WPI

Multi-objective Optimization by Learning Space Partitions

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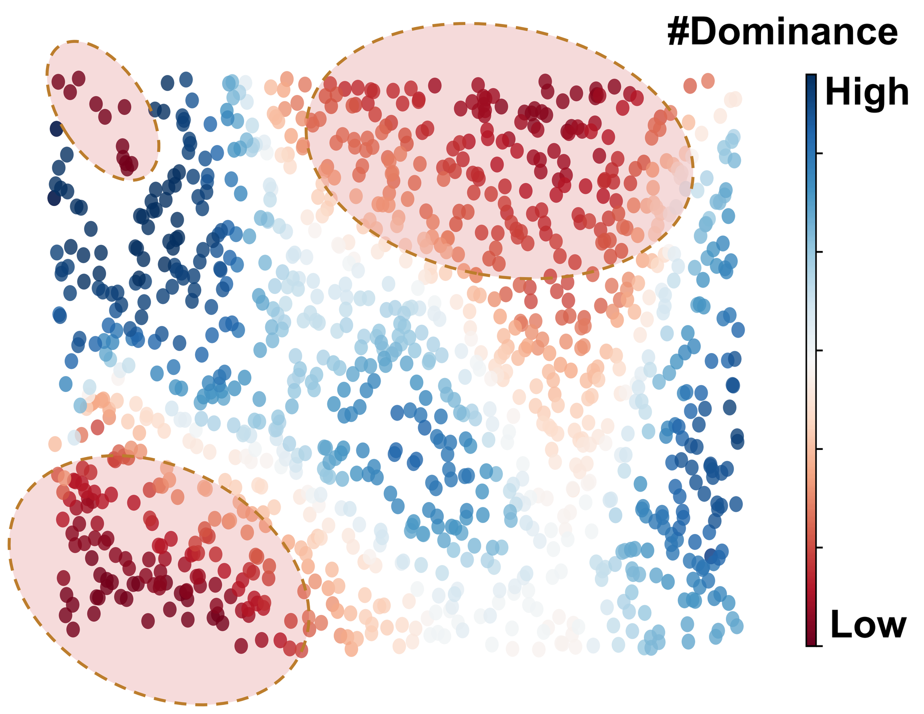
Motivation

Problem: Branin-Currin

$$f^{(1)}(x_1,x_2) = \left(15x_2 - \frac{5.1(15x_1-5)x^2}{4\pi^2} + \frac{75x_1-25}{\pi} - 5\right)^2 + \left(10 - \frac{10}{8\pi}\right) * cos(15x_1 - 5)$$

$$f^{(2)}(x_1,x_2) = [1 - exp(\frac{-1}{2x_2})] \frac{2300x_1^3 + 1900x_1^2 + 2092x_1 + 60}{100x_1^3 + 500x_1^2 + 4x_1 + 20} \quad , where\ (x_1,x_2) \in [0,1]$$



Observation:

- The good samples are gathering in small regions(shaded areas).

Intuition :

- The search space can be learned to partition by samples.

Learning Space Partitions

Algorithm 1 LaMOO Pseudocode.

