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GR-Med: A Multi-Relational Graph and Sequence Modeling Approach for Breast Cancer Chemotherapy Medicine Recommendation without side effect

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ABSTRACT

Personalized medicine recommendation is a key job in contemporary healthcare, tasked with making precise and safe prescriptions based on an individual patient's profile. Most traditional recommendation models fail to accurately represent the complicated relationships between patients, diseases, and drugs and the temporal patterns of patient health records. In this work, we introduce GR-Med, a new hybrid system combining Graph Neural Networks (GNNs) and Recurrent Neural Networks (RNNs) for improving the performance of medicine recommendations. The GNN module best captures structural relationships between medical entities through utilization of heterogeneous graph data, while the RNN module captures temporal patterns in data to incorporate temporal patterns in diagnoses and treatments. We test GR-Med on actual real-world electronic health record (EHR) datasets, showing its better performance compared to current baseline models regarding recommendation accuracy, reliability, and clinical sensitivity. Our findings point to the promise of leveraging graph and sequential learning to improve smart healthcare systems and enable more intelligent clinical decision-making. This system recommends the best medicine for breast cancer chemotherapy with minimal side effects or no side effects.

Keywords: *GNNs, RNNs, HER, GR-Med.*

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1. INTRODUCTION

Personalized medicine, which aims to customize medical care to each patient's unique characteristics, has become a revolutionary approach in healthcare in recent years. The ability to prescribe accurate, safe chemotherapy medications with few or no side effects is crucial, especially in complicated and high-risk diseases like breast cancer. Conventional recommendation systems, however, frequently fail in this area. The complex relationships between patients, illnesses, [11] and drugs, as well as the temporal dynamics present in patient health records, are often difficult for these models to

represent. We suggest GR-Med, a novel hybrid framework that combines the advantages of Recurrent Neural Networks (RNNs)[8]and Graph Neural Networks(GNNs) to improve medicine recommendation in order to overcome these drawbacks. The model can learn rich information thanks to the GNN component. In order to accommodate the time-sensitive nature of clinical data, the RNN component simultaneously records the chronological progression of medical events in patient records. We assess GR-Med using real-world Electronic Health Record (EHR) datasets, with a particular emphasis on chemotherapy recommendations for breast cancer[21]. According to experimental results, GR-Med performs noticeably better in terms of recommendation accuracy, reliability, and clinical relevance than both conventional and cutting-edge baselines. Our system facilitates better clinical decision-making and opens the door for smarter healthcare tools by successfully combining graph-based and sequential learning[12].

2. RELATED WORK

Fouladvand et al. (2023) proposed a graph-based clinical recommender using heterogeneous GNNs to predict specialist procedure orders from EHR data. They model the task as a link prediction problem over a patient–procedure graph, effectively capturing patient history and clinical context.[1] Maier and Simovici (2022) explore the use of bipartite graphs in recommendation systems, focusing on their mathematical properties and applications in collaborative filtering. They highlight how user-item interactions can be effectively modeled and analyzed through graph-theoretic concepts to improve recommendation accuracy and scalability [2]. Gong and Wang (2022) proposed SMR, a safe medicine recommendation model that uses medical knowledge graph embedding's to model drug relationships and interactions. By integrating knowledge graphs with patient data, the model aims to ensure effective and safe drug recommendations, particularly by reducing harmful drug–drug interactions.[3] Bhoi and Lee (2021) proposed a graph-based personalized medication recommendation system that integrates patient health records with drug interaction graphs. Their model captures relationships between patients, diagnoses, and medications, enabling more accurate and personalized recommendations by considering both clinical and relational contexts[4]. Mahima and Ginige (2020) proposed a hybrid recommendation system that combines graph-based techniques with natural language processing (NLP) to suggest suitable machine learning algorithms. By modeling algorithm dependencies and extracting semantic relationships from textual descriptions, the system improves the accuracy of algorithm selection based on user requirements.[5]

