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PyBOP: A Python package for battery model optimisation and parameterisation

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Summary

The Python Battery Optimisation and Parameterisation (PyBOP) package provides methods for parameterising and optimising battery models, offering both deterministic and stochastic approaches with example workflows to assist users. PyBOP enables parameter identification of various battery models, including the electrochemical and equivalent circuit models provided by the popular open-source PyBaMM package (Sulzer et al., 2021).

Similarly, PyBOP can be used for design optimisation under user-defined operating conditions across a variety of model structures and design goals. PyBOP facilitates model parameterisation using a range of methods, with diagnostics for examining the performance and convergence of the resulting parameters. Identified parameters can be used for prediction, on-line control, and design optimisation, supporting improved battery utilisation and development.

Statement of need

PyBOP is a Python package that provides 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. PyBOP is intended to serve a broad audience including students, engineers, and researchers in academia and industry, enabling the use of battery models for performance prediction where previously this was not possible without specialised knowledge of both modelling, parameter inference and software development. PyBOP emphasises clear and informative diagnostics and workflows to support users with varying expertise, and provides access to a wide range of different optimisation and sampling algorithms. These methods are provided through interfaces to PINTS (Clerx et al., 2019), SciPy (Virtanen et al., 2020), and PyBOP's own 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 battery parameter sets. These parameter sets are typically costly to obtain due to the specialised equipment and time required for characterisation experiments, the need for battery domain knowledge, and the computational cost of parameter estimation. PyBOP reduces these costs by providing fast parameter estimation, standardised workflows, and parameter set interoperability (via BPX).

This package 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 numerical impedance spectroscopy, since the identified parameters from PyBOP are easily exportable to these other packages.

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Architecture

PyBOP has a layered structure designed to compute forward model predictions, process the results, and package the necessary information for the optimisation and sampling algorithms. The forward model is solved using the popular battery modelling package, 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 models and optimisers. The statistical methods and optimisation algorithms are constructed to interface cleanly with the forward model predictions. Furthermore, identifiability metrics are provided with the estimated parameters (through Hessian approximation of the cost functions in frequentist workflows, and posterior distributions in Bayesian workflows).

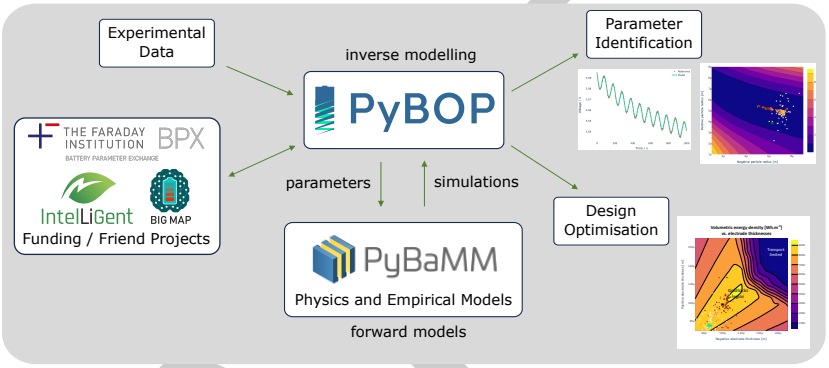

Figure 1: PyBOP's interface to supporting funding agencies, alongside a visualisation of the general workflow for parameterisation and optimisation.

PyBOP formulates the inference process into four key classes, namely the model, the problem, the cost, and the optimiser/sampler, as shown in Figure 2. Each of these objects represents a base class with child classes constructing specialised functionality for inference or optimisation workflows. The model class constructs a PyBaMM forward model for a given set of model equations provided by PyBaMM, initial conditions, spatial discretisation, and numerical solver. By composing PyBaMM directly into PyBOP, specialised models can be constructed alongside the standard models, which can be modified, and optimally constructed for the inference tasks. One such example is spatial rediscretisation, which is performed when geometric parameters are optimised. In this situation, PyBOP minimally rediscretises the PyBaMM model while maintaining the problem, cost, and optimiser objects, providing improved performance benefits to users. Alongside construction of the forward model, PyBOP's model class provides methods for obtaining sensitivities from the prediction, enabling gradient-based optimisation algorithms. This 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 corresponding cost function or the negative log-likelihood if a likelihood class is provided. Bayesian inference is provided by Monte Carlo sampling 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 2 are constructed in sequence.

