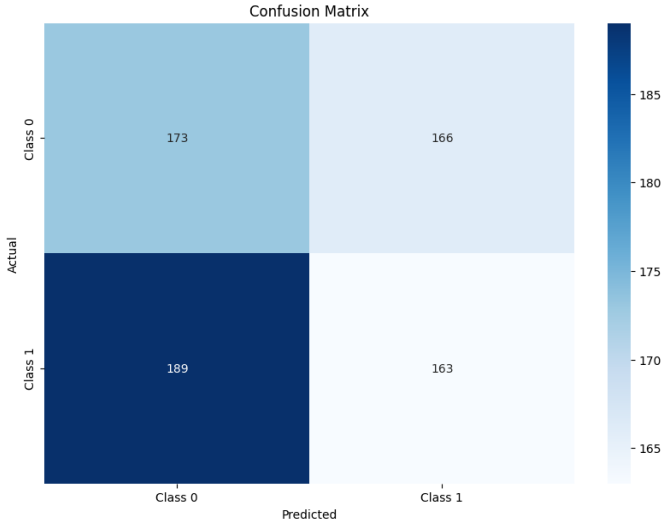

Fig. 14. Confusion Matrix of SDNE Embedding model combined with *Fully Connected Neural Network* model on the BACE dataset

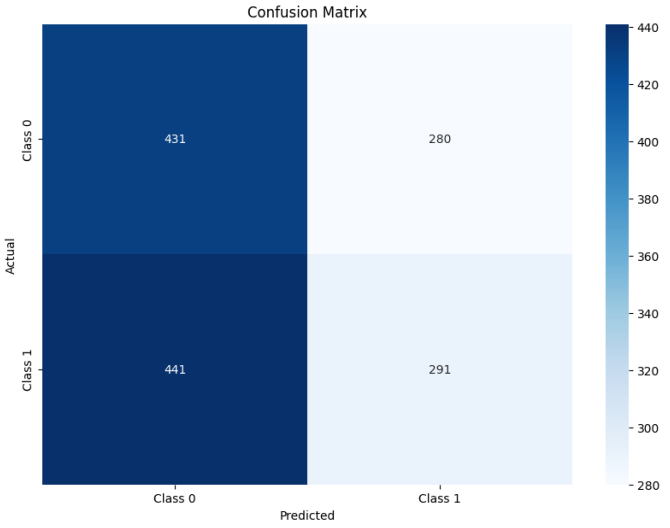

Fig. 13. Confusion Matrix of SDNE Embedding model combined with *Fully Connected Neural Network* model on the HIV dataset

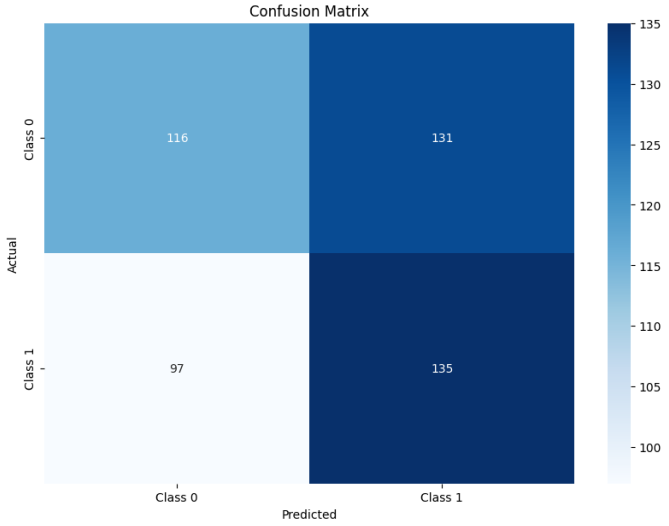

Fig. 15. Confusion Matrix of SDNE Embedding model combined with *Fully Connected Neural Network* model on the BBBP dataset

