COMPARATIVE EVALUATION OF LSTM AND GRAPH NEURAL NETWORKS FOR ADVERSE DRUG REACTION PREDICTION

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Introduction and Problem

Fatalities from adverse drug reactions pose a major challenge, with hospital death rates ranging from 0.1% to 10%

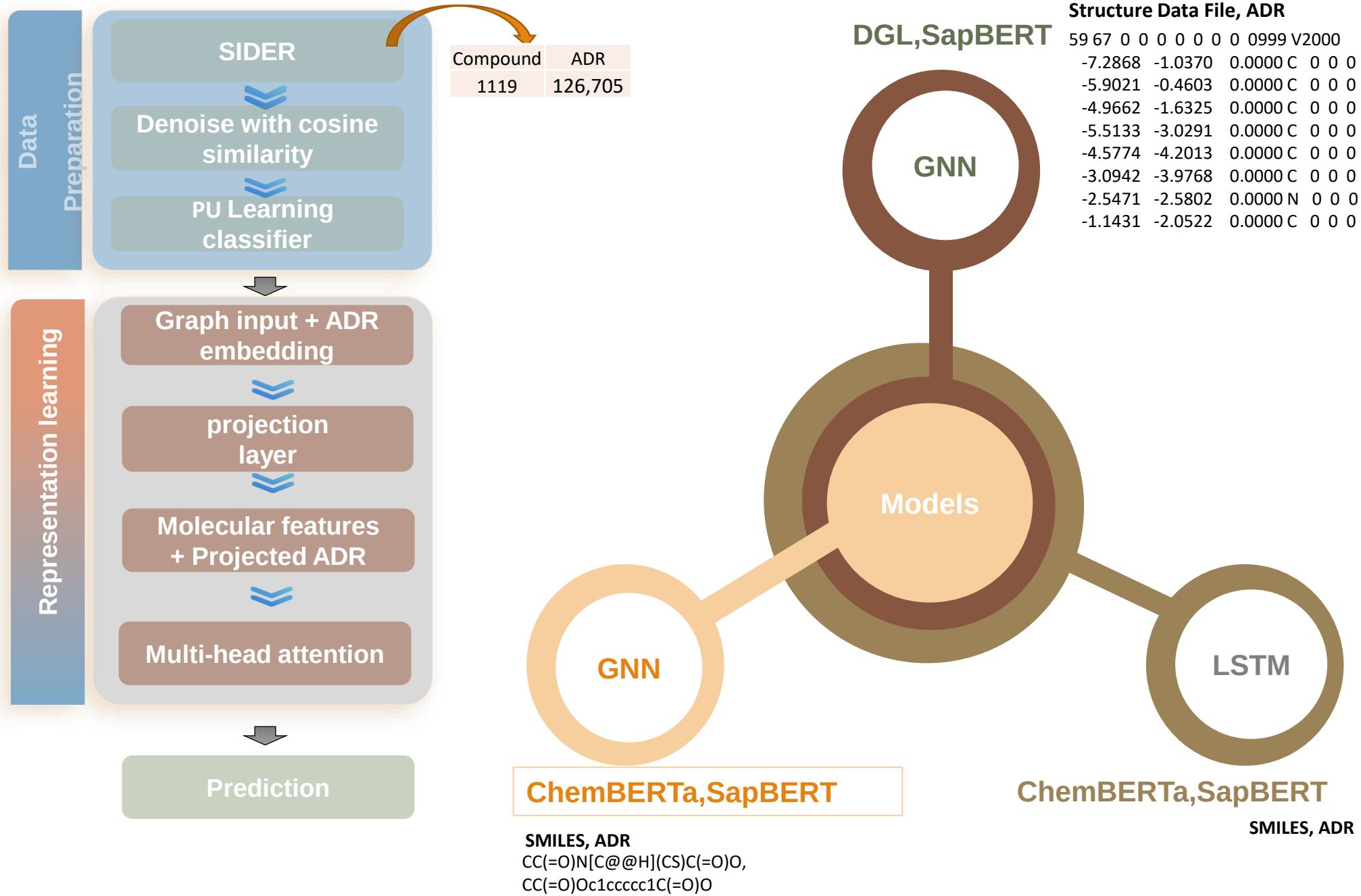
Adverse drug reactions related hospitalizations range from 0.2% to 54.5% globally

Clinical trials are limited in their ability to detect rare or long-term reactions because of their restricted duration and sample size

