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PyBOP: A Python package for battery model optimisation and parameterisation

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DOI: 10.xxxxxx/draft

Software

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Editor: Open Journals

Reviewers:

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Submitted: 01 January 1970
Published: unpublished

Summary

The Python Battery Optimisation and Parameterisation (PyBOP) package provides methods for estimating and optimising battery model parameters, offering both deterministic and stochastic approaches with example workflows to assist users. PyBOP enables parameter identification from data for various battery models, including the electrochemical and equivalent circuit models provided by the popular open-source PyBaMM package (Sulzer et al., 2021). Using the same approaches, PyBOP can also be used for design optimisation under user-defined operating conditions across a variety of model structures and design goals. PyBOP facilitates optimisation with a range of methods, with diagnostics for examining optimiser performance and convergence of the cost and corresponding parameters. Identified parameters can be used for prediction, on-line estimation and control, and design optimisation, accelerating battery research and development.

Statement of need

PyBOP is a Python package providing a user-friendly, object-oriented interface for optimising battery model parameters. PyBOP leverages the open-source PyBaMM package (Sulzer et al., 2021) to formulate and solve battery models. Together, these tools serve a broad audience including students, engineers, and researchers in academia and industry, enabling the use of advanced models where previously this was not possible without specialised knowledge of battery modelling, parameter inference, and software development. PyBOP emphasises clear and informative diagnostics and workflows to support users with varying levels of domain expertise, and provides access to a wide range of optimisation and sampling algorithms. These are enabled through interfaces to PINTS (Clerx et al., 2019), SciPy (Virtanen et al., 2020), and PyBOP's own implementations of algorithms such as adaptive moment estimation with weight decay (AdamW), gradient descent, and cuckoo search.

PyBOP supports the battery parameter exchange (BPX) standard (Korotkin et al., 2023) for sharing parameter sets. These are typically costly to obtain due to the specialised equipment and time required for characterisation experiments, the need for domain knowledge, and the computational cost of estimation. PyBOP reduces the requirements for the latter two by providing fast parameter estimation methods, standardised workflows, and parameter set interoperability (via BPX).

PyBOP complements other lithium-ion battery modelling packages built around PyBaMM, such as `liionpack` for battery pack simulation (Tranter et al., 2022) and `pybamm-eis` for fast numerical computation of the electrochemical impedance of any battery model. Identified PyBOP parameters are easily exportable to other packages.

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Architecture

PyBOP has a layered structure enabling the necessary functionality to compute forward predictions, process results, and run optimisation and sampling algorithms. The forward model is solved using the battery modelling software PyBaMM, with construction, parameterisation, and discretisation managed by PyBOP's model interface to PyBaMM. This provides a robust object construction process with a consistent interface between forward models and optimisers. Furthermore, identifiability metrics are provided along with the estimated parameters (through Hessian approximation of the cost functions around the optimum point in frequentist workflows, and posterior distributions in Bayesian workflows).

PyBOP formulates the inference process into four key classes: model, problem, cost (or likelihood), and optimiser (or sampler), as shown in Figure 1. Each of these objects represents a base class with child classes constructing specialised functionality for different workflows. The model class constructs a PyBaMM forward model with a specified set of equations, initial conditions, spatial discretisation, and numerical solver. By composing PyBaMM directly into PyBOP, specialised models can be constructed alongside the standard models that can also be modified for different inference tasks. One such example is spatial re-discretisation, which is required when one or more geometric parameters are being optimised. In this situation, PyBOP rebuilds the PyBaMM model a minimum number of times while maintaining the problem, cost, and optimiser objects, providing improved performance. Alongside construction of the forward model, PyBOP's model class provides methods for obtaining sensitivities from the prediction, enabling gradient-based optimisation. A forward prediction, along with its corresponding sensitivities, is provided to the problem class for processing and exception control. A standardised data structure is then provided to the cost classes, which then computes a distance, design, or likelihood-based metric for optimisation. For deterministic optimisation, the optimisers minimise the cost function or the negative log-likelihood if a likelihood class is provided. Bayesian inference is provided by sampler classes, which accept the LogPosterior class and sample from it using PINTS-based Monte Carlo algorithms at the time of submission. In the typical workflow, the classes in Figure 1 are constructed in sequence, from left to right in the figure.

