Polytechnique Montréal
Department of Mathematics and Industrial Engineering

Introduction to Multiobjective Optimization

Ludovic Salomon

Prerequites

- Basic notions in numerical analysis: gradient, hessian, vector space.
- Basic notions in optimization: solution, objective function, constraints, or convexity.

Objectives

At the end of this tutorial, you will be able to:

- Describe what a solution in multiobjective optimization is; and its main properties.
- List some general multiobjective resolution methods.

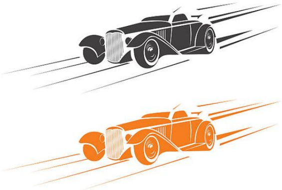
How to choose a car ? (drawn from [Ehrgott, 2005])

Your dilemna

How to choose a car ? (drawn from [Ehrgott, 2005])

Your dilemna

Your criteria



How to choose a car ? (drawn from [Ehrgott, 2005])

A market study (drawn from [Ehrgott, 2005])

Brand	VW	Opel	Ford	Toyota
Price ($)	16200	14900	**14000**	15200
Consumption (l/100 km)	7.2	**7.0**	7.5	8.2
Power (kW)	66.0	62.0	55.0	**71.0**

Conclusion

No choice is optimal : life is about making compromises ...

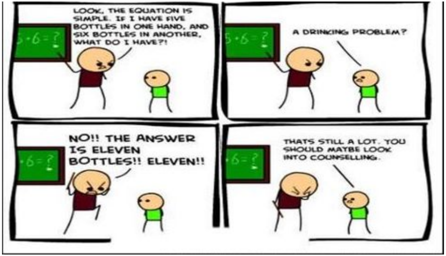
Applications

Various applications of multiobjective optimization

- Machine learning [Alexandropoulos et al., 2019, Jin, 2006]
- Chemical engineering [Sharma and Rangaiah, 2013]
- Bioinformatics and computational biology [Handl et al., 2007]
- Discrete optimization [Ehrgott, 2005]
- Economics [Tapia and Coello, 2007]
- And so on ...

Last remarks before to start

Pros



Last remarks before to start

Cons

Hard, hard, hard... More difficult to solve than single-objective optimization problems !

The general problem

The problem

$$\begin{array}{ll} \text{minimize} & f(x) = [f_1(x), f_2(x), \ldots, f_m(x)]^\top \\ x \in \Omega & \end{array}$$

where:

- $f : \Omega \to \mathbb{R}^m$ is the objective function, composed of $m \geq 2$ **objective functions** $f_1, f_2, \ldots, f_m$ for $i = 1, 2, \ldots, m$.
- $\Omega \subseteq \mathbb{R}^n$ is the **feasible decision space**.
- $f(\Omega)$ is designed as the **feasible objective space**.
- $\mathbb{R}^n$ is designed as the **decision space**, $\mathbb{R}^m$ as the **objective space**.

Order relations : definitions

Pareto dominance

Given two decision vectors x^1 and x^2,

- x^1 **weakly dominates** x^2 (denoted as $x^1 \preceq x^2$) if and only if $f_i(x^1) \leq f_i(x^2)$ for all $i = 1, 2, \ldots, m$.
  ex : when $f(x^1) = [2, 1]^\top$ and $f(x^2) = [2, 2]^\top$, $x^1 \preceq x^2$.
- x^1 **dominates** x^2 (denoted as $x^1 \prec x^2$) if and only if $f_i(x^1) \leq f_i(x^2)$ for all $i = 1, 2, \ldots, m$ and there exists index $j \in \{1, 2, \ldots, m\}$ such that $f_j(x^1) < f_j(x^2)$.
  ex : for $f(x^1) = [1, 0]^\top$ and $f(x^2) = [1, 1]^\top$, $x^1 \prec x^2$.
- x^1 **strictly dominates** x^2 (denoted as $x^1 \prec\prec x^2$) if and only if $f_i(x^1) < f_i(x^2)$ for all $i = 1, 2, \ldots, m$.
  ex : when $f(x^1) = [1, 0]^\top$ and $f(x^2) = [5, 6]^\top$, $x^1 \prec\prec x^2$.
- x^1 and x^2 are **incomparable** (denoted as $x^1 \parallel x^2$) if and only if x^1 does not weakly dominate x^2 nor x^2 does not weakly dominate x^2.
  ex : when $f(x^1) = [-1, 3]^\top$ and $f(x^2) = [7, -2]^\top$, $x^1 \parallel x^2$.

