An Introduction to Graph Neural Networks for Drug Discovery

Graph Neural Networks (GNNs) have revolutionized the field of drug discovery. Traditional drug design relied heavily on feature engineering and domain-specific knowledge. However, GNNs allow for end-to-end learning on molecular graphs.

Methodologies:

Early GNN models like GCN and GAT were applied to predict molecular properties. These models propagate node features via message passing, capturing the local structural context.

Datasets:

The QM9 and MoleculeNet datasets are among the most widely used in training GNNs for drug-like molecules. These contain molecular graphs annotated with physical and chemical properties.

Performance:

GNNs outperform classical models in virtual screening tasks and molecular property prediction. However, challenges remain in scalability and interpretability.