NEURAL INFORMATION PROCESSING SYSTEMS

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MOBO-OSD: Batch Multi-Objective Bayesian Optimization via Orthogonal Search Directions

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Paper Code

Multi-Objective Bayesian Optimization (MOBO)

Goal: MOBO finds the Pareto optimal solutions of expensive black-box vector-valued objective functions $\boldsymbol{f} = [f_1 \quad \dots \quad f_M]$,

$$\mathcal{P}_f = \min_{x \in \mathcal{X}} (f_1(x) \quad \dots \quad f_M(x)),$$

where $\mathcal{X}$ is the search space, M is the number of objective.

- In MOBO, no single best solutions, find the set of Pareto optimal f(x) (*Pareto front*) and x (*Pareto set*) in a sample-efficient manner.

Motivation

Drawbacks of current MOBO solutions:

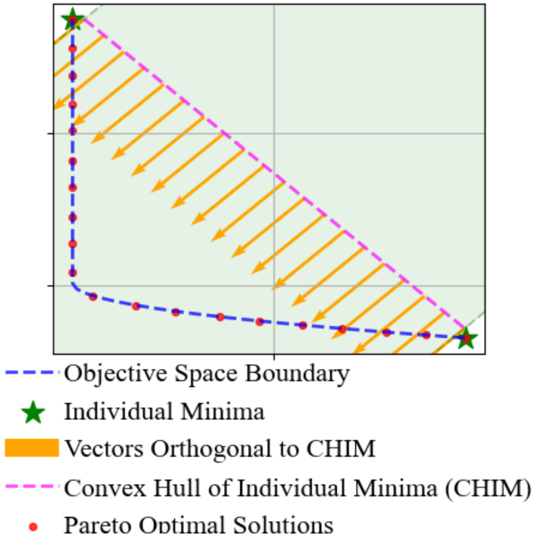
- Scalarization (ParEGO [1]): bad diversity on concave Pareto Front
- DGEMO [2] (NeurIPS 2020): cannot scale to M>3
- EHVI [3] (NeurIPS 2020): computationally expensive

→ Focus on Pareto Front diversity while maintaining scalability and feasibility

Key Ideas

Inspiration:

- Insight from the Normal Boundary Intersection (NBI) technique [4]
- The *intersection points* between the boundary of the objective space and the vectors orthogonal to the CHIM → Pareto optimal solutions



Proposed Solutions MOBO-OSD:

1. Propose the *Approximated CHIM* and the well-distributed *Orthogonal Search Directions* (OSD) → The MOBO-OSD Components
2. Find the intersection points (Pareto optimal solutions) using the proposed OSD → The MOBO-OSD Subproblems
3. Enrich the set of Pareto optimal solutions → Pareto Front Estimation
4. Select next data points for evaluations → Batch Selection Policy

Batch Multi-Objective Bayesian Optimization via Orthogonal Search Directions (**MOBO-OSD**)

The Proposed MOBO-OSD Algorithm

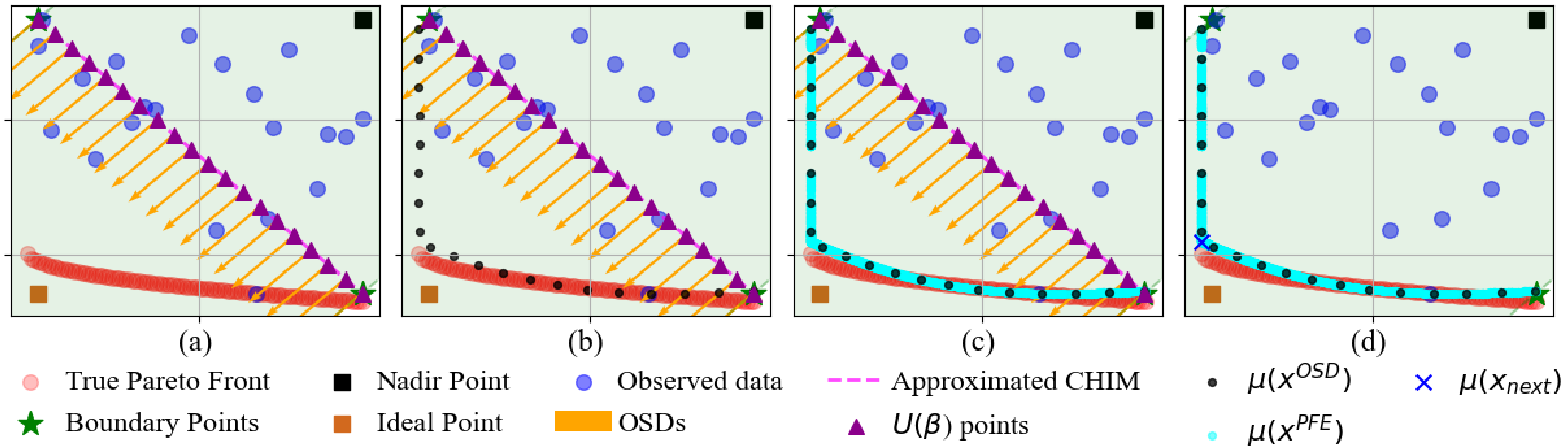
Overall Process: MOBO-OSD iteration:

(a) Compute the components (Approximated CHIM + OSDs)

(b) Solve MOBO-OSD subproblems for candidates

(c) Approximate the PF for additional candidates

(d) Select optimal candidates for evaluations.



Experimental Results

Baselines

qParEGO [1]

USeMO [7] – AAAI 2020

PDBO [8] – AAAI 2024

DGEMO [2] – NeurIPS 2020

qEHVI [3] – NeurIPS 2020

JES [9] – NeurIPS 2022

State-of-the-art MOBO methods

NSGA-II [10] → A well-known Multi-Objective Evolutionary Algorithm

NBI [4] → The original Normal Boundary Intersection method

Experimental Results

Benchmark Problems

Synthetic Functions:

- DTLZ (D=5, M=2,3,4)
- ZDT (D=5, M=2)
- VLMOP2 (D=5, M=2)

Real-world Problems:

- Speed Reducer (D=7, M=3)
- Car Side Design (D=7, M=4)
- Marine Design (D=6, M=4)
- Water Planning (D=3, M=6)

Comparison metrics:

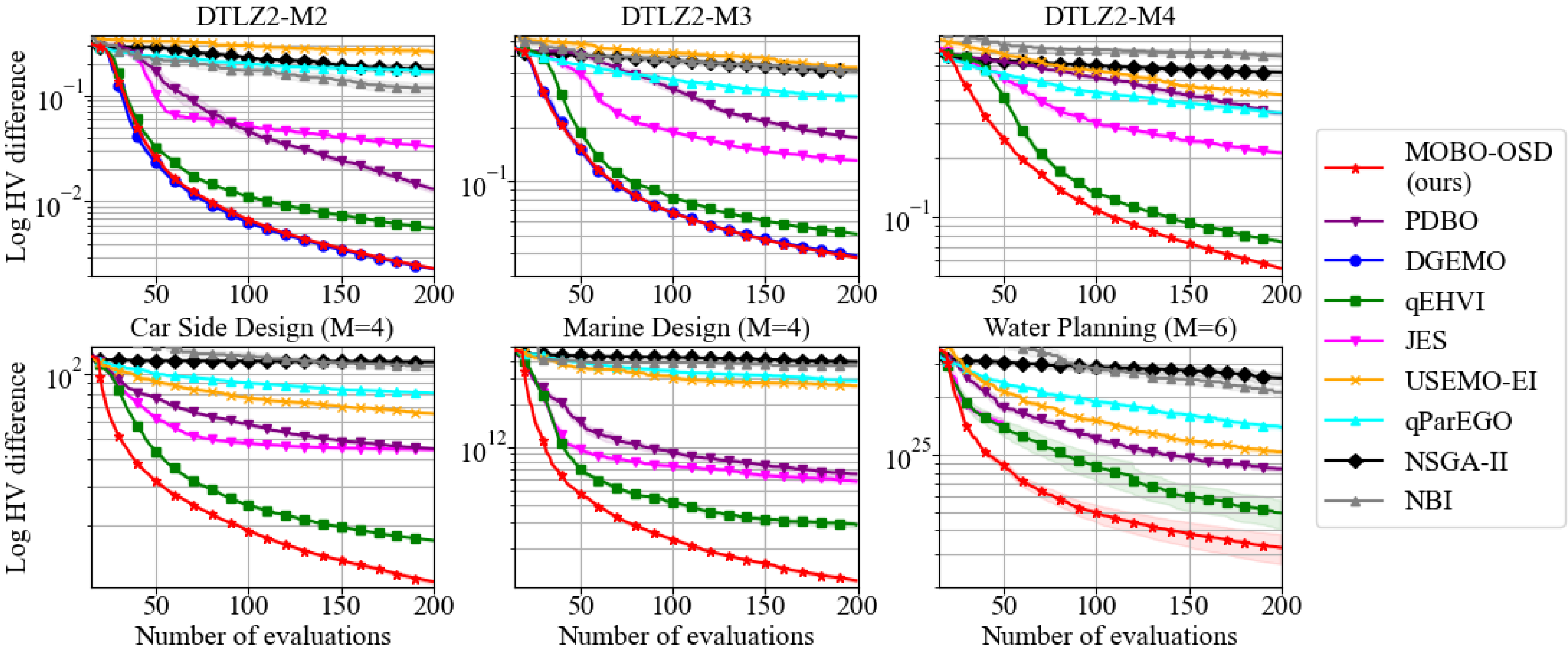
- Hypervolume (the most common in MOBO)
- We run each problem 10 times and report the accumulated best results (mean and standard errors).

