Identification of drug interactions with a graph autoencoder

(Gyógyszer kölcsönhatások azonosítása gráf autoenkóderrel)

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*Abstract*—The goal of this project is to realize a learning based on Variational Graph AutoEncoders. The motivation was the fact that certain medicines applied together can have adverse reaction on each other, meaning one drug can increase or decrease the effect of another. The following steps was followed to reach the wanted results: extract the features from the DrugBank database, eliminate the validation and test edges from the graph, modelling the interaction graph with an autoencoder. The challenge of this project was to modell the graph datas, create the model so it will reaches an accuracy of at least 80%, to extract features and then to illustrate the results with ROC curve and AUC.

Keywords—Variational Graph AutoEncoder, features, drug, edges, graph, modell, effect

Absztrakt – A projekt célja egy Variational Graph AutoEncoderen alapuló tanulás megvalósítása. A motiváció az volt a projekt megvalósítására, hogy bizonyos gyógyszerek együttes alkalmazása nemkívánatos reakciót válthat ki egymásra nézve, vagyis az egyik gyógyszer növelheti vagy csökkentheti a másik hatását. A kívánt eredmény elérése érdekében a következő lépések lettek alkalmazva: a jellemzők kinyerése a DrugBank adatbázisból, a validációs és teszt élek eltávolítása a gráfból, az interakciós gráf modellezése autoencoderrel. A projekt kihívása a gráf adatok modellezése, a modell létrehozása volt úgy, hogy az legalább 80%-os pontosságot érjen el, hogy kivonja a jellemzőket, majd az eredményeket ROC görbével és AUC-val illusztrálja.

Kulcsszavak – Variational Graph AutoEncoder, jellemzők, gyógyszer, élek, gráf, modell, hatás

Introduction

Drug–drug interactions (DDIs) are an essential attention in each drug improvement and medical utility, specially for co-administered medicines. Whilst it'sfar important to perceive all possible DDIs during clinical trials, DDIs are often mentioned after the medication are accepted for clinical use, and they are a commonplace cause of damaging drug reactions (ADR) and increasing healthcare expenses. Computational prediction may additionally help in identifying potential DDIs in the course of medical trials.

State of Art

Recent studies show that drugs have combined effects. These days this is a very interesting topic to study, so does many investigators in the last 40 years.

Their methods of generating and reading records have changed dramatically through the years but the primary problem has not. [1] Many different methods were considered to solve the question, including three-dimensional models for synergetic and antagonistic drug interactions in antiviral and anticancer chemotherapy.

Other articles explains the absorption of drugs and the basic concept how they interact, from a pharmacokinetic point of view, from these articles can be seen the extent of interactions, which is also important. [2]

In [3] another method is applied to analyze drug-drug interactions. A heterogeneous network-assisted inference (HNAI) framework to assist with the prediction of DDIs. First, was built a comprehensive DDI community that contained 6946 particular DDI pairs connecting 721 accepted capsules primarily based on DrugBank facts. next, was calculated drug–drug pair similarities the usage of four functions: phenotypic similarity primarily based on a comprehensive drug–ADR community, healing similarity based totally at the drug Anatomical healing Chemical category device, chemical structural similarity from SMILES facts, and genomic similarity primarily based on a big drug–goal interplay network constructed the usage of the DrugBank and therapeutic goal Database. sooner or later, then was implemented five predictive models within the HNAI framework: naive Bayes, selection tree, okay-nearest neighbor, logistic regression, and aid vector system, respectively.

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Identify applicable funding agency here. If none, delete this text box.

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*a**b* 

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* The subscript for the permeability of vacuum **0, and other common scientific constants, is zero with subscript formatting, not a lowercase letter “o”.
* In American English, commas, semicolons, periods, question and exclamation marks are located within quotation marks only when a complete thought or name is cited, such as a title or full quotation. When quotation marks are used, instead of a bold or italic typeface, to highlight a word or phrase, punctuation should appear outside of the quotation marks. A parenthetical phrase or statement at the end of a sentence is punctuated outside of the closing parenthesis (like this). (A parenthetical sentence is punctuated within the parentheses.)
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1. Table Type Styles

| Table Head | Table Column Head | | |
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1. A three-dimensional model to analyze drug-drug interactions

By Mark N. Prichard, Charles Shipman Jr.,  
[Antiviral Research](https://www.sciencedirect.com/journal/antiviral-research)

[Volume 14, Issues 4–5](https://www.sciencedirect.com/journal/antiviral-research/vol/14/issue/4), October–November 1990, Pages 181-205  
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2. Machine learning-based prediction of drug–drug interactions by integrating drug phenotypic, therapeutic, chemical, and genomic properties

By Feixiong Cheng, Zhongming Zhao  
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