World Academy of Science, Engineering and Technology
International Journal of Bioengineering and Life Sciences
Vol:18, No:03, 2024

Graph Clustering Unveiled: ClusterSyn - A Machine Learning Framework for Predicting Anti-Cancer Drug Synergy Scores

Authors : Babak Bahri, Fatemeh Yassaee Meybodi, Changiz Eslahchi

Abstract : In the pursuit of effective cancer therapies, the exploration of combinatorial drug regimens is crucial to leverage synergistic interactions between drugs, thereby improving treatment efficacy and overcoming drug resistance. However, identifying synergistic drug pairs poses challenges due to the vast combinatorial space and limitations of experimental approaches. This study introduces ClusterSyn, a machine learning (ML)-powered framework for classifying anti-cancer drug synergy scores. ClusterSyn employs a two-step approach involving drug clustering and synergy score prediction using a fully connected deep neural network. For each cell line in the training dataset, a drug graph is constructed, with nodes representing drugs and edge weights denoting synergy scores between drug pairs. Drugs are clustered using the Markov clustering (MCL) algorithm, and vectors representing the similarity of drug pairs to each cluster are input into the deep neural network for synergy score prediction (synergy or antagonism). Clustering results demonstrate effective grouping of drugs based on synergy scores, aligning similar synergy profiles. Subsequently, neural network predictions and synergy scores of the two drugs on others within their clusters are used to predict the synergy score of the considered drug pair. This approach facilitates comparative analysis with clustering and regression-based methods, revealing the superior performance of ClusterSyn over state-of-the-art methods like DeepSynergy and DeepDDS on diverse datasets such as Oniel and Almanac. The results highlight the remarkable potential of ClusterSyn as a versatile tool for predicting anti-cancer drug synergy scores.

Keywords : drug synergy, clustering, prediction, machine learning., deep learning
Conference Title : ICBB 2024 : International Conference on Bioinformatics and Biomedicine
Conference Location : Hanoi, Vietnam
Conference Dates : March 18-19, 2024

Open Science Index, Bioengineering and Life Sciences Vol:18, No:03, 2024 publications.waset.org/abstracts/179301.pdf