In addition to the core architecture, PyBOP provides several specialised inference and optimisation features. One example is parameter inference from electrochemical impedance spectroscopy (EIS) simulations, where PyBOP discretises and linearises the EIS forward model into a sparse mass matrix form with accompanying auto-differentiated Jacobian. This is then translated into the frequency domain, giving a direct solution to compute the input-output impedance. In this situation, the forward models are constructed within the spatial re-discretisation workflow, allowing for geometric parameter inference from EIS simulations and data.

A second specialised feature is that PyBOP builds on the JAX (Bradbury et al., 2018) numerical solvers used by PyBaMM by providing JAX-based cost functions for automatic forward model differentiation with respect to the parameters. This functionality provides a performance improvement and allows users to harness many other JAX-based inference packages to optimise cost functions, such as Numpyro (Phan et al., 2019), BlackJAX (Cabezas et al., 2024), and Optax (DeepMind et al., 2020).

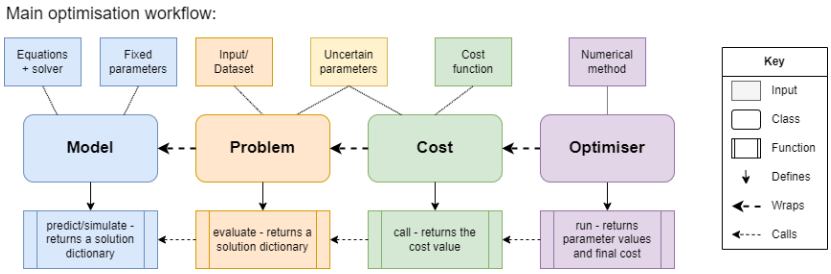

Figure 1: The core PyBOP architecture with base class interfaces. Each class provides a direct mapping to a step in the optimisation workflow.

The currently implemented subclasses for the model, problem, and cost classes are listed in Table 1. The model and optimiser classes can be selected in combination with any problem-cost pair.

Table 1: List of available model, problem and cost (or likelihood) classes.

Battery Models	Problem Types	Cost / Likelihood Functions
Single-particle model (SPM)	Fitting problem	Sum-squared error
SPM with electrolyte (SPMe)	Design problem	Root-mean-squared error
Doyle-Fuller-Newman (DFN)	Observer	Minkowski
Many-particle model (MPM)		Sum-of-power
Multi-species multi-reaction (MSMR)		Gaussian log likelihood
Weppner Huggins		Maximum a posteriori
Equivalent circuit model (ECM)		Volumetric energy density
		Gravimetric energy density
		Unscented Kalman filter

Similarly, the current algorithms available for optimisation are presented in Table 2. It should be noted that SciPy minimize includes several gradient and non-gradient methods. From here on, the point-based parameterisation and design-optimisation tasks will simply be referred to as optimisation tasks. This simplification can be justified by comparing Equation 5 and Equation 7; deterministic parameterisation is just an optimisation task to minimise a distance-based cost between model output and measured values.

Table 2: Currently supported optimisers classified by candidate solution type, including gradient information.

Gradient-based	Evolutionary	(Meta)heuristic
Weight decayed adaptive moment estimation (AdamW)	Covariance matrix adaptation (CMA-ES)	Particle swarm (PSO)
Improved resilient backpropagation (iRProp-)	Exponential natural (xNES)	Nelder-Mead
Gradient descent	Separable natural (sNES)	Cuckoo search
SciPy minimize	SciPy differential evolution	

In addition to deterministic optimisers Table 1, PyBOP also provides Monte Carlo sampling routines to estimate distributions of parameters within a Bayesian framework. These methods construct a posterior parameter distribution that can be used to assess uncertainty and practical identifiability. The individual sampler classes are currently composed within PyBOP from the PINTS library, with a base sampler class implemented for interoperability and direct integration

with PyBOP's model, problem, and likelihood classes. The currently supported samplers are listed in Table 3.

