ParMOO: A Python library for parallel multiobjective simulation optimization

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SIAM CSE 23

Outlines

Introduction to MOSO + my experience

3 challenges + solutions

ParMOO software design + release

Example Problems

Conclusions + some closing thoughts

Multiobjective Optimization Problems

$$\min_{x \in \mathcal{X}} F(x)$$

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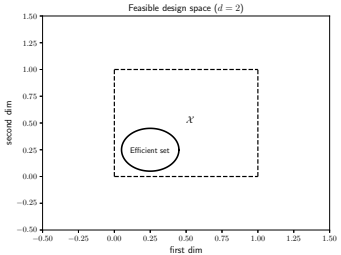
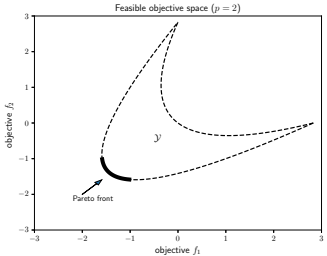


$$F : \mathcal{X} \to \mathcal{Y}$$



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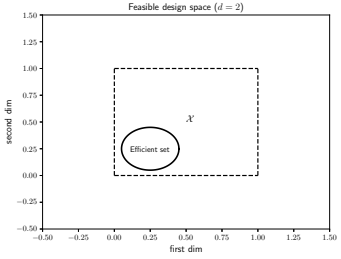

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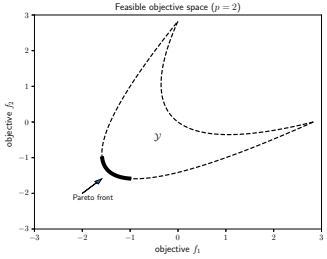
expensive
blackbox process



Multiobjective Response Surface Methodology

or Model-Based Optimization or Active Learning

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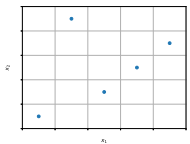

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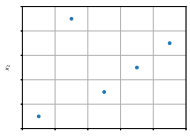

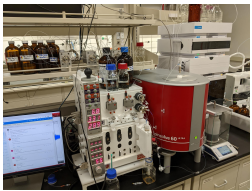

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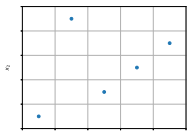

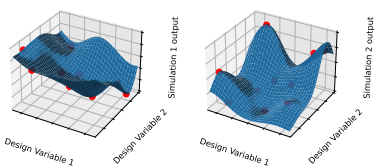

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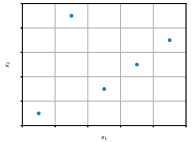

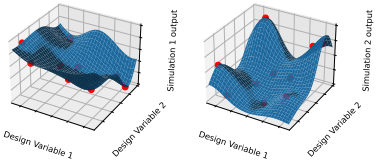

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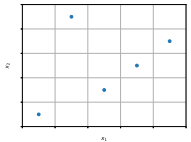
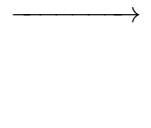
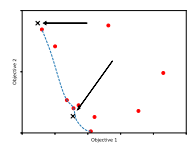
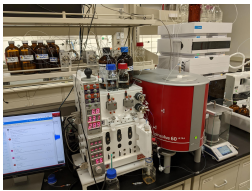
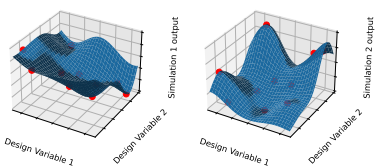


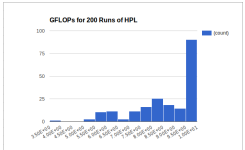








Example: HPC Performance Tuning



VT VarSys Project – 40 runs of HPL

ANL – LCRC Computing Resources: Bebop

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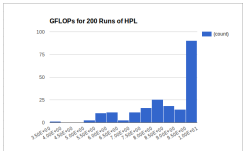

