Bayesian Optimization for Parameterization of Battery Cell Models

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We want to automatically parameterize battery cell models for the model-based evaluation of experimental databases. Today's manual standard approach requires cell disassembly and individual measurements on the various cell components [1]. Measurement techniques include galvanostatic intermittent titration technique (GITT) [2] or impedance spectroscopy [3]. They are complicated by their long run-time and considerably noise sensitivity. This calls for the adoption of Bayesian algorithms which can directly incorporate the inherent uncertainties of model and measurement. The standard approach for parameterization is Markov-Chain Monte Carlo (MCMC) [4]. But for complex 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 the experience of battery researchers. However, the algorithm does not rely on approximative formulas and can be applied to a broad range of techniques. In this way, our algorithm becomes fast, reproducible, and flexible. 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.

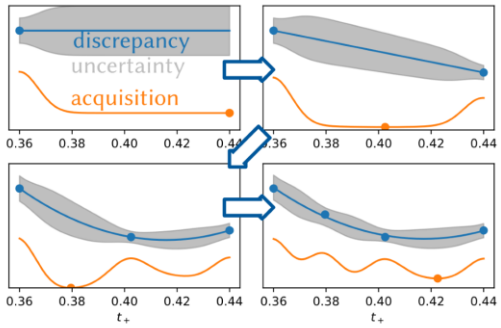

Figure 1: Scheme of Bayesian Optimization

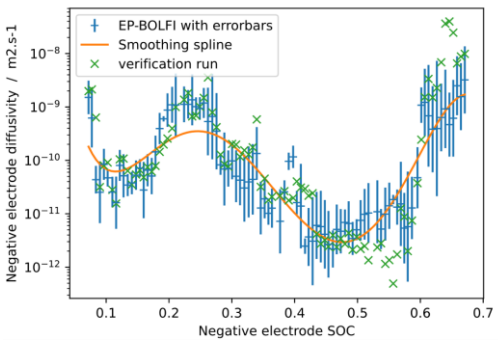

Figure 2**:** Automated fitting of anode diffusivity to GITT

1. Chen, C.; Planella, F. et al. Journal of The Electrochemical Society **2020**, 167 (8), 080534. DOI: 10.1149/1945-7111/ab9050.
2. Weppner, W.; Huggings, R. A. Journal of The Electrochemical Society **1977**, 124 (10), 1569-1578. DOI: 10.1149/1.2133112.
3. Single, F.; Horstmann, B.; Latz, A. The Journal of Physical Chemistry C **2019**, 123(45), 27327-27343. DOI: 10.1021/acs.jpcc.9b07389.
4. Aitio, A.; Marquis, S. et al. IFAC-PapersOnLine **2020**, 53 (2), 12497-12504. DOI: 10.1016/j.ifacol.2020.12.1770.
5. Gutmann, M. U.; Corander, J. Journal of Machine Learning Research (JMLR) **2016**, 17, 1-47. arXiv ID: 1501.03291.
6. Barthelmé, S.; Chopin, N.et al. Handbook of Approximate Bayesian Computation (ABC) **2018**, Chapter 13. DOI: 10.1201/9781315117195.