Combining bottom up and top down approaches for Drug-Target-Interaction prediction

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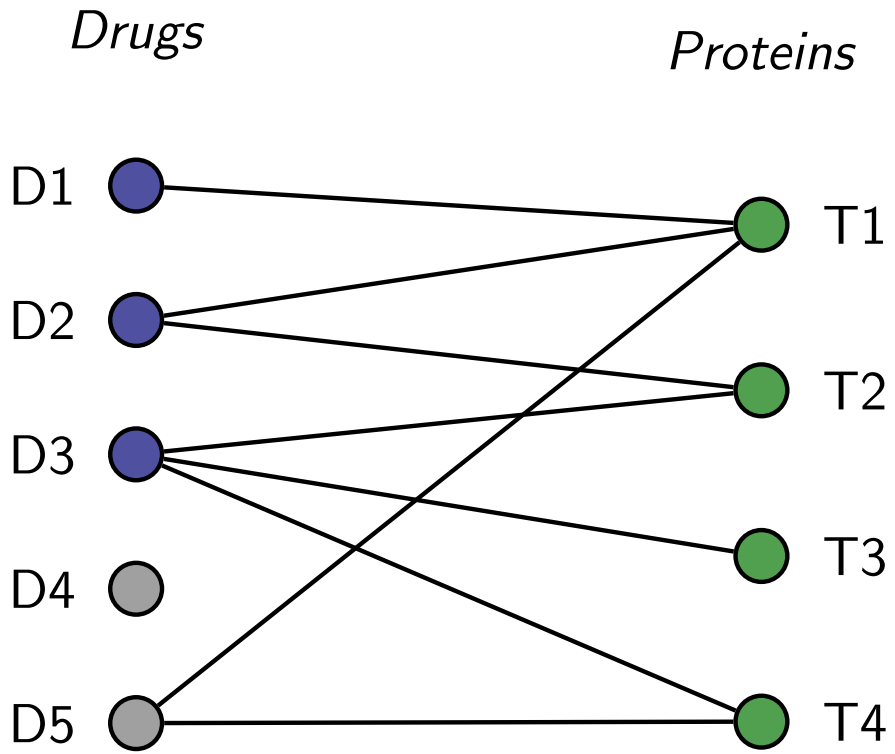
December 09, 2019

Outline

Problem Description

Prediction over bipartite graph:



Classification of recent approaches[1][2]

	Drugs	Protein
bottom-up	▶ GCN over molecules ▶ drug similarity	▶ secondary structure prediction ▶ contact prediction ▶ convolution over amino acid sequences
top-down	▶ network approaches ▶ drug similarity	▶ protein similarity

[1] Chen Wang et al., Briefings in Bioinformatics, 2018
[2] Yu Ding, Briefings in Bioinformatics, 2019

Problems of recent approaches

Main issues:

- lack of generalization
- Usually only top-down or bottom-up

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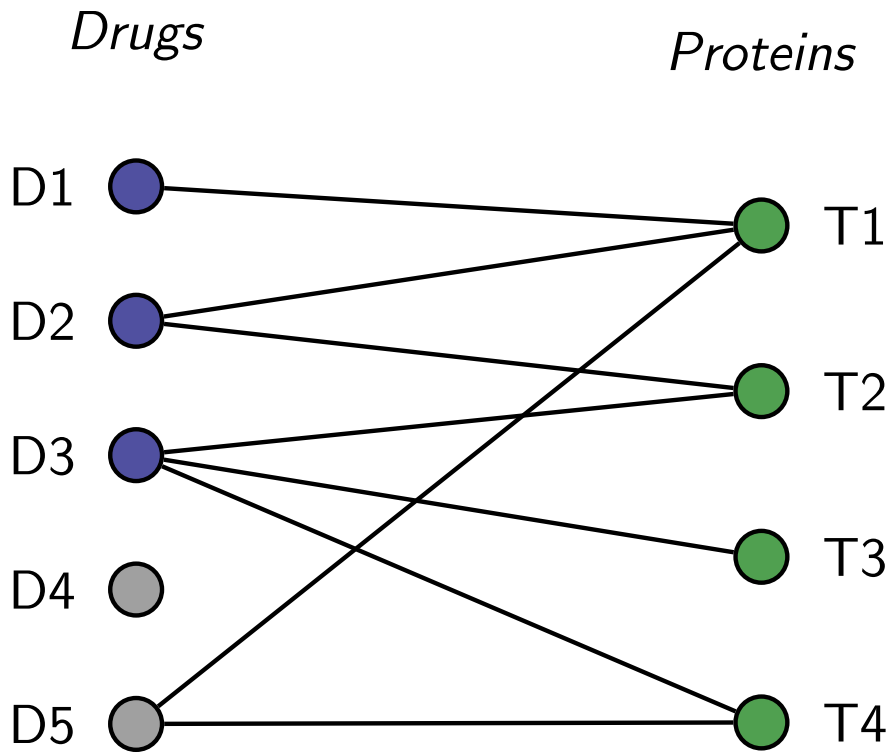

Full citations

- Yu Ding, Hong Wang, Hewei Zheng, Lianzong Wang, Guosi Zhang, Jiaxin Yang, Xiaoyan Lu, Yu Bai, Haotian Zhang, Jing Li, Wenyan Gao, Fukun Chen, Shui Hu, Jingqi Wu, Liangde Xu, Evaluation of drug efficacy based on the spatial position comparison of drug–target interaction centers, Briefings in Bioinformatics, , bbz024, https://doi.org/10.1093/bib/bbz024
- Chen Wang, Lukasz Kurgan, Review and comparative assessment of similarity-based methods for prediction of drug–protein interactions in the druggable human proteome, Briefings in Bioinformatics, , bby069, https://doi.org/10.1093/bib/bby069