In addition to the core architecture, PyBOP provides several specialised inference and optimisation processes. One such instance is parameter inference from EIS forward model predicitions. PyBOP discretises the EIS forward model inso sparse mass matrix form with accompanying auto-differentiated Jacobian. These objects are then translated into the frequency domain with a linear solution used to compute the battery model impedance. In this situation, the forward models are constructed within the spatial rediscretisation workflow, allowing for geometric parameter inference from EIS forward model predictions. Furthermore, PyBOP builds on the

JAX (Bradbury et al., 2018) numerical solvers provided 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 use many other JAX-based inference packages in order to optimise their cost function, such as Numpyro (Phan et al., 2019), BlackJAX (Cabezas et al., 2024), and Optax (DeepMind et al., 2020).

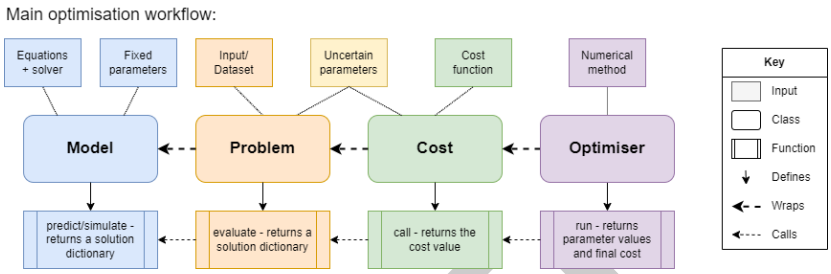

Figure 2: The core PyBOP architecture, showcasing the base class interfaces. Each class provide direct mapping to a classical step in the optimisation workflow.

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 tasks are presented in Table 2. It should be noted that SciPy minimize has gradient and non-gradient methods. From now on, the point-based parameterisation and design optimisation tasks will simply be referred to as optimisation tasks. This simplification can be justified by examining Equation 5 and Equation 7 and confirming that deterministic parameterisation can be viewed as an optimisation task to minimise a distance-based cost function.

Table 2: The currently supported optimisation algorithms 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

Gradient-based	Evolutionary	(Meta)heuristic
SciPy minimize	SciPy differential evolution	

As discussed above, PyBOP provides both point-based optimisation estimates Table 1 in addition to Monte Carlo sampling routines in order to recover distributions of likely parameter values. The Monte Carlco methods construct a posterior distribution on the inference parameters, which can be used for uncertainty and practical identifiability. The individual sampler classes are currently composed within PyBOP from the PINTS library, with a base sampling class implemented for interoperability and direct integration with the PyBOP 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:

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

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

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

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 capabilities at a 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 battery 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 measurable outputs (Andersson et al., 2022; Miguel et al., 2021; Wang et al., 2022). A complete parameterisation often requires a 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).

A generic data fitting optimisation problem may be formulated as:

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

where $\mathcal{L} : \boldsymbol{\theta} \mapsto [0, \infty)$ is a cost function that quantifies the agreement between the model, $\mathbf{y}(t_i)$ and a sequence of measured 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 `FittingCost` classes for the computation of the specific cost function. For gradient-based optimisers, the Jacobian of the cost function with respect to the unknown parameters, $(\frac{\partial \mathcal{L}}{\partial \theta})$ 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 problem, we use `PyBaMM`'s implementation of the single particle model (SPM) with an added contact resistance submodel. We assume that the battery model is already parameterised except for two dynamic parameters, namely the lithium diffusivity of the negative electrode active material particle (denoted "negative particle diffusivity") and the contact resistance. We generate synthetic data from a one-hour discharge from 100% state of charge, to 0% (denoted as 1C rate), followed by 30 minutes of relaxation. This data is then corrupted with zero mean Gaussian noise of amplitude 2mV, shown by the dots in Figure 3 (left). The initial states are assumed known, although such an assumption is not generally necessary. The `PyBOP` repository contains multiple example notebooks that follow a similar inference process for readers that would like further information. The underlying cost landscape to be explored by the optimiser is shown in Figure 3 (right) with the initial position denoted alongside the known system parameters for this synthetic inference task. In general, the true parameters are not known a priori.

