

A simple pipeline for Multi-Objective and Multi-Modal optimization problems

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ABSTRACT

This work proposes a pipeline and a dedicated algorithm for exploring multimodal solutions in multi-objective optimization (MOO). The approach is based on the premise that, after approximating a Pareto front, the decision-maker can define a trade-off of interest and specify thresholds for equivalence in the objective space and distinctiveness in the decision space. A second algorithm, based on Differential Evolution, then searches for alternative decision variable configurations achieving equivalent objective performance. The proposed method was validated on a classic beam design problem through 51 independent runs, analyzing the algorithm's sensitivity to hyperparameter settings. Results demonstrate the algorithm's ability to identify diverse solutions with equivalent performance, enhancing the decision-making process by offering alternatives for practical implementation.

KEYWORDS. Multiobjective optimization. Multimodal optimization. Decision Making.

Multiobjective Optimization

1. Introduction

Multi-objective optimization (MOO) addresses problems characterized by the simultaneous optimization of conflicting objectives [Miettinen, 1999]. In such cases, it is generally not possible to identify a single optimal solution; instead, a set of trade-off solutions, known as the Pareto front, is approximated. This Pareto front provides the decision-maker with a range of alternatives, each representing a different balance between the competing objectives. MOO techniques have demonstrated significant applicability across various fields of engineering [Rangaiah et al., 2020; Pereira et al., 2022; Stewart et al., 2021; Cerda-Flores et al., 2022; Sawik, 2023], where complex design problems often involve conflicting performance metrics that must be carefully balanced to achieve effective and practical solutions.

Once the Pareto front has been approximated, a decision-making process must take place to select the most appropriate solution for implementation. This process may involve objective criteria, such as performance indicators, cost, or reliability, but also subjective or experience-driven considerations that are often specific to real-world engineering practice [Bonissone et al., 2009]. While most decision-making activities are conducted in the objective space, it is also possible (and sometimes necessary) to involve the decision variable space. Ultimately, it is the decision variables that define the concrete implementation of a solution, directly impacting feasibility, manufacturing processes, and operational constraints.

One key concept that can be explored within the decision variable space is multimodality. In the context of optimization, multimodality refers to the existence of multiple distinct decision variable vectors that lead to the same or nearly the same objective vector [Das et al., 2011]. This implies that there are several alternative ways to achieve a given performance level. From the perspective of Pareto optimization, multimodality indicates that multiple design configurations can lead to the same trade-off region of interest for the decision maker.

This research is motivated by the research question *how to explore and exploit multimodality in multi-objective optimization?* Specifically, in this work we propose a pipeline to identify multimodal solutions associated with trade-off regions that are of interest to the decision-maker. This approach introduces an additional dimension to the decision-making process by offering alternative solutions that achieve similar trade-offs, providing greater flexibility in the final design selection and supporting decisions based on factors beyond the objectives initially modeled.

The remainder of this paper is organized as follows. Section 2 presents the theoretical background required to support the proposed approach. Section 3 describes the proposed pipeline and algorithm for multimodal solution search. Section 4 provides a case study to validate the methodology. Finally, Section 5 concludes the paper and discusses future research directions.

2. Background

Next, a brief background on multi-modal optimization and multi-objective optimization is presented. At the end of the section, a contextualization is commented.

2.1. Multi-Modal Optimization

Multi-modal optimization involves finding multiple optimal solutions in a search space that contains several local optima. An optimization problem can be defined as follows:

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}) \quad (1)$$

where $\mathbf{x} \in \mathbb{R}^n$ is a vector of decision variables in an n -dimensional real-valued space, and $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is the objective function to be minimized. In the case of multi-modal optimization, there are multiple equivalent decision vectors in $\mathbb{R}^n$ that are optimal. Two decision vectors $\mathbf{x}_1, \mathbf{x}_2$ are equivalent if $\|f(\mathbf{x}_1) - f(\mathbf{x}_2)\| \leq \delta$ [Tanabe and Ishibuchi, 2019]. This concept is depicted in Figure 1.

