1st Online Developer Meeting

(Pending new logo)

The PyBOP Team

21st March 2024

Agenda

- Presentation on current version of PyBOP (Nicola, 15 min)
- Quick introduction from everyone (5 min)
- Discussion of open issues (30 min)
- Planning and assignment of tasks (10 min)

Introduction

With thanks to:

- the PyBaMM developers PyBaMM
- the PINTS developers

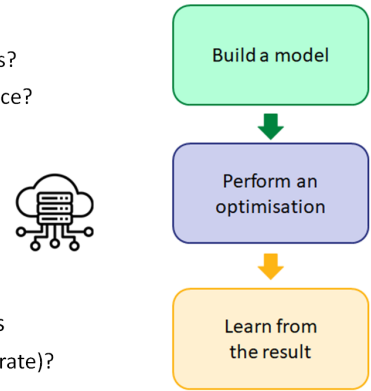
Aims

PyBOP

1. Parameter estimation from cell data
   - How will my battery respond to different excitations?
   - How is degradation affecting my battery performance?

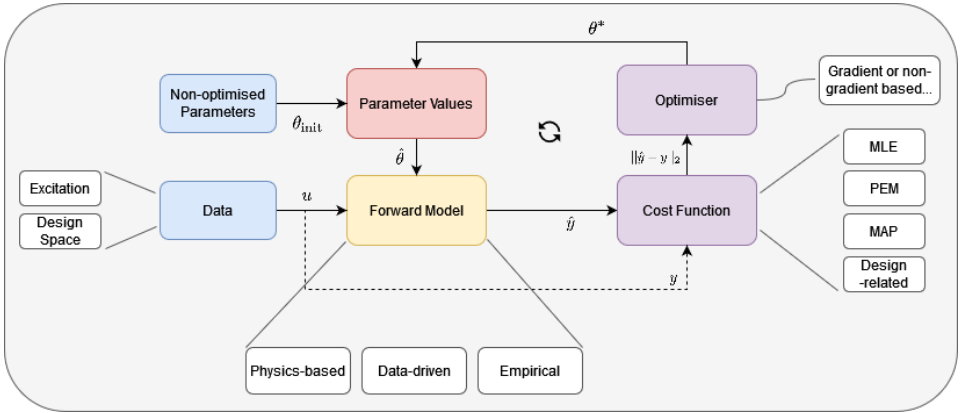
2. Model comparison
   - What can I learn from a more detailed model?
   - Is it worth the extra computational effort?

3. Design optimisation within practical constraints
   - How energy dense can I make my battery (at some rate)?

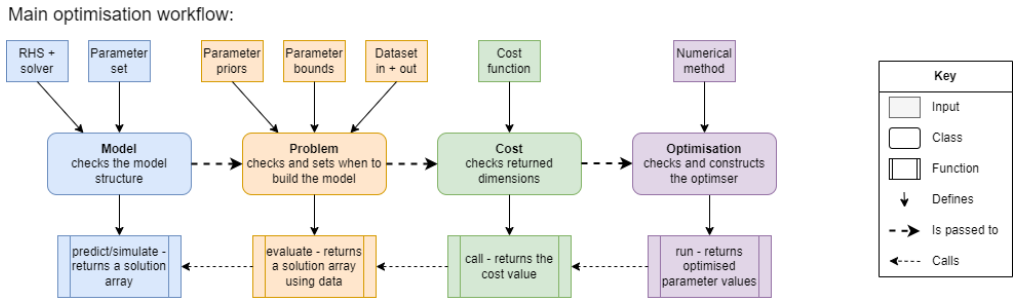


Icons made by Uniconlabs, RaftelDesign and Freepik from www.flaticon.com

PyBOP


θ^*
Non-optimised Parameters
θ_{init}
Parameter Values
$\hat{\theta}$
Optimiser
Gradient or non-gradient based...
$\|\hat{y} - y\|_2$
Excitation
Design Space
Data
u
Forward Model
$\hat{y}$
Cost Function
y
MLE
PEM
MAP
Design -related
Physics-based
Data-driven
Empirical

Python objects



Demo/examples

- Parameterisation
- Design optimisation

1. Define a model (PyBaMM's SPM) and fitting parameters

```
import pybop
import numpy as np

# Define model
parameter_set = pybop.ParameterSet.pybamm("Chen2020")
model = pybop.lithium_ion.SPM(parameter_set=parameter_set)

# Fitting parameters
parameters = [
    pybop.Parameter(
        "Negative particle radius [m]",
        prior=pybop.Gaussian(6e-06, 0.1e-6),
        bounds=[1e-6, 9e-6],
    ),
    pybop.Parameter(
        "Positive particle radius [m]",
        prior=pybop.Gaussian(4.5e-06, 0.1e-6),
        bounds=[1e-6, 9e-6],
    ),
]
```