Dominance, dominated and indifferent zones

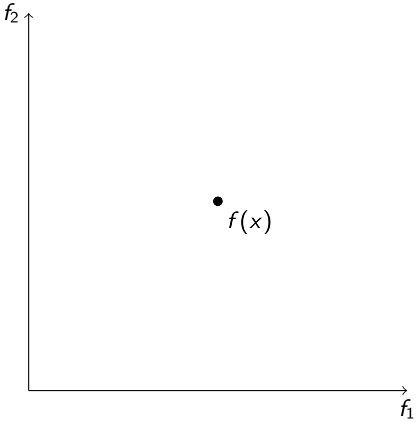
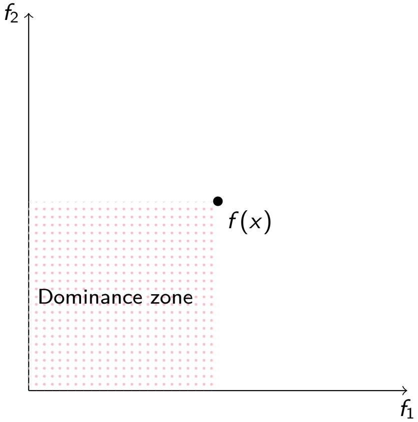


Figure: Principal search zones for a biobjective minimization problem in the objective space.

Dominance, dominated and indifferent zones



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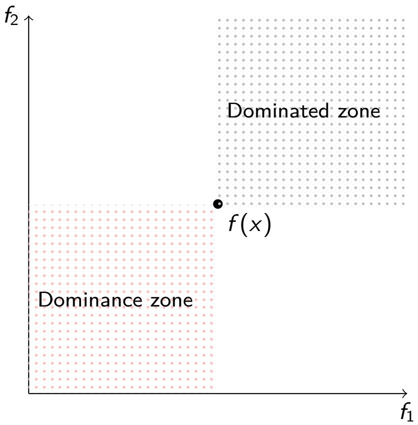

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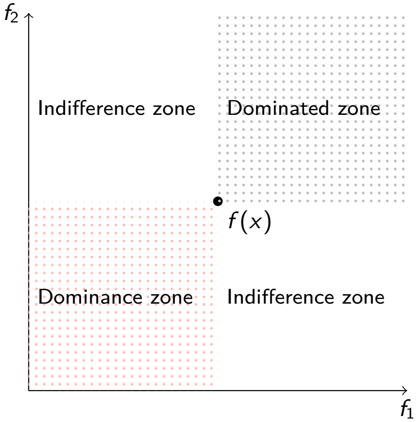


Figure: Principal search zones for a biobjective minimization problem in the objective space.

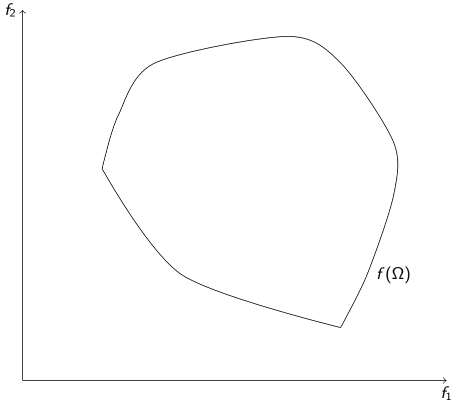
Pareto front and Pareto set

Definition

The decision vector $x^* \in \Omega$ is said to be **Pareto-optimal** if there does not exist any other decision vector $x \in \Omega$ such that $x \prec x^*$.
The set of all Pareto optimal solutions is called the **Pareto set** denoted as $\mathcal{X}_P$ and its image by the objective function is called the **Pareto front** denoted as $\mathcal{Y}_P$.

Pareto front and Pareto set

An illustration,



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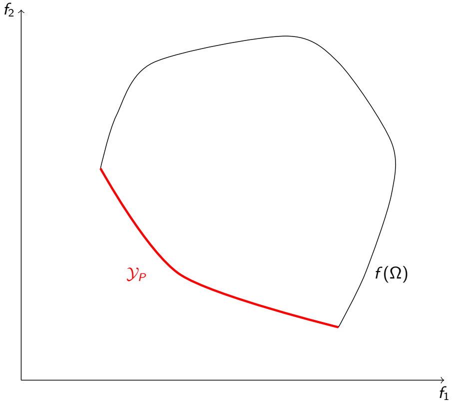
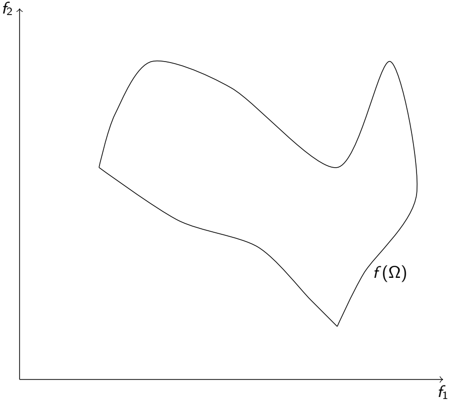


Figure: Objective space and convex Pareto front for a biobjective minimization problem.