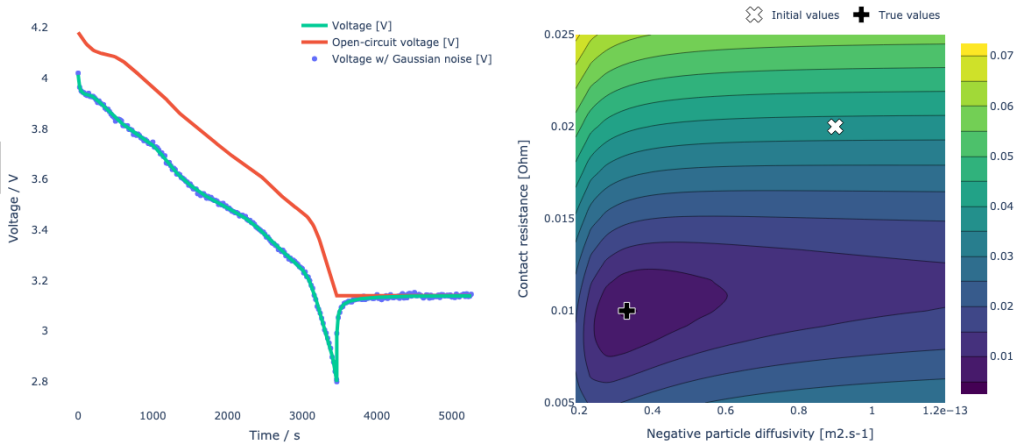

Figure 3: The cost landscape for the time-series parameterisation problem with a root mean squared error cost function.

As mentioned above, PyBOP also provides inference and optimisation capabilities through numerical impedance spectroscopy. This is based on the methods presented in the pybamm-eis package and allows fast impedance computation by inversion of the sparse PyBaMM mass matrix after scaling and subtraction of the auto-differentiated Jacobian matrix. More information about this procedure is available in (Dhoot et al., n.d.). The Figure 4 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.

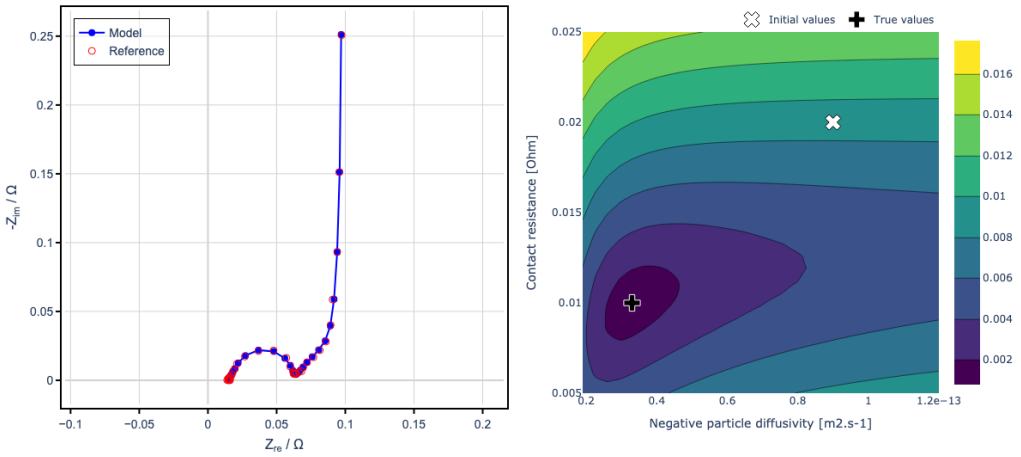

Figure 4: The cost landscape for the frequency domain impedance parameterisation problem with a root mean squared error cost function at 5% SOC.

