Bayesian Optimization of Simulation Components

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Simulations consist of many numerical components that affect the simulation accuracy and the required resources. Components such as models, discretization, solvers and floating point accuracy, all influence the simulation behavior. But, a user of the software is not primarily interested in specific choices of components, but rather in the final simulation accuracy and resource cost. Finding an optimal combination of these components that balances accuracy and computational resources can be a difficult and time-consuming process. Model-based Bayesian optimization methods are a useful tool to tackle such problems [1]. Many existing optimization approaches treat the optimization function as a black-box. We present a Bayesian approach that uses existing knowledge about the simulation components and that is tailored to optimize simulation parameters for a minimal error under run time constraints and vice versa.

The Bayesian optimization consists of three major steps that are visualized in Figure 1: First, we build surrogate models for the objective and constraint using existing data from simulation runs. Here, we rely on known asymptotic behavior, such as convergence theorems, to ensure that the model is able to extrapolate further away from the data. Modeling on a logarithmic scale allows the model to represent typical data, such as errors or run times, that spans over multiple orders of magnitude. Second, the models are used to evaluate a so-called acquisition function to select a new evaluation point most suited to improve the models and the current optimum. Selecting a good evaluation point is crucial as each data point corresponds to an expensive full simulation and we, thus, have to ensure that it leads to a maximal knowledge gain. When optimizing simulations, the evaluation cost for different simulation parameters can vary significantly, e.g. due to different discretization widths. Therefore, we present cost-aware acquisition functions that do not only take the constrained structure of the optimization problem into account, but also put the knowledge, that is gained by an evaluation

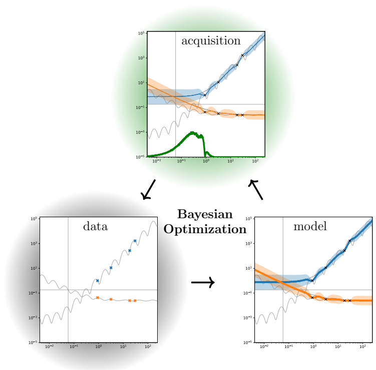

Figure 1: Constrained Bayesian optimization for a one-dimensional example problem. The objective function is blue, the constraint is orange, and the acquisition function is green.

in relation to the evaluation cost. Third, the run is actually executed, data are added to our already existing data set, and we proceed with the first step again in the next iteration.

We present modeling and optimization aspects and show our findings on the multi-scale multi-physics muscle simulation framework OpenDiHu [2].

References

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