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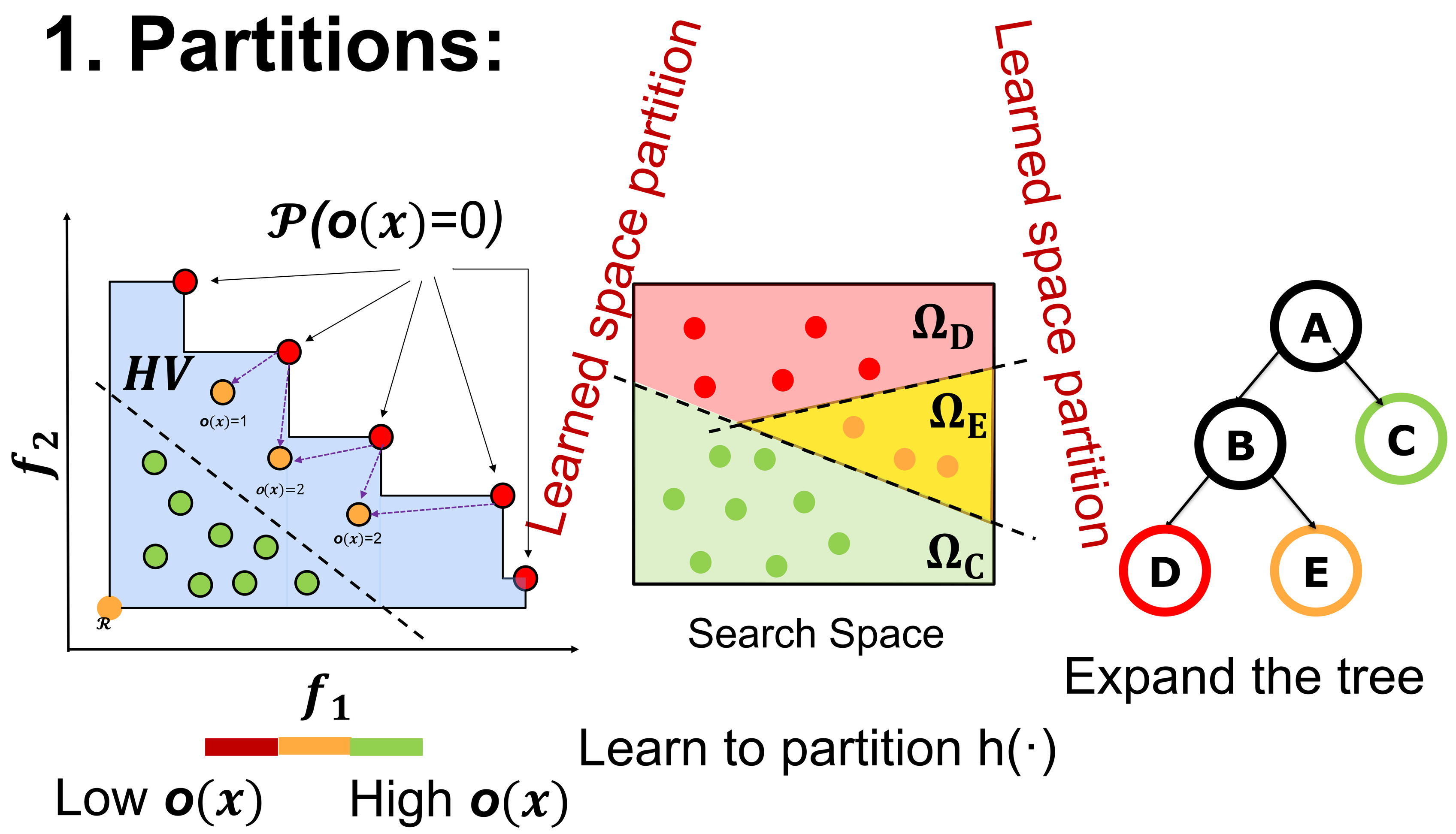
Inputs: Initial D_0 from uniform sampling, sample budget T.
for t = 0, ..., T do
    Set L ← {Ω_root} (collections of regions to be split).
    while L ≠ ∅ do
        Ω_j ← pop_first_element(L),  D_{t,j} ← D_t ∩ Ω_j,  n_{t,j} ← |D_{t,j}|.
        Compute dominance number o_{t,j} of D_{t,j} using dominance numbers and train SVM model h(·).