Pareto front and Pareto set

Another illustration,



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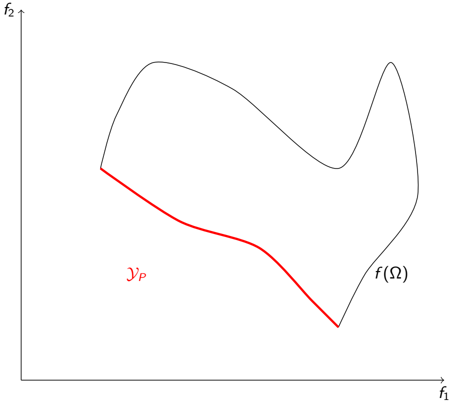
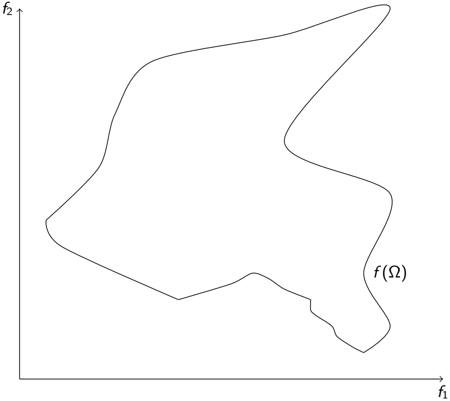


Figure: Objective space and non convex Pareto front for a biobjective minimization problem.

Pareto front and Pareto set

And a last one !



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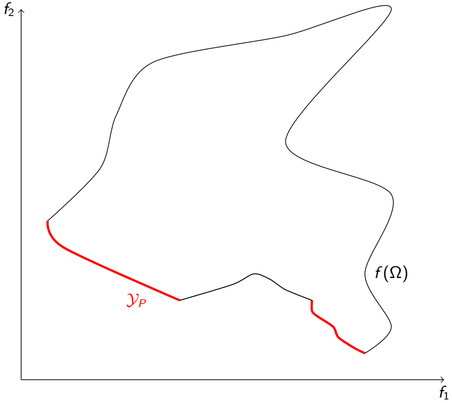

Figure: Objective space and piecewise-continuous Pareto front for a biobjective minimization problem

Bounds on the Pareto front

Definition

The **ideal objective vector** y^I is defined as

$$y^I = \left[\min_{x\in\Omega} f_1(x), \min_{x\in\Omega} f_2(x), \ldots, \min_{x\in\Omega} f_m(x)\right]^\top$$

Definition

The **nadir objective vector** y^N is defined as

$$y^N = \left[\max_{x\in\mathcal{X}_P} f_1(x), \max_{x\in\mathcal{X}_P} f_2(x), \ldots, \max_{x\in\mathcal{X}_\mathcal{P}} f_m(x)\right]^\top$$

Definition

The **utopian objective vector** y^U is defined as

$$y^U = \left[y_1^I - \epsilon_1, y_2^I - \epsilon_2, \ldots, y_m^I - \epsilon_m\right]^\top$$

where $\epsilon_i > 0$ for $i = 1, 2, \ldots, m$.

Bounds on the Pareto front

An illustration

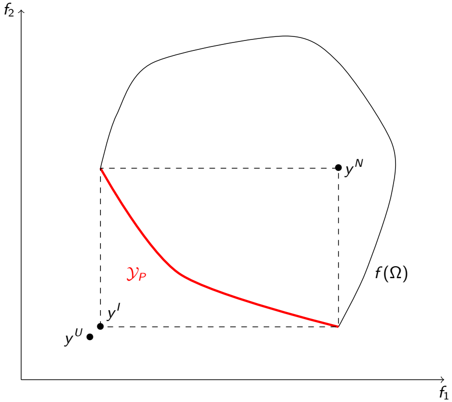

Figure: Objective space, ideal, utopian and nadir objective vector for a biobjective minimization problem.

Limits

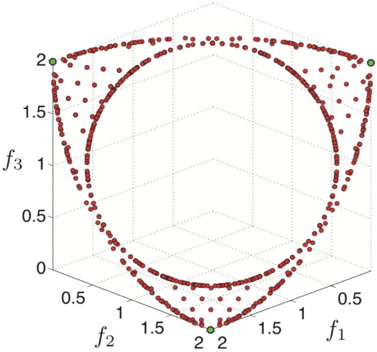

Figure: An exemple of a Pareto front approximation [Burachik et al., 2017].

Scalarization methods: the main idea

- Rely on single-objective optimization methods.
- Convert the multiobjective optimization problem (MOP) into a succession of parameterized single-objective subproblems (SOP_j).

