

Master thesis project "Explainable ML for drug 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 efficiency of a given drug for a certain disease profile. Some of them like RefDNN [1] are based on deep learning to provide accurate predictions. The price for this is inability to understand why the model makes various predictions.

To make predictions from deep learning models more interpretable, methods from explainable ML, like LIME [2] have been proposed. Your task will be to adopt LIME or similar model to understand predictions of RefDNN.

Data

- Drug related data such as chemical properties is freely available from the repositories cited in [1]
- Disease related data such as gene expressions are freely available from the repositories cited in [1]

Research questions

- Which methods for explainable AI are able to extract rule-based decisions explaining predictions of RefDNN locally, i.e in the context of a given patient?
- How can these rule-based decisions be extracted from the RefDNN model?
- Are the rule-based decisions obtained for the most popular drugs for a certain disease make sense biologically?
- How uncertain are predictions delivered by the rule-based decisions?

Prerequisites

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

Research Team

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Contact and application

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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] Ribeiro, M. T., Singh, S., & Guestrin, C. (2016, August). "Why should i trust you?" Explaining the predictions of any classifier. In *Proceedings of the 22nd ACM SIGKDD international conference on*