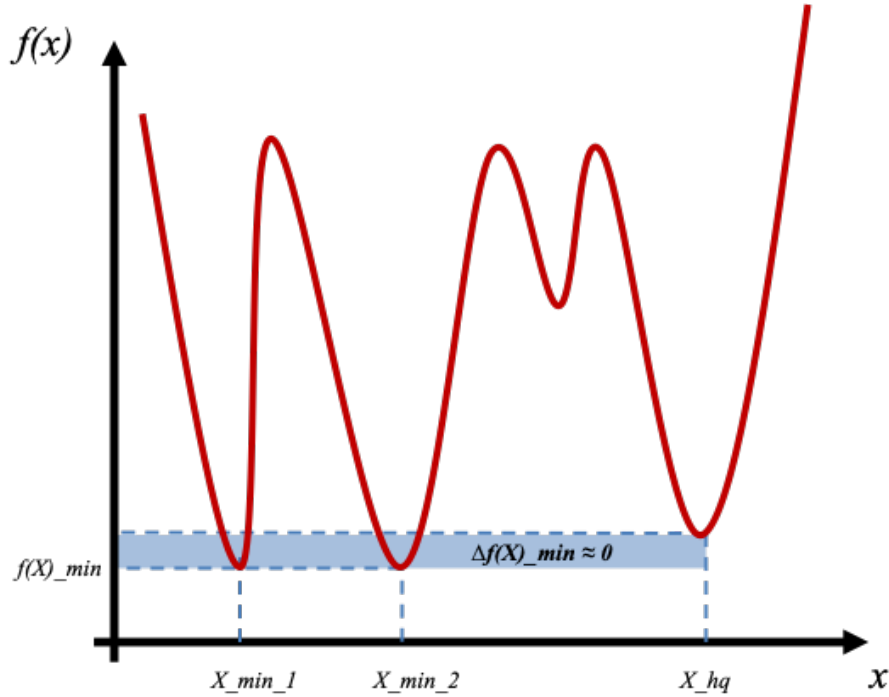


Figure 1: Concept of multimodality. Two solutions are equal (X_{min_1} and X_{min_2}) and therefore, equivalent. A third solution, X_{hq} is identified as equivalent with a certain $\Delta f(X)$ and thus, as of equivalent quality to the other two.

2.2. Multi-Objective Optimization

Multi-objective optimization extends the concept to problems involving more than one objective function, each to be optimized simultaneously. Such a problem can be represented as:

$$\min_{x \in \mathbb{R}^n} \mathbf{F}(x) = [f_1(x), f_2(x), \dots, f_m(x)]^T, \quad (2)$$

where $\mathbf{F}(x)$ is a vector of m objective functions. A solution x^* is considered Pareto optimal if there is no other solution x such that:

$$f_i(x) \leq f_i(x^*) \quad \forall i \in \{1, \dots, m\}, \quad (3)$$

and at least one strict inequality holds.

In order to have success employing such ideas in engineering design, at least three fundamental steps [Reynoso Meza et al., 2017] must be carried out:

- **Multi-Objective Problem (MOP) Statement:** In this step, the parametric model, the cost function, the design concept (decision variables), and the constraints must be defined.
- **Multi-Objective Optimization (MOO) Process:** This step involves applying a multi-objective optimization algorithm to simultaneously optimize all design objectives defined in the previous step. As a result, an approximation of the Pareto front is obtained.
- **Multi-Criteria Decision Making (MCDM) Analysis:** This step involves analyzing and selecting the most preferable solution from the Pareto optimal set for implementation.

