AUTOMATED EXPERIMENTAL PLANNING

Context

Automated Experimental Planning is aimed to be a fully automated human-out-of-the-loop workflow to find an optimal design as fast as possible. Using (Bayesian) statistical machine learning techniques like GPR or BNN, we get a more complete picture about the possibility of reaching certain target value.

This problem consists of a two-way interaction between prediction and prescription. The first part is the forward problem, predicting from a set of input variables what the outcome will be. The inverse problem is much harder and more interesting. The inverse problem should recommend which products or processes to test next, and when a target is actually reached. It should thus function as a self-supervised search algorithm.

Knowing in advance if and how a target can be reached or not, is highly valuable in a large range of use-cases. It can materially improve any design workflow, from yoghurt and plastic polymers to fleet chamber matching.

Internship overview

- Master Student
- Internship and/or Graduation Assignment
- Mathware
- Location: Eindhoven

Technologies

- Machine Learning
- Bayesian Optimization
- Gaussian Process Regression
- Prescriptive Modelling
- MLOps
- Adaptive Experimental Design
- Experimental Workflow Simulation

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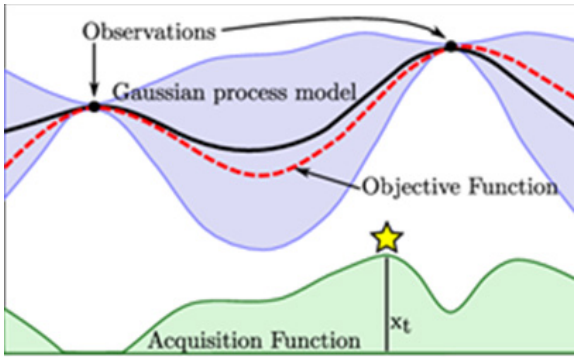
Assignment

Developing new products or processes takes dozens of design iterations with choices based on expert feedback. This process is costly and time-consuming, and doesn't necessarily converge towards the optimal solution. On top of that, checking all possible combinations of ingredients quickly becomes intractable.

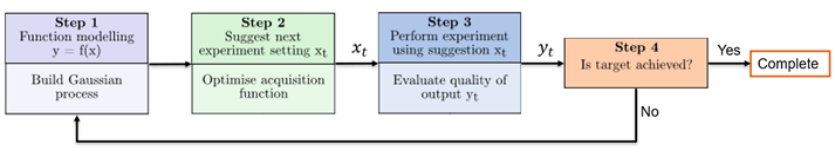


Bayesian Optimization is a design strategy that optimizes black-box functions globally without any knowledge about the underlying model. It is thus an ideal candidate to, quickly and easily, incorporate learnings from historical data when predicting new recipes that fulfill certain target criteria.
In this project, we aim to create a generalizable framework for Automated Experimental Planning based on the global concepts of Bayesian Optimization. This should then also be part of an Adaptive Experimental Design simulation to test the interactive capabilities of the optimization framework. The scope of this framework is from the initial experiment where there is no data yet, to the large data regime.

Activities

You will investigate and apply different Bayesian techniques (among which GPR and potentially BNN) aimed at experimental planning.

Furthermore, a testing environment for interactive testing of the algorithm should be developed. This framework should work for a variety of use-cases with as little adaptations as possible.



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Would you like to know more about this student assignment?

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