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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 a set of methods for the parameterisation and optimisation of battery models, offering both Bayesian and frequentist approaches with example workflows to assist the user. PyBOP can be used for parameter identification of various models, including the electrochemical and equivalent circuit models provided by the popular open-source package PyBaMM (Sulzer et al., 2021). Similarly, PyBOP can be used for design optimisation under user-defined operating conditions for a given parameter. PyBOP allows the user to parameterise battery models using a variety of methods and provides diagnostics on the performance and convergence of the optimisation. The identified parameters can be used for prediction, on-line control and design optimisation, all of which support improved battery utilisation and development.

Statement of need

PyBOP is designed to provide a user-friendly, object-oriented interface for the optimisation of battery models which have been implemented in existing battery modelling software, e.g. PyBaMM (Sulzer et al., 2021). PyBOP is intended to serve a broad audience of students, engineers, and researchers in both academia and the battery industry. PyBOP prioritises clear and informative diagnostics and workflows for both new and experienced users, while also leveraging advanced optimisation algorithms provided by SciPy (Virtanen et al., 2020), PINTS (Clerx et al., 2019), and internal implementations such as the adaptive moment estimation with weight decay (AdamW), as well as Cuckoo search.

PyBOP supports the Battery Parameter eXchange (BPX) standard (Korotkin et al., 2023) for sharing battery parameter sets. These parameter sets are costly to obtain due to a number of factors: the equipment cost and time spent on characterisation experiments, the requirement of battery domain knowledge, and the computational cost of parameter estimation. PyBOP reduces the barrier to entry and ongoing costs by providing an accessible workflows' that efficiently connects battery models with numerical optimisers, as well as explanatory examples of battery parameterisaton and design optimisation.

This package complements other tools in the field of lithium-ion battery modelling built around PyBaMM, such as liionpack for simulating battery packs (Tranter et al., 2022) as the identified parameters are easily exportable from PyBOP into such packages aimed at predictive forward modelling.

- PyBOP incorporates a PDE solver, and parameterisation/optimisation workflows into a single package.

- PyBOP provide identifiablity estimates for the identified parameter set (Hessian approximation, fisher information?, Posterior variance, CI upper/lower)

Architecture

PyBOP is a Python package provided through PyPI, currently available for Python versions 3.9 to 3.12. The package composes the popular battery modelling package PyBaMM for forward modelling, while providing classes for parameterisation and optimisation. These workflows are constructed through a mixture of internal algorithms, as well as popular optimisation packages such as Pints and SciPy. PyBOP formulates the optimisation workflow through four main classes, namely the model, problem, cost, and optimiser or sampler, as shown in **??**. Each of these objects has a base class and example subclasses that combine to form a flexible and extensible codebase. The typical workflow would be to define an optimisation problem by constructing the objects in sequence.

PyBOP's high level interface.

Figure 1: PyBOP's high level interface.

Furthermore, to construct this workflow, the following classes represent the process required. The current instances for each class are listed in Table 1 and Table 2.

Table 1: List of preset subclasses for the model, problem and cost classes.

Battery Models	Problem Types	Cost / Likelihood Functions
Single particle model (SPM)	Fitting Problem	Sum of Squared Error
SPM with electrolyte (SPMe)	Design Problem	Root Mean Squared Error
Doyle-Fuller-Newman (DFN)	Observer	Gaussian Log Likelihood
Many particle model (MPM)		Maximum a Posteriori
Multi-species multi-reaction (MSMR)		Unscented Kalman Filter
Weppner Huggins		Gravimetric Energy Density
Equivalent circuit model (ECM)		Volumetric Energy Density

Table 2: List of available optimisers. (*) Scipy Minimize provides gradient and non-gradient methods.

Gradient-based	Non-gradient-based
Adaptive Moment Estimation with Weight Decay (AdamW)	Covariance Matrix Adaptation Evolution Strategy (CMA-ES)
Improved Resilient Backpropagation (iRProp-)	Exponential Natural Evolution Strategy (xNES)
Gradient Descent	Separable Natural Evolution Strategy (sNES)
SciPy Minimize (*)	Particle Swarm Optimization (PSO)
	SciPy Differential Evolution
	Nelder-Mead
	Cuckoo Search

The cost functions are grouped by problem type, while each of the models and optimisers may be selected in combination with any problem-cost pair. As previously discussed, PyBOP offers Bayesian inference methods such as Maximum a Posteriori (MAP) presented alongside the frequentist methods in Table 2. A full Bayesian framework is available from a Markov-chain Monte Carlo implemented within PyBOP, capable of providing uncertainty on the inferred

parameters. These samplers are currently composed within PyBOP from the Pints' library, with a base class implemented for interopability and direct application to the PyBOP model, problem, and likelihood classes. The currently support MCMC samplers is shown in Table Table 3.