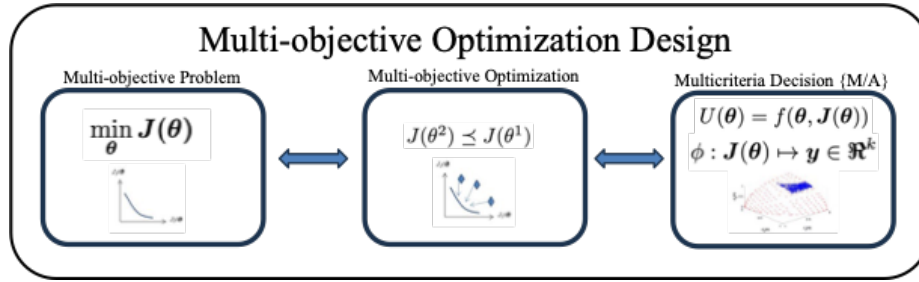


Figure 2: Multi-objective Optimization Design

Such steps are depicted in the Figure 2. This overall process was named Multi-objective Optimization Design (MOOD).

2.3. Contextualization

Traditional techniques for solving multi-modal optimization problems include crowding distance, niching methods, and clustering techniques [Tanabe and Ishibuchi, 2019]. Crowding distance [Yue et al., 2021] is used to maintain diversity among solutions by ensuring that solutions are spread out in the objective space. Niching methods [Cao et al., 2024], such as fitness sharing, reduce the reproductive potential of solutions that are too close to each other, thus promoting exploration of different peaks. Clustering techniques [Gu et al., 2025] group similar solutions together, allowing the algorithm to focus on different regions of the search space.

Previous techniques discussed for determining multimodal solutions typically operate within the same execution of the optimization algorithm, enabling the approximation and presentation of multiple Pareto fronts for the decision-maker. In contrast, the approach proposed in this work aligns with the hypothesis that, from an engineering design perspective, the initial step is to approximate a Pareto front representing the problem scenario. Once this front has been identified, and the solutions with trade-offs of interest to the designer are selected, a second algorithm is employed to explore the multimodal solutions associated with the specified trade-off region. Such approach is identified as an *post-processing approach* by Tanabe and Ishibuchi [2019].

This allows the decision-maker to define the minimum acceptable δ in the objective space to consider a solution equivalent to the selected one, as well as the minimum distance in the decision space to classify a solution as distinct. In this way, solutions of high or equivalent quality to the selected trade-off are identified, enabling a detailed analysis within the decision space.

3. Proposal, tools and methods

As commented before, the pipeline proposed here is based on a *a posteriori* approach. It is depicted in Figure 3. It involves three steps: (1) decision maker preferences for the multi-modal process; (2) optimization process to search for multimodal solutions; (3) new pareto set with multimodal solutions for decision making.

3.1. Step 1: Decision maker preferences

A posteriori methods involve decision making after an approximate Pareto front has been obtained. Once the Pareto front approximation is available, the decision maker selects a subset of design alternatives x^{dm} with a preferred trade-off among the objectives $J(x^{dm})$ in the objective space. Such solutions will constitute a list L that will be used by the multimodal algorithm. Also, the decision maker will define the maximum distance δ for a solution be considered equivalent in the objective space, and the minimum distance Δ to be considered different in the decision space.

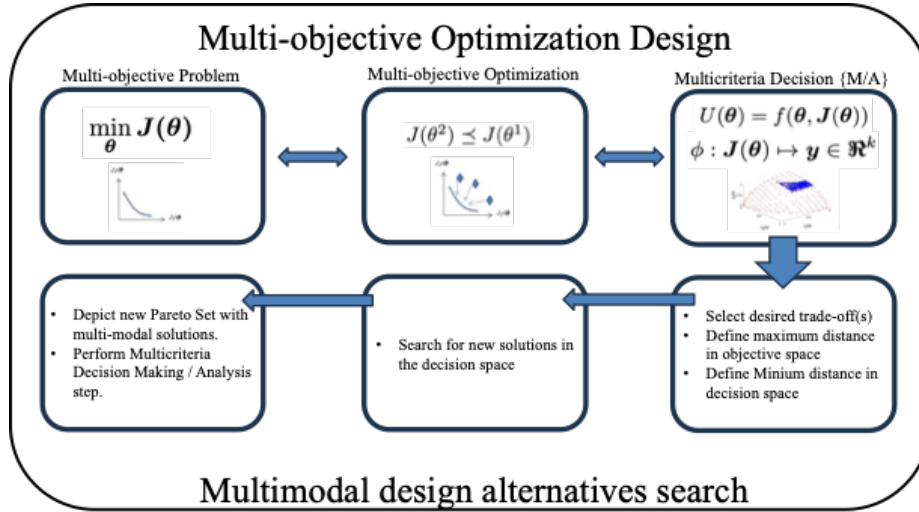


Figure 3: Pipeline proposal for *a posteriori* multi-modal multi-objective optimization.