2. Generate synthetic data and define problem, cost and optimisation

```
# Generate data
sigma = 0.001
t_eval = np.arange(0, 900, 2)
values = model.predict(t_eval=t_eval)
corrupt_values = values["Voltage [V]"].data + np.random.normal(0, sigma, len(t_eval))

# Form dataset
dataset = pybop.Dataset(
    {
        "Time [s]": t_eval,
        "Current function [A]": values["Current [A]"].data,
        "Voltage [V]": corrupt_values,
    }
)

# Generate problem, cost function, and optimisation class
problem = pybop.FittingProblem(model, parameters, dataset)
cost = pybop.SumSquaredError(problem)
optim = pybop.Optimisation(cost, optimiser=pybop.CMAES)
optim.set_max_iterations(100)
```

3. Run the optimisation and plot the results

```
# Run the optimisation
x, final_cost = optim.run()
print("True parameters:", true_x)
print("Estimated parameters:", x)

# Plot the timeseries output
pybop.quick_plot(problem, parameter_values=x, title="Optimised Comparison")

# Plot convergence and parameter traces
pybop.plot_convergence(optim)

# Plot the parameter traces
pybop.plot_parameters(optim)

# Plot the cost landscape with optimisation path
pybop.plot2d(optim, steps=15)
```

Parameterisation results

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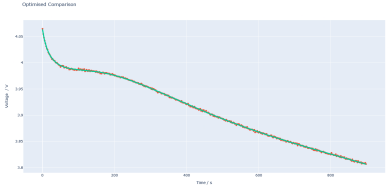

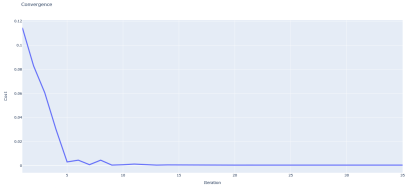

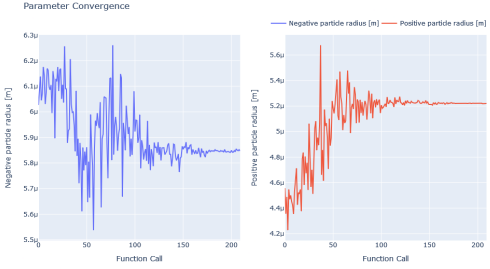

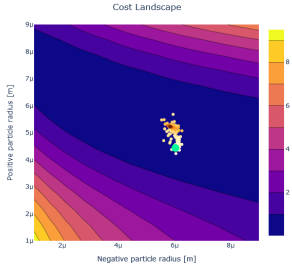

1. Define a model (PyBaMM's SPMe) and design parameters

```
# Define parameter set and model
parameter_set = pybop.ParameterSet.pybamm("Chen2020")
model = pybop.lithium_ion.SPMe(parameter_set=parameter_set)

# Fitting parameters
parameters = [
    pybop.Parameter(
        "Positive electrode thickness [m]",
        prior=pybop.Gaussian(7.56e-05, 0.05e-05),
        bounds=[65e-06, 10e-05],
    ),
    pybop.Parameter(
        "Positive particle radius [m]",
        prior=pybop.Gaussian(5.22e-06, 0.05e-06),
        bounds=[2e-06, 9e-06],
    ),
]
```

2. Set the target experiment and define problem, cost and optimisation

```
# Define test protocol
experiment = pybop.Experiment(
    ["Discharge at 1C until 2.5 V (5 seconds period)"],
)
init_soc = 1  # start from full charge
signal = ["Voltage [V]", "Current [A]"]

# Generate problem
problem = pybop.DesignProblem(
    model, parameters, experiment, signal=signal, init_soc=init_soc
)

# Generate cost function and optimisation class:
cost = pybop.GravimetricEnergyDensity(problem)
optim = pybop.Optimisation(
    cost, optimiser=pybop.PSO, verbose=True, allow_infeasible_solutions=False
)
optim.set_max_iterations(15)
```

3. Run the optimisation and plot the results

```
# Run optimisation
x, final_cost = optim.run()
print("Estimated parameters:", x)
print(f"Initial gravimetric energy density: {-cost(cost.x0):.2f} Wh.kg-1")
print(f"Optimised gravimetric energy density: {-final_cost:.2f} Wh.kg-1")

# Plot the timeseries output
if cost.update_capacity:
    cost.problem._model.approximate_capacity(x)
pybop.quick_plot(problem, parameter_values=x, title="Optimised Comparison")

# Plot the cost landscape with optimisation path
pybop.plot2d(optim, steps=3)
```

