Meta-Learning for Graph Abstractions

Predicting Drug-Drug Interaction Using GNN

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Problem Statement

Predicting Drug-Drug Interaction Using GNN

- Due to its enormous relevance, drug-drug interaction is one of the most sought-after research areas.
- Its definition is the result of an interaction between two or more medicines. These interactions may have beneficial effects or they may have unfavourable outcomes.

Uniqueness

The distinction of the aforementioned remark comes from its emphasis on the use of graph neural networks (GNNs) in the study of drug-drug interactions. The remark implies that conventional manual procedures can be improved to recognise intricate connections and interactions between medications by utilising GNNs. The statement also emphasises how crucial it is to evaluate many GNN models side by side in order to discover which ones function best in certain situations. Overall, the statement outlines an original and cutting-edge method for employing machine learning to solve a medical problem.

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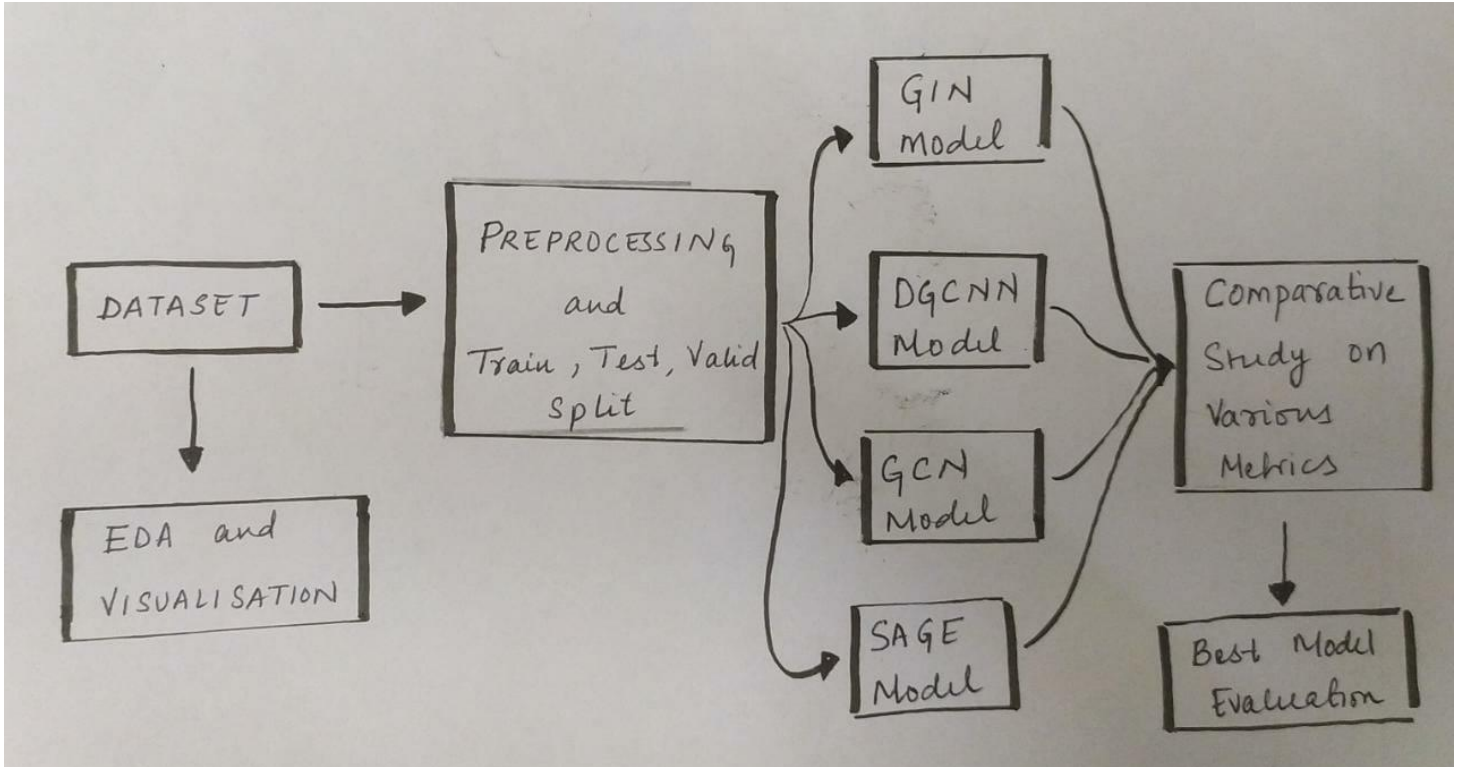
Overall design and approach



