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Drug-Drug Interactions Predictions Using BiLSTM

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Abstract: ***Various methods are innovated in the field of bioinformatics and drug discovery. The recent papers on drug discovery [23,25], insisted many ideas to the researchers of that field. In the field of drug discovery, ANN plays a vital role to differentiate drug discovery, Machine Learning and Deep Learning. These methods were used to predict interactions between D-D, T-T, D-T means Drug-Drug, Target-Target, Drug-Target interactions. In Machine Learning prediction is made by use of the Multilayer Perceptron, Decision Trees, Random Forest, Support Vector Machines and Naïve Bayes methods. In the other hand, Deep Learning make use of LSTM (Long Short Term Memory), GRUs and Transformers. Among all the methods, we are planned to implement BiLSTM with RDkit to predict the interactions between any two drugs.***
Keywords: Deep Learning, Drug-Drug interactions, BiLSTM.

I. INTRODUCTION

To understand the basics of the neural networks, graph neural networks, graph representation learning and deep learning we have referred the following books [1-9]. DDI Net model is utilized to predict the DDI Interaction in a sequential learning architecture in [10]. Graph convolutional network with fully connected layers is used for binary classification of toxicity in [11]. MPNN based GAT is used for Drug-Drug interaction prediction in this comprehensive review [12]. The AI technology on black box models and other AI are utilized in this paper [13] of drug discovery. A substructure aware graph neural network using Graph Self Adaptive Pooling and a substructure aware interaction module incorporating relation features(RSAM) and GSP-DMPNN is used for Drug-Drug interactions in [14]. A simple but effective model is discussed not only for DDI but also for DDA in [15]. GNN-MGSEP means Graph Neural Network Molecular graph side effect prediction is constructed for drug effect interaction prediction in [16]. In the survey paper of [17], a broad review of deep learning algorithms for modelling drug interaction is discussed clearly. In [18], similarity based Support Vector Machine is used for prediction process. However, wastage of a large number of unselected negative samples remain the same. In [19], SSF-DDI is discussed for deep learning prediction of drug interactions. It shows that using inductive setting is more challenging than the transductive setting. A BiLSTM is used for side effect prediction in [20]. Protein-Protein or drug interactions using graph neural networks is discussed in [21,24]. DPDDI deep predictor for drug-drug interactions are used in [22].

II. MATERIALS AND METHODS

In this phase we discussed the data and methodologies used in this paper. In 2.1, we discuss about the datasets, and in 2.2, we discuss about experimental process, section 3 presents the experimental results.

A. Dataset Construction

In this work, we have collected the dataset from the drug bank. By using the SMILES notation and the UNIQUE ID and name of the chemical structure of the respective drugs/targets/proteins we are going to utilize only two drug/target/protein. In this paper, we have selected two drugs among the list of database. By using that respective two drug we have planned to do prediction by using the deep learning model. i.e., splitting any two required drugs/targets/ proteins from the entire databases.

