Division of Statistics and Machine Learning Department
of Computer and Information Science Linköping
University

Master thesis project ”Biologically informed graph neural networks for drug effect prediction”

Background

More than 40% of patients do not respond to standard treatments in common diseases. Accordingly, methods from personalized medicine aim to identify and propose the best treatments for a patient with given characteristics.

Many advanced methods have been developed for prediction of sensitivity of samples to drugs. Some of these methods, like RefDNN [1], are based on deep learning to provide accurate predictions. However, these methods are not taking into account information about the known molecular interactions between genes. In this project, we aim to apply Graph Neural Networks and information from prior knowledge networks such as Omnipath [2] to predict drug effects.

Data

- GDSC database contains drug sensitivities for various drug and sample combinations [3].

Research questions

- Which graph neural network (GNN) models are most appropriate for predicting drug sensitivities from gene expression data and information about drug targets?
- How accurately can GNN models predict the drug sensitivities for new samples and for unseen drugs?
- How much do predictions obtained through the the GNN models differ from predictions of some published ML models that only uses gene expressions but not the network structure (for ex. RefDNN)?

Prerequisites

- Good knowledge of Machine learning and Statistics
- Good programming skills

Contact and application

- Oleg Sysoev, oleg.sysoev@liu.se

References

[1] Choi, J., Park, S., & Ahn, J. (2020). RefDNN: a reference drug based neural network for more accurate prediction of anticancer drug resistance. *Scientific reports*, *10*(1), 1-11.
[2] Türei, D., Korcsmáros, T., & Saez-Rodriguez, J. (2016). OmniPath: guidelines and gateway for literature-curated signaling pathway resources. *Nature methods*, *13*(12), 966-967.
3] Yang, W., Soares, J., Greninger, P., Edelman, E. J., Lightfoot, H., Forbes, S., ... & Garnett, M. J. (2012). Genomics of Drug Sensitivity in Cancer (GDSC): a resource for therapeutic biomarker discovery in cancer cells. *Nucleic acids research*, *41*(D1), D955-D961.