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Biomedical Knowledge Graph Embedding with Capsule Network for Multi-label Drug-Drug Interaction Prediction

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ABSTRACT: A relationship between two medications in which one drug's pharmacological actions are altered by another is known as a drug-drug interaction (DDI). Positive DDIs typically help patients have better therapeutic outcomes, however negative DDIs are the main cause of bad drug reactions, and can potentially lead to the drug being taken off the market and patient death. As a result, DDI identification has become crucial to the development of new drugs and the management of disease. We present a unique approach to predict DDIs in this paper that integrates similarity and semi-supervised learning (DDI-IS-SL). The cosine similarity method is used by DDI-IS-SL to combine the drug's chemical, biological, and phenotypic data in order to determine how similar the medications' features are. Additionally, the kernel similarity of medicines' Gaussian Interaction Profiles is determined using known DDIs. To determine the ratings for potential drug interactions, supervised learning is employed.

I. INTRODUCTION

An relationship between two medications in which one drug's pharmacological actions are altered by another is known as a drug-drug interaction (DDI).

Positive DDIs typically help patients have better therapeutic outcomes, however negative DDIs are the main cause of bad drug reactions, and can potentially lead to the drug being taken off the market and patient death.

DDI identification has become crucial to the development of new drugs and the management of disease.

II. LITERATURE SURVEY

Pharmacokinetic drug-drug interactions (DDIs), affecting the systemic exposure of drugs, may result in a lack of efficacy, or increase in severe adverse reactions. Sometimes, because of the unexpected lethal adverse reactions caused by DDI, drugs are withdrawn from the market. To avoid such serious DDIs in the patients, it is now strongly recommended that the magnitude of DDIs with new chemical entities that act as victims (substrates) or perpetrators (inhibitors) be evaluated before drugs are marketed [1].

The aim was to develop a drug-drug interaction database (SFINX) to be integrated into decision support systems or to be used in website solutions for clinical evaluation of interactions [2].

III. PROPOSED SYSTEM

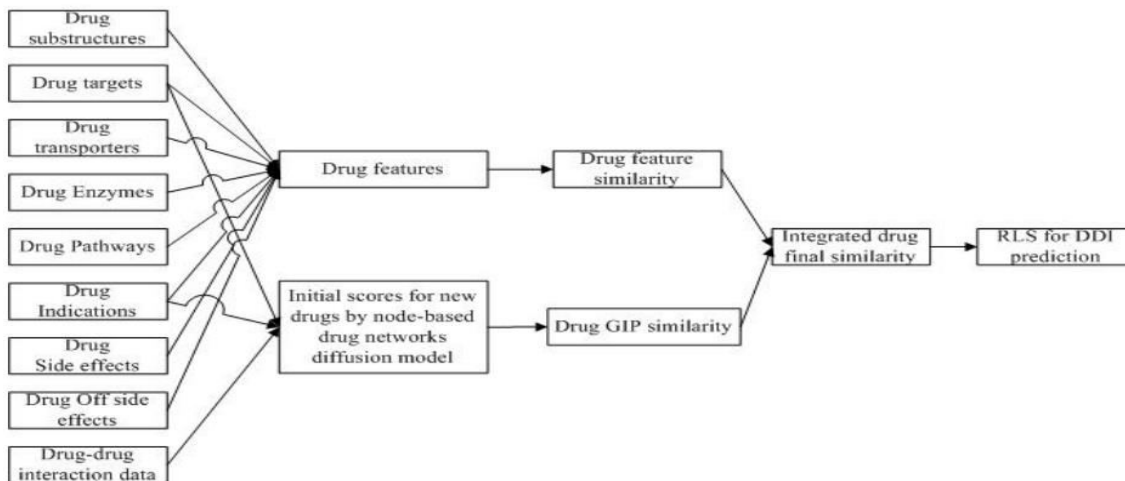
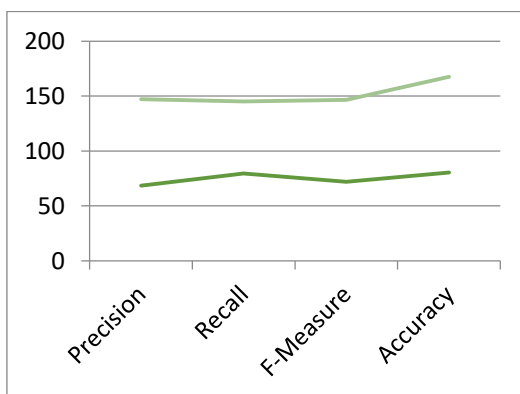


Figure 1 System Architecture

Our proposed DDI-IS-SL for predicting DDIs. First, DDI-IS-SL finds the new drug set which has no known DDIs. Second, based on the drug-target interactions, drug-indication interactions and known DDIs, DDIIS-SL computes the initial interaction scores between these new drugs and other drugs which have known DDIs by the node-based drug network diffusion method.

IV. RESULTS AND DISCUSSION

We compared the proposed system accuracy on number of samples and show the result graphically. Let see the following graph and table shows the prediction accuracy result based on machine learning technique.



	Existing system	Proposed System
Precision	69.75	79.88
Recall	82.45	64.99
Accuracy	78.99	90.91

V. CONCLUSION

In order to increase the effectiveness of treatment and lessen the burden on patients, multidrug therapies have been frequently employed to treat illnesses, particularly complex disorders like cancer. Multi-drug therapy do, however,



sometimes have unfavourable side effects that might result in serious problems or even patient death. Consequently, finding drug-drug interactions aids in bettering the treatment of diseases and lessens the complexity of developing new drugs. In particular, it is imperative to create new computational techniques for DDI identification.

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