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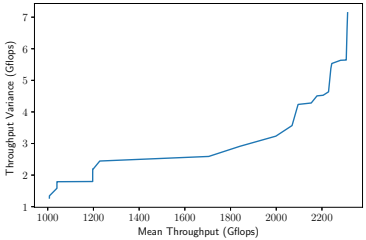
VTMOP solver



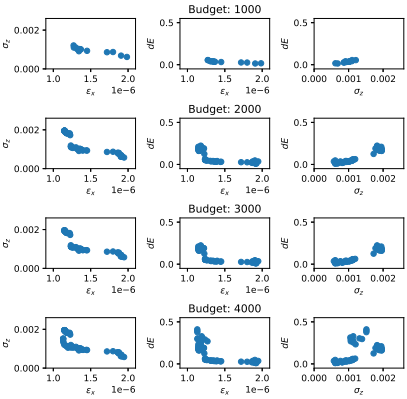
[1] Chang, Larson, and Watson. Multiobjective optimization of the variability of the high-performance LINPACK solver. In Proc. WSC 2020.

Challenge 1:
mixed vars + problem types

Example: Particle Accelerator Design

OPAL-t
(Object Oriented Parallel Accelerator Library for beam-lines + linacs)

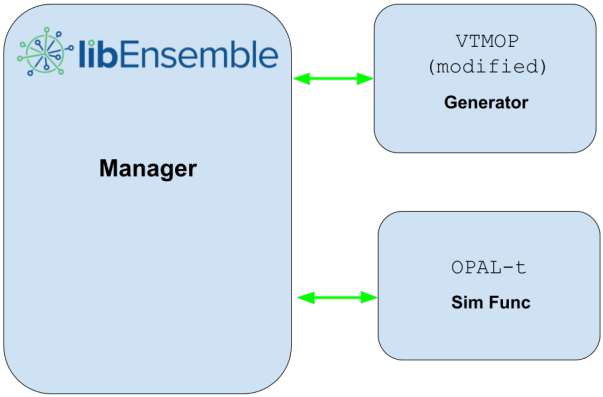
VTMOP solver



[2] Chang et al. Algorithm 1028: VTMOP: Solver for blackbox multiobjective optimization problems. ACM TOMS 48(3):36 (2022).

[3] Neveu et al. Comparison of multiobjective optimization methods for the LCLS-II photoinjector. CPC 283:108566 (2023).

Handling parallel evals



[4] Chang et al. Managing computationally expensive blackbox multiobjective optimization problems with libEnsemble. In Proc. SpringSim 2020.

Challenge 2:

parallel evals + computing environments

Commercial solutions

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"Using Bayesian optimization for balancing metrics in recommendation systems" by Yunbao Ouyang et al. on LinkedIn Engineering Blog.

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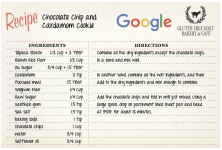

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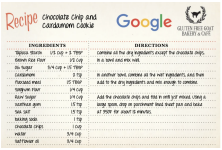

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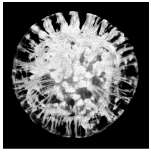

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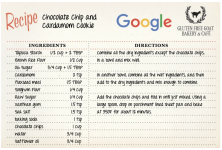

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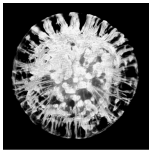

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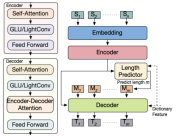

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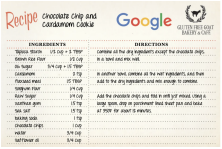

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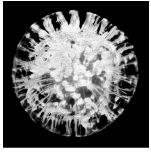

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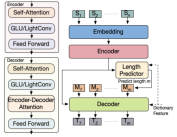

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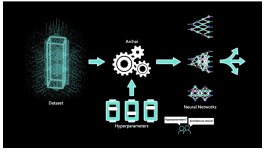

"Archai can design your neural network with state-of-the-art NAS" by Shital Shah et al. on Microsoft Research Blog.