Goal

Solve $(SOP_j) \Rightarrow$ One non dominated point.

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Goal

$$\text{Solve } (SOP_j) \Rightarrow \text{One non dominated point.}$$

The Weighted-sum scalarization method [Miettinen, 1999]

Principle

Given a set of positive weights w_i for $i = 1, 2, \ldots, m$ such that

$$\sum_{i=1}^{m} w_i = 1,$$

solve the subproblem

$$\underset{x \in \Omega}{\text{minimize}} \quad \sum_{i=1}^{m} w_i f_i(x)$$

Pros

- Intuitive to understand and easy to interpret.
- The global solution of this problem is weakly Pareto optimal.

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Cons

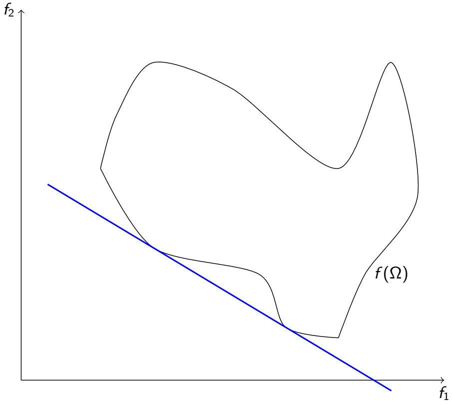

Figure: The weighted sum approach may generate only a subset of the Pareto front.

The ε-constraint method [Chankong and Haimes, 1983]

Principle

Solve the following subproblem

$$\begin{array}{ll} \text{minimize} & f_l(x) \\ x \in \Omega(\varepsilon) & \end{array}$$

where

$$\Omega(\varepsilon) = \{x \in \Omega : f_j(x) \leq \varepsilon_j,\ j = 1, 2, \ldots, m,\ j \neq l\}$$

The ε-constraint method [Chankong and Haimes, 1983]

Functioning

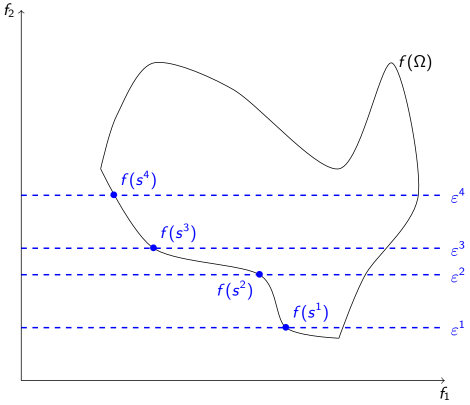

Figure: Generation of non dominated points using the ε constraint method.

The ε-constraint method [Chankong and Haimes, 1983]

Pros

- Easy to understand.
- Easy to interpret.

Cons

- Numerical issues.
- Difficulties to solve the single-objective optimization subproblem.

The Normal Boundary Intersection (NBI) method [Das and Dennis, 1998]

Principle

Solve the following subproblem

$$\begin{array}{ll} \text{maximize} & t \\ \text{s.t} & f(x) = \Phi w + tn \\ & x \in \Omega, t \in \mathbb{R} \end{array}$$

where:

- w is a vector of weights: $w_i \geq 0$ and $\sum_{i=1}^{m} w_i = 1$.
- n is an unit vector orthogonal to the CHIM simplex (Convex Hull of Individual Minima) pointing to the origin.
- Φ the $m \times m$ matrix whose columns are $f(x^{j,\star}) - y^I$ with

$$x^{j,\star} \in \arg\min_{x \in \Omega} f_j(x).$$

The Normal Boundary Intersection (NBI) method [Das and Dennis, 1998]

Illustration

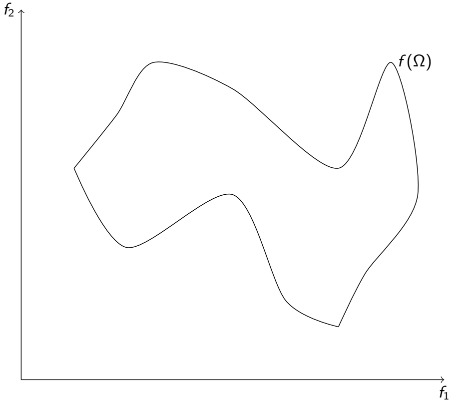

Figure: Generation of non dominated points using the NBI method.

