Graph Neural Networks for Drug Discovery

Abstract

This paper explores the application of Graph Neural Networks (GNNs) in the field of drug discovery.

1. Introduction

Drug discovery involves identifying compounds that can modulate biological targets. Machine learning models, particularly Graph Neural Networks (GNNs), have emerged as effective tools for molecular property prediction.

2. Methodologies

We discuss key GNN architectures such as Graph Convolutional Networks (GCNs), Graph Attention Networks (GATs), and Message Passing Neural Networks (MPNNs). These models can learn from molecular graphs to predict drug-like properties.

3. Datasets

Popular datasets include MoleculeNet, PubChemBioAssay, and ChEMBL. These datasets provide molecular structures and activity labels for benchmarking.

4. Benchmarks and Performance

Benchmark studies show that GNNs outperform traditional fingerprint-based methods in QSAR tasks. We present performance metrics across datasets.

5. Conclusion

GNNs hold great promise for accelerating drug discovery by leveraging molecular graph representations.