To avoid over complicating this example, we will continue with identification in the time-domain; however, in general these two forward-model prediction 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 different magnitudes of the two parameters, we apply the logarithmic parameter transformation offered by PyBOP. This transforms the optimisers 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 5 (left) shows the rate of convergence for each of the distance-minimising cost functions, while Figure 5 (right) shows analogous results for maximising a likelihood. The optimisation is performed with SciPy Minimize using the gradient-based L-BFGS-B method.

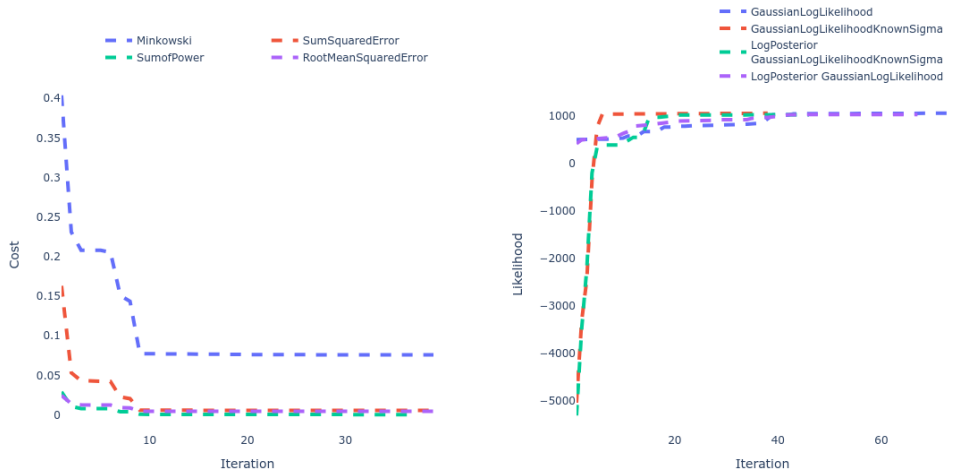

Figure 5: Convergence in the likelihood functions obtained using various likelihood functions and the L-BFGS-B algorithm.

Next, the performance of the various optimisation algorithms is presented by category: gradient-based in Figure 7 (left), evolutionary strategies in Figure 7 (middle) and (meta)heuristics in Figure 7 (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.

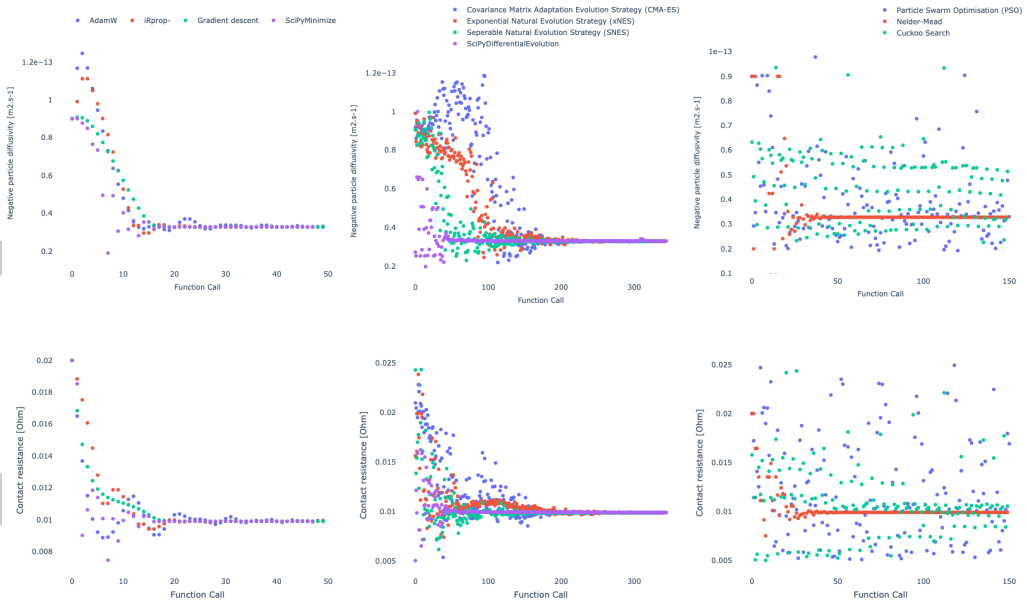

Figure 6: Convergence in the parameter values obtained for the various optimisation algorithms provided by PyBOP.