The Normal Boundary Intersection (NBI) method [Das and Dennis, 1998]

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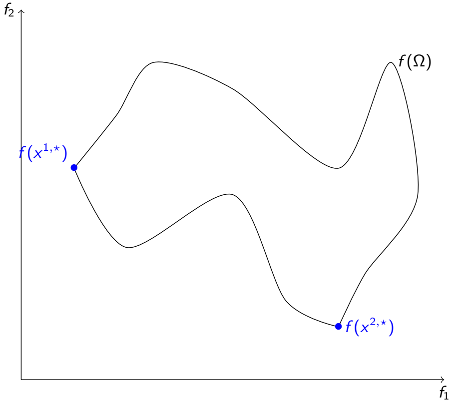

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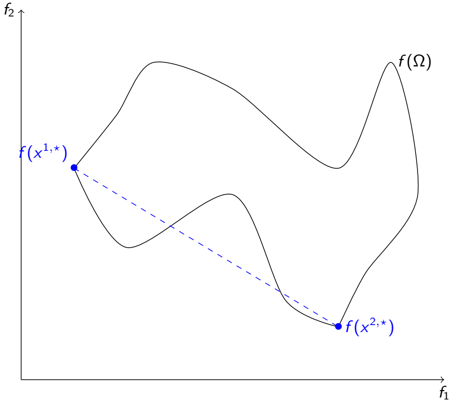

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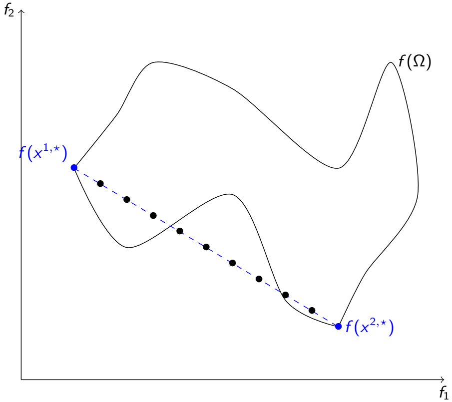

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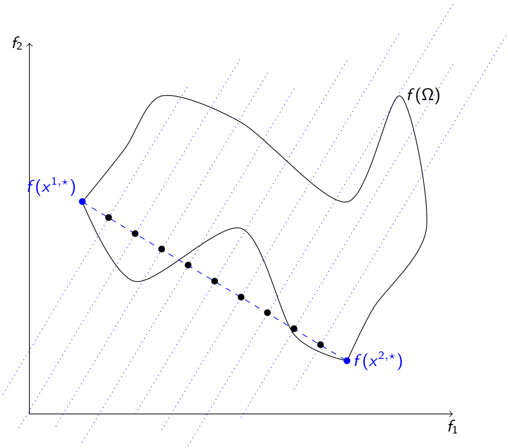

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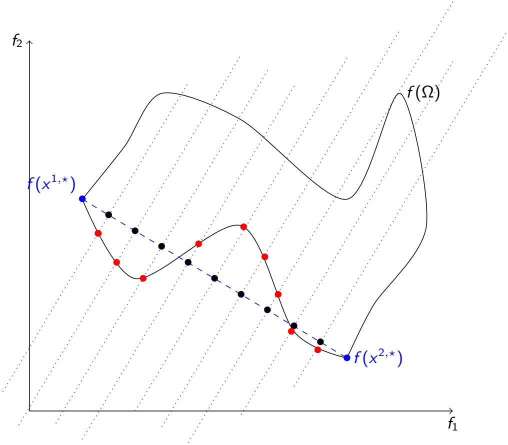

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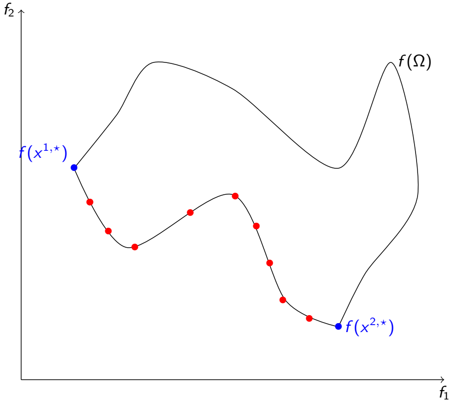

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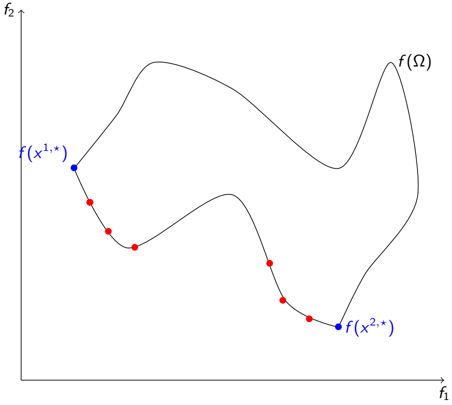

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The Normal Boundary Intersection (NBI) method [Das and Dennis, 1998]

A limitation of NBI

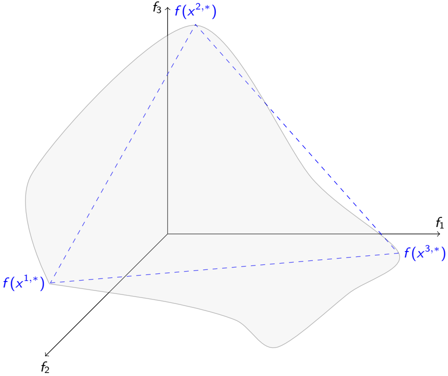


Figure: The NBI method can miss some parts of the Pareto front (inspired by [Das and Dennis, 1998]).