Table 3: List of available Monte Carlo samplers.

Gradient-based	Non-gradient-based
Adaptive Moment Estimation with Weight Decay (AdamW)	Covariance Matrix Adaptation Evolution Strategy (CMA-ES)
Improved Resilient Backpropagation (iRProp-)	Exponential Natural Evolution Strategy (xNES)
Gradient Descent	Separable Natural Evolution Strategy (sNES)
SciPy Minimize (*)	Particle Swarm Optimization (PSO)
	SciPy Differential Evolution
	Nelder-Mead
	Cuckoo Search

- Performance (multiprocessing)
- Construction of PyBaMM models (geometric and non-geometric identification)
- Feasability checks on identified parameters
- Spatial identification methods?
- Documentation supported at X
- Benchmarks provided at X
- Plotting available via Plotly (cost landscapes, gradient landscapes)
- Test suite provided by pytest (~98% coverage)
- Standalone implementations (Bring your own model)

Background

Battery models

In general, battery models can be written in the form of a differential-algebraic system of equations:

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

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

with initial conditions

$$\mathbf{x}(0) = \mathbf{x}_0(\boldsymbol{\theta}). \tag{3}$$

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

Common battery models include various types of equivalent circuit model (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) (Planella et al., 2022), as well as the multi-scale, multi-reaction (MSMR) model (Verbrugge et al., 2017).

Simplified models that retain good prediction capabilities at a lower computational cost are widely used, for example within battery management systems, while physics-based models are required to understand the impact of design parameters on battery performance.

Examples

Parameterisation

Battery model parameterisation is difficult due to the high ratio of the number of parameters to measurable outputs (Andersson et al., 2022; Miguel et al., 2021; Wang et al., 2022). A complete parameterisation often requires a step-by-step identification of smaller groups of parameters from a variety of different datasets (Chen et al., 2020; Chu et al., 2019; Kirk et al., 2023).

A generic data fitting optimisation problem may be formulated as:

$$\min_{\boldsymbol{\theta}} \ \mathcal{L}_{(\mathbf{y}_i)}(\boldsymbol{\theta}) \quad \text{subject to equations (1)-(3)} \tag{4}$$

in which $\mathcal{L} : \boldsymbol{\theta} \mapsto [0, \infty)$ is a cost (or likelihood) function that quantifies the agreement between the model and a sequence of data points $(\mathbf{y}_i)$ measured at times t_i. For gradient-based optimisers, the Jacobian of the cost function with respect to the unknown parameters, $(\frac{\partial L}{\partial \theta})$ is used as a directional metric for the algorithm when exploring the parameter space.

By way of example, we next demonstrate the fitting of some synthetic data for which we know the true parameter values.

Design optimisation

Design optimisation is supported within PyBOP to guide future development of the battery design by identifying parameter variations which may unlock improvements in battery performance. This optimisation task can be viewed similarly to the parameterisation workflows described above, however, with the aim of increasing the distance metric instead of minimising it. In the case of design optimisation for maximising 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, instead it is the integrated energy from the vector normalised with the corresponding cell mass. This is typically quantified for operational conditions such as a 1C (the applied current required to discharge the cell in one hour) capacity.

Design optimisation can be written in the form of a constrained optimisation problem as:

$$\min_{\boldsymbol{\theta} \in \Omega} \ \mathcal{L}(\boldsymbol{\theta}) \quad \text{subject to equations (1)-(3)} \tag{5}$$

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

As an example, let us consider the target of maximising gravimetric energy density subject to constraints on the geometric electrode parameters (Couto et al., 2023).

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References

Andersson, M., Streb, M., Ko, J. Y., Löfqvist Klass, V., Klett, M., Ekström, H., Johansson, M., & Lindbergh, G. (2022). Parametrization of physics-based battery models from input-output data: A review of methodology and current research. *Journal of Power Sources*, *521*(November 2021), 230859. https://doi.org/10.1016/j.jpowsour.2021.230859

Chen, C.-H., Brosa Planella, F., O'Regan, K., Gastol, D., Widanage, W. D., & Kendrick, E. (2020). Development of experimental techniques for parameterization of multi-scale lithium-ion battery models. *Journal of The Electrochemical Society*, *167*(8), 080534. https://doi.org/10.1149/1945-7111/ab9050

