Optimization on the Pareto set

Geometry of multi-objective optimization

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Multi-objective optimization

Decision

Buying a home

Objectives

Multi-objective optimization

Decision

Buying a home

Objectives

Cost

Location

Value

Noise

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Solution concept: Pareto efficiency/optimality

A Pareto efficient decision makes an optimal trade off: improving one objective necessarily comes at the cost of worsening another.

Multi-objective optimization problem

The (unconstrained) multi-objective optimization problem:

$$\min_{x \in \mathbb{R}^d} F(x).$$

- $F \equiv (f_1, \ldots, f_n) : \mathbb{R}^d \to \mathbb{R}^n$ is a collection of objectives.

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- x is a decision variable.
- $F(x)$ is the outcome of the decision x.

Pareto optimal solutions

Definition

A decision $x \in \mathbb{R}^d$ *is* ***Pareto optimal*** *if for all* $x' \in \mathbb{R}^d$ *and* $i \in [d]$,

$$f_i(x') < f_i(x)$$

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Notation: let $\mathrm{Pareto}(F)$ be the set of Pareto optimal solutions.

Making a single decision

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However, Pareto optimal solutions are generally:

- not unique: there can be many optimal trade offs,
- not totally ordered: there is usually no ‘best’ optimal trade off.

Thus, the problem is not very well-posed yet.

Multi-objective optimization: current approaches

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Construct a representative subsample of the set of Pareto efficient solutions.

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Example: a realtor selects a small collection of homes for you to inspect.

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Example: quantify how much each additional mile to work is worth to you.

Pareto-constrained optimization

This work:

- Let $F \equiv (f_1, \ldots, f_n) : \mathbb{R}^d \to \mathbb{R}^n$ be n objective functions.
- Suppose we are given an additional preference function $f_0 : \mathbb{R}^d \to \mathbb{R}$.

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Goal: optimize f_0 constrained to the Pareto set of F,

$$\min_{x \in \mathrm{Pareto}(F)} f_0(x).$$

Challenges of Pareto-constrained optimization

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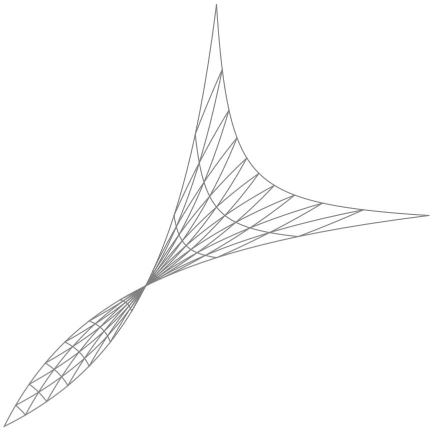
1. The Pareto set is defined implicitly.
2. The Pareto set is generally non-smooth and non-convex.
   - This is true even when the objectives are very nice.
   - Even defining an appropriate solution concept can be non-trivial.

Non-smoothness and non-convexity of Pareto set



Example

The Pareto set of three quadratics,

$$f_i(x) = \frac{1}{2}(x - c_i)^\top A_i (x - c_i).$$

$$A_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad c_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

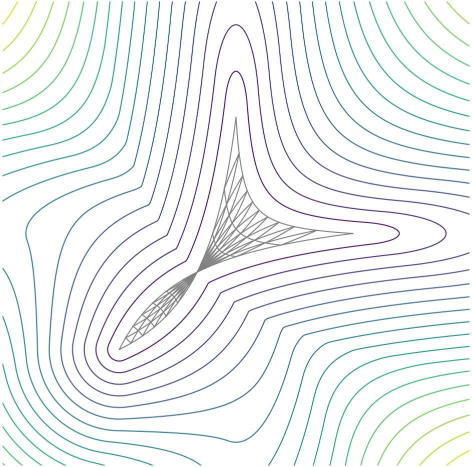
$$A_2 = \begin{bmatrix} 0.25 & 0 \\ 0 & 1 \end{bmatrix} \qquad c_2 = \begin{bmatrix} 1 \\ 0.5 \end{bmatrix}$$

$$A_3 = \begin{bmatrix} 1 & 0 \\ 0 & 0.25 \end{bmatrix} \qquad c_2 = \begin{bmatrix} 0.5 \\ 1 \end{bmatrix}$$