The Normal Boundary Intersection (NBI) method [Das and Dennis, 1998]

Pros

- Generate a good distribution of Pareto objective vectors
- Adaptive for many types of problems.

Cons

- The equality constraints can complexify the resolution of the subproblem.
- The method can generate dominated points.
- Can miss some part of the Pareto front for more than 2 objectives [Das and Dennis, 1998].

Other Variant

- Normal Constraint Method [Messac and Mattson, 2004]

Weighted Tchebycheff methods [Miettinen, 1999]

Weighted Tchebycheff method

Given a set of weights w_i for $i = 1, 2, \ldots, m$ with $\sum_{i=1}^{m} w_i = 1$, solve the subproblem

$$\begin{array}{ll} \text{minimize} & \max\limits_{1 \le i \le m} w_i |f_i(x) - r_i| \\ x \in \Omega & \end{array}$$

where $r \in \mathbb{R}^m$ is a reference objective vector. Generally, $r \in \{y^I, y^U\}$.

Weighted Tchebycheff methods [Miettinen, 1999]

Weighted Tchebycheff augmented methods

Given a set of weights w_i for $i = 1, 2, \ldots, m$ with $\sum_{i=1}^{m} w_i = 1$, solve the subproblem

$$\begin{array}{ll} \text{minimize} & \left[\max\limits_{1\leq i\leq m} w_i(f_i(x) - r_i)\right] + \rho \sum_{i=1}^{m} f_i(x) - r_i \\ x \in \Omega & \end{array}$$

where

- $r \in \mathbb{R}^m$ is a reference objective vector. Generally, $r \in \{y^I, y^U\}$.
- $\rho > 0$ is an external parameter.

Another variant is

$$\begin{array}{ll} \text{minimize} & \max\limits_{1\leq i\leq m} w_i \left[f_i(x) - r_i + \rho \sum\limits_{i=1}^{m} f_i(x) - r_i\right] \\ x \in \Omega & \end{array}$$

Weighted Tchebycheff methods [Miettinen, 1999]

Pros

- Can capture non convex parts of the Pareto front.

Cons

- Choice of the weights
- Require a reformulation.

The goal programming scalarization method

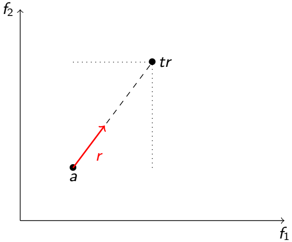
Pascoletti and Serafini scalarization [Pascoletti and Serafini, 1984]

Solve the following subproblem

$$\begin{array}{ll} \text{minimize} & t \\ \text{s.t.} & f(x) \leq a + tr \\ & (x,t) \in \Omega \times \mathbb{R} \end{array}$$

with $r \in \mathbb{R}^m$ and $a \in \mathbb{R}^m$.

Interpretation



The goal programming scalarization method

Illustration (inspired by [Ghosh and Chakraborty, 2015, Khorram et al., 2014])

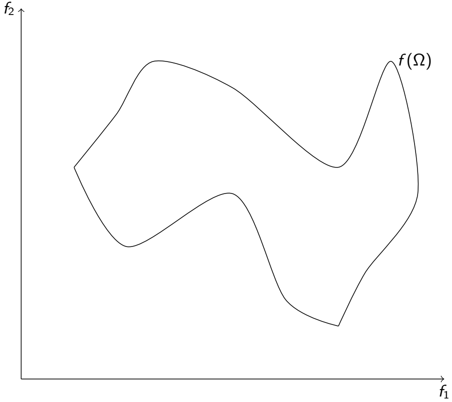


Figure: Generation of non dominated points using the Pascoletti and Serafini approach.

