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Ensemble Models of Tensor Decomposition and Multi-layer Perceptron for Drug Repositioning

Jong-Hoon Park[1], and Young-Rae Cho[1,2,*]

[1]*Department of Software, Yonsei University Mirae Campus*
[2]*Department of Digital Healthcare, Yonsei University Mirae Campus*
**Corresponding author: youngcho@yonsei.ac.kr*

Since developing new drugs is a time- and money-consuming endeavor, the research of drug repositioning is expending which discovers new therapeutic indications for existing drugs. For effective repositioning of drugs, it is crucial to utilize the information of drug-targeted proteins or disease-causing genes, as drugs function by inhibiting or activating specific genes. Recently, computational methods which leverage a network are gaining interest for identifying possible drug-disease associations based on drug, gene, and disease networks. In this research, we present a network-based drug repositioning approach to predict drug-gene-disease associations through the tensor decomposition process. Our approach integrates drug-disease, drug-gene, and disease-gene associations into a drug-gene-disease tensor and models drug-gene-disease triple associations by generalized tensor decomposition. It also learns the features of drugs, genes, and diseases through multi-layer perceptron (MLP). In our experiment, we measured drug-drug similarities by drug chemical structures and ATC codes from DrugBank, disease-disease similarities by the phenotypic annotations from both OMIM and Human Phenotype Ontology (HPO), and gene-gene similarities by the annotations from Gene Ontology (GO) and protein-protein interactions from BioGRID. We also used drug-disease associations from the Cdataset, drug-gene associations from Comparative Toxicogenomic Database (CTD), and disease-gene associations from OMIM, as the training dataset. By 10-fold-cross-validation, our method achieved an accuracy of 96% in predicting drug-gene-disease associations for new drugs, surpassing the results of previous algorithms.