

Development, Analysis, and Parameterization of Physics-based Battery Models via Bayesian Model Selection

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This primer on Bayesian Model Selection (BMS) introduces its benefits to model-based battery characterization. With the uniquely limited experimental accessibility of the critical electrode-electrolyte interphase processes, we require first-principles models to study them via proxy measurements. Due to the typically low signal-to-noise ratio, evidence to support one possible mechanism explanation over another may be slight and easily missable or disputable. So we propose BMS as a quantifiable, reproducible, and self-assessing method to evaluate how well a dataset supports a model. The algorithms SOBER [1] and BASQ [2] have been developed to make BMS applicable to use cases like battery simulators, and already shown at earlier iterations of OBMS. Here, we showcase how to apply them in practice, in particular on electrolyte parameter identifiability from pulse tests as shown in Figure 1 and Electrochemical Impedance Spectroscopy (EIS) interpretation via continuum model simulators [3].

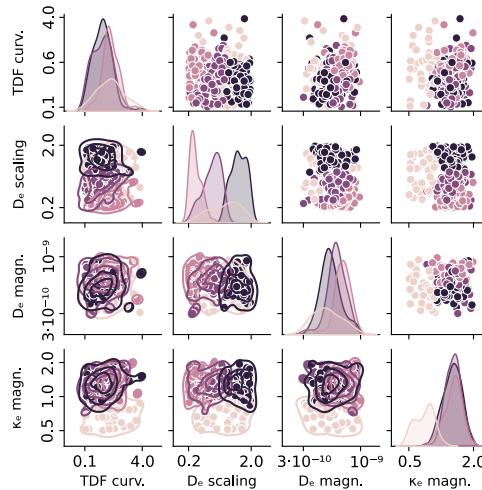


Figure 1: Optimally chosen training data for rapid electrolyte parameterization. The four grouped parameter sets represent the portions of parameter space to verify other parameterization methods on.

References

- [1] Adachi, M. & Hayakawa, S. & Jørgensen, M. & Hamid, S. & Oberhauser, H. & Osborne, M. A Quadrature Approach for General-Purpose Batch Bayesian Optimization via Probabilistic Lifting. *CoRR*. (2024), <https://doi.org/10.48550/arXiv.2404.12219>
- [2] Adachi, M. & Hayakawa, S. & Oberhauser, H. & Jørgensen, M. & Osborne, M. Fast Bayesian Inference with Batch Bayesian Quadrature via Kernel Recombination. *Advances in Neural Information Processing Systems*. **35**, 16533-16547 (2022), <https://doi.org/10.48550/arXiv.2206.04734>
- [3] Hallemans, N. & Courtier, N. & Please, C. & Planden, B. & Dhoot, R. & Timms, R. & Chapman, S. & Howey, D. & Duncan, S. Physics-based battery model parametrisation from impedance data. *Journal of The Electrochemical Society*. (2025), <https://doi.org/10.1149/1945-7111/add41b>