Indian Academy of Sciences, Bengaluru
Indian National Science Academy, New Delhi
The National Academy of Sciences India, Prayagraj

SUMMER RESEARCH FELLOWSHIPS — 2022

Format for the four-week Report*,^,@

Name of the candidate : .....

Application Registration no. : .....

Date of joining : .....

Name of the guide : .....

Guide's institution : .....

Place of stay during the tenure of the fellowship : Hostel provided by _____
Guide _____
Own arrangement
Other (Specify) _____

....

Signature of the candidate Signature of the guide

Date: _____ Date: _____

INSPIRE/KVPY FELLOWSHIP (please fill this box)#			
1.	I am currently a recipient of	INSPIRE FELLOWSHIP	☐ Yes / ☐ No
		KVPY FELLOWSHIP	☐ Yes / ☐ No
		If, YES, fill cols. 2, 3 & 4	
2.	**INSPIRE/KVPY** Fellowship is from _____[month]/_____[yr] to _____[month]/_____[yr]		
3.	I receive a monthly fellowship of Rs. _____ from INSPIRE/KVPY towards my living expenses		
4.	I also receive towards contingencies a sum of Rs. _____ per year		
	I affirm that the information given above is correct.		
	Signature of the candidate		

IMPORTANT NOTES:

*** The four-week report could be between 300 and 350 words.**

^ This format should be the first page of the report and should be stapled with the main report.

 # Mandatory to fill this section, this should be filled and signed by you even if you are not an INSPIRE/KVPY Fellow. Otherwise release of fellowship amount will be withheld.

@ The hard copy of the duly signed report should reach the Academy office within 10 days of completing the first month fellowship. If delayed the fellowship amount will not be paid.

(For office use only; do not fill/tear)

Candidate's name:		Fellowship amount:
Student:	Teacher:	Deduction:
Guide's name:		Amount to be paid:
KVPY Fellow:	INSPIRE Fellow:	A/c holder's name:
Others		

Modelling polypharmacy side effects with graph convolution networks

SRFP 2022 4-week report

Application ID: ENGS3188

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August, 2022

Abstract:

The following report highlights the modelling of polypharmacy side effects using graph convolution networks. The decagon model predicts the side effects for a pair of given drug combinations. The goal is to implement decagon paper.

1. Introduction

Polypharmacy is the administration of two or more drugs as a single effective medication which can improve the therapeutic efficacy by overcoming redundancy in underlying biological processes. Even though polypharmacy is a good practice, it comes with a much higher risk of side effects due to drug-drug interactions, which are subject to patient mortality and morbidity.

Polypharmacy side effects are difficult to identify because, firstly, they are rare secondly, it is impossible to test all possible pairs of drugs. And thirdly, small-scale clinical tests are ineffective in identifying side effects.

Researchers in the past have developed several approaches, but they could only predict the strength of a drug-drug interaction but couldn't predict the exact side effects.

1.1 Problem Statement

The goal is to study the decagon paper and implement it using the DGL library.

2. Decagon Paper

The problem is modelled by constructing a two-

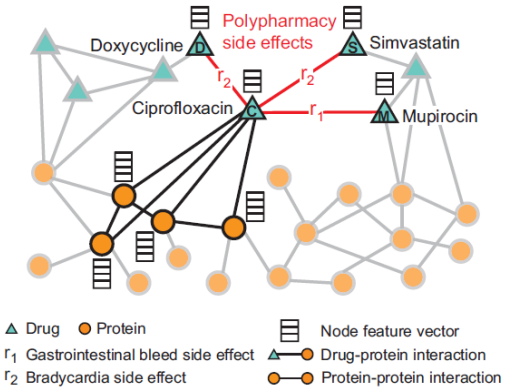

Figure 1: An example graph of polypharmacy side effects derived from genomic and patient population data.

layer multimodal graph of protein-protein interactions, drug-protein interactions and drug-drug interactions. Each drug-drug interaction is labelled by an edge type, which signifies the type of the side effect. Then a multi-relational edge prediction model that uses the multimodal graph to predict drug-drug interactions and their types is developed.

3. Graph Representational Learning

We view the graph representation learning problem in the encoder-decoder framework. It involves two fundamental operations. First, an encoder model maps each node in the graph into a low-dimensional vector or embedding. Next a decoder model that takes the low-dimensional node embeddings and uses them to reconstruct information about each node's neighbourhood in the original graph.

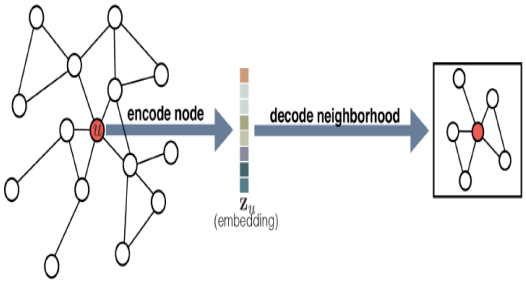

Figure 2: Overview of encoder-decoder approach.

Graph representational learning can solve problems related to node classification, relation prediction, clustering and community detection, graph classification, regression and clustering.

4. Conclusion

Graph representational learning is learnt. Studied Decagon paper and understood the multi-relational link prediction model. Learnt the implementation of neural networks using PyTorch.

In the coming four weeks, expect to learn the DGL library and implement the decagon paper using the same.

5. References

[1] Modeling polypharmacy side effects with graph convolutional networks. Marinka Zitnik, Monica Agrawal and Jure Leskovec. Bioinformatics, 2018.

[2] Deep Graph Library (https://www.dgl.ai/)