        If (D_{t,j}, o_{t,j}) is splittable by SVM, then L ← L ∪ Partition(Ω_j, h(·)).
    end while
    for k = root, k is not leaf node do
        D_{t,k} ← D_t ∩ Ω_k,  v_{t,k} ← HyperVolume(D_{t,k}),  n_{t,k} ← |D_{t,k}|.
        k ← arg max_{c ∈ children(k)} UCB_{t,c}, where UCB_{t,c} := v_{t,c} + 2C_p sqrt(2 log(n_{t,k}) / n_{t,c})
    end for
    D_{t+1} ← D_t ∪ D_new, where D_new is drawn from Ω_k based on qEHVI or CMA-ES.
end for
```

Learning Partitions:

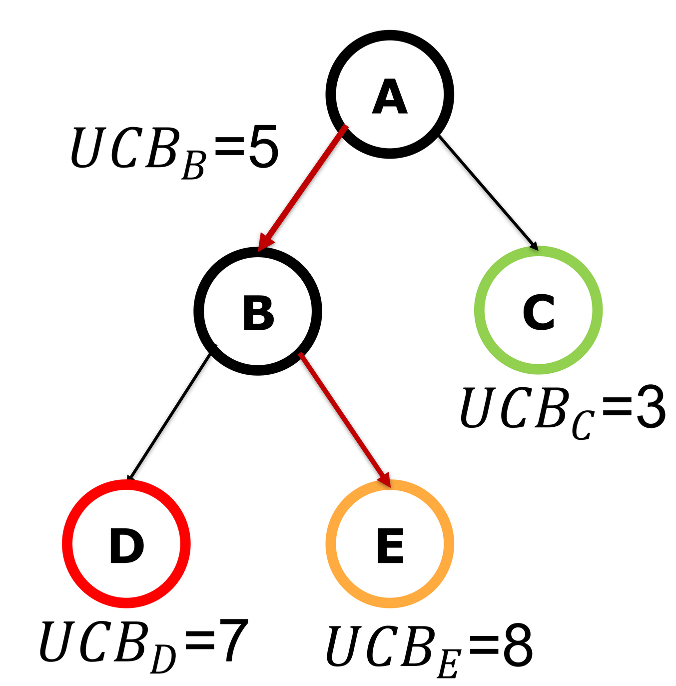
- Sort the dominance numbers of samples $\boldsymbol{o}(x)$ to get two groups of samples, i.e., good, bad.
- Leverage a SVM classifier to learn a boundary to partition the search space.

Methodology

1. Partitions:



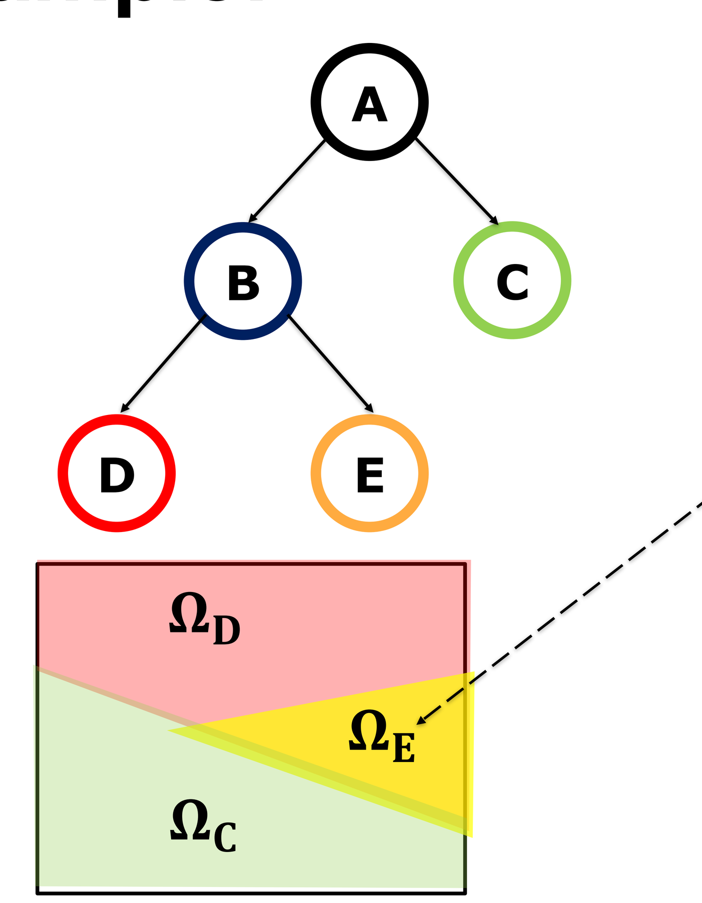
2. Select:



Select the leaf node with most UCB value to trade off the exploration and exploitation.

