Abstract

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Title :Drug-Drug Interaction Prediction by Recommender System Approach

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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 or not one drug interacts with another, but neglect their enhancive (positive) and depressive (negative) changes of pharmacological effects. Moreover, these comprehensive DDIs do not occur at random, and derived from the structural features of the graph of DDIs. Revealing such a relationship is very important, because it is able to help understand how DDIs occur. Both the prediction of comprehensive DDIs and the discovery of structural relationship among them play an important guidance when making a co-prescription.

In this work, treating a set of comprehensive DDIs as a signed network, we design a novel model (SNF-CNN) for the prediction of enhancive and degressive DDIs based on similarity network fusion and 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 it superiority. Finally, this new approach is not only able to predict comprehensive DDI, but also predicts conventional DDI.

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