ISSN: 1391-8796
Proceedings of 7th Ruhuna International Science & Technology Conference
University of Ruhuna, Matara, Sri Lanka
January 22, 2020

Inferring drug repositioning candidates using subnetwork identification

Hameed P.N.[1*], Verspoor K.[2] and Halgamuge S.[3]

[1]*Department of Computer Science, Faculty of Science, University of Ruhuna, Matara, Sri Lanka*
[2]*Department of Computing and Information Systems, University of Melbourne, Parkville, Australia*
[3]*Department of Mechanical Engineering, University of Melbourne, Parkville, Australia*

Computational drug repositioning can reduce the cost, time and risks of drug development. This study demonstrates the benefits of identifying subnetworks from large-scaled drug similarity networks (DSNs) and the use of Anatomical Therapeutic Chemical (ATC) classification for inferring plausible drug repositioning candidates.

The subnetwork identification algorithms used in this study aim to infer drug repositioning candidates for a single disease at a time. The use of ATC classification enables analysis of multiple subnetworks to prioritize useful drug repositioning candidates. Here, the drugs related to the nervous system are chosen from ATC class-N to construct the drug similarity networks. Moreover, the hierarchy of the ATC classification is used to construct multiple meaningful DSNs. Since sparse graphs are known to be effective for subnetwork identification, we used a two-tiered clustering approach to construct sparse DSNs.

Our results suggest 'Physarum-inspired Subnetwork Identification Algorithm', a subnetwork identification algorithm inspired by the biological properties of the physarum organism, is effective in identifying subnetworks for DSNs that are 14.5% sparse. Further, an average Rand Index of 82.1% and an average Precision of 57.9% were observed in the identified subnetworks in relation to the drugs that are already in ATC class-N. These subnetworks can be analyzed further to investigate plausible drug repositioning candidates for nervous system diseases. Furthermore, using various subnetwork identification algorithms and various sparse graph generation methods would be beneficial in prioritizing plausible drug repositioning candidates.

Keywords: drug repositioning, ATC classification, subnetwork identification and sparse graphs

*Corresponding author: nusrath@dcs.ruh.ac.lk