Table 3: Sampling methods supported by PyBOP, classified according to the proposed method.

Gradient-based	Adaptive	Slicing	Evolutionary	Other
Monomial gamma	Delayed rejection adaptive	Rank shrinking	Differential evolution	Metropolis random walk
No-U-turn	Haario Bardenet	Doubling		Emcee hammer
Hamiltonian	Haario	Stepout		Metropolis adjusted Langevin
Relativistic	Rao Blackwell			

Background

Battery models

In general, battery models (after spatial discretisation) can be written in the form of a differential-algebraic system of equations,

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = f(t, \mathbf{x}, \boldsymbol{\theta}), \tag{1}$$

$$0 = g(t, \mathbf{x}, \boldsymbol{\theta}), \tag{2}$$

$$\mathbf{y}(t) = h(t, \mathbf{x}, \boldsymbol{\theta}), \tag{3}$$

with initial conditions

$$\mathbf{x}(0) = \mathbf{x}_0(\boldsymbol{\theta}). \tag{4}$$

Here, t is time, $\mathbf{x}(t)$ are the (spatially discretised) states, $\mathbf{y}(t)$ are the outputs (e.g. the terminal voltage) and $\boldsymbol{\theta}$ are the unknown parameters.

Common battery models include various types of equivalent circuit models (e.g. the Thévenin model), the Doyle–Fuller–Newman (DFN) model (Doyle et al., 1993; Fuller et al., 1994) based on porous electrode theory, and its reduced-order variants including the single particle model (SPM) (Brosa Planella et al., 2022) and the multi-species multi-reaction (MSMR) model (Verbrugge et al., 2017). Simplified models that retain acceptable predictive accuracy at lower computational cost are widely used, for example in battery management systems, while physics-based models are required to understand the impact of physical parameters on performance. This separation of complexity traditionally results in multiple parameterisations for a single battery type, depending on the model structure.

Examples

Parameterisation

The parameterisation of battery models is challenging due to the large number of parameters that need to be identified compared to the number of measurable outputs (Andersson et al., 2022; Miguel et al., 2021; Wang et al., 2022). A complete parameterisation often requires stepwise identification of smaller sets of parameters from a variety of excitations and different data sets (Chen et al., 2020; Chu et al., 2019; Kirk et al., 2023; Lu et al., 2021).

A generic data-fitting optimisation problem may be formulated as:

$$\min_{\boldsymbol{\theta}} \ \mathcal{L}_{(\hat{\mathbf{y}}_i)}(\boldsymbol{\theta}) \quad \text{subject to equations (1)-(4)} \tag{5}$$

where $\mathcal{L} : \boldsymbol{\theta} \mapsto [0, \infty)$ is a cost function that quantifies the agreement between the model output $\mathbf{y}(t)$ and a sequence of observations $(\hat{\mathbf{y}}_i)$ measured at times t_i. Within the PyBOP framework, the `FittingProblem` class packages the model output along with the measured observations, both of which are then passed to the cost classes for the computation of the specific cost function. For gradient-based optimisers, the Jacobian of the cost function with respect to unknown parameters, $\partial\mathcal{L}/\partial\theta$, is computed for step-size and directional information.

Next, we demonstrate the fitting of synthetic data where the system parameters are known. In this example, we use PyBaMM's implementation of the single particle model with an added contact resistance submodel. We assume that the model is already parameterised except for two dynamic parameters, namely, the lithium diffusivity of the negative electrode active material particles (denoted "negative particle diffusivity") and the contact resistance. We generate synthetic data with a one-hour discharge from 100% to 0% state of charge, denoted as 1C rate, followed by 30 minutes of relaxation. This dataset is then corrupted with zero-mean Gaussian noise of amplitude 2 mV, with the resulting signal shown by the blue dots in Figure 2 (left). The initial states are assumed known, although this assumption is not generally necessary. The PyBOP repository contains several other example notebooks that follow a similar inference process. The underlying cost landscape to be explored by the optimiser is shown in Figure 2 (right), with the initial position denoted alongside the known true system parameters for this synthetic inference task. In general, the true parameters are not known.

