PyBOP: Python Battery Model Optimisation and Parameterisation

Brady Planden, Nicola Courtier, David Howey

Engineering Science
University of Oxford

Faraday ECR, March 2024

Battery
Intelligence
Lab

Battery models are useful for:

Physical Insight

How well does the model predict future evolution?

How does parameter X affect variable Y?

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Operational Improvements

What is the current state of the cell?

How fast can I charge the cell?

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How well does the model predict future evolution?
How does parameter X affect variable Y?

Operational Improvements
What is the current state of the cell?
How fast can I charge the cell?

Design Optimisation
How energy dense can the cell be?
What is the best configuration for this operation?

Well then, why isn't everyone modelling?

Parameter values

Geometric & non-geometric

Requires cell disassembly

Observability can be unclear

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Domain expertise

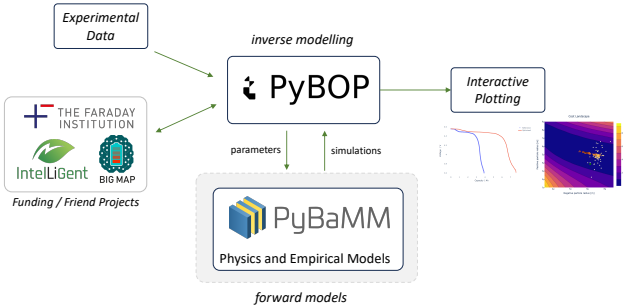
Is a more complex model needed?

Where should the complexity be added?

PyBOP is a platform to solve these challenges

Provides workflows for parameter identification and exploitation:

- Physics-based parameter identification
- Frequentistic and Bayesian methods
- Fast empirical model fitting
- Optimised cell designs