Experimental Results

Comparisons against Baselines – Sequential Optimization (batch = 1)

MOBO-OSD overall outperforms all baselines:

- Best HV performance
- Scalability to any number of objective



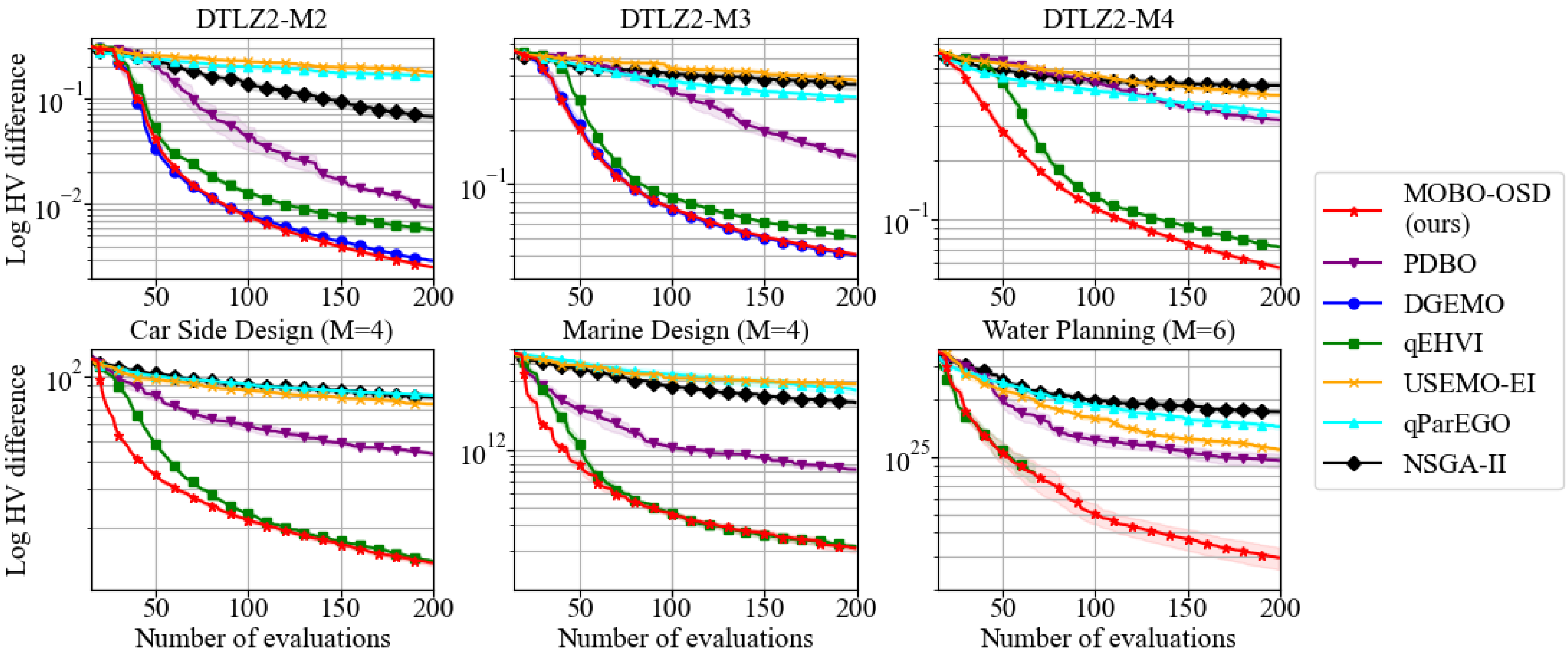
Smaller values indicate better methods

Experimental Results

Comparisons against Baselines – Batch Optimization (batch = 8)

MOBO-OSD overall outperforms all baselines :

- qEHVI: scales expensively with number of objectives and batch size → cannot finish Water Planning (M=6).



Smaller values indicate better methods

Summary

MOBO-OSD: Batch Multi-objective BO via Orthogonal Search Directions (OSD)

- Methodology:
  - Compute the MOBO-OSD components
  - Solve MOBO-OSD subproblems for the candidates (intersection points)
  - Generate additional candidates
  - Select next observations via HV-based AF
- Validate with extensive experiments (HV performance, scalability and cost)

Thank You

Poster Session: Wed 3 Dec (Exhibit Hall C,D,E)

References

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