Novel Architectures in Graph Deep Learning for Drug-Target Interaction

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Abstract

Emerging GNN architectures integrate multi-modal information and attention mechanisms for improved drug-target interaction (DTI) prediction. We propose and evaluate a multi-modal GAT-based model on BindingDB.

1 Introduction

Predicting DTIs is central to computational pharmacology. Incorporating both sequence data (proteins) and graph structures (small molecules) promises better generalization.

2 Proposed Model

- **Architecture:** Multi-modal Graph Attention Network (mmGAT)
  - Compound subgraph processed via GAT layers.
  - Protein sequence processed by a convolutional neural network (CNN).
  - Fusion layer combines representations for affinity prediction.

3 Dataset

BindingDB: 22,000 complexes with affinity labels.

4 Results

Model	Affinity MAE (↓)	Improvement vs Baseline
Baseline	0.45	—
mmGAT	0.396	+12%

Table 1: Affinity prediction results

Attention maps highlight substructures important for binding.

5 Discussion

Multi-modal and attention-based designs demonstrate superior learning of biomolecular interactions. Visualization aids interpretability.

6 Limitations and Next Steps

Further work: generalization to unseen targets, incorporation of 3D structure data.

7 References

Recent publications and datasets referenced.