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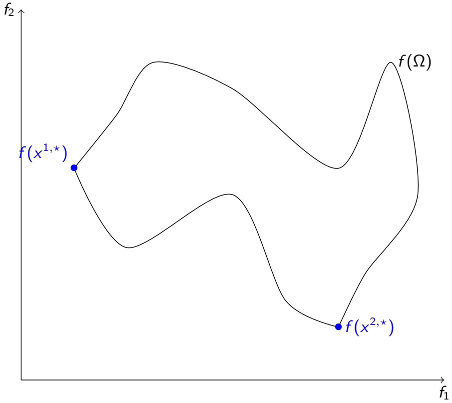

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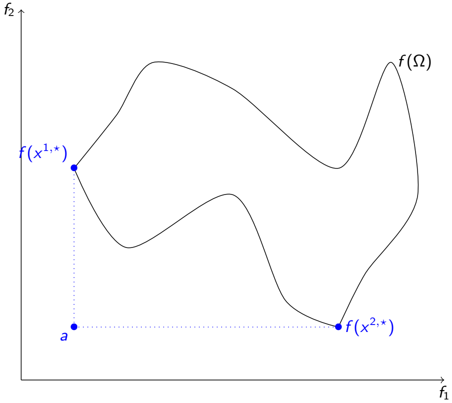

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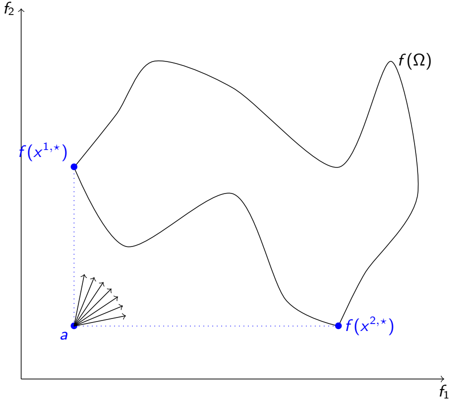

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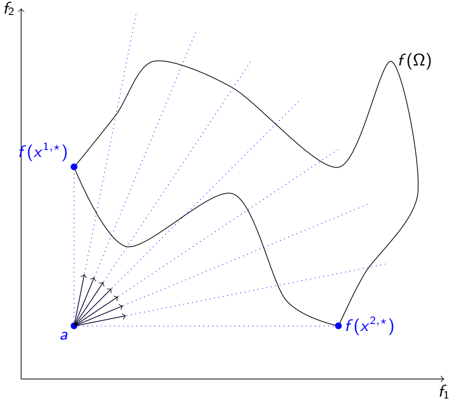

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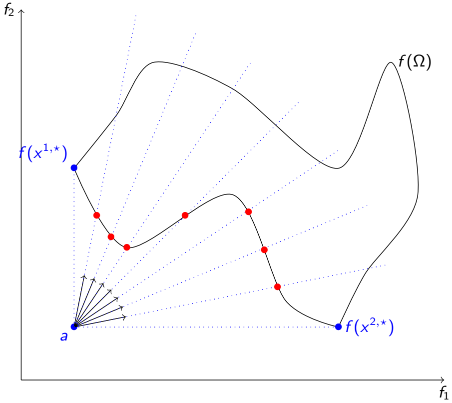

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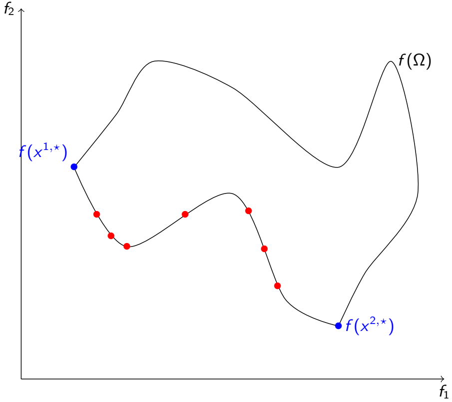

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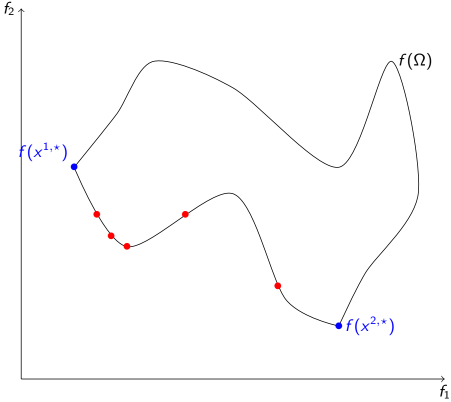

Figure: Generation of non dominated points using the Pascoletti and Serafini approach.

To go further

- Some general references on scalarization methods [Miettinen, 1999, Wiecek et al., 2016].
- How to deal with $m \geq 3$ objectives ? Some works [Mueller-Gritschneder et al., 2009, Burachik et al., 2017] explore this path.
- Recently, methods using a combination of scalarization approaches and branch and bound techniques have been proposed [Eichfelder et al., 2021, Niebling and Eichfelder, 2019].

A reminder

The problem

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

where $f : \mathbb{R}^n \to \mathbb{R}$ is a **scalar-valued** function and continuously differentiable.