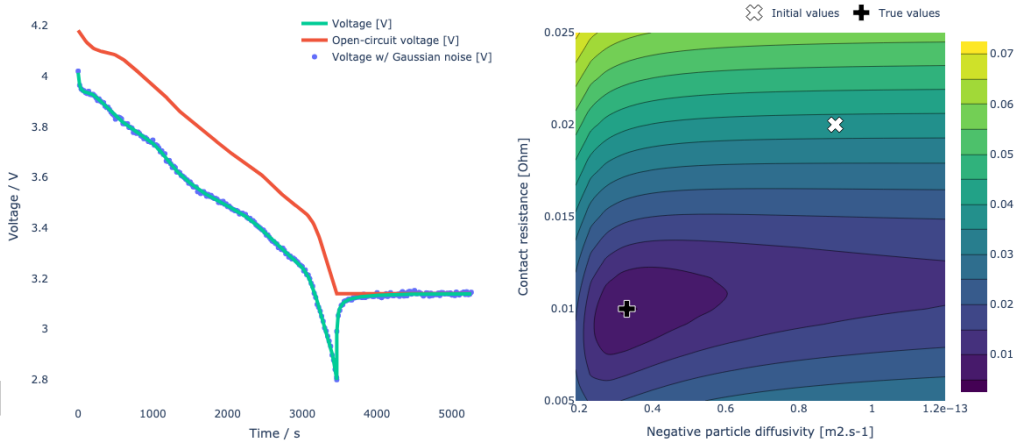

Figure 2: The fitted synthetic dataset (left) and cost landscape (right) for an example time-series battery model parameterisation using a root-mean-squared error cost function.

In a second example, we now showcase PyBOP's capability to fit electrochemical impedance data using methods within `pybamm-eis` that enable fast impedance computation of battery models (Dhoot et al., n.d.). The Figure 3 below shows the numerical impedance prediction available in PyBOP alongside the cost landscape constructed for the inference task. At the time of publication, gradient-based optimisation and sampling methods are not available when using an impedance workflow.

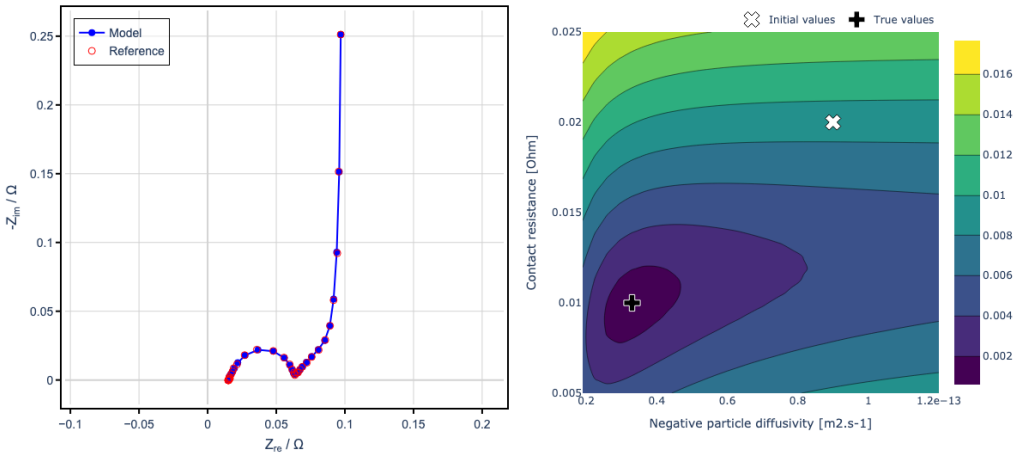

Figure 3: The data and model fit (left) and cost landscape (right) for a frequency-domain impedance parameterisation with a root-mean-squared error cost function, at 5% SOC.