Chu, Z., Plett, G. L., Trimboli, M. S., & Ouyang, M. (2019). A control-oriented electrochemical model for lithium-ion battery, Part I: Lumped-parameter reduced-order model with constant phase element. *Journal of Energy Storage*, *25*(August), 100828. https://doi.org/10.1016/j.est.2019.100828

Clerx, M., Robinson, M., Lambert, B., Lei, C. L., Ghosh, S., Mirams, G. R., & Gavaghan, D. J. (2019). Probabilistic inference on noisy time series (PINTS). *Journal of Open Research Software*, *7*(1), 23. https://doi.org/10.5334/jors.252

Couto, L. D., Charkhgard, M., Karaman, B., Job, N., & Kinnaert, M. (2023). Lithium-ion battery design optimization based on a dimensionless reduced-order electrochemical model. *Energy*, *263*(PE), 125966. https://doi.org/10.1016/j.energy.2022.125966

Doyle, M., Fuller, T. F., & Newman, J. (1993). Modeling of Galvanostatic Charge and Discharge of the Lithium/Polymer/Insertion Cell. *Journal of The Electrochemical Society*, *140*(6), 1526–1533. https://doi.org/10.1149/1.2221597

Fuller, T. F., Doyle, M., & Newman, J. (1994). Simulation and optimization of the dual lithium ion insertion cell. *Journal of The Electrochemical Society*, *141*(1), 1. https://doi.org/10.1149/1.2054684

Kirk, T. L., Lewis-Douglas, A., Howey, D., Please, C. P., & Jon Chapman, S. (2023). Nonlinear electrochemical impedance spectroscopy for lithium-ion battery model parameterization. *Journal of The Electrochemical Society*, *170*(1), 010514. https://doi.org/10.1149/1945-7111/acada7

Korotkin, I., Timms, R., Foster, J. F., Dickinson, E., & Robinson, M. (2023). Battery parameter eXchange. In *GitHub repository*. The Faraday Institution. https://github.com/FaradayInstitution/BPX

Miguel, E., Plett, G. L., Trimboli, M. S., Oca, L., Iraola, U., & Bekaert, E. (2021). Review of computational parameter estimation methods for electrochemical models. *Journal of Energy Storage*, *44*(PB), 103388. https://doi.org/10.1016/j.est.2021.103388

Planella, F. B., Ai, W., Boyce, A. M., Ghosh, A., Korotkin, I., Sahu, S., Sulzer, V., Timms, R., Tranter, T. G., Zyskin, M., Cooper, S. J., Edge, J. S., Foster, J. M., Marinescu, M., Wu, B., & Richardson, G. (2022). A Continuum of Physics-Based Lithium-Ion Battery Models Reviewed. *Progress in Energy*, *4*(4), 042003. https://doi.org/10.1088/2516-1083/ac7d31

Sulzer, V., Marquis, S. G., Timms, R., Robinson, M., & Chapman, S. J. (2021). Python Battery Mathematical Modelling (PyBaMM). *Journal of Open Research Software*, *9*(1), 14. https://doi.org/10.5334/jors.309

Tranter, T. G., Timms, R., Sulzer, V., Planella, F. B., Wiggins, G. M., Karra, S. V., Agarwal, P., Chopra, S., Allu, S., Shearing, P. R., & Brett, D. J. l. (2022). Liionpack: A python package for simulating packs of batteries with PyBaMM. *Journal of Open Source Software*, *7*(70), 4051. https://doi.org/10.21105/joss.04051

Verbrugge, M., Baker, D., Koch, B., Xiao, X., & Gu, W. (2017). Thermodynamic model for substitutional materials: Application to lithiated graphite, spinel manganese oxide, iron phosphate, and layered nickel-manganese-cobalt oxide. *Journal of The Electrochemical Society*, *164*(11), E3243. https://doi.org/10.1149/2.0341708jes

Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D., Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, M., Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E., … SciPy

1.0 Contributors. (2020). SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python. *Nature Methods*, *17*, 261–272. https://doi.org/10.1038/s41592-019-0686-2

Wang, A. A., O'Kane, S. E. J., Brosa Planella, F., Houx, J. L., O'Regan, K., Zyskin, M., Edge, J., Monroe, C. W., Cooper, S. J., Howey, D. A., Kendrick, E., & Foster, J. M. (2022). Review of parameterisation and a novel database (LiionDB) for continuum Li-ion battery models. *Progress in Energy*, *4*(3), 032004. https://doi.org/10.1088/2516-1083/ac692c