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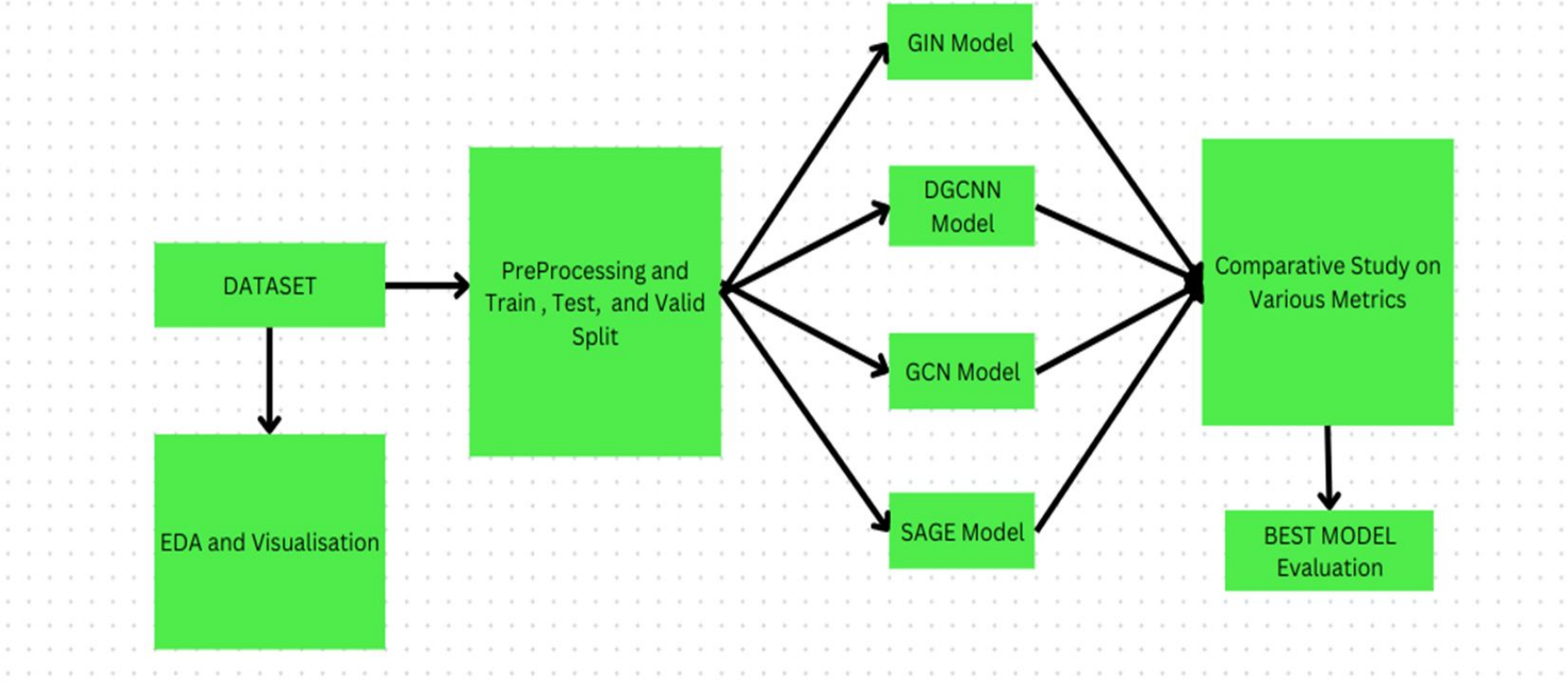
Overall design or approach in uml diagram



Use cases

Adverse Effect Prediction: GNN predicts potential adverse effects from drug interactions, assisting healthcare providers in avoiding harmful combinations.

Optimizing Medication Regimens: GNN suggests adjustments to dosages or alternative medications to maximize therapeutic benefits while minimizing the risk of negative drug interactions.

Early Detection System: GNN acts as an early warning system, identifying potential drug interactions before clinical manifestations, enabling proactive intervention.

Personalized Treatment Plans: GNN tailors treatment plans based on individual patient data, ensuring personalized medication regimens that balance efficacy and safety.

Application

Clinical Decision Support: *GNN aids healthcare decisions, especially in complex cases, improving prescription accuracy.*

Drug Development Acceleration: *GNN expedites drug development by predicting interactions early, streamlining the identification of safe treatment options.*

Real-time Healthcare Monitoring: *GNN integrates into continuous monitoring, enabling adaptive treatment plans and early detection of emerging drug interactions.*

Public Health Surveillance: *GNN monitors population-wide medication data for trend analysis, aiding public health surveillance.*

Feasibility

Abundant Data Sources: *Feasible with rich healthcare databases and drug interaction datasets becoming more available.*

Computational Efficiency: *Feasible with GNN models adaptable to modern hardware, ensuring scalability and speed.*

Interdisciplinary Collaboration: *Feasible through collaboration among computer scientists, pharmacologists, and healthcare professionals.*

Model Trust and Interpretability: *Feasible by enhancing GNN model interpretability, ensuring trust and facilitating integration into clinical workflows.*

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Dataset

- Obl-ddi from Open Graph Benchmark.
  Nodes - 4267
  Edges - 13,34,889
- It is a Homogenous, Undirected, Unweighted Graph representing drug-drug interactions
- Source - link

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Reference Papers

Paper Title	Authors
Link Prediction Based on Graph Neural Network	Muhan Zhang, Yixin Chen
DGCNN: Disordered Graph Convolutional Neural Network Based on the Gaussian Mixture Model	Bo Wu, Yang Liu, Bo Lang, Lei Huang
Semi-Supervised Classification with Graph Convolutional Networks	Semi-Supervised Classification with Graph Convolutional Networks

THANK YOU

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