3.2. Step 2: Optimization process

The proposed optimization process uses the information defined in the previous step as input and formulates a new multi-objective optimization problem with the following goals:

1. Minimize the distance to the preferred solutions $\mathbf{J}(\mathbf{x}^{dm})$ in the list L while considering the equivalence threshold δ .
2. Maximize the diversity among the solutions in the decision space by considering the distance Δ .

The new optimization problem can be expressed as:

$$\min_{\mathbf{x} \in \mathbb{R}^n} \mathbf{G}(\mathbf{x}) = \left[\text{dist}(\mathbf{x}, \mathbf{F}(\mathbf{x}^{dm})), -\text{diversity}(\mathbf{x}, \mathbf{F}(\mathbf{x}^{dm})) \right] \quad (4)$$

where $\text{dist}(\mathbf{x}, \mathbf{F}(\mathbf{x}^{dm}))$ is the distance between the solution $\mathbf{x}$ and the elements $\mathbf{x}^{dm}$ in the list L , defined as:

$$\text{dist}(\mathbf{x}, \mathbf{F}(\mathbf{x}^{dm})) = \begin{cases} 0 & \text{if } \|\mathbf{F}(\mathbf{x}) - \mathbf{F}(\mathbf{x}^{dm})\| \leq \delta, \\ \|\mathbf{F}(\mathbf{x}) - \mathbf{F}(\mathbf{x}^{dm})\| & \text{otherwise,} \end{cases} \quad (5)$$

and $\text{diversity}(\mathbf{x}, \mathbf{F}(\mathbf{x}^{dm}))$ is a measure of how spread out the solutions are, typically calculated as the average distance between the solutions in the subset $J(X)$. That is:

$$\text{dist}(\mathbf{x}, \mathbf{x}^{dm}) = \begin{cases} 0 & \text{if } \text{dist}(\mathbf{x}, \mathbf{x}^{dm}) \geq \Delta, \\ \text{dist}(\mathbf{x}, \mathbf{x}^{dm}) & \text{otherwise,} \end{cases} \quad (6)$$

By minimizing the distance to the preferred solutions while maximizing diversity, the algorithm generates a set of solutions that not only align with the decision-maker's preferences but also maintain a high degree of diversity, ensuring a comprehensive exploration of the objective space. The algorithm utilizes Differential Evolution (DE) [Piotrowski et al., 2023] for generating new solutions, adapting dynamically by incorporating the multimodal solutions found so far (See Annex 1 for details on the DE algorithm).

Below is the pseudocode incorporating these principles:

Algorithm 1 Dynamic Multi-Objective Differential Evolution (DMODE)

```

1: Initialize population  $P$  with  $N$  individuals
2: Initialize list of discovered solutions  $L = \emptyset$ 
3: Evaluate fitness of each individual in  $P$ 
4: while stopping criterion not met do
5:   for each individual  $\mathbf{x}_i$  in  $P$  do
6:     Mutation: Generate mutant vector  $\mathbf{v}_i$  using Equation (1)
7:     Crossover: Generate trial vector  $\mathbf{u}_i$  using Equation (2)
8:     Selection: Select the next generation individual  $\mathbf{x}_i^{(t+1)}$  using Equation (3)
9:     if  $\mathbf{u}_i$  is a new multi-modal solution then
10:       Add  $\mathbf{u}_i$  to list  $L$ 
11:     end if
12:   end for
13:   Dynamic Cost Function Adjustment:
14:   for each individual  $\mathbf{x}_i$  in  $P$  do
15:     Calculate  $\text{dist}(\mathbf{x}_i, L)$  as the distance to the minimum cost in  $L$ 
16:     Update the fitness value of  $\mathbf{x}_i$  based on  $\text{dist}(\mathbf{x}_i, L)$ 
17:   end for
18:   Evaluate fitness of each individual in the new population
19: end while
20: return the best individual found

```

3.3. Decision Making

Finally, the new set of solutions approximated is provided to the decision maker to perform a selection. This is essentially, a similar step than in the MOOD procedure.