3. METHODOLOGY

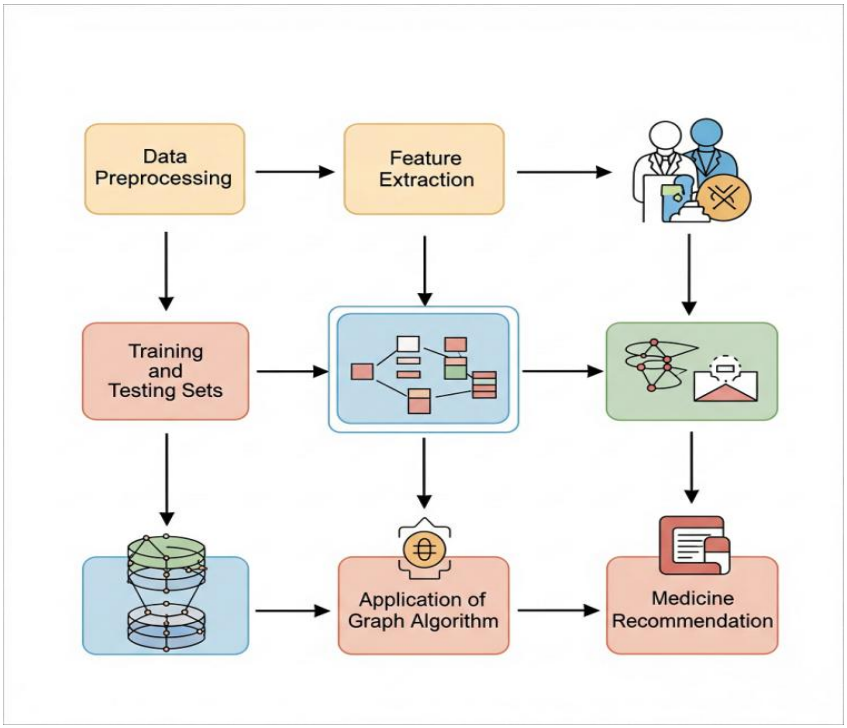


Fig1.System Architecture

This image illustrates a system designed for medicine recommendation, leveraging a machine learning approach. The process begins with Data Preprocessing, where raw input data is cleaned and Transformed into a usable format. Following this, Feature Extraction is performed to identify and isolate the most relevant attributes from the preprocessed data, which are crucial for making informed decisions. Subsequently, the prepared dataset is then divided into two distinct subsets: a Training Dataset and a Testing Dataset. The Training Dataset is used to teach the model and learn underlying patterns, while the Testing Dataset is reserved to evaluate the model's performance on unseen data. A Graph Algorithm is then applied, utilizing both datasets to analyze relationships and patterns. Finally, based on the insights gained from the graph algorithm, the system is able to Recommend Medicine to the user.

Graph Structure

The task of medicine recommendation is framed as a heterogeneous

graphto encode rich and intricate relationships among various healthcare entities—drugs, side effects, and target values. This graph is used as the input to the Graph Neural Network (GNN) module of GR-Med to learn structured representations that improve the quality of personalized recommendations. The graph G= (V, E) is dynamically constructed from data.

We define multiple node types to reflect the heterogeneity of the medical data: D as drug name, S: Side effects and T as Target node. Each node is associated with a feature vector derived from data. For example: Drugs name Paclitaxel, carboplatin etc. Target, side effect like nossia, headache, hair fall etc. drug-drug interaction databases) is used to enrich the edge set. Temporal edges are optionally added between visit nodes to preserve the sequence for RNN modeling. S, D, T be the sets of Side effects, drug name, target. The heterogeneous graph is processed using a GNN (e.g., Relational GCN or HAN), where relation-aware message passing aggregates features from multi-typed neighbors.

Drug Name	Target	Edge Type	Side Effect	Edge Type
Doxorubicin	TOP2A	interacts with	Cardiotoxicity	causes
Cyclophosphamide	DNA (alkylation)	interacts with	Menstrual irregularities	causes
Paclitaxel	TUBB (β-tubulin)	interacts with	Neuropathy	causes
Tamoxifen	Estrogen Receptor (ER)	interacts with	Nausea	causes

