[BIOINFO 2023]

Graph Convolutional Network Model based on Drug-gene-disease Network for Drug Repurposing

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The traditional de novo drug discovery is time-consuming and expensive. As a result, identifying new indications for already approved drugs, known as "drug repurposing," has gained considerable attention in pharmaceutical research. The advantage of drug repurposing over de novo drug discovery is that it can substantially decrease the risk of side effects since it starts from clinically approved compounds. Therefore, many computational methods for drug repurposing have been studied to identify novel drug-disease relationships. However, it is very challenging to integrate the heterogenous data such as chemical structure of compounds, genomic sequence or expression profiles and process for a model due to the data inconsistency and sparseness problems. Recently, deep learning techniques have been applied to predict the novel drug-disease relationships.

In this study, we have proposed a Graph Convolutional Networks (GCN) model to predict the novel drug-disease interactions by integrating heterogenous interactions between drugs, genes, and diseases into the graph model. Here, drugs, genes, and diseases are represented as nodes, while their interactions are denoted as edges. Chemical structure information is utilized as the feature for drug nodes, whereas disease phenotype information serves as the feature for disease nodes. Our model exhibited superior performance compared to traditional machine learning methods such as SVM or Random Forest. Furthermore, it outperformed the state-of-the-art drug repurposing deep learning models, DeepDR. GCN model based on drug-protein-disease network allows us to identify novel indications for approved drugs, drug repurposing, ultimately contributing to more efficient and effective drug discovery for emerging medical challenges.