4. Experimental setup

Next, the proposed pipeline will be evaluated in a classical multi-objective optimization problem.

4.1. Case Study: I-BEAM Design Problem

The I-BEAM design problem is a classical benchmark in engineering optimization, originally presented by Huang et al. [2006]. It consists of minimizing structural objectives under stress constraints to determine optimal cross-sectional parameters for an I-shaped beam subjected to static loads. The design involves four decision variables:

- x_1 : Total height of the beam cross-section [$10 \leq x_1 \leq 80$ cm],
- x_2 : Width of the flange [$10 \leq x_2 \leq 50$ cm],
- x_3 : Thickness of the web [$0.9 \leq x_3 \leq 5$ cm],
- x_4 : Thickness of the flange [$0.9 \leq x_4 \leq 5$ cm].

The multi-objective optimization problem is defined as:

$$\begin{aligned}
 \min_x \quad & J_1(x) = 2x_2x_4 + x_3(x_1 - 2x_4), & (\text{Cross-sectional area [cm}^2\text{)}) \\
 \min_x \quad & J_2(x) = \frac{PL^3}{48EI(x)}, & (\text{Vertical deflection [cm]}) \\
 \text{subject to} \quad & C_1(x) \leq S_b, & (\text{Bending stress constraint [kN/cm}^2\text{)})
 \end{aligned} \tag{7}$$

where the second moment of area $I(x)$ is computed as:

$$I(x) = \frac{1}{12} \left[x_3 (x_1 - 2x_4)^3 + 2x_2x_4 (4x_4^2 + 3x_1 (x_1 - 2x_4)) \right], \quad (8)$$

and the bending stress constraint is given by:

$$C_1(x) = \frac{300Px_1}{x_3 (x_1 - 2x_4)^3 + 2x_2x_4 (4x_4^2 + 3x_1 (x_1 - 2x_4))} + \frac{300Qx_2}{(x_1 - 2x_4)x_3^3 + 2x_4x_2^3}. \quad (9)$$

The model parameters are defined as follows:

- Beam length: $L = 200$ cm,
- Central force $P = 600$ kN,
- Lateral force $Q = 50$ kN,
- Young's modulus: $E = 2 \times 10^4$ kN/cm²,
- Maximum allowable bending stress: $S_b = 16$ kN/cm².

This problem represents a trade-off between material usage (minimizing cross-sectional area) and mechanical performance (minimizing vertical deflection), under strict structural constraints. It serves as a challenging test case for evaluating the capability of optimization algorithms to handle multi-objective and constraint-handling scenarios.

A Pareto front was approximated for this problem. From this point, the decision-maker must select a trade-off solution that best aligns with their design preferences. Without loss of generality, let's suppose the decision maker select the solution $\mathbf{F}\mathbf{x}^{dm} = [247.8000, 0.0186]$.

Once this preferred trade-off has been identified, the decision-maker must define two critical thresholds to guide the search for multimodal solutions:

- The maximum deviation $\delta_{obj}^{\max}$ in the objective space to consider two solutions as equivalent is set to 1% of the maximum observed values in the Pareto front.
- The minimum distance $\Delta_{dec}^{\min}$ in the decision space to classify solutions as distinct is set to 5% of the maximum value for each decision variable:

4.2. Results and discussions

Based on these criteria, the proposed Algorithm 1 is executed to identify the set of multimodal solutions. These solutions provide alternative design configurations that achieve equivalent performance in the objective space while exhibiting significant differences in the decision space. This information supports the decision-maker in performing a detailed exploration of the design alternatives, taking into account manufacturing feasibility, cost considerations, or other practical factors beyond the objectives initially modeled.