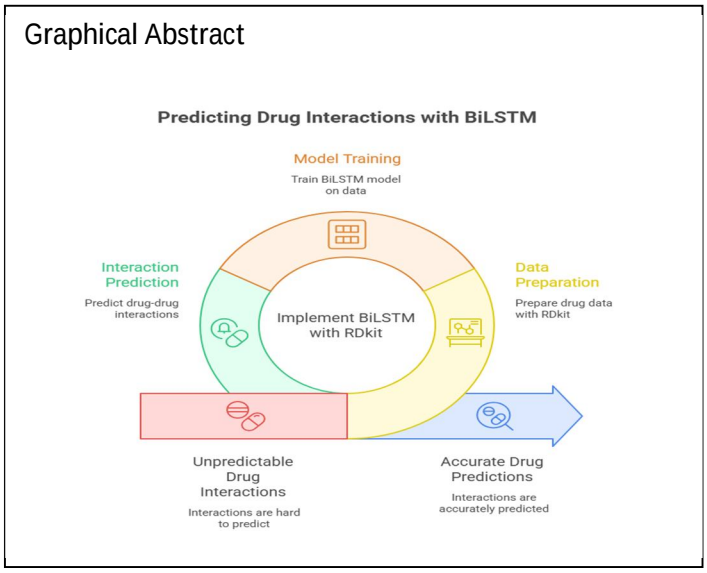
B. Experimental Setup

We have planned to make use of Blood Brain Barrier Penetration datasets from the drug bank database. After fetching the CSV file named BBBP, we have seperated two drug among the entire dataset. The two drug A and B were discussed with two different drug/chemical name/unique id and chemical structures from SMILES notation. First of all, we load the csv file in the python code to get few rows and to get the basic information about the entire dataset. After viewing basic information, we have collected two drugs and their SMILES notation. To generate the fingerprints of the SMILES notation, we are using the Morgan fingerprints by using the SMILES string. After fetching the SMILES fingerprint we have got the learned vector representation. Then we setup a sequential model to make dense layers (=9) with max pooling and dropout, along with 1D convolutional layers with different values.

Then we have focused on the BiLSTM model to preprocess, train and to predict the accurate values/ probabilities of the two required drugs.

The dense layer consists of input layer, hidden layer with ReLU as an activation function and Softmax function with an output layer. Then the visualization is performed with fully connected layer with 10-fold classification along with Adam optimizer and categorical cross entropy loss. In the output layer, Softmax function acts as an activation function and ReLU acts as an activation function for input and hidden layers along with epoch, batch size, and validation splits.

Then the performance metrics is calculated with accuracy score, F1 score, Area under the curve and confusion matrix. And the accuracy, F1 score, AUC, Average specificity,and average sensitivity are calculated in the validation metrics in the form of heatmap and others through graph plot.



C. Experimental Results

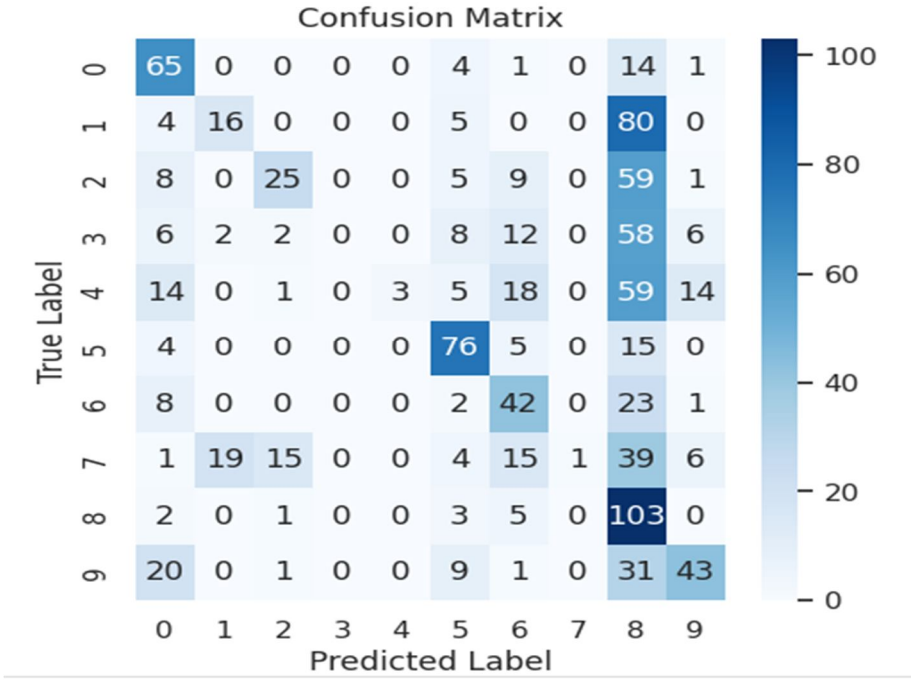


Fig 3.1 represents the confusion matrix

PERFORMANCE METRICS SCORES ARE LISTED BELOW :	
Accuracy	0.3740
F1 Score (Macro)	0.3201
AUC (OvR)	0.8647466817518522
Avg Sensitivity	0.3813
Avg Specificity	0.9300

