TECHNISCHE UNIVERSITÄT DARMSTADT

Bayesian optimization for the characterization of synthetic circuits

Pro-/ Project Seminar, Bachelor-/ Master Thesis

Fachbereich 18
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Bioinspirierte Kommunikationssysteme

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Motivation

Synthetic logic gates are basic boolean functions expressed using a biological process. For example an AND-gate can be build by using a synthetic biological circuit, with two inputs and one output. The inputs are expressed by two distinct molecules and a third molecule is used for the output. For implementing an AND-gate, the output should be high, if both inputs are high. In all other cases the output should be low. The biological system is subject to different parameters which can be set before starting an experiment run with the synthetic gate. These parameters should be set optimally, such that the AND-Gate has the desired functionality.

The problem is that one experiment can take hours. Even when speeding up the system utilizing parallel experiments with a robotic platform, a full grid search for all possible parameter combinations can take very long.

Instead of doing a grid search we use a learning algorithm, which proposes the new experiment setups in order to find the optimal configuration.

Approach

The score of how good a parameter set is can be described by a function, which maps the parameters to the score. The function can only be accessed by performing an experiment, which takes hours. Therefore, a Gaussian process model [1] is used. This model can be optimized using classical optimization techniques. However, there is an inherent trade-off between ”Should I exploit my current knowledge?” or ”Should I probe the system to learn more about how it behaves?”. Here, Bayesian optimization [2] is used to solve problems of hard to evaluate black box functions.

For more information on the topic of Bayesian optimization, have a look at the YouTube video [3].

Goals

Goals can be different, dependent on the experience of the student. Implementation of a Bayesian optimization algorithm on the robotic platform is one possibility. Another possibility is to come up with a better model for Bayesian optimization. Here, for example a stochastic differential equation model [4] might be a good candidate.

Prerequisites

There are no hard prerequisites for the task. However, for the theoretical work good mathematical skills are required, as well as programming skills in a high level programming language, such as Python. Basic skills helpful for the task are:

- Knowledge of inference algorithms, e.g., maximum likelihood, Bayesian inference, Hidden-Markov-Models.

- (Convex) Optimization algorithms, such as gradient descent.
- Basic knowledge of differential equations

For further information, please contact M.Sc. Bastian Alt.

References

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[4] Simo Särkkä and Arno Solin. *Applied stochastic differential equations*, volume 10. Cambridge University Press, 2019. https://users.aalto.fi/~asolin/sde-book/sde-book.pdf.