To validate the performance of the proposed algorithm, a total of 51 independent runs were conducted using the following combinations of hyperparameter settings: a scaling factor $F = [0.3, 0.5, 0.7]$, and crossover rate $Cr = [0.2, 0.5, 0.9]$. Initial population size is set to 50 decision vectors randomly distributed in the decision space, and a total of 100,000 generations per run. No initial population was provided.

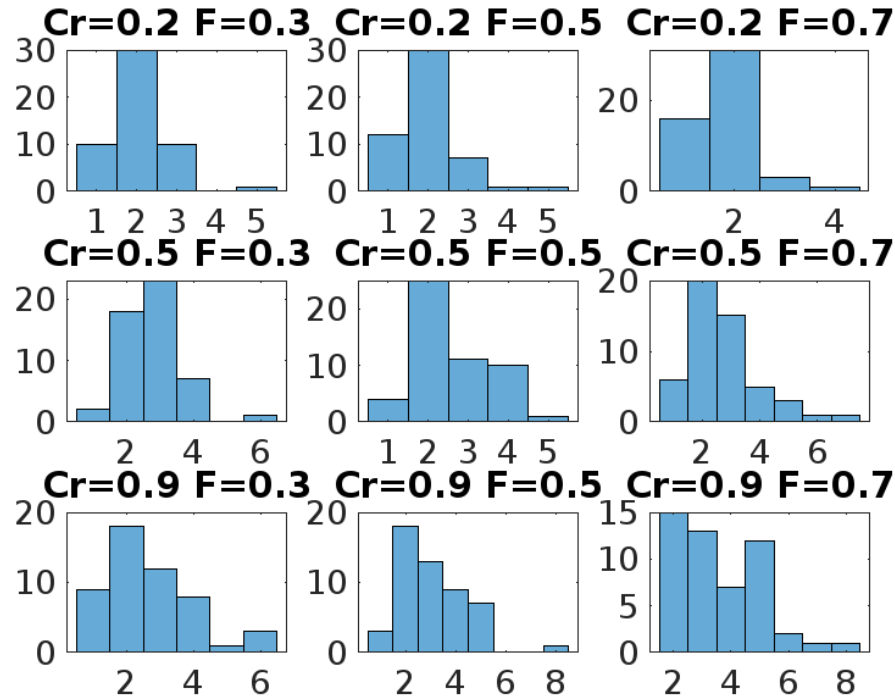


Figure 4: Number of multimodal solutions approximated by each hyperparameter setting.

Figure 4 depicts the number of multimodal solutions approximated by the algorithm for each combination of hyperparameters. It is possible to appreciate that it is highly sensitive to the hyperparameter set. This suggests that a deeper study on its selections is required. As the best hyperparameter setting is selected the combination $F = 0.7$ and $Cr = 0.9$.

Figure 5 presents the distribution of the number of multimodal solutions identified across the 51 runs. The Magenta star represents the original decision vector selected by the decision maker. As it can be notice, the remainder solutions (black squares) are different front this one. Figure 6 depicts the original approximated Pareto front (red diamonds) and the region where the multimodal solutions are (black squares). All multimodal solutions are equivalent, in terms of the information provided from the decision maker, to the desired trade-off.

This capability allows the decision maker to further explore the design space and apply additional selection criteria, such as manufacturability, cost, or robustness to determine which decision variable configurations are most suitable for implementing the preferred trade-off solution or an alternative of comparable quality.

5. Conclusions

The objective of this work was to propose a pipeline and a dedicated algorithm for the search of multimodal solutions in the context of multi-objective optimization. The proposed pipeline establishes that a multi-objective algorithm should first approximate a Pareto front for a given problem. Subsequently, during the multi-criteria decision-making phase, once the designer selects a solution or set of solutions corresponding to an interesting trade-off, a second algorithm is employed to search for multimodal solutions. This search is guided by the decision-maker's definitions regarding the maximum acceptable distance in the objective space to consider solutions equivalent and the minimum distance in the decision space to classify solutions as distinct.

