

Simple Problems

The Simplicial Gluing Structure of Pareto Sets and Pareto Fronts

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ABSTRACT

Quite a few studies on real-world applications of multi-objective optimization reported that their Pareto sets and Pareto fronts form a topological simplex. Such a class of problems was recently named the *simple problems*, and their Pareto set and Pareto front were observed to have a gluing structure similar to the faces of a simplex. This paper gives a theoretical justification for that observation by proving the gluing structure of the Pareto sets/fronts of subproblems of a simple problem. The simplicity of standard benchmark problems is studied.

CCS CONCEPTS

• **Applied computing** → **Multi-criterion optimization and decision-making**; • **Mathematics of computing** → **Evolutionary algorithms**; **Nonconvex optimization**; **Geometric topology**;

KEYWORDS

multi-objective optimization, problem class, stratification

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1 INTRODUCTION

The success of evolutionary multi-objective optimization (EMO) is widely spreading over various academic and industrial fields. Recent numerical studies showed that decomposition-based EMO algorithms such as MOEA/D [5], NSGA-III [1], and AWA [3] have an ability to approximate the entire Pareto set and Pareto front of many-objective problems.

In contrast to their abundance of experimental successes, the theory shedding light on why they work is still under developing. Especially, the problem class in which decomposition-based EMO algorithms can cover the entire Pareto set/front has not been understood. Recently, Hamada et al. [3] defined a class of problems called the *simple problem*. They pointed

out, without rigorous proofs, that the Pareto set and Pareto front of a simple problem are both homeomorphic to a simplex and the faces of the simplex correspond to the Pareto sets and their images of the subproblems. They also discussed that this property is closely related to scalarization. This paper mathematically refines their arguments. The full version of the paper, which contains rigorous proofs, is provided in the supplementary material as well as in arXiv.

2 SIMPLE PROBLEM

Definition 2.1 (simple problem [3]). A multi-objective optimization problem \mathbf{f} is *simple* or has *simplicity* if every subproblem $\mathbf{g} \subseteq \mathbf{f}$ satisfies the following conditions: if \mathbf{g} is a k -objective problem, then

- (S1) $X^*(\mathbf{g})$ is homeomorphic to Δ^{k-1} ,
- (S2) $\mathbf{g}|_{X^*(\mathbf{g})} : X^*(\mathbf{g}) \rightarrow \mathbb{R}^k$ is an embedding.

Here, we abuse \mathbf{f} to denote a mapping $\mathbf{f} = (f_1, \dots, f_m) : X \rightarrow \mathbb{R}^m$ and a set $\mathbf{f} = \{f_1, \dots, f_m\}$. For a subproblem $\mathbf{g} \subseteq \mathbf{f}$, i.e., a subset of \mathbf{f} , the Pareto set and its image are denoted by $X^*(\mathbf{g})$ and $\mathbf{f}X^*(\mathbf{g})$, respectively. $\Delta^{k-1} = \{(x_1, \dots, x_k) \in [0, 1]^k \mid \sum x_i = 1\}$ is the $(k-1)$ -simplex.

2.1 Main Result

The solutions to a simple problem have a simplicial gluing structure as shown in Figs. 1 and 2.

THEOREM 2.2. *For a simple problem \mathbf{f} and a subproblem $\mathbf{g} \subseteq \mathbf{f}$, it holds that*

$$\partial X^*(\mathbf{g}) = \bigsqcup_{\mathbf{h} \subset \mathbf{g}} \text{int } X^*(\mathbf{h}), \quad (1)$$

$$\partial \mathbf{f}X^*(\mathbf{g}) = \bigsqcup_{\mathbf{h} \subset \mathbf{g}} \text{int } \mathbf{f}X^*(\mathbf{h}), \quad (2)$$

$$\mathbf{f}\partial X^*(\mathbf{g}) = \partial \mathbf{f}X^*(\mathbf{g}), \quad (3)$$

$$\mathbf{f} \text{int } X^*(\mathbf{g}) = \text{int } \mathbf{f}X^*(\mathbf{g}). \quad (4)$$

2.2 Relation to Scalarization

Equations (1)–(4) together define a gluing structure of the Pareto sets and their images of subproblems of a simple problem. This structure induces a natural stratification of the Pareto set (resp. the Pareto front) where each stratum is the interior of the Pareto set (resp. its image) of a subproblem. Therefore, we can numerically compute the stratification by solving each subproblem. Points spreading over all strata can be a good covering of the Pareto set/front.

