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Opinion Article

Using Heterogeneous Networks for Computational Drug Repositioning, Drug-Disease Association Prediction

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DESCRIPTION

Drug repositioning, which entails finding new therapeutic indications for already-approved medications, significantly cuts the time and expense of creating new medications. Heterogeneous networks are used in recent computational drug repositioning strategies to find drug-disease connections. This study identifies existing deep learning, matrix factorization, and matrix completion network-based methods for predicting drug-disease correlations. To compare the prediction abilities of the eleven approaches from the three categories. Separate homogenous datasets for the medication and illness sides were used for the experiment. Using drug-drug similarities based on chemical structures and ATC codes, disease-disease similarities based on ontologies, and drug-disease correlations, scientists created heterogeneous networks. As positive connections are often rare, an enhanced assessment metric was utilized to indicate the data imbalance. The prediction outcomes showed that techniques in the areas of matrix factorization or completion and graph mining did well in the overall evaluation. Furthermore, drug-related predictions were more accurate than disease-related ones. To enhance disease-side prediction, drug-drug similarity assessment must carefully choose and include useful drug properties. The creation of new medications is a time-consuming, costly, and dangerous process. From medication development to preclinical studies, clinical testing, and regulatory approval, the drug release process necessitates a significant amount of work and expenditure. New medication development takes 13.5 years on average and costs more than USD 1.8 billion.

The number of new pharmaceuticals entering the market is declining even if spending in medical development is continually rising. Therefore, improving drug research's success rate is essential for reducing time and expense. Drug repositioning, which includes finding new therapeutic indications for medicines that have previously received approval, has recently attracted interest since it significantly cuts down on the time and expense of finding new medicines. Additionally, clinical trials have previously shown that current medications are safe. In the past several decades, there have been several successful examples of pharmacological repositioning. For instance, sildenafil was originally created to treat coronary artery disease but was later relocated to treat erectile dysfunction. The need for efficient treatment medicines increased during the COVID-19 pandemic, and remdesivir was effectively repositioned to treat COVID-19. Although clinical observations have mostly guided therapeutic repositioning attempts, computational approaches have lately been presented to forecast potential medicines for successful repositioning. Additionally, they are scaleable to genome-wide data for medications, illnesses, and genes or proteins from a variety of perspectives. The majority of computational techniques make use of networks created by the connections between biological elements and enable systematic study of the systems. This article offers a thorough analysis of current network-based methods for computerized medication repositioning. Discovering interactions between a medication and its molecular targets was the main goal of computational drug repositioning in its early stages. On the premise that various medications interact with various targets, evidence of Drug-Target Interactions (DTIs) offers important hints for therapeutic repositioning. For each medication, new targets were inferred using networks, such as a drug-target bipartite network, in the majority of prior DTI prediction approaches. Up until recently, a number of network-based techniques for DTI prediction were suggested. This study focused solely on predicting connections between medications and illnesses because numerous other studies have previously reviewed such methodologies.

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