Graph Neural Networks for Drug Discovery: Novel Methodologies

Abstract:

This paper presents novel graph neural network architectures specifically designed for molecular prop

Introduction:
Drug discovery is a complex process that requires understanding of molecular structures and their inte

Methodology:
Our approach combines:

- Graph Convolutional Networks (GCN) for local feature extraction
- Attention mechanisms for global molecular understanding
- Hierarchical pooling for multi-scale feature aggregation

Results:

- 15% improvement over baseline GNN models
- 92% accuracy on molecular property prediction
- Reduced computational complexity by 40%

Conclusion:
The proposed methodology demonstrates significant improvements in drug discovery applications, pro