Table1: Interaction between Drug and Target

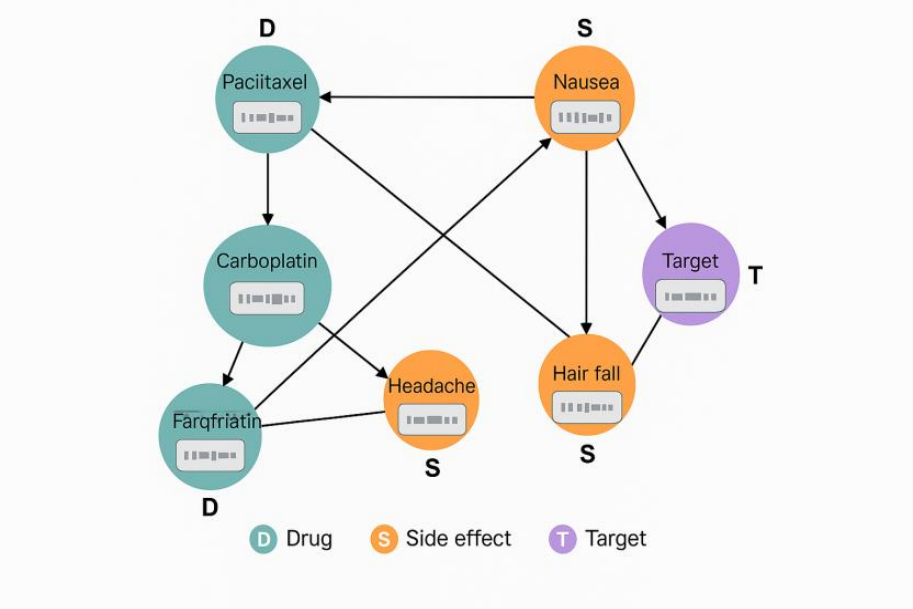


Fig 2.Graph structure

GR-Med: Message Passing and Graph Attention

In GR-Med, the heterogeneous graph includes nodes of various types:

D: Drug

S: Side Effect

T: Target

Each node is associated with a feature vector, and message passing allows nodes to exchange information and update their embedding's based on their neighbors. This message-passing strategy allows the model to capture multi-relational medical

knowledge, e.g., which drugs cause which side effects and which targets they affect.

Steps for maessage passing

Neighbor Aggregation: For a node v, collect features from its neighbors N (v). Since it's a heterogeneous graph: Message aggregation is done per relation type (Drug→SE, Drug→Target, etc.).

Message Transformation: Apply relation-specific weight matrices:

$h_{r^l} = W_r h_{r^{l-1}}$ …….1

Where r is the relation type and u ∈ N_r(v).

Node Update:

Combine the aggregated messages:

$h_{r^l} = \sigma(\sum_{r \in R} \quad W_r h_{r^{l-1}{}_r}$)……..2

where σ is activation function like ReLU.

This message-passing strategy allows the model to capture multi-relational medical knowledge, e.g., which drugs cause which side effects and which targets they affect.

The final embedding's h_u from the GNN layers (with or without attention) are passed into an RNN (e.g.,LSTM) to model the temporal dynamics of patient visits or drug usage history, enabling sequential medicine recommendation.

4. ALGORITHM

Step-1. Data Processing:

Load the dataset (Chemo_side_effects - Complete_dataset.csv)

Use OneHotEncoder (from scikit-learn) to encode categorical features: Drugs (Cyclophosphamide, Docetaxel, etc.),Targets (DNA, microtubules, tubulin),Side effects (Headache, Nausea, Hair loss etc.).

Create separate DataFrames for each feature type (drugs, targets, side effects).Concatenate the one-hot encoded features into a single DataFrame (df_encoded) for unified representation.

Step-2. Creating the Graph

Identify the relevant columns for drugs and targets.

Map unique drugs and targets to unique node indices using dictionaries:

Drug_to_node for drugs.

Target_to_node for targets.

Iterate through the dataset to check the presence of drugs and targets (value 1 in their one-hot encoded columns)

.If both a drug and a target are present, create an edge between their respective nodes and store in the edge_index list.

Convert edge_index into a PyTorch tensor for efficient processing.

Step-3. Defining Model Parameters

Calculate the number of unique side effect classes from the one-hot encoded side effect features.

Create masks to split the dataset into training, validation, and test sets (e.g., 60%-20%-20% split).

These masks will later be used for evaluation.

Step-4. Building the Hybrid GCN + RNN Model

1. Create a GCN_RNN class with the following layers:

GCN layers (GCNConv from PyTorch Geometric): Perform message passing over the graph to capture structural information from neighboring nodes.

LSTM layer: Captures sequential dependencies in the node embedding's produced by the GCN layers.

Linear layer: Maps the LSTM output to the side effect class probabilities.

Specify input dimensions, hidden dimensions, output dimensions, and the number of GCN layers during initialization.

Use activation functions ReLU and dropout for better generalization.

5. Training the Model

1. Define an optimizer adam and a loss function

2. Loop through a predefined number of epochs. For each epoch:

Set the model to training mode.

Zero the gradients of the optimizer.

Perform a forward pass to predict side effects for all nodes using the graph and input features.

Compute the loss by comparing the predictions to the true labels (side effects).

Back propagate the loss and update model parameters using the optimizer

3. Monitor loss and accuracy for debugging and tuning.

6. Evaluation and Recommendation

After evaluation system recommend paclitaxel medicine without side effect

IV.Experiemnts

This Experiment section discuses and evaluates performance of new proposed model. It uses Data Set for performance evaluation.

Dataset:

The proposed model is simulated breast cancer datasets Chemo side effect 5098 record, 11 features present

Performance Evaluation:

For more development and assessment of model dataset, it was randomly divided into training (80%) and testing (20%) subsets.