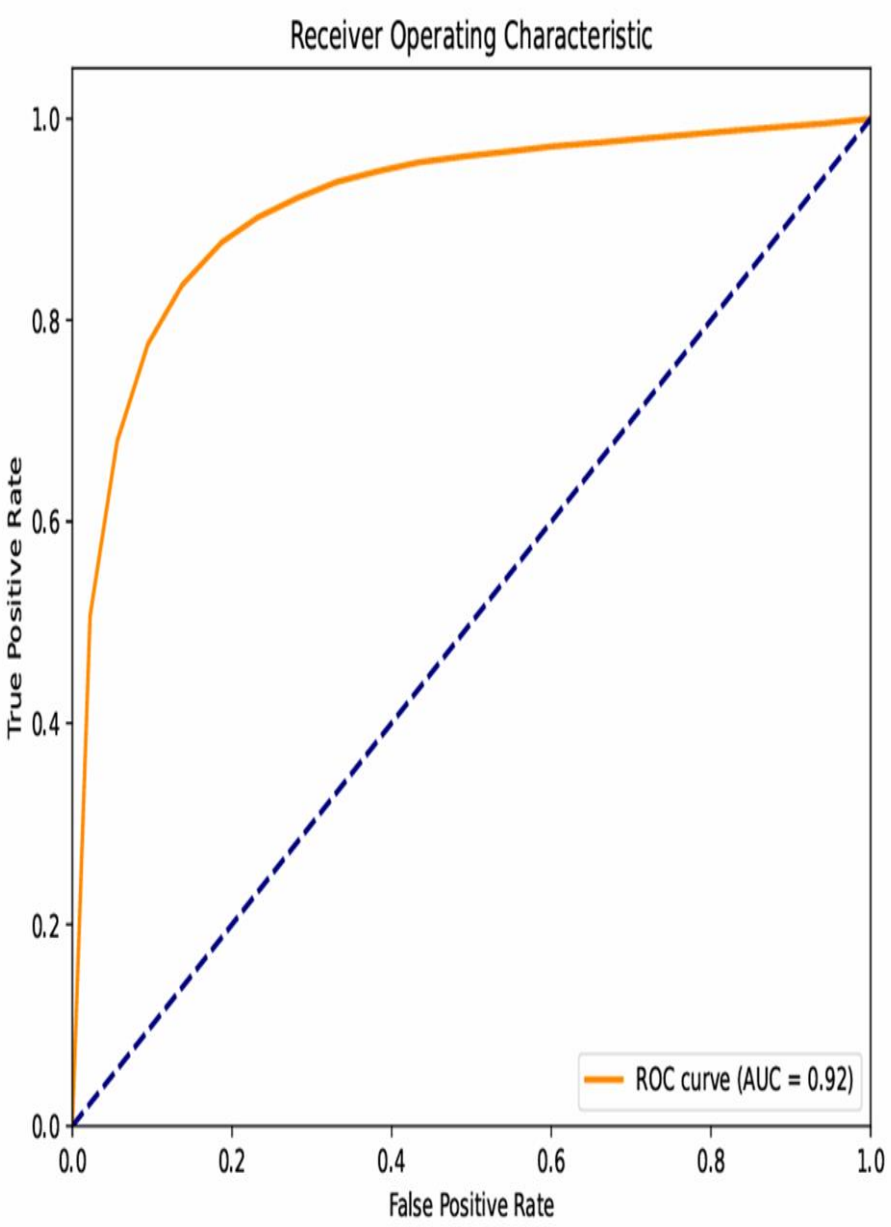
ML is making progress however hindered by noisy training data and insufficient methods for chemical structure representation

How differently do sequence and graph embeddings represent drug structures in ADR prediction? Can GNN on PU-optimized data lead to measurable performance improvements?

Qiu et al. (2025). Bio-K-Transformer for ADR Prediction. Computer Methods and Programs in Biomedicine



Kuhn et al. (2016). The SIDER Database of Drugs and Side Effects. Nucleic Acids Research



RESULTS

Model	Accuracy	Precision	Recall	AUC	F1-Score
LSTM	0.67	0.66	0.70	0.73	0.68
GNN (ChemBERTa)	0.84	0.82	0.87	0.91	0.84
GNN (DGL)	0.86	0.87	0.85	0.92	0.86

Compound	Adverse Drug Reaction	Prediction
Tazarotene	Abdominal distension	1.00
Enasidenib	Abdominal discomfort	1.00
Fenfluramine (Dexfenfluramine)	Agitation	0.99
Diclofenac Etalhyaluronate	Abdominal pain	0.99
Enalapril	Anaemia	0.98
Sevoflurane	Anaesthesia	0.98
Tafenoquine	Alanine aminotransferase increased	0.97
Dipotassium phosphate	Anxiety	0.97
Vinblastine	Angina pectoris	0.96
Penicillin G	Agranulocytosis	0.96
Zaleplon	Aggression	0.92
Azelaic acid	Acne	0.92
Calcitriol	Altered state of consciousness	0.92
Glycopyrronium bromide	Accommodation disorder	0.91
Celecoxib	Alanine aminotransferase	0.88
Dihydrocodeine-6-glucuronide (Metabolite)	Apnoea	0.87
Pirenzepine	Abnormal dreams	0.82
Olanzapine	Akathisia	0.75

We accessed the generalizability of the model by making predictions using data from ADReCS

Cai et al. (2015). ADReCS: An Ontology Database for Adverse Drug Reaction Terms. Nucleic Acids Research

GNN Training Efficiency: Accelerating Discovery

The significant reduction in training time translates directly into faster iteration cycles and lower computational costs

8h

LSTM Training Time

Time required to process a single epoch of training data using the sequence-based

3m

GNN Trained DGL

Time required to process a single epoch using the optimized Graph Neural Network model

160x

Improved Speed

The relative speed-up achieved by leveraging structural embeddings and GNN architecture

Conclusion

Metrices

GNNs outperform LSTMs in both accuracy and efficiency. AUC and F1-score 0.9242, 0.8559 against 0.7338, 0.6826

Scalability

High scalability and faster training with structure data file compared to SMILES

Positive and Unlabeled (PU)

PU-optimized data on GNN demonstrated improved performance

Thank you for your attention!

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