Select w.r.t ucb

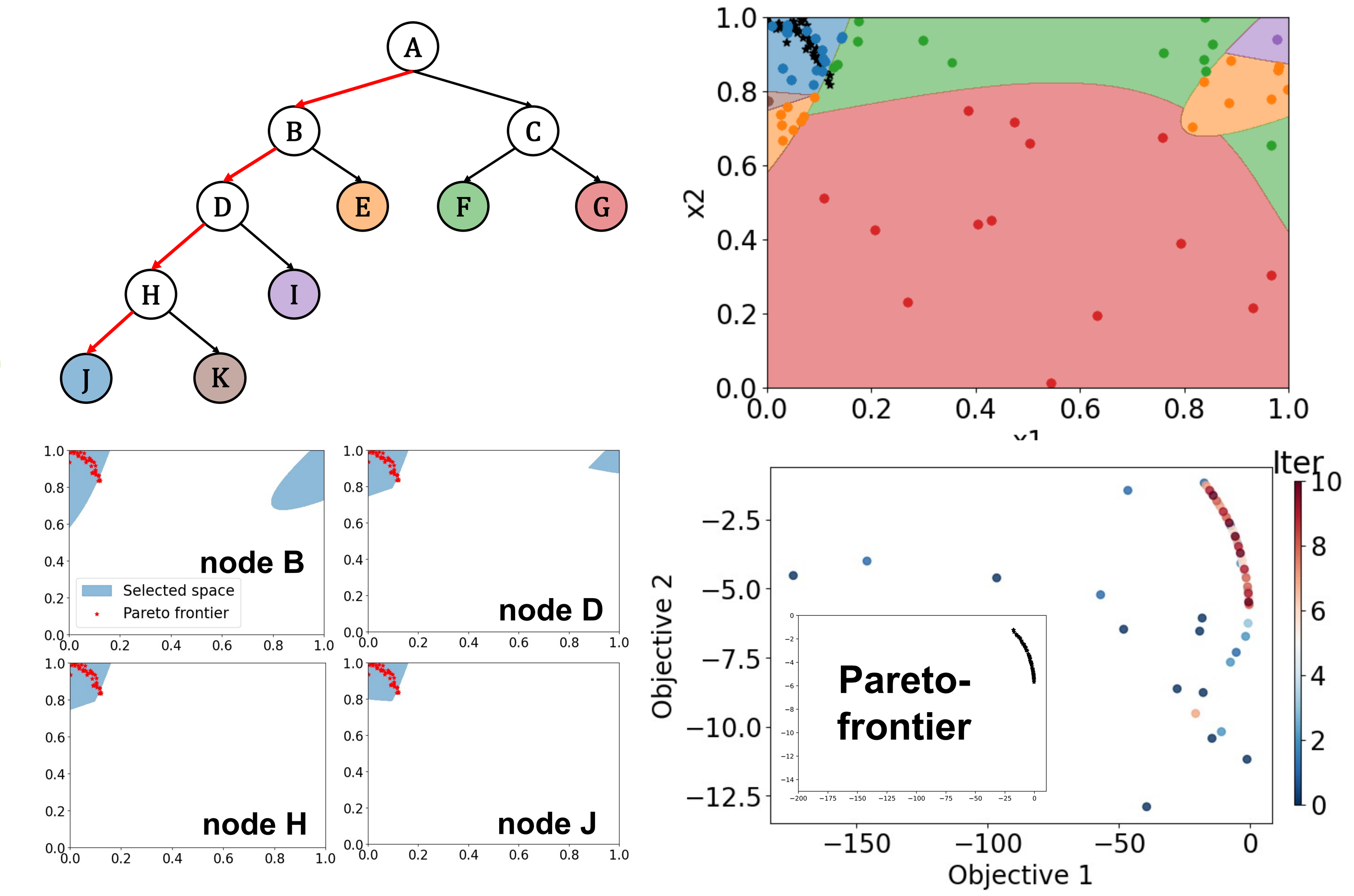
3. Sample:



Only samples from Ω_E based on sample methods

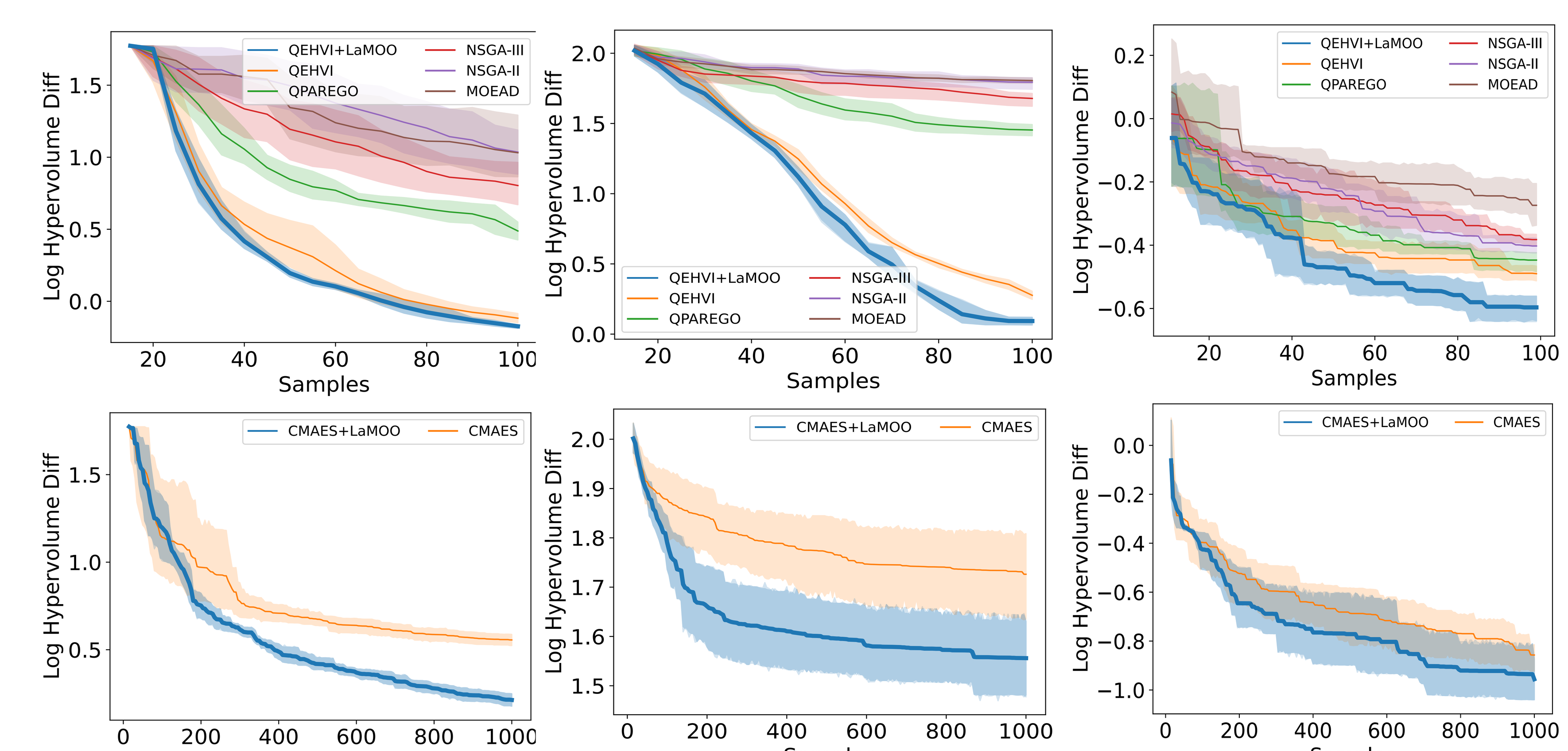
Visualization of LaMOO

Problem: Branin-Currin



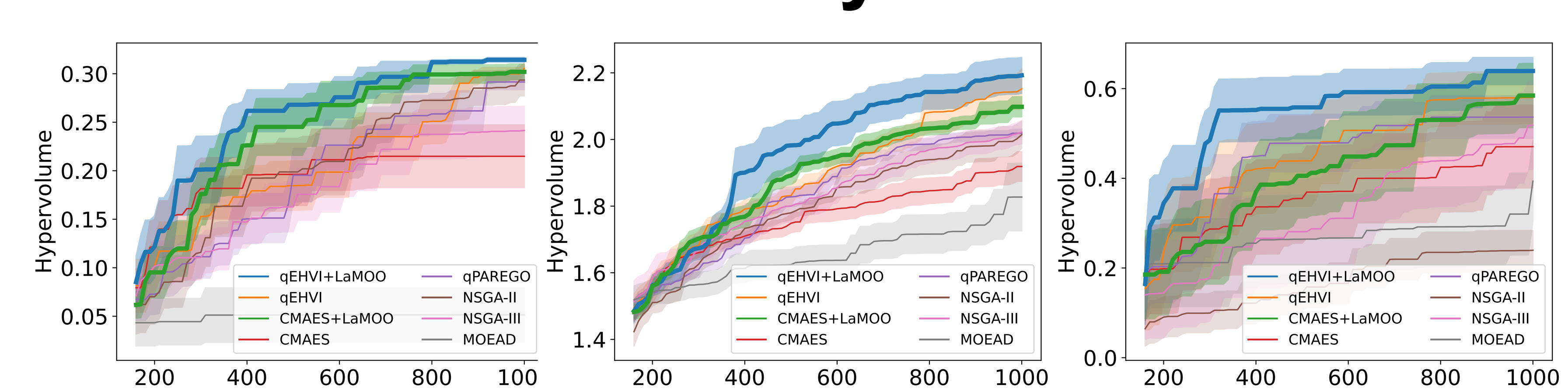
Experiment Results

1. Small-scale Problems



Branin-Currin **VehicleSafety** **NasBench201**

2. Molecule Discovery



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