Previously observed unruliness

- singularities or self-crossings (Sheftel et al., 2013)
- needle-like extensions and knees (Kulkarni et al., 2023)

A failed attempt



Approach. Find a potential Φ where:

- $\Phi(x) \geq 0$
- $x \in \text{Pareto}(F) \iff \Phi(x) = 0.$

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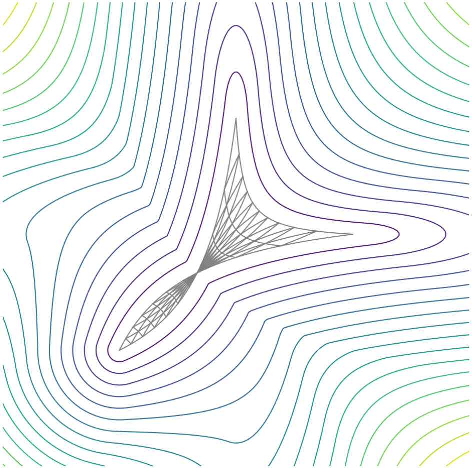

Approach. Find a potential Φ where:

- $\Phi(x) \geq 0$
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Difficulty. Non-smoothness of Pareto set carries over to the potential.

- Φ is not analytic near singularity; Taylor series a poor approximate.

Geometry of the Pareto set

Pareto stationarity

Definition

Let $f_1, \ldots, f_n$ be smooth. A point $x \in \mathbb{R}^d$ is Pareto stationary if zero is a convex combination:

$$\sum_{i \in [n]} w_i \nabla f_i(x) = 0,$$

for some $w_1, \ldots, w_n \geq 0$ such that $w_1 + \cdots w_n = 1$.

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$$f_w(x) := \sum_{i \in [n]} w_i f_i(x).$$

Therefore, x is Pareto stationary if and only if $\nabla f_w(x) = 0$ for some $w \in \Delta^{n-1}$.

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Claim. If x is not Pareto stationary, then there is a descent direction for all objectives.

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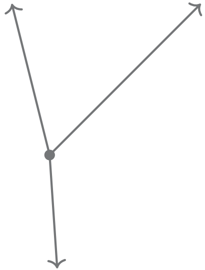

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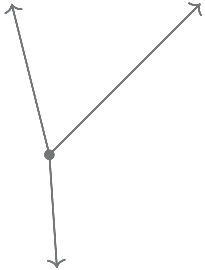

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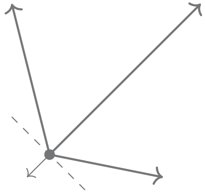

All vectors lie in some half-space:

$$u^\top v_i < 0.$$

Strict convexity + Pareto stationarity $\implies$ Pareto optimality

Claim. If $f_1, \ldots, f_n$ are strictly convex and x is Pareto stationary, then x is Pareto optimal.

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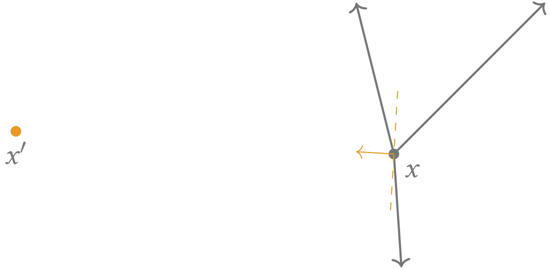

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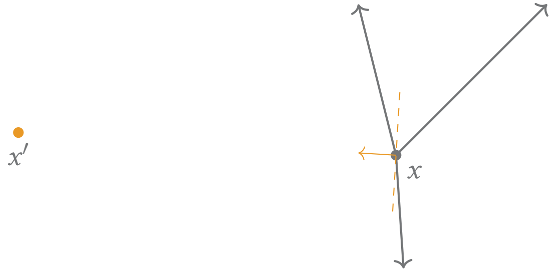

If x is Pareto stationary, then moving toward any direction $x' - x$ will increase one of the objectives. By strict convexity, the increase is strictly monotonic.