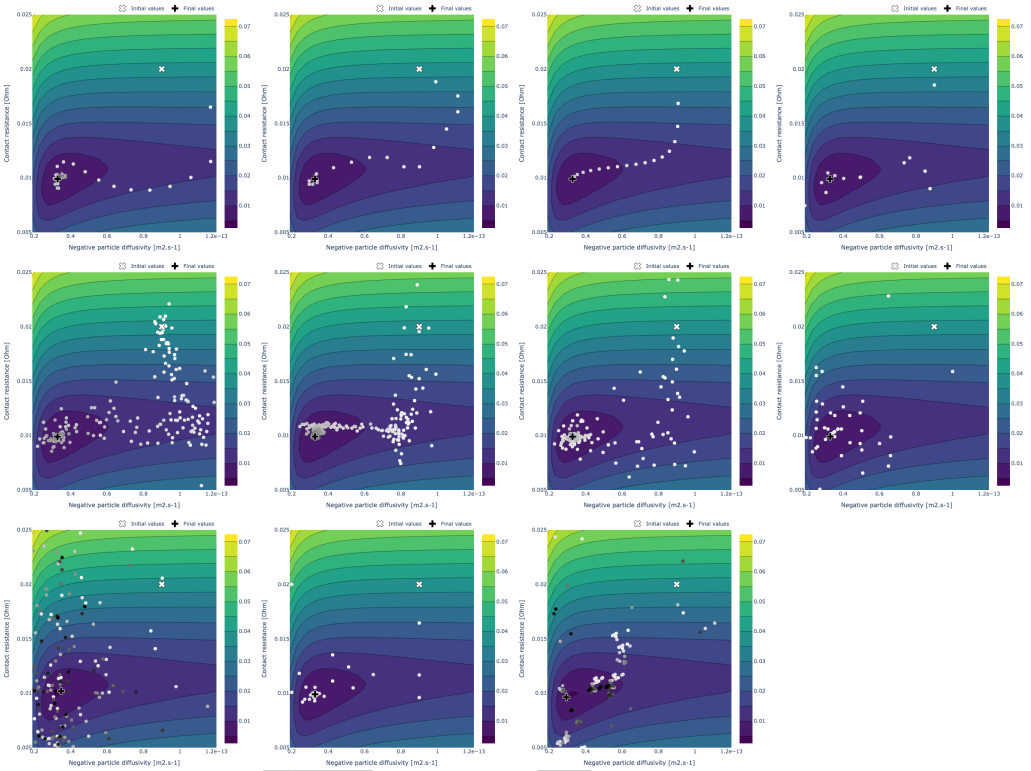

Figure 7: Cost landscape contour plot with corresponding optimisation traces. The top row represents the gradient-based optimisers, the middle row is the evolution-based, and the bottom row is the (meta)heuristics. The order from left to right corresponds to the entries in Table 2.

This parameterisation task can also be approached from a Bayesian perspective, which we will present below using PyBOP's sampler methods. The optimisation equation presented in Equation 5 does not represent the Bayesian parameter identification task, and as such we introduce the Bayes theorem as,

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

where, $P(\theta|D)$ is the posterior and represents the probability density function of the parameter. $P(D|\theta)$ is the likelihood function and assesses the parameter values alongside a noise model. $P(\theta)$ encapsulates the prior knowledge about the parameters, and finally $P(D)$ is the model evidence and acts as a normalising constant so that the final posterior is a correctly scaled density function. Our goal in parameter inference is to identify the parameter values with the highest probability, which can be represented as a point-based metric or as the posterior distribution, which provides additional information about the uncertainty of the identified parameters. Monte Carlo sampling methods are available to obtain this posterior distribution. These methods sample from the posterior using a variety of methods, including 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 finally conventional methods based on random sampling with rejection criteria (Metropolis et al., 1953). PyBOP offers a sampling class that provides an interface to these samplers, which are supported by the Probabilistic Inference of Noise Time-Series (PINTS) package. Figure 8 below shows the sampled posterior for the synthetic workflow described above, using an adaptive covariance-based sampler, Haario Bardenet (Haario et al., 2001).

