

# Drug Recommendation System using Hetionet Dataset

## 1. Introduction

In this report, the model aims to develop a drug recommendation system, specifically referring to two tasks: an alternative drug for disease and drugs with side effect constraints. The Hetionet dataset is here for use in one's modelling between the two.

## 2. Methodology

### 2.1 Data Set

Data were extracted from the Hetionet dataset, which is a heterogeneous network of biological information. The data were processed to get drug-disease relationships that spell out as triples (head, relation, tail).

### 2.2 Task 1: Drug Recommendation

#### Method 1:

**Model:** TransE, a knowledge graph embedding model.

**Process:** The model is trained on the Hetionet dataset. It learns the embeddings for the diseases and drugs. For a given disease, it recommends drugs that have the most similar embeddings with that disease.

**Evaluation:** The best method of performance evaluation is Hits@5, wherein the first five results will be compared with the reference data.

#### Method 2:

**Model:** TransE

**Process:** Similar to Method-1 but does not take into account the drugs having direct connections with disease under the dataset.

**Evaluation:** NDCG@10 and Hits@10 are used, thereby assessing relevance and ranking quality of the top 10 recommendations.

## 2.3 Task 2: Drug Recommendations with Side Effect Constraints

### Method 1:

#### Model: Graph Convolutional Network (GCN)

**Process:** A model is created for GCN, which will predict interaction between drugs and diseases. The predicted side effect constraints will apply afterward, where screened out drugs are above a given similarity threshold.

**Evaluation:** As it compares recommendations with reference data, the specific metric for this is not mentioned in the provided output.

### Method 2:

#### Model: Relational Graph Convolutional Network (R-GCN)

**Process:** An R-GCN is used to consider the different kinds of relationships of the Hetionet dataset. Side effect risks are precomputed and then recommendations are done on top of those risks.

**Evaluation:** The measure used here is Hits@3.

## 3. Results

### 3.1 Task 1

**Method 1:** Sample showing recommendations for the top 5 connections is provided for three diseases. The actual scores reached for Hits@5 are not printed in full but are calculated for the purposes of evaluation.

**Method 2:** The top 10 alternatives for 2 diseases are listed against similarity scores. The Hits@10 score is 1.0 for disease Id 85, while the NDCG@10 score is 1.0 for disease Id 131, meaning perfect matching is done on both recommendations.

### 3.2 Task 2

**Method 1:** Sample recommendations show up for 3 diseases and their top 5 drugs with similarity scores given under constraints of side effects. The evaluation metric and scores are not specified.

**Method 2:** Top 3 drug recommendations for 3 diseases with relevant scores and candidate IDs are produced, and the evaluation is done using the Hits@3 metric.

## 4. Conclusion

The project has successfully demonstrated various methodologies applicable to drug recommendation. The comparison indicates that one of these models, TransE, shows a high success rate in recommending alternate drugs.