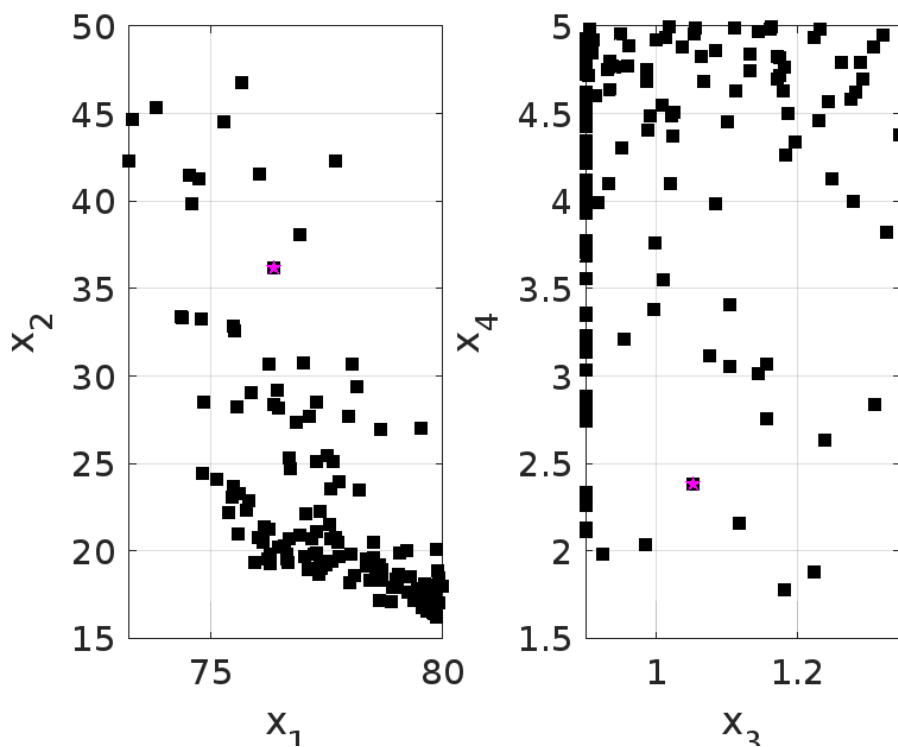


Figure 5: Distribution of the multimodal solutions (black squares) found in 51 runs using the setting $F = 0.7$, $Cr = 0.9$. Magenta star is the original solution selected by the decision maker.

