Department of Computer Science

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Presents

DTGNNS: Drug-Target Deep Graph Neural Networks
by

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Annex 23A

Several machine learning methods have been developed in cheminformatics to investigate the molecular property, develop new drugs, and predict interactions of drug-protein. Among them, graph neural networks (GNNs) represent a quite new and fast-evolving field in deep learning applications and research along other domains such as social networks, graphs, and molecular descriptions. Exploring drug-protein interactions (DPIs) performance and their predictions is crucial in drug discovery. By exploiting GNNs, I directly build molecular graphs that work on node-level, edge-level, and graph-level as input to the GNN. In this thesis, I propose a novel architecture that will take the graph properties of the molecule and generate interactions of DPIs. In particular, I discuss a GNN model that uses graph neural networks to predict drug-protein interactions (DPIs) while representing both drugs and proteins in a single homogenous graph. The results demonstrated the use of deep learning models for the prediction and binding of drugs to proteins, as well as the potential benefits of representing drugs and proteins as graphs for future advancements in the pharmaceutical sector.