Table 3.1 represents the performance metrics score

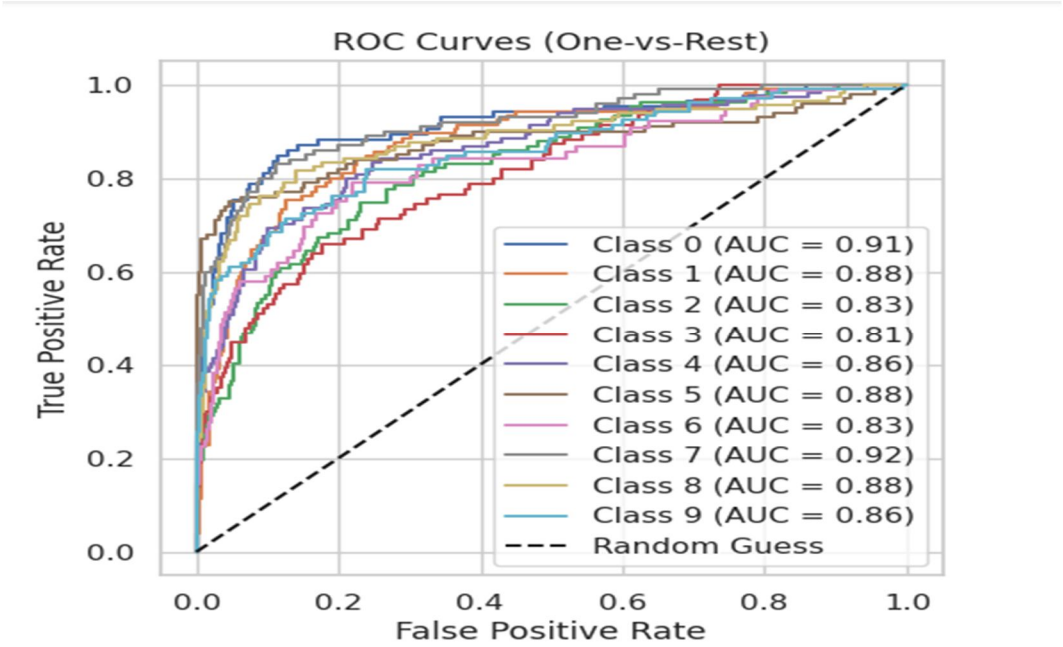


Fig 3.2 represents the ROC Curves (One-vs-Rest)

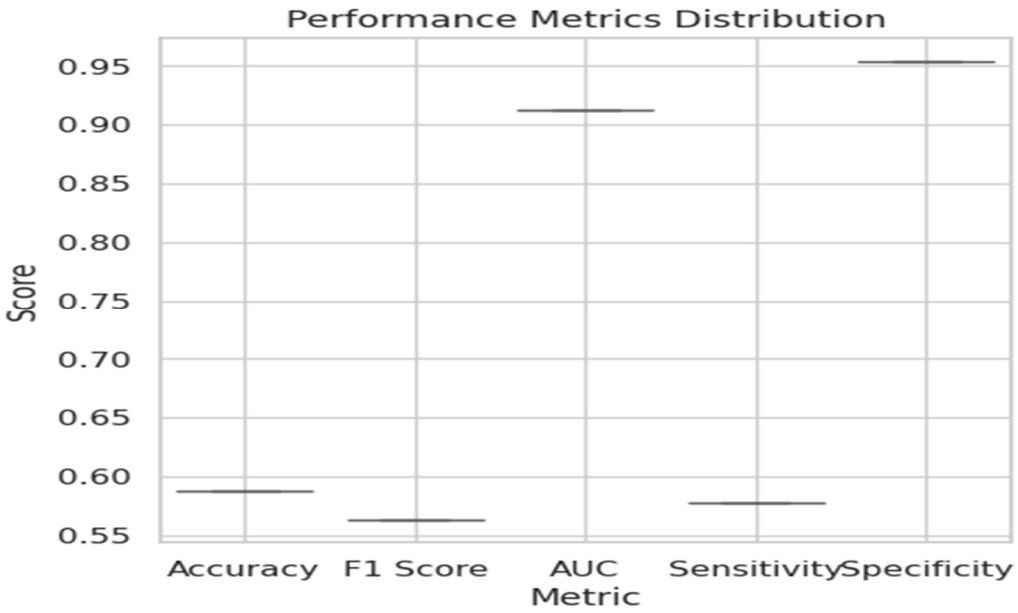


Fig 3.3 represents the Performance metrics distribution

III. CONCLUSIONS

A lot of different varieties of topics are discussed in the paper mentioned above. In our study, performance metrics is measured accurately with most effective scores. In future work, Graph Attention Network (GAT) and transformers might be used by the future researchers.

