AUTOMATED BATTERY MODEL SELECTION WITH BAYESIAN QUADRATURE AND BAYESIAN OPTIMIZATION

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MOTIVATION AND AIM

- Many models are available for each process in a battery cell:
  - intercalation,
  - SEI growth,
  - cracking, …
- Selection from many combinations leads to a vast zoo of possible models to describe a particular battery cell.
- Bayesian methods are best suited to perform honest parameterization and selection in the face of uncertainty.
- Aim: a model selection algorithm that is both flexible and stable enough to handle the variety in battery models.

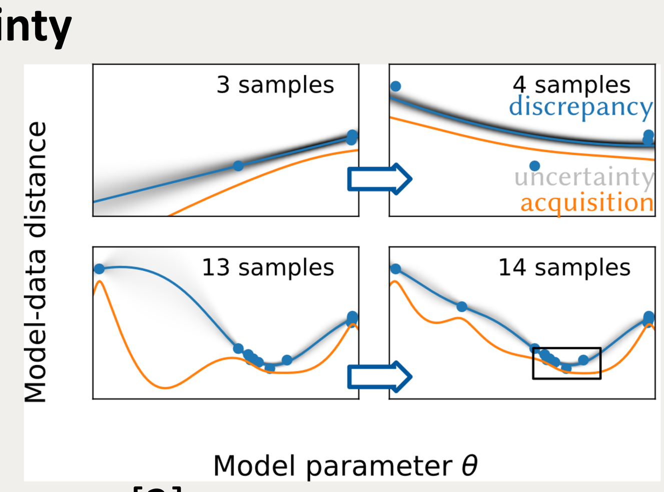
BAYES' THEOREM

- P(parameter | data) ∝ P(data | parameter) · P(parameter)
- Read: „The Likelihood of the model parameters matching the data updates the Prior knowledge to Posterior knowledge.“

BAYESIAN MACHINE LEARNING

Learn a function describing uncertainty

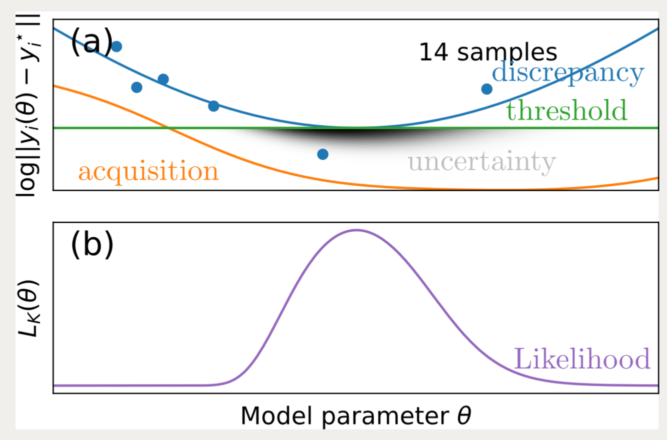
- The target to learn from will be ||model(parameter) – data||.
- Active Learning: leverage the included uncertainty to decide on the most informative next parameter sample.
- Choice of fit function: Gaussian Process [2].



BAYESIAN OPTIMIZATION (LFI)

Substitute Likelihood with ML function

- Likelihood is often intractable.
- Approximation: integral of ML fit function below a certain threshold.
- Optimal threshold can be calculated from ML fit function automatically [2].



BAYESIAN QUADRATURE

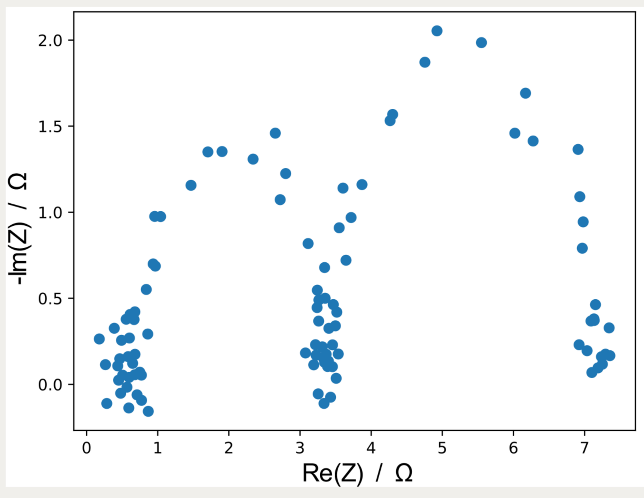
Evidence calculation for model selection

- Bayes' Theorem hides a normalizing factor, the so-called Evidence: ∫ P(data | parameter) · P(parameter) d(parameter).
- The Evidence is a reliable measure for the question „Could this data have originated from this model?“ [1].
- BQ can efficiently calculate the Evidence.

EXAMPLE APPLICATION: ECM

The simplest ECM to model arbitrarily many time constants is a chain of RC pairs (to infinity: DRT).