SOA and structure-exploiting blackbox optimization

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SOA and structure-exploiting blackbox optimization

SciPy

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TAO

SOS structure can be exploited by DFO solver POUNDERS in TAO [6].

[5] Wild. Optimization and learning with zeroth-order stochastic oracles. SIAM News 56(1):1,3 (2023).

[6] Wild. Solving derivative-free nonlinear least squares problems with POUNDERS. Adv. and Trends in Optimization with Engineering Applications, Ch. 40, pp. 529–540 (2017).

Challenge 3:

SOA optimization + exploiting problem structure

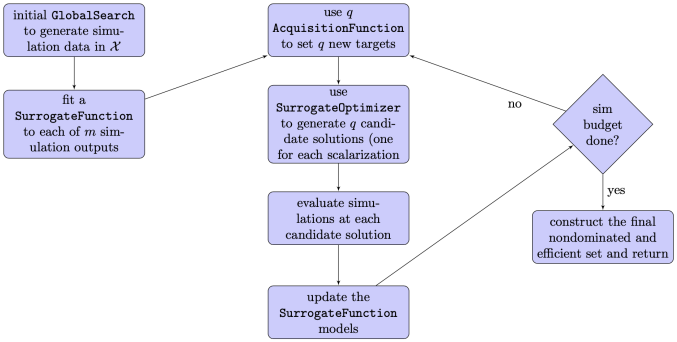
ParMOO Design Criteria

Design goals:

1. Highly customizable framework for multiobjective RSM
2. Flexible problem types (mixed-variables, constraints, etc.)
3. Easy to use, deploy, and extend (unforeseen use-cases and environments)
4. Exploit structure and domain knowledge

Customizability

ParMOO uses an object-oriented framework:



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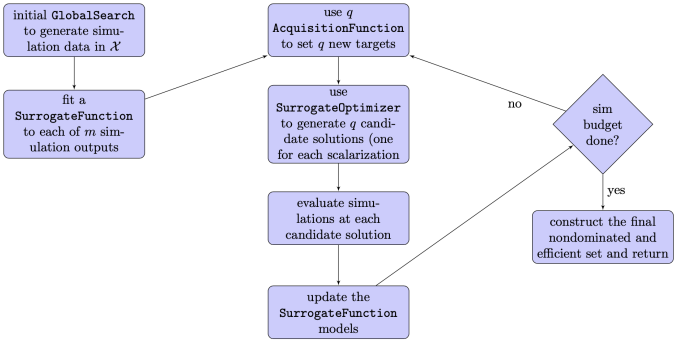
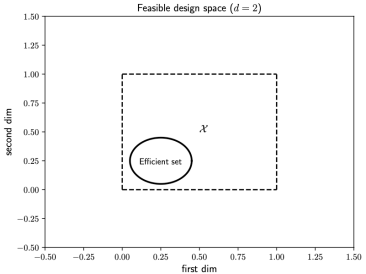
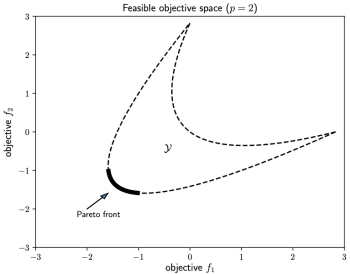


- Search/DOE
- Surrogate model
- Acquisition function
- Single-obj solver

Simulation Structure

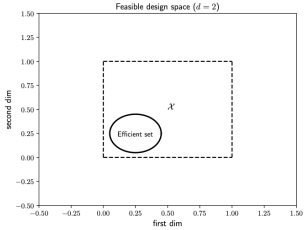


Objective Functions

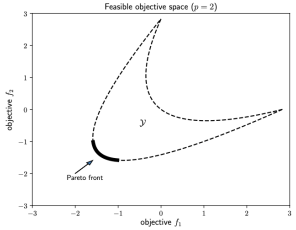


Design space *Objective space*

Simulation Structure



Simulations $\mathcal{S}$ Objectives



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Sum-of-squares structure:

$$h_i(x, S(x)) = \sum_{j \in N_i} \left(S_j(x)\right)^2$$

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

Increases order of approximation $\Rightarrow$
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Increases order of approximation $\Rightarrow$ increases order of convergence