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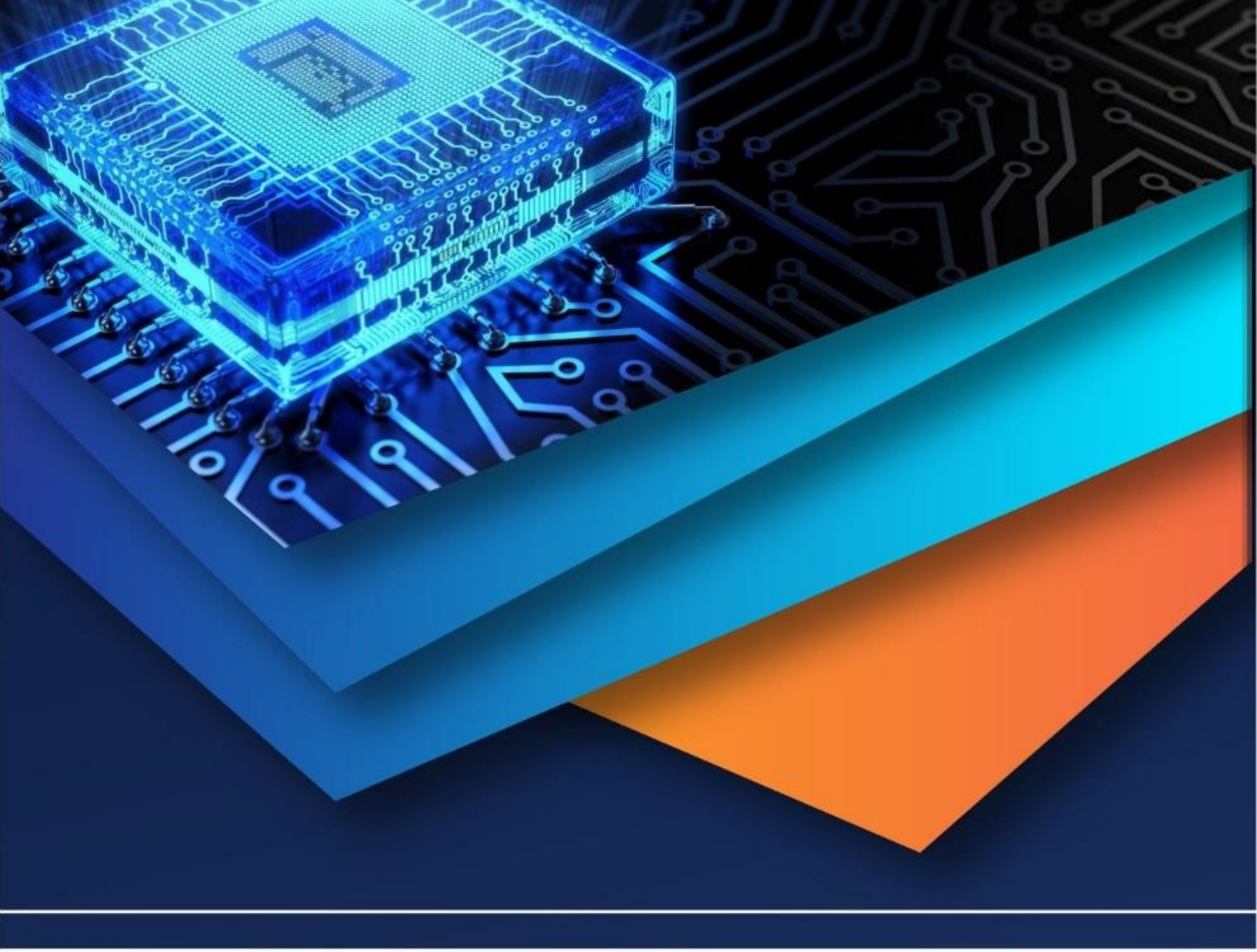

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