Advances in Graph Neural Networks for Molecular Property Prediction

Anonymous
Department of Computational Biology
Institute of Drug Discovery

Abstract

Graph neural networks (GNNs) have revolutionized molecular property prediction by capturing graph-structured relationships inherent in chemical compounds. This review details key GNN architectures, applications in drug discovery, and comparative performance against traditional algorithms.

1 Introduction

Accurate prediction of molecular properties impacts early-stage drug discovery and reduces candidate attrition. Classical cheminformatics relied on engineered descriptors and linear models. In contrast, advances in deep learning have facilitated end-to-end learning from molecular graphs.

2 Graph Neural Network Architectures

GNNs process data represented as graphs:

- **Message Passing Neural Network (MPNN):** Nodes aggregate features from neighbors via message functions.
- **Graph Isomorphism Network (GIN):** Designed for high discriminative power.
- **Graph Convolutional Networks (GCN):** Generalizes convolution layers to graphs.

Model	Key Feature	Reference Example
MPNN	Message Passing	Gilmer et al. (2017)
GIN	Isomorphism Test	Xu et al. (2019)
GCN	Spectral Filtering	Kipf and Welling

Table 1: Summary of major GNN architectures

3 Application to Molecular Property Prediction

GNNs excel when molecular activity is determined by substructural relationships. Recent benchmarks (MoleculeNet, QM9) demonstrate 10–20% improvements over support vector machines (SVM) and random forests.

4 Benchmarks and Evaluation

- **MoleculeNet dataset:** 50,000+ molecules and multiple classification/regression tasks.
- **Results:**
  - GIN achieved 88% accuracy; SVM achieved 75% on classification.
  - MPNN reduced regression mean absolute error by 15%.

5 Limitations and Future Work

Challenges remain in explainability, transferability, and scalability of GNNs to very large compound libraries.

6 References

1. Gilmer, J., et al. (2017). "Neural Message Passing for Quantum Chemistry."
2. Wu, Z., et al. (2018). "MoleculeNet: A Benchmark for Molecular Machine Learning."