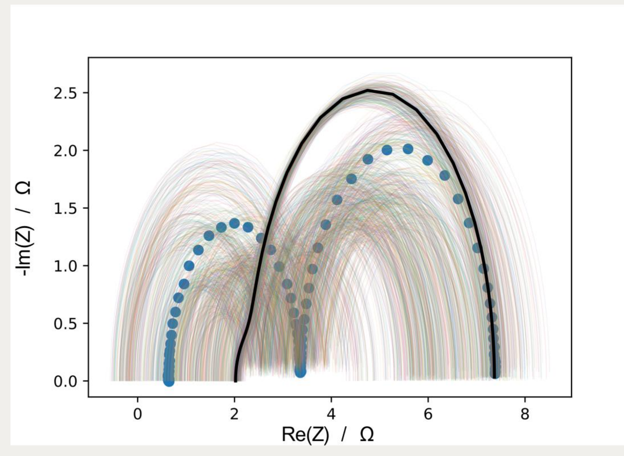
- Question: how many time constants / RC pairs are visible in any given impedance spectrum?
- High amount of noise makes classical optimization inaccurate [1].
- Overlapping time constants further complicate the task.



Impedance spectrum of a R-RC-RC-RC circuit with one RC element “hidden” in the noise at high frequency

BQ ISSUE: SENSITIVITY TO RANDOM INITIALIZATION

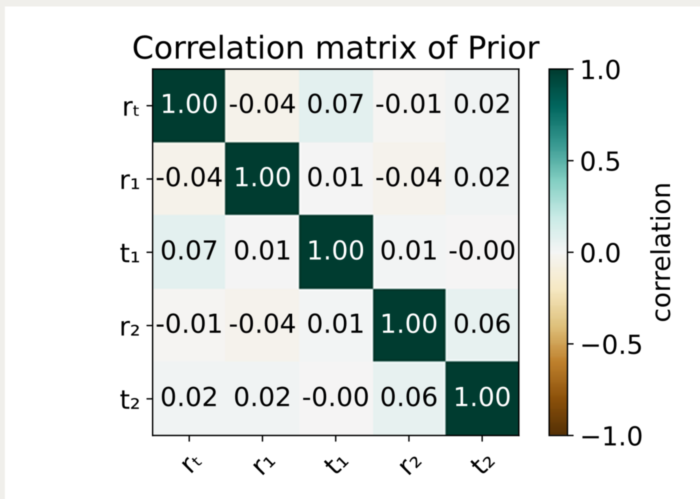
- The randomly chosen initial samples greatly affect BQ convergence.
- There is no “best” design of experiment to counteract this.
- While parameterization consistency is acceptable, model selection consistency is not.



Predictive posterior visualization after failed parameterization

BO PRECONDITIONING OF BQ

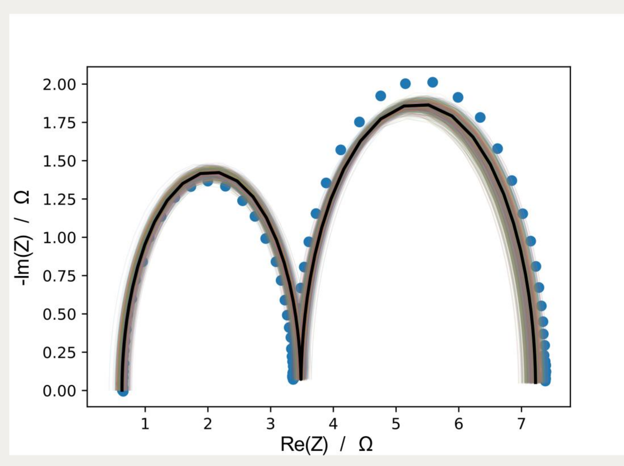
- Preemptively ended Bayesian Optimization gives a Posterior that is not much narrower, but greatly increases BQ success rate if used as a “preconditioned” Prior.
- Tests with a simply narrower Prior did not improve results.



Correlation matrix computed by EP-BOLFI [2]; variances barely changed

MODEL SELECTION

- With data from R-RC-RC, Evidence is computed once for R-RC-RC-RC.
- Without BO preconditioning, only 1 out of 6 times the Evidence for the correct R-RC-RC is higher.
- With BO preconditioning, 6 out of 6 times R-RC-RC scores higher.



Predictive posterior visualization after successful parameterization

SUMMARY

We suggest that Bayesian Quadrature as a model selection algorithm synergizes perfectly with Bayesian Optimization to reliably deliver automated model selection in complex scenarios.

[1] Adachi, M., et al., *IFAC-PapersOnLine* (2022), DOI 10.48550/arXiv.2210.17299
[2] Kuhn, Y., et al., *Batteries & Supercaps* **6** (2023), DOI 10.1002/batt.202200374