To avoid overcomplicating this example, we will continue with identification in the time-domain; however, in general these two simulation methods can be combined for improved system excitation. As gradient information is available for this problem, the choice of distance-based cost function and optimiser is not constrained. Due to the difference in magnitude between the two parameters, we apply the logarithmic parameter transformation offered by PyBOP. This transforms the search space of the optimiser to allow for a common step size between the parameters, which is generally is not required, but improves convergence in this problem. As a demonstration of the parameterisation capabilities of PyBOP, Figure 4 (left) shows the rate of convergence for each of the distance-minimising cost functions, while Figure 4 (right) shows analogous results for maximising a likelihood. The optimisation is performed with SciPy Minimize using the gradient-based L-BFGS-B method.

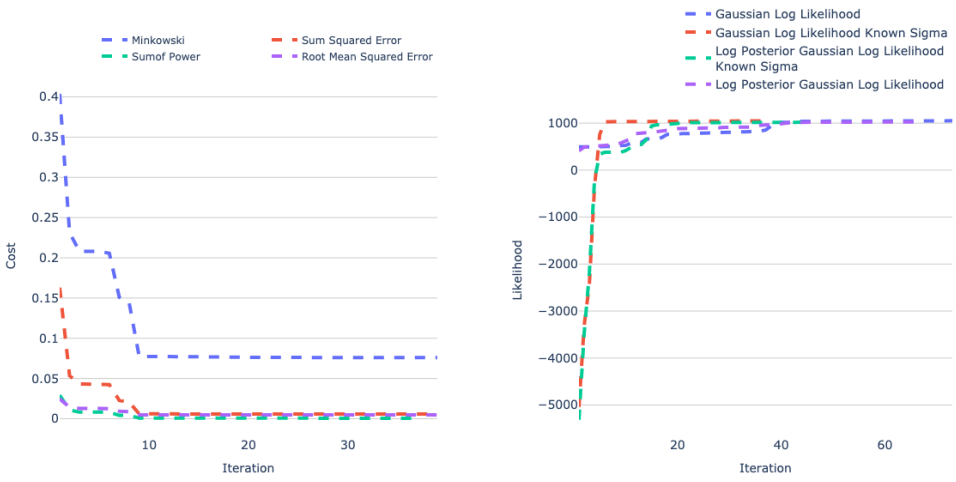

Figure 4: Convergence in the likelihood functions obtained using various likelihood functions and the L-BFGS-B algorithm.

Next, example performance of various optimisation algorithms is presented by category: gradient-based methods in Figure 6 (left), evolutionary strategies in Figure 6 (middle) and

(meta)heuristics in Figure 6 (right) for a mean squared error cost function. Note that the performance of the optimiser depends on the cost environment, prior information and corresponding hyperparameters for each specific problem.

Figure 5: Convergence in the parameter values obtained for the various optimisation algorithms provided by PyBOP.

