GNN Based Food-Drug Interaction Prediction

고려대학교 KOREA UNIVERSITY

Team 논알콜제로디카페인소주

18th Junhyeok Won, 20th Minseok Kwon, GunYoung Lee, 21st YunKyung Ko

KUBIG(Korea University Data Science & AI Society), Korea University

8th CONFERENCE

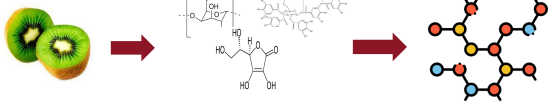
Introduction

Drug-Drug Interaction **Food - Drug Interction**

→ Idea : Food is a collection of compounds

Data

1. Molecule Data



kiwi **Compounds** **node: Molecule, edge: contain ratio**

2. Knowledge Graph(DRKG based)

FOOD Entity

3. Interaction Labeling

Food, Drug type

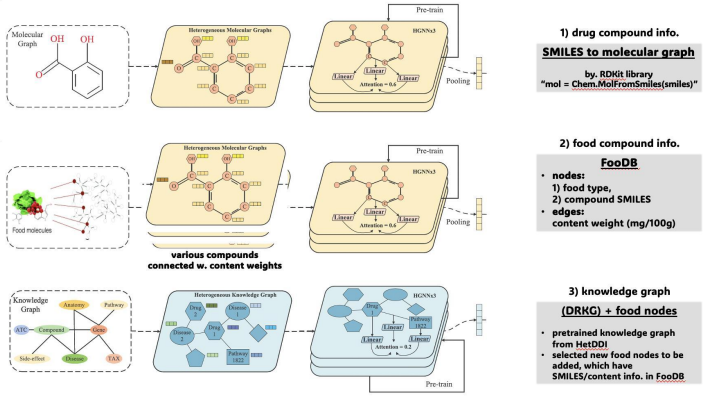
→ Mapped and filtered using SapBERT

Food-drug interaction

Drugbank : Expert defined text type label

→ Mapped to DrugBank interaction labels using S-PubMedBERT

Method



Baseline : HetDDI

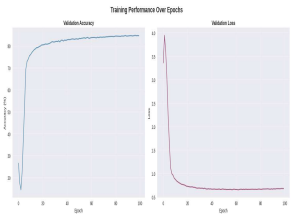
- **Drug to drug interaction multi class prediction**
- **smilter structure knowledge graph embedding**
- **Interaction Labeling**
- **pre-training, graph representation to supervised learning**

Our Method : Baseline + Food Information

- **Used weighted sum of compound SMILES (like drugs) as food SMILES**
- **Applied the same predicton using a knowledge graph with food and FDI labels**

Result

Loss



Fold

```
=== Training Summary (Fold 1) ===
                Metric  Initial  Final  Best  Improvement
Validation Accuracy      11.81  84.94 85.06        73.14
     Validation Loss      3.42   0.67  0.65         2.75
       Validation F1      0.54  61.94 62.44        61.39
    Validation Kappa      2.16  83.02 83.14        80.86

Total epochs: 100
Best score updates: 29
Final validation accuracy: 84.94%
Best validation accuracy: 85.06%
```

Food	Drug	Interaction Result
Port	Calcium Chloride	Drug and Food co-administration may lower clacium levels
Protein supplement	Ibrutinib	Drug may reduce serum levels of Food's active metabolites, decreasing efficacy

Conclusion

Significance

- **Extends DDI to complex food structure**
- **potential for presonalized food, drug interaction studies using patient data**

Limitation

- **Reduced accuracy by label assumption**
- **limited food coverage**