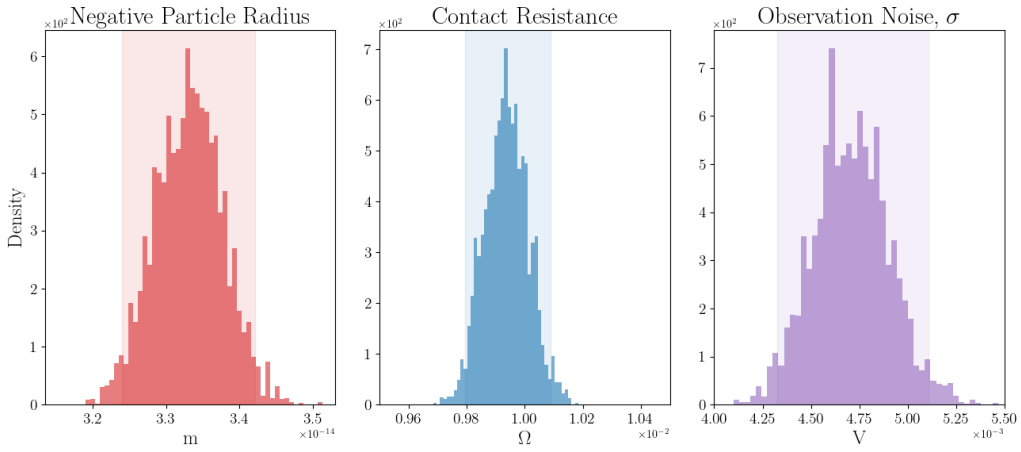

Figure 8: Posterior distributions for model parameters alongside identified noise on the observations. Shaded area denotes confidence bounds for each parameter.

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 distance metric rather than minimising it. In the case of design optimisation to maximise gravimetric energy density, PyBOP minimises the negative of the cost function, where the cost metric is no longer a distance between two time series vectors, but the integrated energy of the vector normalised by with the corresponding cell mass. This is typically quantified for operating conditions such as a 1C discharge, at a given temperature.

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 thePyBaMM 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.

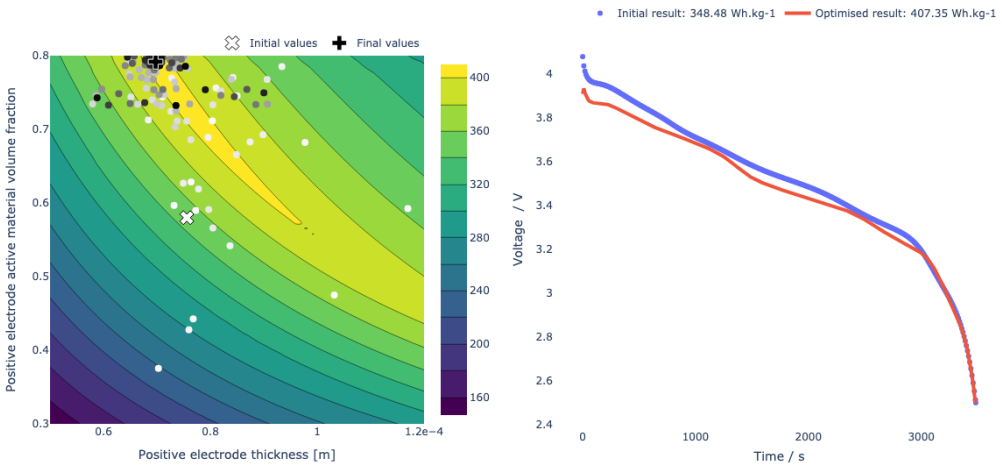

Figure 9: The gravimetric landscape alongside the corresponding initial and optimised voltage profiles for a 1C discharge.

Figure 9 (left) shows the optimiser's search over the gravimetric energy density parameter space. The predicted improvement in the discharge profile between the initial and optimised parameter values (right) for their respective applied 1C current.

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