Recent GNN Architectures for Drug Molecule Prediction

Recent architectures like DimeNet, SchNet, and Graphormer have pushed the boundaries of GNNs for molecular learning.

Methodologies:

DimeNet incorporates directional message passing, while Graphormer introduces transformer-style attention over molecular graphs. These innovations improve accuracy on 3D property prediction tasks.

Datasets:

ZINC and PCBA datasets are commonly used benchmarks for evaluating drug-likeness and bioactivity.

Performance:

Graphormer achieved state-of-the-art results on the Open Graph Benchmark (OGB), especially on the ogbg-molhiv task. It outperformed all previous GNN baselines.