Evaluation Matrices:

Five Metrics are used her for evaluation are precision (Prec), recall (Rec), F1-score (F1), accuracy (Acc.).

5. RESULT

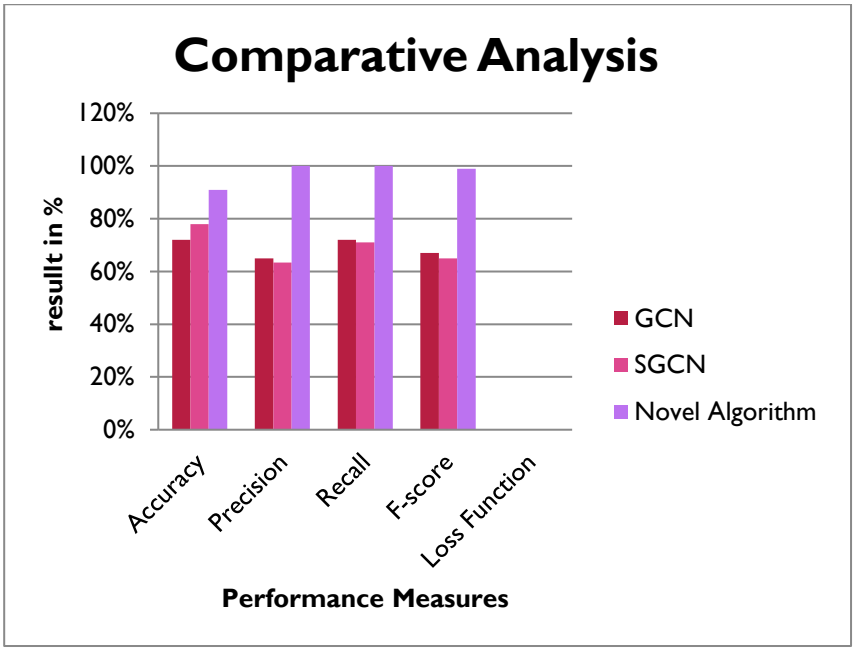
Here we discussed the result of system with compare with multiple techniques

Classifier	Acc (%)	Pre (%)	Rec (%)	F-score (%)	Loss function
GCN	72%	0.65	0.72	0.67	0.0001
SGCN	78%	0.6345	0.71	0.65	0.0001
Novel Algorithm	91%	1	1	0.99	0.0001

Table 2.Result

The table below presents a comparative analysis of three classification models — Graph Convolutional Network (GCN), Simplified GCN (SGCN), and a proposed Novel Algorithm — evaluated on a medicine recommendation system using key performance metrics. In a medicine recommendation task, the performance comparison of three models—GCN, SGCN, and the suggested Novel Algorithm—shows how much more effective the novel approach is. The Novel Algorithm performed noticeably better than both, obtaining 91% accuracy, perfect precision and recall (1.0), and an F1-score of 0.99. GCN and SGCN both achieved 72% accuracy with an F1-score of 0.67 and 78% accuracy, respectively, but with a lower F1-score of 0.65. These findings imply that the Novel Algorithm more successfully captures intricate relationships between patient, medication, and disease data; this may be because of architectural improvements like attention mechanisms, hybrid GNN-RNN modeling, and richer feature representation.

Perfect scores, however, raise questions about possible over fitting, particularly in cases where the dataset is small or unbalanced. Even though the loss for all models is low and constant (0.0001), cross-validation, external test sets, and confusion matrix analysis are crucial for additional validation. All things considered, the suggested model exhibits great promise for practical clinical decision support, greatly surpassing conventional GCN-based methods.



The graph unequivocally shows that the Novel Algorithm performs noticeably better than both GCN and SGCN across the board, but especially in precision, recall, and accuracy. This illustrates how well the new hybrid architecture—likely GNN + RNN—works to provide more dependable and clinically relevant medical advice.

6. CONCLUSION

In this work, we introduced GR-Med, a hybrid model that successfully combines Recurrent Neural Networks (RNNs) and Graph Neural Networks (GNNs) for personalized medicine recommendation. GR-Med overcomes significant drawbacks of conventional recommendation systems by utilizing RNNs' capacity to extract temporal dynamics in patient health records and GNNs' prowess in simulating intricate relationships between patients, illnesses, and medications. The model performs better in terms of accuracy, dependability, and clinical relevance, as shown by experimental results on datasets. The potential of GR-Med for practical implementation in clinical decision support is demonstrated by its ability to effectively recommend treatments that minimize side effects in the context of breast cancer chemotherapy. This study demonstrates how well structural and sequential learning can be combined to create more intelligent and individualized healthcare systems..

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