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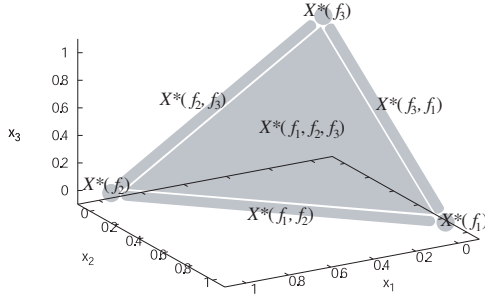


Figure 1: The gluing structure of Pareto sets.

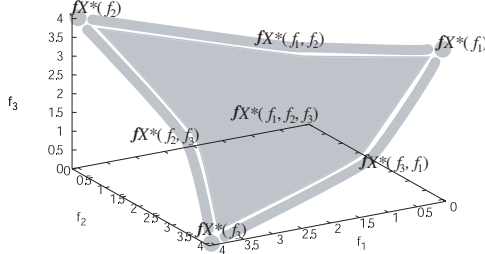


Figure 2: The gluing structure of Pareto set images.

To see why this structure enables decomposition-based EMO algorithms to cover the Pareto set/front, consider the Chebyshev-norm scalarization

$$\underset{x \in X}{\text{minimize}} \ f_w(x) = \max_i w_i (f_i(x) - z_i) \quad (5)$$

where the weight $w = (w_1, \dots, w_m)$ is chosen from Δ^{m-1} and the ideal point is fixed to be $z_i = \min_{x \in X} f_i(x)$. Let e_i be the i -th standard base in \mathbb{R}^m whose i -th coordinate is one and the other coordinates are zero. The standard $(m-1)$ -simplex is rewritten as $\Delta^{m-1} = [e_1, \dots, e_m]$. Using the notation of the weight-optima correspondence

$$S(W) = \bigcup_{w \in W} X^*(f_w),$$

a well-known fact of the optima to (5) can be written as

$$S([e_{i_1}, \dots, e_{i_k}]) = X^w(f_{i_1}, \dots, f_{i_k}) \quad (6)$$

for any choice of an arbitrary number of indices $i_1, \dots, i_k \in \{1, \dots, m\}$. If the problem is simple, then we can go further: the simplicity extends (6) to

$$S([e_{i_1}, \dots, e_{i_k}]) = X^*(f_{i_1}, \dots, f_{i_k}),$$

and we have

$$S(\partial[e_{i_1}, \dots, e_{i_k}]) = \partial X^*(f_{i_1}, \dots, f_{i_k}).$$

Therefore, a weight on each face gives a boundary point of each stratum with corresponding indices.

Unfortunately, the Chebyshev-norm, as well as other existing scalarization methods including the weighted sum, the augmented Chebyshev-norm, and PBI [5], does NOT give the correspondence between the interiors:

$$S(\text{int}[e_{i_1}, \dots, e_{i_k}]) \neq \text{int} X^*(f_{i_1}, \dots, f_{i_k}).$$

Nevertheless, once boundary points of a stratum are obtained, we can find new weights corresponding to interior points of the stratum by interpolating the weights used for the boundary points. Thus, the grid arrangement or divide-and-conquer generation of weights over $[e_{i_1}, \dots, e_{i_k}]$ practically often hit interior points of $X^*(f_{i_1}, \dots, f_{i_k})$.

3 SIMPLICITY OF BENCHMARKS

THEOREM 3.1. *The simplicity of benchmark problems are:*

ZDT1–6 [6] *are non-simple.*

DTLZ1–9 [2] *are non-simple.*

WFG2, 4, 5, 9 [4] *are non-simple.*

WFG1, 3, 6–8 [4] *are simple if and only if they have one position-related variable and two objectives.*

MED [3] *is simple.*

4 CONCLUSIONS

In this paper, we have discussed the simple problem and showed that the Pareto sets of its subproblems (resp. their images) constitute a stratification of its Pareto set (resp. its Pareto front). This topological property gives a theoretical guarantee that decomposition-based EMO algorithms can obtain an entire approximation of the Pareto set as well as the Pareto front. We have also investigated the simplicity of benchmark problems widely-used in the EMO community. All problems in the ZDT and DTLZ suites are non-simple. The WFG suite contains five simple problems under a very restrictive situation but usually does not, whereas the MED problem is always simple.

We believe that the absence of simple problems in the standard benchmark suites is a considerable gap between the benchmark and the real-world since there are many evidences that a large portion of nowadays applications seems to be simple. Additionally, real-world applications involving simulations can be black-box; it would be important to develop an estimation method for the simplicity of black-box problems from a finite set of approximate solutions.

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