ParMOO: A Python library for parallel multiobjective simulation optimization

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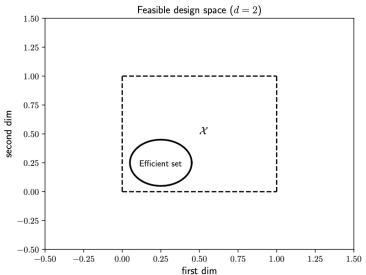
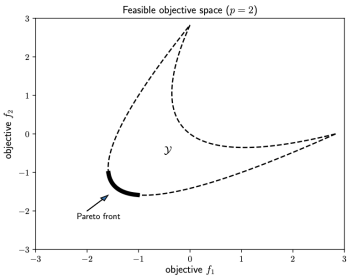
Multiobjective *Simulation* Optimization

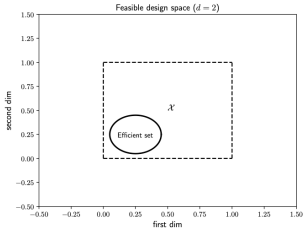


Objective Functions



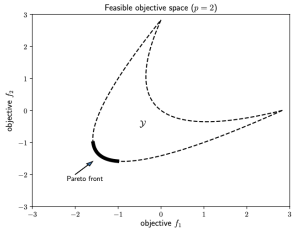
Design space *Objective space*

Multiobjective *Simulation* Optimization



Design space

Simulations $\longrightarrow$ $\mathcal{S}$ Objectives $\longrightarrow$



Objective space

Simulation Structure

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where each $N_1, \ldots, N_o$ is an index set.

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Heterogeneous MOOPs:

$$h_1(x, S(x)) = S_1(x)$$
$$h_2(x, S(x)) = \|x\|^2$$

Use expensive surrogate models for h_1 (i.e., S_1) but not for h_2

Example 1: Fayans EDF Model Calibration

Find params $x \in [0,1]^{13}$ to fit the Fayans model to data d_i:

$$M(\xi_i; x) \approx d_i \qquad i = 1, \ldots, 198$$

ParMOO simulation:

$$S_i(x) = M(\xi_i; x) - d_i, \qquad i = 1, \ldots, 198;$$

Min SOS across 3 observable classes

$$F_t = \sum_{i=1}^{m_t} \left(S_{t,i}(x)\right)^2$$

Example 2: Material Manufacturing with ParMOO

Choose optimal settings for material manufacturing in a continuous flow reactor (CFR)

We know how to make a desired material, need to produce at scale:

1. **Maximize the product** (battery electrolyte: TFML)
2. Can increase temperature to **reduce reaction time**
3. Too much heat activates a side reaction; need to **minimize unwanted byproduct**

Product and **byproduct** are the result of expensive experiment,
reaction time is a controllable input

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ParMOO is under review with JOSS

GitHub: github.com/parmoo/parmoo
Docs: parmoo.readthedocs.io
PyPI: pip install parmoo
Conda Forge: conda install --channel=conda-forge parmoo

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