Drug-Drug Interaction Prediction by Deep Learning Approach

Mohammad.Amin Khodamoradi [1,2], Bahareh Levian [1,2], Changiz Eslahchi[1,2,*]

[1]Department of Computer Science, Faculty of Mathematical Science, Shahid Beheshti University, Tehran, Iran.

[2] School of Bioinformatics, IPM - Institute for Research in Fundamental Sciences, Tehran, Iran.

*** Correspondence:**
Changiz Eslahchi
ch-eslahchi@sbu.ac.ir

Keywords: Drug-Drug Interaction, Drug Similarity, Drug Similarity Integration, Feature Selection, Recommender System Abstract

Drug-drug interactions (DDIs) always cause unexpected and even adverse drug reactions. It is important to identify DDIs before drugs are used in the market. However, preclinical identification of DDIs requires much money and time. Computational approaches have exhibited their abilities to predict potential DDIs on a large scale by utilizing premarket drug properties. Nevertheless, most of them only predict whether one drug interacts with another but neglects their enhancive (positive) and depressive (negative) changes of pharmacological effects. Moreover, these comprehensive DDIs do not occur at random and are derived from the DDI graph's structural features. Revealing such a relationship is very important because it can help to understand how DDIs occur. Both the prediction of comprehensive DDIs and the discovery of structural relationships play important guidance when making a co-prescription.

In this work, creating a set of comprehensive DDIs as a signed network, we design a novel model (SNF-CNN) to predict enhancive and degressive DDIs based on similarity network fusion convolutional neural networks. SNF-CNN achieves the depressive DDI prediction AUC=0/9747 ±0/0033 and AUPR=0/9666 ±0/0045, enhancive DDI prediction AUC=0/9686 ±0/0028 and AUPR=0/8221 ±0/0184, and the Unknown DDI prediction AUC=0/9714 ± 0/0040 and AUPR=0/9480 ±0/0083. Compared with two state-of-the-art approaches, SNF-CNN shows its superiority. Finally, this new approach is not only able to predict comprehensive DDI but also predicts conventional DDI.

Code and data are available at: https://github.com/aminkhod/DDI-Project

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9 Acknowledgments

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1 Data Availability Statement

Code and data are available at: https://github.com/aminkhod/DDI-Project