Pareto optimality $\iff$ Pareto stationarity (under strict convexity)

Proposition

Let $f_1, \ldots, f_n$ be smooth and strictly convex. Then:

$$\text{Pareto}(F) = \left\{x : \nabla f_w(x) = 0 \text{ for some } w \in \Delta^{n-1}\right\}.$$

Pareto manifold

Definition

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Let $f_1, \ldots, f_n$ be smooth and strictly convex. The ***Pareto manifold*** $\mathcal{P}(F)$ *is defined:*

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where (x, w) *ranges over* $\mathbb{R}^d \times \Delta^{n-1}$.

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- $\mathcal{P}(F)$ is a smooth submanifold of $\mathbb{R}^d \times \Delta^{n-1}$.
- In fact, it is diffeomorphic to Δ^{n-1}.

Proof of smoothness structure

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$$(x, w) = \big(x^*(w), w\big), \qquad \forall (x, w) \in \mathcal{P}(F).$$
4. In fact, we can also deduce x^* and ∇x^* (albeit implicitly):
$$x^*(w) \equiv x_w := \operatorname*{arg\,min}_{x \in \mathbb{R}^d} f_w(x) \qquad \text{and} \qquad \nabla x^*(w) = -\nabla^2 f_w(x_w)^{-1} \nabla F(x_w).$$

Pareto-constrained optimization

$$\min_{x \in \text{Pareto}(F)} f_0(x)$$

Pareto-constrained optimization: high-level idea

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$$\min_{(x,w) \in \mathcal{P}(F)} f_0(x)$$

Pareto-constrained optimization: high-level idea

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- However, the problem remains implicit, since $x^*(w)$ is implicitly defined.
  - This is an instance of a bilevel optimization problem:

$$\min_{w \in \Delta^{n-1}} f_0\left(\arg\min_{x \in \mathbb{R}^d} f_w(x)\right).$$

Solution concepts

Given objectives $f_1, \ldots, f_n$ and a preference function f_0, we say:

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  2. for all $w' \in \Delta^{n-1}$,

$$-\nabla(f_0 \circ x^*)(w)^\top (w' - w) \leq 0.$$

Preference optimality $\Longrightarrow$ preference stationarity

Proposition (Necessary condition)

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Proof.

Standard from convex optimization, see Nesterov (2013) for example. □

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Expanding out the preference stationarity condition, we obtain:

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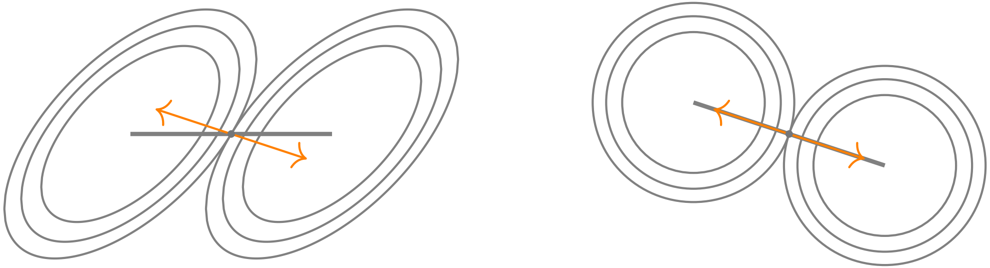
Question: is second-order information necessary?

- Yes. First order information ∇F doesn't tell us how the Pareto set curves.

Necessity of second-order information



Two Pareto sets (thick gray) with the same first-order information (orange vectors).

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(i) reject Pareto optimal points at times, or

(ii) are uninformative.