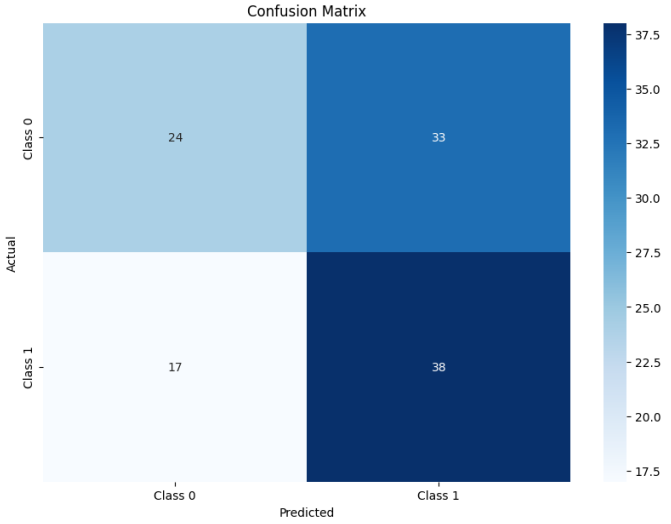

Fig. 16. Confusion Matrix of SDNE Embedding model combined with *Fully Connected Neural Network* model on the CLINTOX dataset

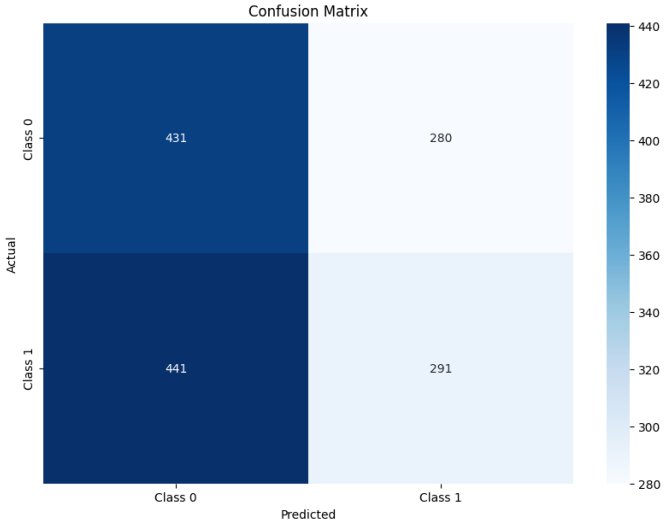

Fig. 17. Confusion Matrix of HOPE Embedding model combined with *Fully Connected Neural Network* model on the HIV dataset

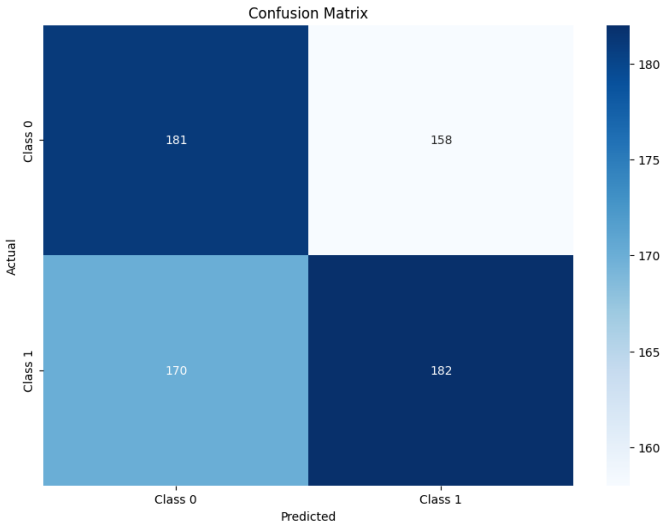

Fig. 18. Confusion Matrix of HOPE Embedding model combined with *Fully Connected Neural Network* model on the BACE dataset

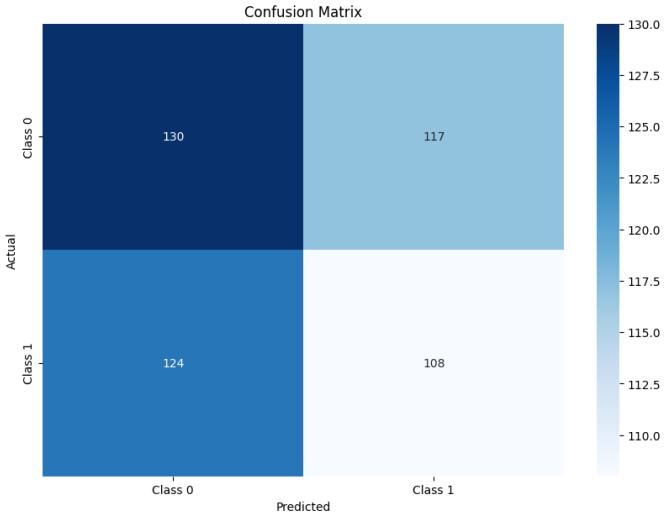

Fig. 19. Confusion Matrix of HOPE Embedding model combined with *Fully Connected Neural Network* model on the BBBP dataset

