Bayesian Optimization for Automated Parameterization of 1+1D Battery Cell Models

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Our goal is the automated parameterizing of battery cell models for model-based evaluation of experimental databases. The manual standard approach requires cell disassembly and individual measurements on the various cell components [1]. Measurement techniques include, e.g., galvanostatic intermittent titration technique (GITT) [2] or impedance spectroscopy [3]. They are complicated by their long run-time and considerably noise sensitivity.

Bayesian algorithms can directly incorporate the inherent uncertainties of model and measurement. The standard approach for parameterization is Markov-Chain Monte Carlo (MCMC) [4]. But with 1+1D battery cell models, their simulation time is too large for the tens of thousands of required samples.

In this contribution, we extend Bayesian Optimization (BOLFI) [5] with Expectation Propagation (EP) [6] to create a black-box optimizer suitable for modular 1+1D battery cell models. The algorithm can exploit a partitioning of the experimental data into features that is motivated by physico-chemcial understanding. However, the algorithm does not rely on approximative formulas and can be applied to a broad range of techniques. This approach reduces the number of required simulations for four parameters from 100,000 [4] to about 500. Furthermore, we can estimate parameter uncertainties and inter-dependencies. As an example, we process GITT full-cell measurements of lithium-ion batteries to non-destructively characterize the diffusivities of both electrodes at the same time.

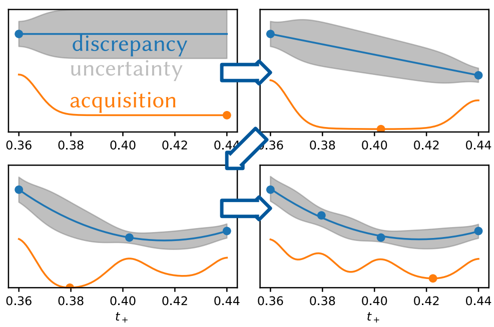

Figure 1: Scheme of Bayesian Optimization

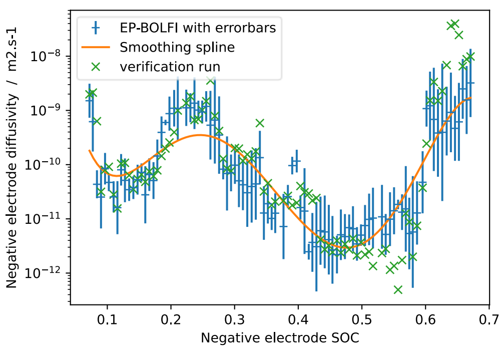

Figure 2**:** automated fitting of anode diffusivity to GITT

***Keywords**:* battery, uncertainty quantification, parameter sensitivity, model parameterization, mesoscale, Bayesian, in situ characterization, volume-averaged cell modelling, data-driven modelling.

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