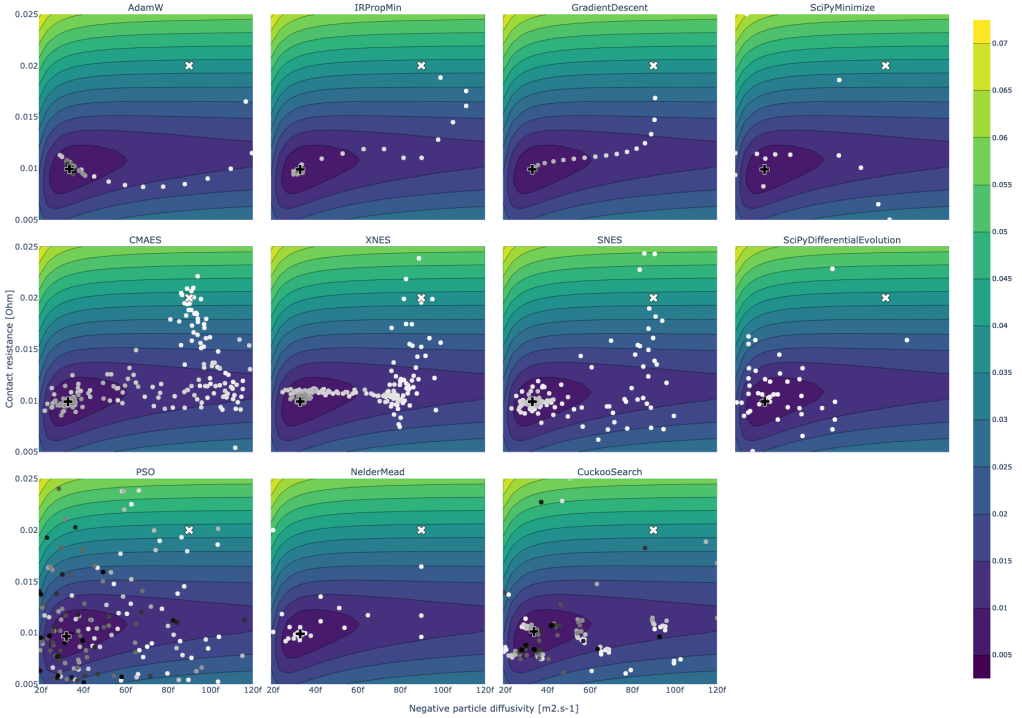

Figure 6: Cost landscape contour plot with corresponding optimisation traces. The three rows show the gradient-based optimisers (top), evolution strategies (middle), and (meta)heuristics (bottom).

This example parameterisation task can also be approached from a Bayesian perspective, solved using PyBOP's sampler methods. First, we introduce Bayes' rule,

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}, \tag{6}$$

where $P(\theta|D)$ is the posterior parameter distribution, $P(D|\theta)$ is the likelihood function, $P(\theta)$ is the prior parameter distribution, and $P(D)$ is the model evidence, or marginal likelihood, which acts as a normalising constant. In the case of maximum likelihood estimation or maximum a posteriori estimation, one wishes to maximise $P(D|\theta)$ or $P(\theta|D)$, respectively, and this may be formulated as an optimisation problem as per Equation 5. However, to estimate the full posterior parameter distribution one must use sampling or other inference methods to reconstruct the function $P(\theta|D)$. The posterior distribution provides information about the uncertainty of the identified parameters, e.g., by calculating the variance or other moments. Monte Carlo methods are used here to sample from the posterior. The selection of Monte Carlo methods available in PyBOP includes gradient-based methods such as no-u-turn (Hoffman & Gelman, 2011) and Hamiltonian (Brooks et al., 2011), as well as heuristic methods such as differential evolution (Braak, 2006), and also conventional methods based on random sampling with rejection criteria (Metropolis et al., 1953). PyBOP offers a sampler class that provides the interface to samplers, the latter being provided by the probabilistic inference on noisy time-series (PINTS) package. Figure 7 below shows the sampled posteriors for the synthetic model described above, using an adaptive covariance-based sampler called Haario Bardenet (Haario et al., 2001).

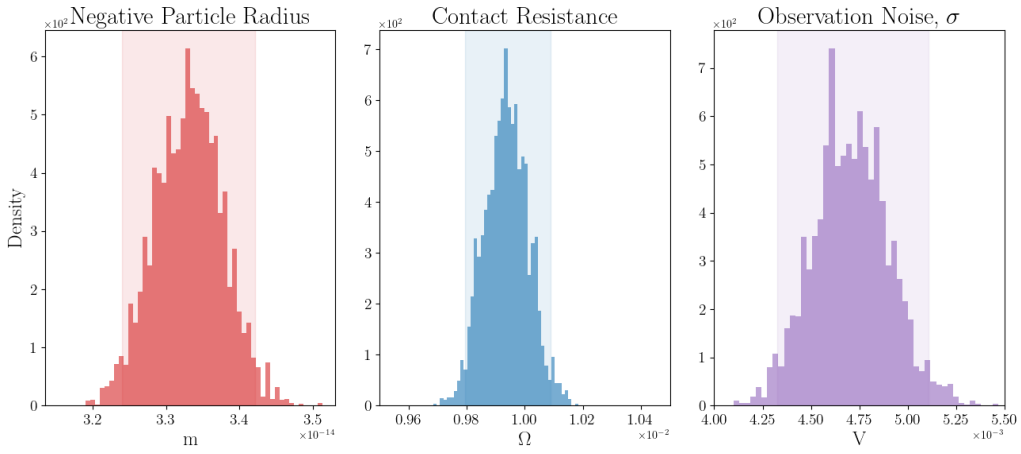

Figure 7: Posterior distributions of model parameters alongside identified noise on the observations. Shaded area denotes the 95th percentile credible interval for each parameter.