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

Flexible Problem Types

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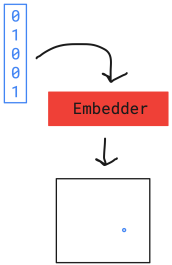
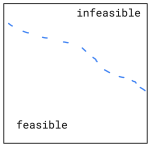


- Mixed variable-types **Ex: categorical variables**
  - Focus on *embedding* into continuous space

- (Nonlinear) constraints
  - Focus on *augmented Lagrangian* penalties (relax to augmented unconstrained problem)



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Easy to deploy:

- Simulation/experiment evaluations are only called in the `MOOP.solve()` method
- Extend `MOOP` class and overwrite `solve()` to deploy in different workflows
- **Ex:** Deploy parallel solvers on HPC systems using `libEnsemble`

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Easy to deploy:

- Simulation/experiment evaluations are only called in the `MOOP.solve()` method
- Extend `MOOP` class and overwrite `solve()` to deploy in different workflows
- **Ex:** Deploy parallel solvers on HPC systems using `libEnsemble`

Easy to maintain and extend:

- OOP + total modularity makes adding new features easy
- Agile development with continuous integration
- Well-documented interface, contributing, and release process

ParMOO Release

Written in `Python` (available on `pip` and `GitHub`)

`https://parmoo.readthedocs.io/en/latest/quickstart.html`

Combine with `libEnsemble` to use parallel solvers

Chang and Wild. ParMOO: A Python library for parallel multiobjective simulation optimization. *JOSS 8(82):4468 (2023).*

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:

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

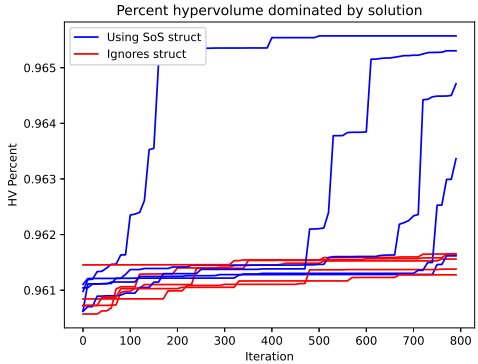
Min SOS across 3 observable classes

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

Bollapragada et al. Journal of Physics G: Nuclear and Particle Physics 48(2), 2020.

Fayans Solution with ParMOO

- Approximated Fayans model using inv dist weighting on existing dataset
- Implemented parallel solver in ParMOO using libEnsemble
- Just **14-25 lines of Python code**
- Ran for **10K** sim evals
- Compared against same solver w/o exploiting SOS structure



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**

Challenges:

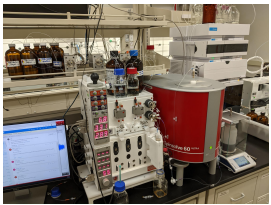
- Mixed variable types
- Heterogeneous objectives
- Must send experiments to run on CFR

CFR Optimization with ParMOO

Extend `MOOP` class to send/receive experiment data using `MDML` library (Apache Kafka)

Used categorical variable embeddings

Modeled Product/Byproduct as simulations and reaction time using algebraic equation of input



Next Release

Coming in v. 0.2

- Interactive post-run visualization tools
- Support for customized embeddings and passing raw (unscaled) inputs
- MDML (Apache Kafka) interface for distributing simulation evalutations
- (Maybe) advanced techniques for design-of-experiments

Resources

E-mail: tchang@anl.gov
E-mail: parmoo@mcs.anl.gov

JOSS 8(82):4468 (2023)

GitHub: github.com/parmoo/parmoo
Docs: parmoo.readthedocs.io
PyPI: pip install parmoo

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