Multi-Objective Bayesian Optimization with Diverse, Cluster-based Solutions (MOBy-DiC)

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MOBy-DiC

Objective

- To generate a **diverse** set of Pareto-optimal solutions for multi-objective optimization problems.

Assumptions

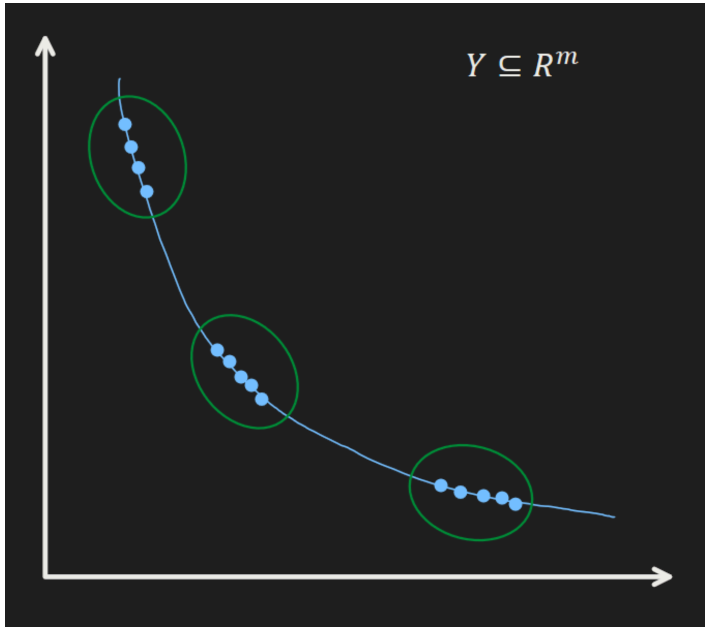
- An initial set of Pareto-optimal solutions is provided as input.
    - These solutions can be sourced from existing algorithms
        - e.g.) MORBO, qNEHVI, NSGA-II
    - Alternatively, in real-world applications, they can be solutions found empirically.

Strategy 1 : Clustering

Cluster the initial solutions in the design space $\mathcal{X} \subseteq \mathbb{R}^d$ to identify distinct promising regions.

Possible Clustering Algorithms

1. DBSCAN
    - Hyperparameters
        - ϵ : maximum distance between each datapoint
            - $\epsilon \approx L_{\min}$ from TuRBO's TR, $\mathcal{T}$
        - MinPts : minimum number of points in a cluster
2. k-Means
    - Hyperparameters
        - k : number of clusters
            - How to choose k?



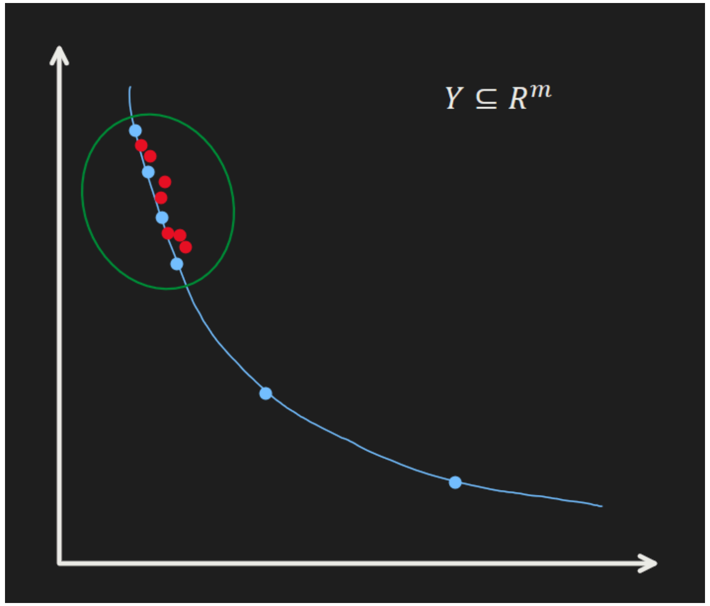
Strategy 2 : Dual Search

Apply a TuRBO-based strategy that operates on two levels:

1. Intra-Cluster Search

Local TuRBO like MORBO within the cluster

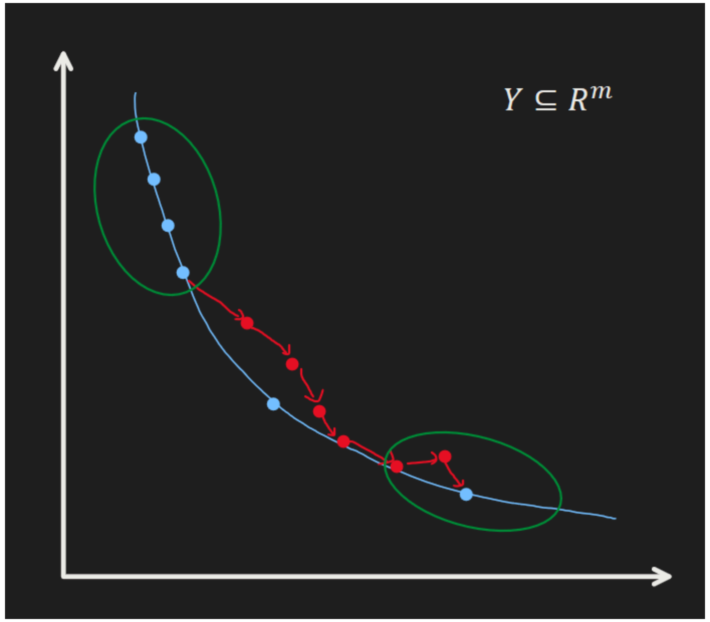
- Input : $\mathbf{x}_1, \mathbf{x}_2 \in C_k \subseteq \mathbb{R}^d$: two intra-cluster points
  - where C_k is the k-th cluster
- Output: $\mathbf{x}^*_{\text{intra}}$
- Procedure
  - Let $\mathbf{x}_0 = \dfrac{\mathbf{x}_1 + \mathbf{x}_2}{2}$: the mid point
  - `return` $\mathbf{x}^*_{\text{intra}}$ = TuRBO($\mathbf{x}_0, \mathcal{L}, \mathcal{GP}$)



2. Inter-Cluster Search

Find a path between two clusters and apply TuRBO on it

- Input : $\mathbf{x}_1 \in C_{k_1},\ \mathbf{x}_2 \in C_{k_2},\ C_{k_1} \neq C_{k_2}$
  - Two points from different clusters
- Output : $\mathbf{x}^*_{\text{inter}}$
- Procedure
  - Find a path between $\mathbf{x}_1$ and $\mathbf{x}_2$ by iteratively solving
    - $\arg\max_{\mathbf{x} \in S} \alpha(\mathbf{x}) = \mathrm{HV}(\mathbf{x}) - \lambda \|\mathbf{x} - \mathbf{x}_2\|,\ \lambda > 0$
    - where S is the set of points within the distance of L from the previous point.



- Procedure
  - $\mathbf{x}^{(0)} = \mathbf{x}_1,\ \mathbf{X}_{\text{cand}} \leftarrow \emptyset$
  - `for` $t = 1, \cdots, T$
    - $S \leftarrow \{\mathbf{x} \mid \mathbf{x} \in \mathbb{R}^d,\ L_{\min} \leq \|\mathbf{x}^{(t-1)} - \mathbf{x}\| \leq L_{\max}\}$
    - $\mathbf{x}^{(t)} = \arg\max_{\mathbf{x} \in S} \alpha(\mathbf{x}) = \mathrm{HV}(\mathbf{x}) - \lambda\|\mathbf{x} - \mathbf{x}_2\|,\ \lambda > 0$
      - Candidate HVs
        - EHVI
        - HV Scalarization by Zhang et al.
    - $\mathbf{x}_{\text{cand}}^{(t)} =$ TuRBO$(\mathbf{x}^{(t)}, \mathcal{L})$
    - $\mathbf{X}_{\text{cand}} \leftarrow \mathbf{X}_{\text{cand}} \cup \{\mathbf{x}_{\text{cand}}^{(t)}\}$
  - $\mathbf{x}_{\text{inter}}^{*} = \arg\max_{\mathbf{x} \in \mathbf{X}_{\text{cand}}} \mathrm{HV}(\mathbf{x})$
    - Or maybe, return $\mathbf{X}_{\text{cand}}$ in batch
  - `return` $\mathbf{x}_{\text{inter}}^{*}$

Related Works

ROBOT

- Props.
  - Suggests diverse solutions using the Bayesian optimization technique
  - Utilizes TuRBO to search the high dimensional design space.
- Differences
  - Solves single objective optimization problems
  - Suggested solutions have priorities.
    - In MOBO, pareto optimality allows various solutions.

Related Works

DGEMO

- Props.
  - Solves multi objective optimization problems
  - Suggests diverse solutions using the Bayesian optimization technique
  - Adapts the batch selection strategy and the First-Order approximation technique
- Limit
  - Does not work on higher dimensional design spaces $(d > 6)$

Related Works

MORBO

- Props.
  - Solves the multi objective optimization problem
  - Works well on higher dimensional design spaces
  - Efficiently finds pareto optimal solutions using TuRBO
- Limit
  - Does not provide diverse solutions along the pareto front