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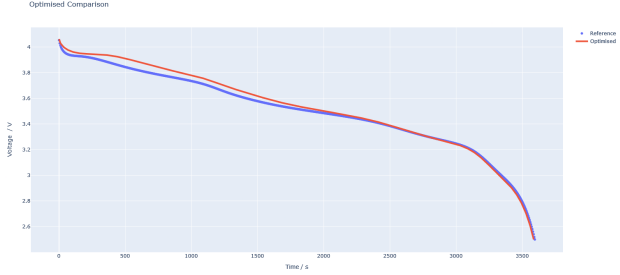
Output

```
Estimated parameters: [6.51159429e-05 2.32340723e-06]
Initial gravimetric energy density: 386.31 Wh.kg-1
Optimised gravimetric energy density: 410.78 Wh.kg-1
```

Results



Choice of optimisers

Gradient-based

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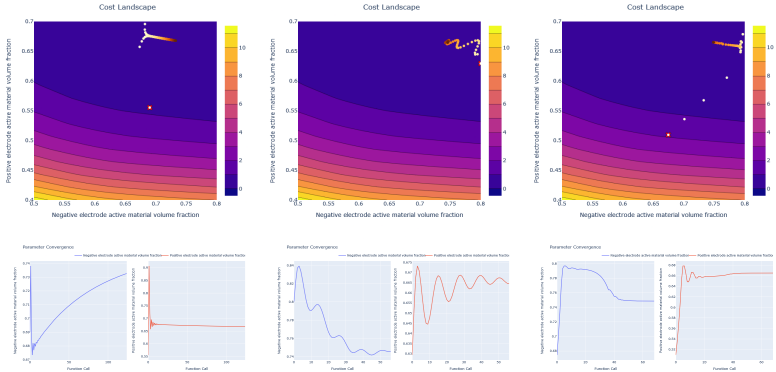
Gradient descent

Adaptive moment (ADAM)

Resilient backpropagation (IRPropMin)



Evolution strategies

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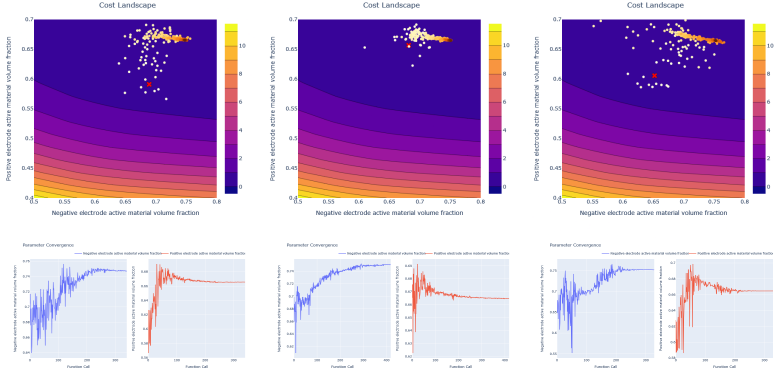
Stochastic natural evolution strategy (SNES)	Exponential natural evolution strategy (SNES)	Covariance matrix adaptation (CMA-ES)



Other optimisers

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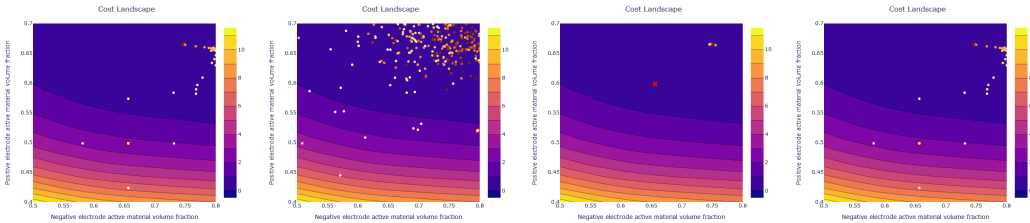
Bound quadratic approx. (BOBYQA)	Particle swarm optimisation	SciPy differential evolution	SciPy minimise (COBYLA)



Questions?

Discussion

Let's introduce everyone:

- Where are you joining from?
- What is your research area of interest?
- How would you like to use/contribute to PyBOP?

Code of Conduct

PyBOP aims to foster a broad consortium of developers and users, both across and outside the Faraday Institution community.

Our values are:

PyBOP

https://github.com/pybop-team/PyBOP

SCAN ME

pybop-docs.readthedocs.io

- Open-source (code and ideas should be shared)
- Inclusivity and fairness (those who want to contribute may and input is appropriately recognised)
- Inter-operability (aiming for modularity to enable maximum impact and inclusivity)
- User-friendliness (putting user requirements first, thinking about user-assistance & workflows)

Icons made by Good Ware, Dewi Sari, Nhor Phai and Vectors Tank from www.flaticon.com

Open issues

https://github.com/pybop-team/PyBOP/issues

Next steps

- How can you contribute?
- Project board: https://github.com/orgs/pybop-team/projects/6/views/1
- Date for next meeting