This is acheived through concise, inuitive design

```
# Generate problem, cost function, and optimisation class
problem = pybop.Problem(model, parameters, dataset)
cost = pybop.SumSquaredError(problem)
optim = pybop.Optimisation(cost, optimiser=pybop.GradientDescent)
x, final_cost = optim.run()
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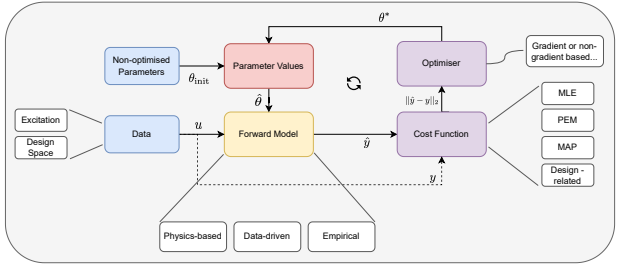

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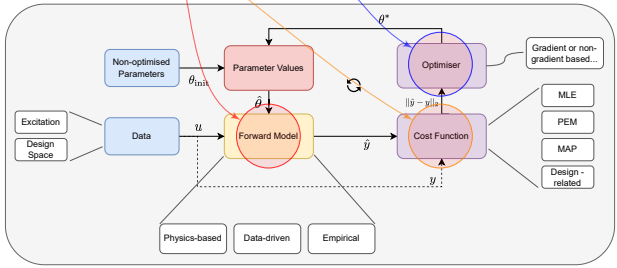


Example: Fast parameter estimation for circuit models

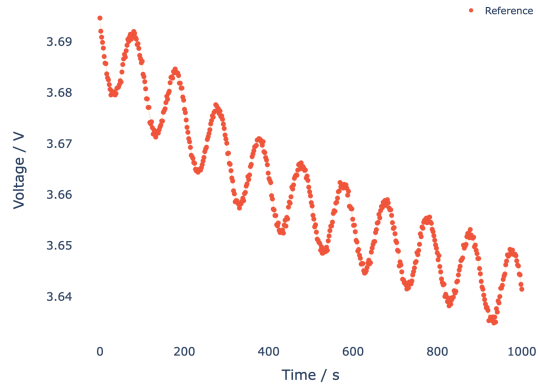
Benefiting from gradient and non-gradient optimisers

Model: 2-RC Thevenin model

Data: Synthetic data w/ unknown parameters

Conditions: discharge biased sinusoid function

Parameters: R_0, R_1, R_2, C_1, C_2



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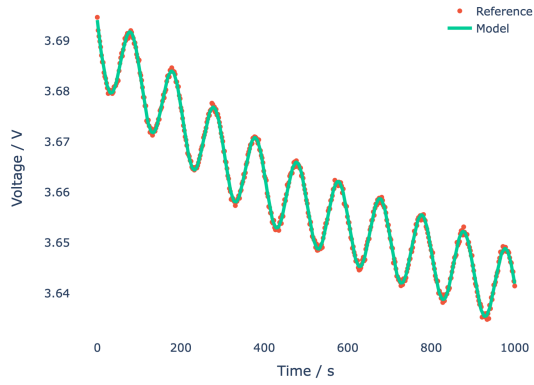
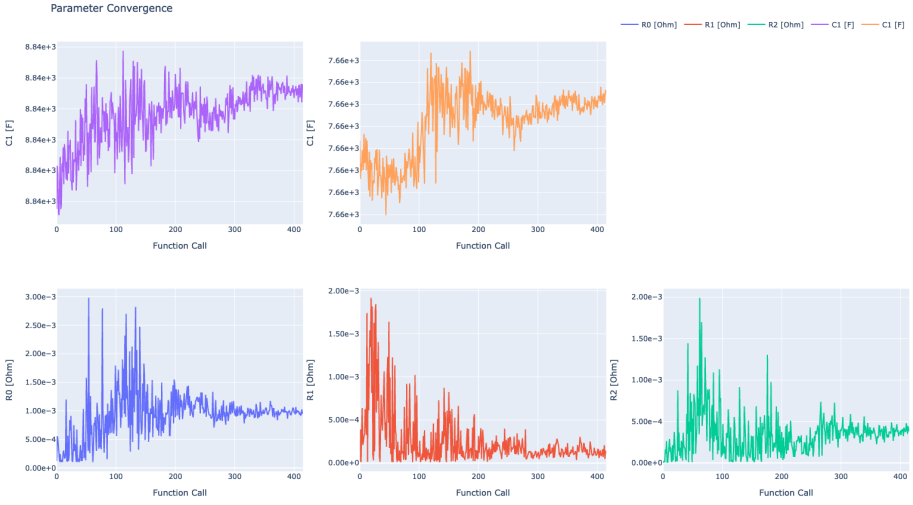


High dimensional parameter spaces still pose a challenge

Low identifiability on capacitance – excitation matters!



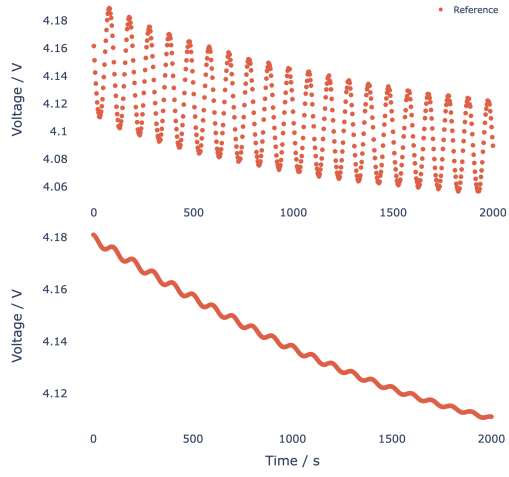
Example: SPM parameter identification

Electrode thickness values for a single particle model[a] are identified from synthetic data.

- Fitting signals: Terminal voltage and predicted OCV
- Initial conditions $\sim \mathcal{N}(\mu, \sigma^2)$
- Maximium iters: 150

Ground truth parameter values:

$$[\mathrm{L_n} = 8.52\text{e-}05,\ \mathrm{L_p} = 7.56\text{e-}05]$$



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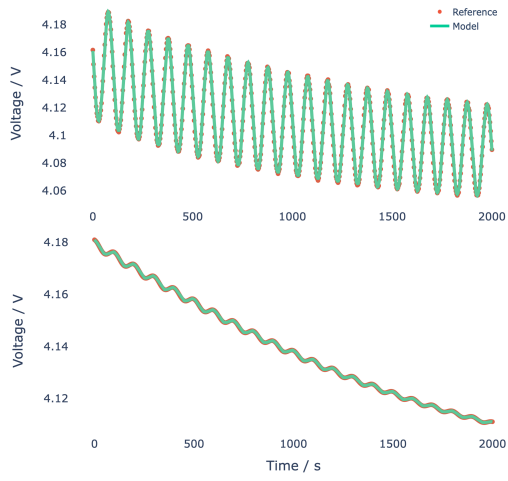

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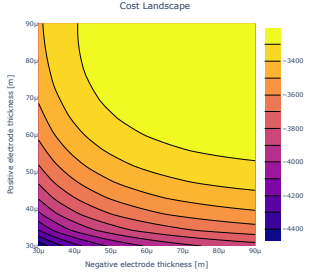
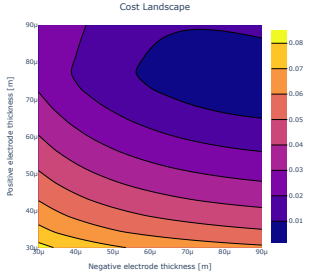
PyBOP provides multiple cost functions for parameter inference

Maximum Likelihood



Root Mean Squared Error



