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PAPER

SNF-CNN: Predicting Comprehensive Drug-Drug Interaction via Similarity Network Fusion and Convolutional Neural Networks

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Abstract

Motivation: This research addresses the critical need to identify drug-drug interactions (DDIs) before market entry. Existing preclinical detection methods are resource-intensive, prompting the use of computational models based on premarket drug properties. However, current models often oversimplify interactions, neglecting nuanced alterations in pharmacological effects. DDIs, rooted in the structural features of the DDI graph, are non-random, and understanding these relationships is vital for making comprehensive predictions and uncovering structural patterns in the DDI graph. This study introduces the Similarity Network Fusion and Convolutional Neural Networks (SNF-CNN) model, treating comprehensive DDIs as a signed network.

Results: SNF-CNN excels in predicting degressive (AUC = 0.975, AUPR = 0.967), enhancive (AUC = 0.969, AUPR = 0.822) and Unknown DDIs (AUC = 0.971, AUPR = 0.948). A comparative analysis against state-of-the-art methods highlights the superiority of SNF-CNN, not only in predicting DDIs but also in accurately forecasting non-DDIs. The graphical abstract of SNF-CNN is provided (Figure 1).

Availability and implementation: The SNF-CNN and data are available as open-source from GitHub at: https://github.com/aminkhod/SNF-CNN.

For inquiries or collaboration, please contact A.khodamoradi@uninova.pt.

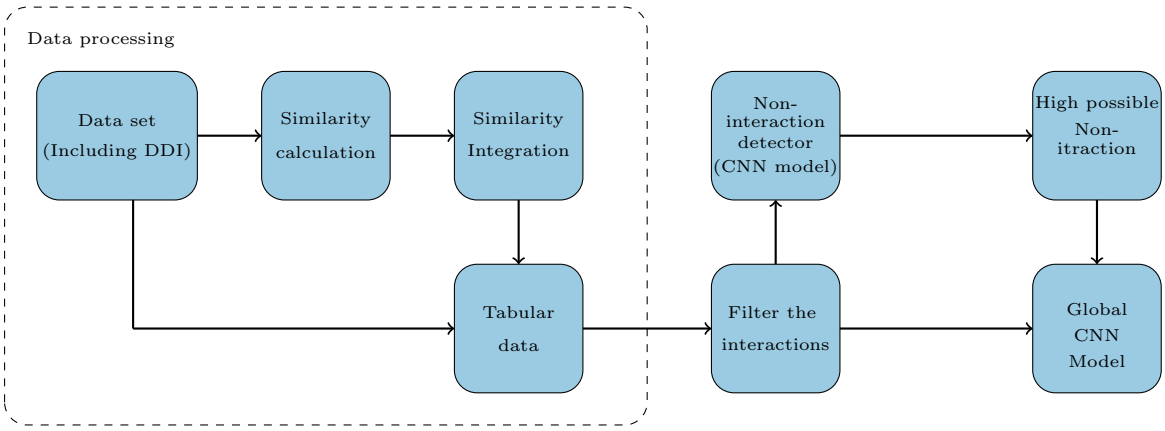

Fig. 1. Graphical abstract

Key words: Drug-Drug Interaction, Drug Similarity, Drug Similarity Integration, Feature Selection, Recommender System

Abbreviations: DDI:Drug-drug interactions; CV:cross-validation; SNF:Similarity Network Fusion