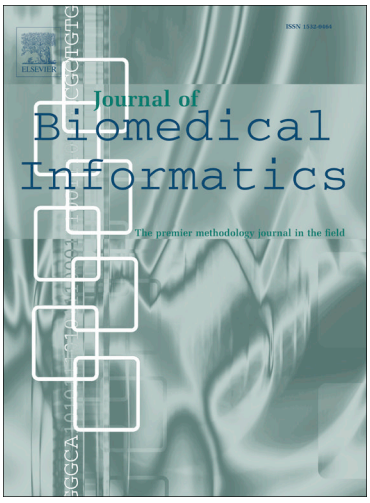

A meta-learning framework using representation learning to predict drug-drug interaction

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A meta-learning framework using representation learning to predict drug-drug interaction

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Abstract

Motivation

Predicting Drug-Drug Interaction (DDI) has become a crucial step in the drug discovery and development process, owing to the rise in the number of drugs co-administered with other drugs. Consequently, the usage of computational methods for DDI prediction can greatly help in reducing the costs of in vitro experiments done during the drug development process. With lots of emergent data sources that describe the properties and relationships between drugs and drug-related entities (gene, protein, disease, and side effects), an integrated approach that uses multiple data sources would be most effective.

Method

We propose a semi-supervised learning framework which utilizes representation learning, positive- unlabeled (PU) learning and meta-learning efficiently to predict the drug interactions. Information from multiple data sources is used to create feature networks, which is used to learn the meta-knowledge about the DDIs. Given that DDIs have only positive labeled data, a PU learning-based classifier is used to generate meta-knowledge from feature networks. Finally, a meta-classifier that combines the predicted probability of interaction from the meta-knowledge learnt is designed.

Results

Node2vec, a network representation learning method and bagging SVM, a PU learning algorithm, are used in this work. Both representation learning and PU learning algorithms improve the performance of the system by 22% and 12.7% respectively. The meta-classifier performs better and predicts more reliable DDIs than the base classifiers.

Keywords: Drug-drug interaction prediction; Positive-Unlabeled learning; Meta-learning; Representation learning

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