SMARTR

Thesis proposal: System response profile visualization in drug discovery with non-linear dimensionality reduction methods from machine learning

About Smartr

Smartr is an expert bureau within data and AI. We work with the entire value chain from data strategy, research, algorithm development, prototyping, validation, software development and data engineering. We have a high level of seniority and we work close to academia. Supervising students at different levels gives us a great opportunity to develop unique skills but also serves as a base for recruitment. We intend to supervise three projects 2020.

Thesis project

This project is a collaboration with IRLAB which is a Biotech company based in Göteborg focusing on discovery and development of drugs to fight Parkinson´s disease. They have a unique data driven and explorative innovation process for finding molecules with a certain effect. IRLAB works very rigorously with data quality and have data from experiments performed for two decades. Old experiments keep creating new insights when combined with data from new experiments. The methods used today are mainly linear dimensionality reduction methods based on partial least squares or principal component analysis. The purpose of this thesis project is to investigate and evaluate non-linear methodology for dimensionality reduction such as self-organizing maps, t-SNE and autoencoders to name a few. The explorative part of the thesis work will consist of testing various methods and see visually and quantitively if the non-linear methods can extract patterns and clusters which the linear methods were unable to detect.

We seek 1-2 students for this project. The students should have a great interest in data and the extraction of useful information from complex data. Good skills in statistics and machine learning methodology are expected. Daytime the thesis work is mainly to be committed at Smartr's office at Vallgatan 3.

Supervisors

Supervisor at Smartr is Mattias Sundén and at Chalmers Rebecca Jörnsten. IRLAB will contribute with their expertise about the data, the application area and the current methodology. There will be frequent meetings at IRLAB where the students report on their progress and get important input. The student(s) can expect an active and interactive supervision.

Contact and application

A complete application contains CV, personal letter and transcripts from university. Please send it to adam.andersson@smartr.se and feel free to ask any questions.