Drug-Target Interactions Prediction Using Network Based Method and Machine Learning

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The lack of effective treatments for many diseases increases the demand for new drug discovery. Consequently, the drug repositioning (DR) strategy is widely used. Drug-Target Interaction (DTI) prediction is a crucial step in DR since it excludes a significant number of experiments on false interactions. Due to their reliability and high success rate, computational methods for prediction are used. In this project, a network-based method is developed to predict novel DTIs using machine learning and a graph embedding technique, namely Node2vec, with high prediction performance. The method constructs a heterogeneous network by integrating three graphs (drug-drug similarity, target-target similarity, and DTIs) that are given within the golden standard Yamanishi datasets. Then Node2Vec is applied to auto-generate feature representation for each drug and target depending on its dataset using the optimum parameters. Subsequently, to obtain the features for each drug-target pair a fusion function was implemented. Finally, the model's performance in drug-target link prediction was evaluated by utilizing multiple classifiers. Compared to previous network-based methods, this method outperformed most of them by achieving the highest accuracy for each dataset, Nuclear receptor: 98%, G Protein-coupled receptor: 99%, Ion channel: 99%, and Enzyme: 99%. The application of the project is to find an efficient treatment in a shorter period because by predicting new DTIs, the search space toward the candidate drugs will be narrowed down.

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