Applications of constrained Bayesian optimization to process systems

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Proposal for specialization project (15 ECTS) and possible continuation for master thesis (30 ECTS).

Optimization of functions which are expensive to evaluate is a relevant limiting factor in the implementation of RTO strategies. In this context, optimization strategies that avoid direct evaluation of the objective function become appealing, and Bayesian optimization is an effective tool for that end. However, most developments have been done for unconstrained optimization problems, and there is still room for improving the available constrained Bayesian optimization procedures, which would be of most relevant to the chemical engineering applications.

The objective of this project is to study constrained Bayesian optimization algorithms, applying them to simple problems of process systems engineering. The student may begin with the use of available packages, and possibly implement custom optimization algorithms. Possible case studies include process optimization under uncertainty and the MPC tuning problem. In this sense, the work can be focused on the development of new algorithms, or on the implementation of existing algorithms in relevant engineering problems.

The student should have interest in programming. Experience with Python is an advantage.