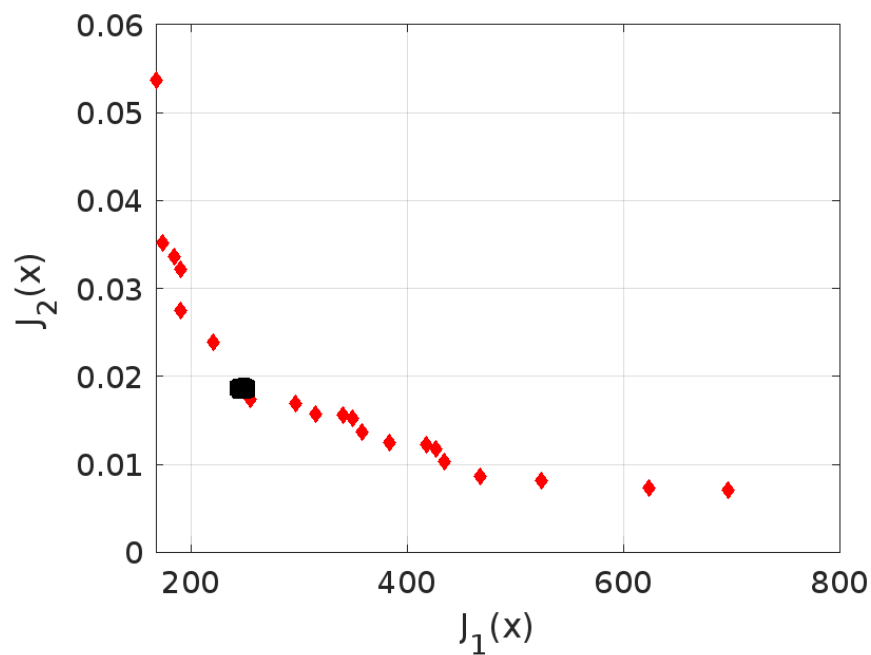


Figure 6: Approximated Pareto front (red diamonds) and multimodal solutions in the objective space (black squares).

The proposed algorithm is based on Differential Evolution and is therefore specifically designed for continuous optimization problems. Future work will focus on developing a variant based on genetic algorithms to extend this approach to combinatorial and discrete optimization problems. Additionally, further research will explore the application of the proposed methodology to more complex scenarios, continuing the validation and refinement of both the pipeline and the algorithm presented in this work.

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Annex: Differential Evolution Algorithm

The Differential Evolution (DE) algorithm is a population-based optimization method widely used for solving complex optimization problems Piotrowski et al. [2023]. It relies on three main operators: mutation, crossover, and selection.

The DE algorithm operates on a population of candidate solutions. Let $P = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ denote the population of N individuals, where each individual $\mathbf{x}_i \in \mathbb{R}^n$ is a vector of decision variables.

Mutation: For each target vector $\mathbf{x}_i$, a mutant vector $\mathbf{v}_i$ is generated using the mutation operator. One common mutation strategy is the DE/rand/1 scheme, defined as:

$$\mathbf{v}_i = \mathbf{x}_{r1} + F \cdot (\mathbf{x}_{r2} - \mathbf{x}_{r3}), \quad (10)$$

where $\mathbf{x}_{r1}, \mathbf{x}_{r2}, \mathbf{x}_{r3} \in P$ are distinct randomly selected individuals from the population, and F is the mutation factor, typically in the range $[0, 2]$.

Crossover: The crossover operator combines the target vector $\mathbf{x}_i$ and the mutant vector $\mathbf{v}_i$ to produce a trial vector $\mathbf{u}_i$. The binomial (uniform) crossover is defined as:

$$u_{ij} = \begin{cases} v_{ij} & \text{if } \text{rand}_j \leq C_r \text{ or } j = j_{rand}, \\ x_{ij} & \text{otherwise,} \end{cases} \quad (11)$$

where u_{ij} , v_{ij} , and x_{ij} are the j -th components of $\mathbf{u}_i$, $\mathbf{v}_i$, and $\mathbf{x}_i$, respectively. C_r is the crossover probability, and j_{rand} is a randomly chosen index to ensure that at least one component is taken from the mutant vector.

Selection: The selection operator determines whether the trial vector $\mathbf{u}_i$ replaces the target vector $\mathbf{x}_i$ in the next generation based on their fitness values. For a minimization problem, the selection operator is:

$$\mathbf{x}_i^{(t+1)} = \begin{cases} \mathbf{u}_i & \text{if } f(\mathbf{u}_i) \leq f(\mathbf{x}_i), \\ \mathbf{x}_i & \text{otherwise,} \end{cases} \quad (12)$$

where f is the objective function to be minimized.

The pseudocoding for the DE algorithm is as follows:

Algorithm 2 Differential Evolution (DE) Algorithm

```

1: Initialize population  $P$  with  $N$  individuals
2: Evaluate fitness of each individual in  $P$ 
3: while stopping criterion not met do
4:   for each individual  $\mathbf{x}_i$  in  $P$  do
5:     Mutation: Generate mutant vector  $\mathbf{v}_i$  using Equation (20)
6:     Crossover: Generate trial vector  $\mathbf{u}_i$  using Equation (21)
7:     Selection: Select the next generation individual  $\mathbf{x}_i^{(t+1)}$  using Equation (22)
8:   end for
9:   Evaluate fitness of each individual in the new population
10: end while
11: return the best individual found

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