Theory and algorithms

Estimating the gradient

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Because x_w is implicit, let us define the (computable) approximation:

$$\widehat{\nabla} x^*(x, w) := -\nabla^2 f_w(x)^{-1} \nabla F(x).$$

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$$\nabla x^*(w) = -\nabla^2 f_w(x_w)^{-1} \nabla F(x_w).$$

Because x_w is implicit, let us define the (computable) approximation:

$$\widehat{\nabla} x^*(x, w) := -\nabla^2 f_w(x)^{-1} \nabla F(x).$$

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- Design of an algorithm that robustly makes use of this approximation.

Assumptions

We assume that the objectives $f_1, \dots, f_n : \mathbb{R}^d \to \mathbb{R}$ satisfy:

- μ-strong convexity and L-Lipschitz smoothness,
- L_H-Lipschitz continuity of the Hessians,
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Implications of assumptions

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2. the approximation error $\left\|\widehat{\nabla} x^*(x, w) - \nabla x^*(w)\right\|$ can also be controlled

Majorizing surrogates

Definition

A ***majorizing surrogate*** $g : \Delta^{n-1} \to \mathbb{R}$ *of the composition* $f_0 \circ x^*$ *is a map:*

$$g(w) \leq (f_0 \circ x^*)(w), \qquad \forall w \in \Delta^{n-1}.$$

A family of majorizing surrogates

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$$g(w'; x, w) := f(x_w) + \nabla f_0(x)^\top \widehat{\nabla} x^*(x, w)(w' - w) + \frac{cn}{2}\|w' - w\|_2^2 + \mathrm{err}(x, w).$$

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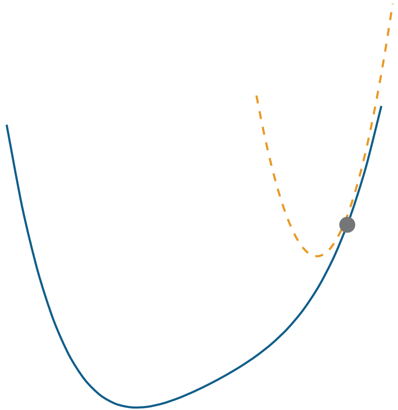
- The constant c and error function $\mathrm{err}(x, w)$ can be computed explicitly.
- As x approaches x_w, the error term shrinks and the upper bound becomes tighter.

Majorization-minimization



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For $k = 0, 1, \ldots$

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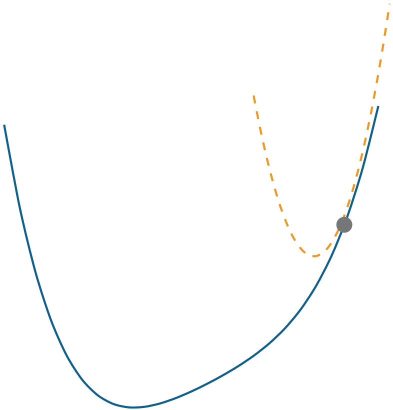

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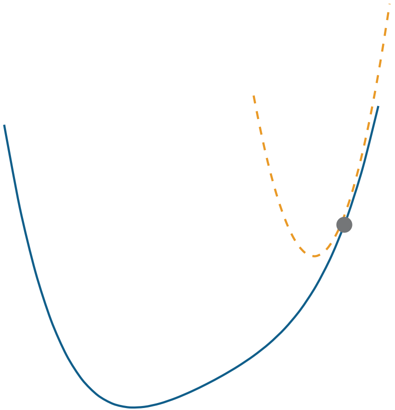

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Initialize $(x_0, w_0) \in \mathbb{R}^d \times \Delta^{n-1}$. For $k = 0, 1, \ldots, K-1$:

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The subroutines are easy: $\operatorname*{arg\,min}_{w \in \Delta^{n-1}} g(w)$ is a quadratic program; $f_w(x)$ is strongly convex.

Convergence result

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- $\arg\min_{w \in \Delta^{n-1}} g(w)$ *achieves ε-stationarity*
- $\arg\min_{x \in \mathbb{R}^d} f_w(x)$ *achieves ε^2-optimality.*

Extensions

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- Sampling from the Pareto set
  - Mirror descent allows for sampling from the simplex.

Collaborators

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Thank you!

Paper at *https://arxiv.org/abs/2308.02145*.

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