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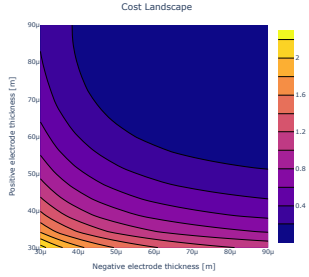

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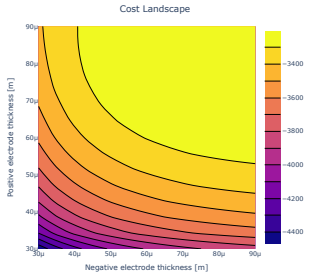

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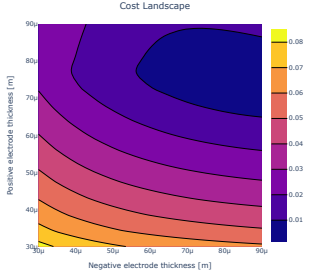

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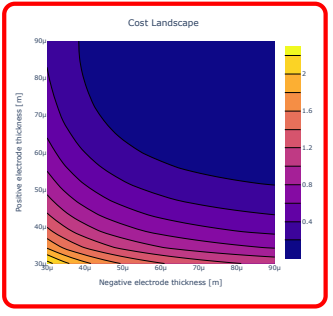
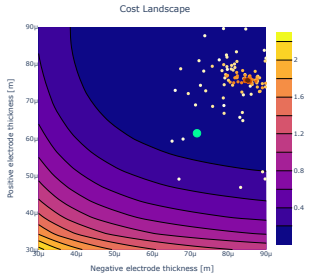
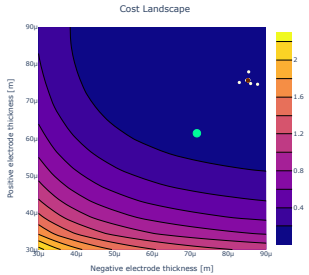


Verfiying optimality with convergence plots

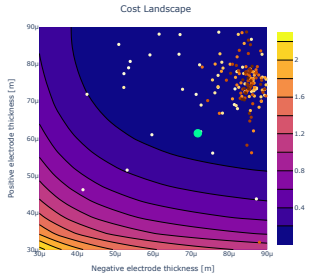
CMA-ES



Differential Evolution



Particle Swam



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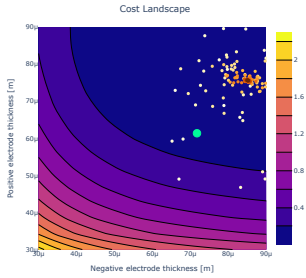

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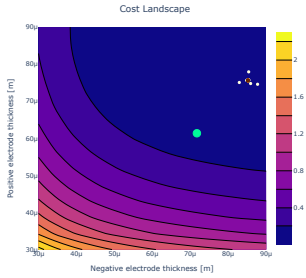

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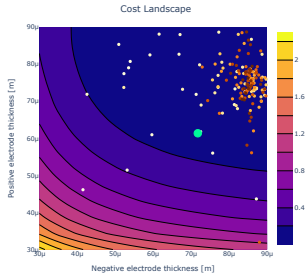


Example: Physics-based design optimisation

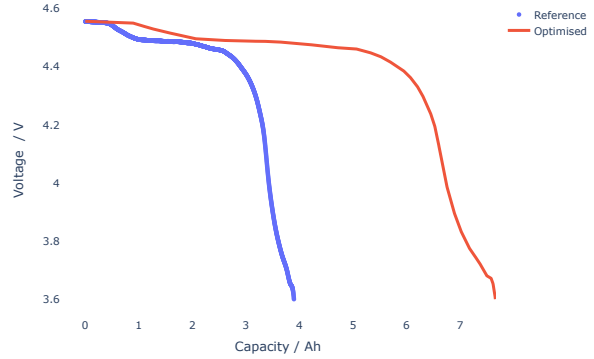
Chemistry: LNMO-Graphite/SiOx

Target: Maximize cell-level specific energy density

Parameters: Electrode coating thickness

Conditions: 1C cycling

Optimal:
$[L_n = 97\text{e-}06,\ L_p = 126\text{e-}06]$



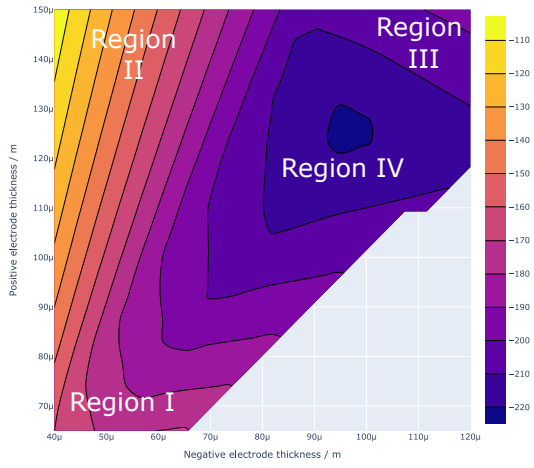
PyBOP enables physical insights into design optimisation

Region I: Electrodes too thin compared to inactive material

Region II: Poor N:P balancing

Region III: Electrodes too thick and cause transport limitations

Region IV: Ideal N:P balance and optimised wrt active material and transport



Get involved and become a developer and/or user!

GitHub Repository:
pybop-team/pybop

Installation:
`pip install pybop`

Examples

Docs

Benchmarks

Future Projects:

- Expansion of Bayesian methods
- New optimisation algorithms
- Improved workflows for battery relevant model optimisation
- Just released v24.3!