Drug-Target and Drug-Drug Interaction Prediction using Knowledge Graph and Graph Neural Network

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Abstract

Understanding drug-drug and drug-target interactions is crucial for developing safe and effective therapeutic strategies. With the rapid growth of pharmaceutical research, traditional methods for identifying these interactions, which heavily rely on experimental data, are often inefficient, costly, and difficult to scale. These limitations can hinder the discovery of new drug candidates and the prediction of harmful drug combinations. Despite advancements in computational techniques, there are still significant challenges in accurately predicting interactions due to the complexity of integrating vast biological datasets. Leveraging advanced data mining, machine learning, and bioinformatics approaches can improve the prediction of DDIs and DTIs. Ultimately, these advancements will help optimize drug development processes and ensure safer, more effective treatments. This paper represents the ways to bridge gaps in current computational techniques by providing insights into safer drug combinations and facilitating personalized medicine, ultimately optimizing the drug development process and contributing to more effective therapeutic strategies.

Keywords

Attention Mechanism, Machine Learning, Multi-layer Framework, Pharmaceutical research.