Benchmarking Graph Neural Networks for Drug Discovery Applications

Abstract

We present a comprehensive benchmarking study comparing various Graph Neural Network architectures for drug discovery tasks. Our evaluation covers multiple datasets and performance metrics to provide insights into the effectiveness of different approaches.

1. Benchmark Framework

We establish a standardized framework for evaluating GNN performance in drug discovery. This framework includes consistent data preprocessing, model training protocols, and evaluation metrics.

2. Model Comparison

We compare various GNN architectures including Graph Convolutional Networks, Graph Attention Networks, and GraphSAGE. Our results show that attention-based models generally outperform traditional convolution-based approaches.

3. Performance Metrics

We evaluate models using multiple metrics including AUC-ROC, precision-recall curves, and mean squared error. These metrics provide comprehensive assessment of model performance across different aspects of drug discovery.