Design optimisation

Design optimisation is supported within PyBOP to guide future battery design development by identifying parameter sensitivities that can unlock improvements in battery performance. This problem can be viewed in a similar way to the parameterisation workflows described above, but with the aim of maximising a cost function rather than minimising it. PyBOP performs maximisation by minimising the negative of the cost function. In design problems, the cost metric is no longer a distance between two time series, but a metric evaluated on a model prediction. For example, to maximise the gravimetric energy (or power) density, the cost is the integral of the discharge energy (or power) normalised by the cell mass. Such metrics are typically quantified for operating conditions such as a 1C discharge, at a given temperature.

In general, design optimisation can be written in the form of a constrained optimisation problem as:

$$\min_{\boldsymbol{\theta}\in\Omega} \mathcal{L}(\boldsymbol{\theta}) \quad \text{subject to equations (1)-(4)} \tag{7}$$

where $\mathcal{L} : \boldsymbol{\theta} \mapsto [0, \infty)$ is a cost function that quantifies the desirability of the design and Ω is the set of allowable parameter values.

As an example, we consider the problem of maximising the gravimetric energy density subject to constraints on two of the geometric electrode parameters (Couto et al., 2023). For this example, we use the`PyBaMM` implementation of the single particle model with electrolyte (SPMe) to investigate the effect of the positive electrode thickness and the active material volume fraction on the target cost. Since the active material volume fraction is related to the electrode porosity, the porosity is defined with a driven constraint from the volume fraction. In this problem, we estimate the 1C rate from the theoretical capacity for each iteration of the design. For this example, we employ the Particle Swarm Optimisation (PSO) algorithm.

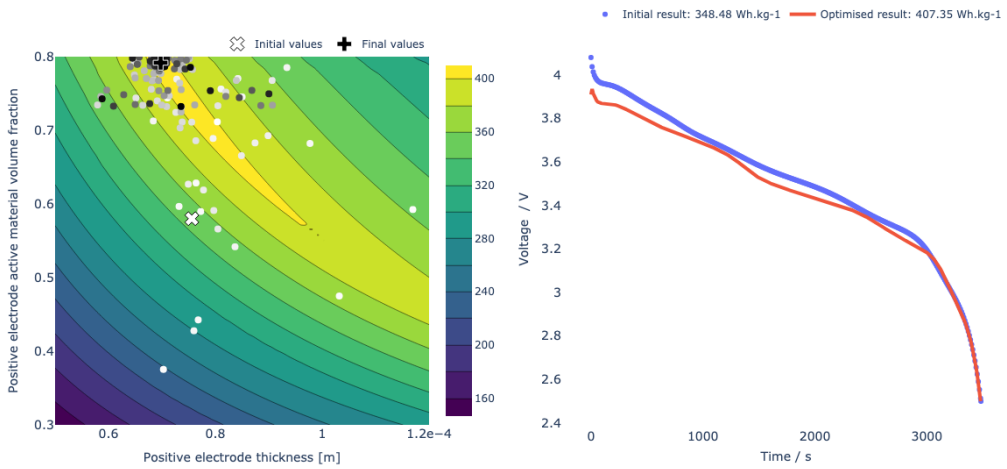

Figure 8: The gravimetric energy density landscape alongside the corresponding initial and optimised voltage profiles for a 1C discharge.

Figure 8 (left) shows the optimiser's search over the parameter space and (right) the predicted improvement in the discharge profile between the initial and optimised parameter values, simulated at their respective 1C rates.

Acknowledgements

We gratefully acknowledge all contributors to this package. This work was supported by the Faraday Institution Multiscale Modelling (MSM) project (ref. FIRG059), UKRI's Horizon Europe Guarantee (ref. 10038031), and EU IntelLiGent project (ref. 101069765).

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