**Identification of drug-target interaction by a random walk with restart method on an interactome network**

## Abstract

### Background

Identification of drug-target interactions acts as a key role in drug discovery. However, identifying drug-target interactions via in-vitro, in-vivo experiments are very laborious, time-consuming. Thus, predicting drug-target interactions by using computational approaches is a good alternative. In recent studies, many feature-based and similarity-based machine learning approaches have shown promising results in drug-target interaction predictions. A previous study showed that accounting connectivity information of drug-drug and protein-protein interactions increase performances of prediction by the concept of ‘guilt-by-association’. However, the approach that only considers directly connected nodes often misses the information that could be derived from distance nodes. Therefore, in this study, we yield global network topology information by using a random walk with restart algorithm and apply the global topology information to the prediction model.

### Results

As a result, our prediction model demonstrates increased prediction performance compare to the ‘guilt-by-association’ approach (AUC 0.89 and 0.67 in the training and independent test, respectively). In addition, we show how weighted features by a random walk with restart yields better performances than original features. Also, we confirmed that drugs and proteins that have high-degree of connectivity on the interactome network yield better performance in our model.

### Conclusions

The prediction models with weighted features by considering global network topology increased the prediction performances both in the training and testing compared to non-weighted models and previous a ‘guilt-by-association method’. In conclusion, global network topology information on protein-protein interaction and drug-drug interaction effects to the prediction performance of drug-target interactions.

(This article has been published as part of BMC Bioinformatics Volume 19 Supplement 8, 2018: Proceedings of the 11th International Workshop on Data and Text Mining in Biomedical Informatics (DTMBIO 2017). The full contents of the supplement are available online at <https://bmcbioinformatics.biomedcentral.com/articles/supplements/volume-19-supplement-8>.)

https://bmcbioinformatics.biomedcentral.com/articles/10.1186/s12859-018-2199-x