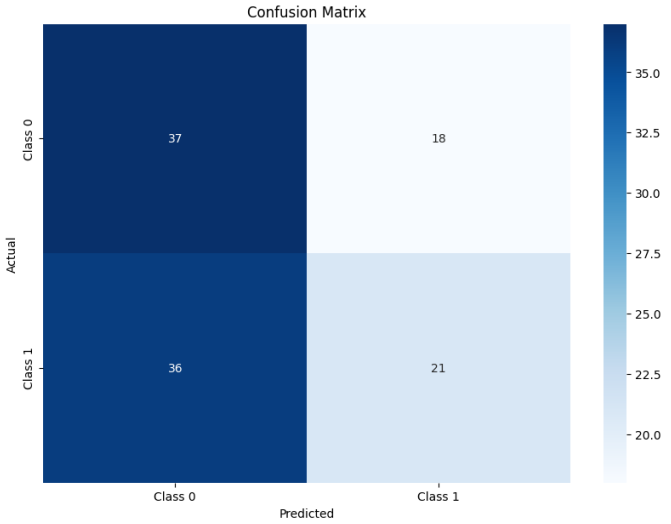

Fig. 20. Confusion Matrix of HOPE Embedding model combined with *Fully Connected Neural Network* model on the CLINTOX dataset

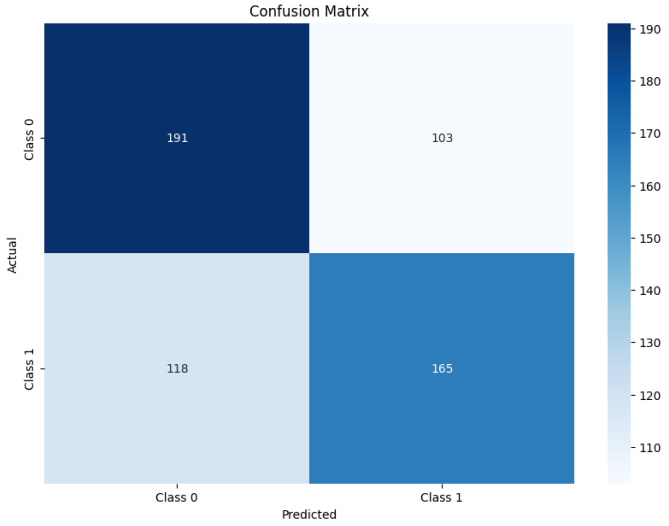

Fig. 22. Confusion Matrix of Node2Vec Embedding model combined with *Fully Connected Neural Network* model on the HIV dataset

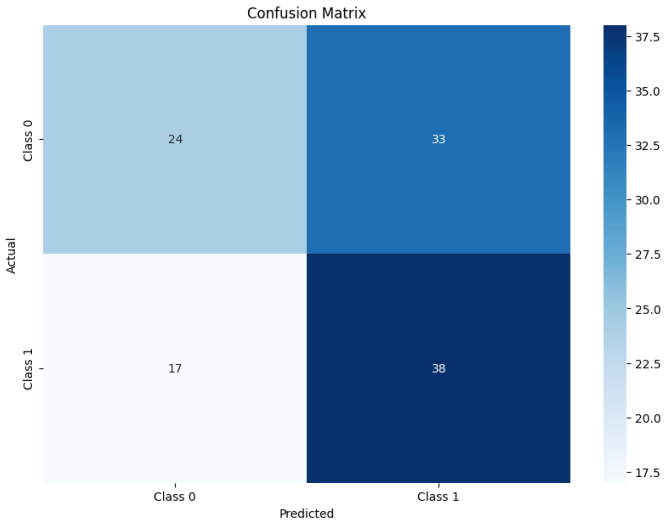

Fig. 21. Confusion Matrix of SDNE Embedding model combined with *Fully Connected Neural Network* model on the CLINTOX dataset

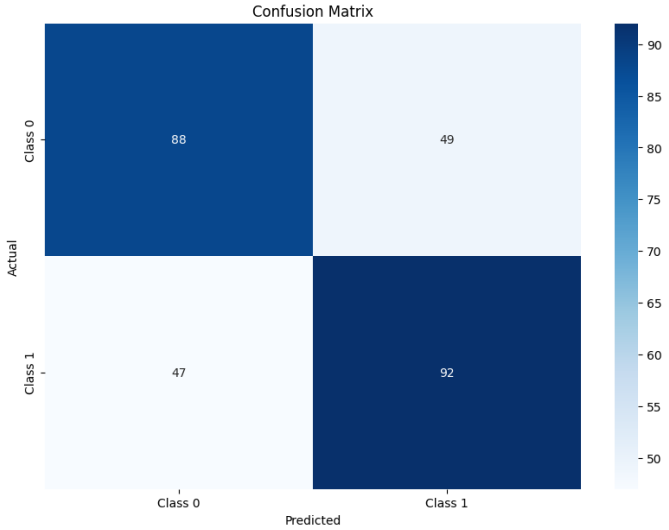

Fig. 23. Confusion Matrix of Node2Vec Embedding model combined with *Fully Connected Neural Network* model on the Bace dataset

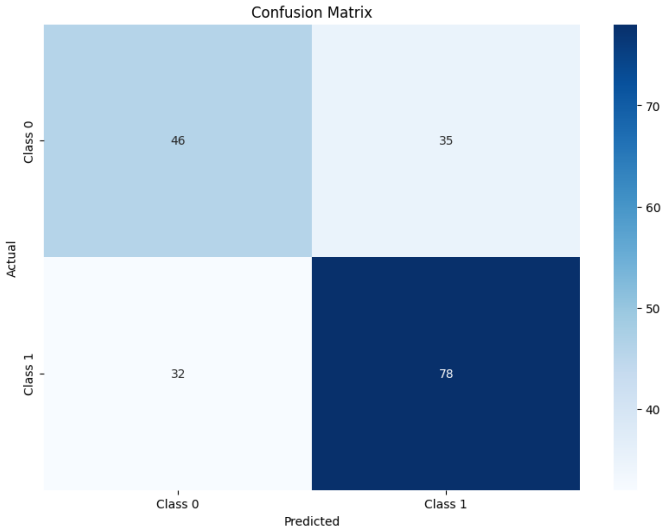

Fig. 24. Confusion Matrix of `Node2Vec` Embedding model combined with *Fully Connected Neural Network* model on the `BBBP` dataset

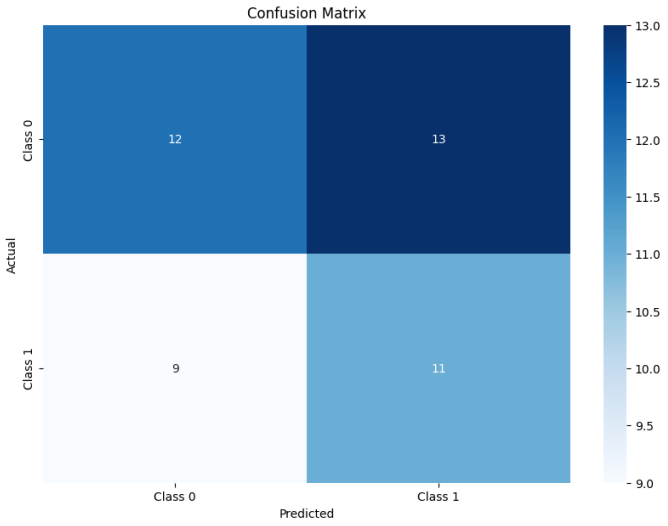

Fig. 25. Confusion Matrix of `Node2Vec` Embedding model combined with *Fully Connected Neural Network* model on the `Clintox` dataset