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A simple minimization optimization algorithm

- **Initialization** : choose a starting point $x^0 \in \mathbb{R}^n$.
- **Main loop** : for $k = 0, 1, \dots$
  1. If x^k satisfies a stopping condition, then stop.
  2. Otherwise, choose a descent direction d^k.
  3. Choose a step length $\alpha^k > 0$.
  4. Set $x^{k+1} := x^k + \alpha^k d^k$.

A reminder

The problem

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

where $f : \mathbb{R}^n \to \mathbb{R}$ is a **scalar-valued** function and continuously differentiable.

Some interesting descent directions

- The **steepest descent direction**

$$d^k = -\nabla f(x^k).$$

- The **Newton direction**

$$d^k = -[\nabla^2 f(x^k)]^{-1} \nabla f(x^k).$$

- The **Quasi-Nexton direction**

$$d^k = -(B^k)^{-1} \nabla f(x^k)$$

  where $B^k \in \mathbb{R}^n$ positive symmetric.

A reminder

Question

Can we define descent directions for multiobjective optimization problems ?

Steepest descent direction for unconstrained multiobjective optimization

The problem

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

where $f:\mathbb{R}^n \to \mathbb{R}^m$ is **continuously differentiable**.

Steepest descent direction for unconstrained multiobjective optimization

The problem

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

where $f : \mathbb{R}^n \to \mathbb{R}^m$ is **continuously differentiable**.

Theorem

If $x^* \in \mathbb{R}^n$ is Pareto optimal, then there does not exist any direction $d \in \mathbb{R}^n$ such that for all indexes $i = 1, 2, \ldots, m$,

$$\nabla f_i(x)^T d < 0.$$

Idea

Study

$$\max_{i=1,2,\ldots,m} \nabla f_i(x)^T d.$$

Steepest descent direction for unconstrained multiobjective optimization

The problem

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

where $f : \mathbb{R}^n \to \mathbb{R}^m$ is **continuously differentiable**.

Steepest gradient descent for unconstrained multiobjective optimization [Fliege and Svaiter, 2000]

$$d(x) \in \arg\min_{d \in \mathbb{R}^n} \max_{i=1,2,\dots,m} \nabla f_i(x)^T d + \frac{1}{2}\|d\|^2$$

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Remarks

- The problem can be reformulated as a smooth one:

$$\begin{array}{ll} \text{minimize} & t + \frac{1}{2}\|d\|^2 \\ \text{s.t.} & \nabla f_i(x)^\top d \leq t, i = 1, 2, \ldots, m \\ & t \in \mathbb{R},\ x \in \mathbb{R}^n \end{array}$$

- If $m = 1$, one gets $d^k = -\nabla f(x^k)$.

Other descent directions for unconstrained multiobjective optimization

Assumption

$f : \mathbb{R}^n \to \mathbb{R}^m$ is $\mathcal{C}^2$, i.e. **twice differentiable** on $\mathbb{R}^n$.

Newton direction for unconstrained multiobjective optimization [Fliege et al., 2009]

$$d(x) \in \arg\min_{d \in \mathbb{R}^n} \max_{i=1,2,\ldots,m} \nabla f_i(x)^\top d + \frac{1}{2} d^\top \nabla^2 f_i(x) d.$$

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Quasi-Newton direction for unconstrained multiobjective optimization [Morovati et al., 2017, Qu et al., 2011]

$$d(x) \in \arg\min_{d \in \mathbb{R}^n} \max_{i=1,2,\ldots,m} \nabla f_i(x)^\top d + \frac{1}{2} d^\top B^{k,i} d$$

where $B^{k,i} \in \mathbb{R}^{n \times n}$ for $i = 1, 2, \ldots, m$ is symmetric.

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where $B^{k,i} \in \mathbb{R}^{n \times n}$ for $i = 1, 2, \ldots, m$ is symmetric.

Advantages and inconveniences

Pros

- Do not require external parameters.
- Intuitive to understand.

Cons

- The subproblem can be difficult to solve.
- Generate only one non dominated point given a starting point.

Heuristics

Principles

- Start from an initial population of points.
- Interaction between them defined by some parameters.
- Mutation and selection along iterations, supposedly toward some Pareto points.
- For more information, see [Deb and Miettinen, 2008].

Classical methods

- Evolutionary algorithms: NSGA-II [Deb et al., 2000], MOEA-D [Zhang and Li, 2007], ...
- Particule-swarm optimization [Poli et al., 2007]: ant, wolf, butterfly, ...

Heuristics

Some software

- jMetal [Durillo and Nebro, 2011, Nebro et al., 2015]: https://github.com/jMetal/jMetal.
- Pagmo2 [Biscani and Izzo, 2020]: https://github.com/esa/pagmo2.
- Pymoo [Blank and Deb, 2020]: https://pymoo.org/.

Heuristics

Pros

- Really versatile (can deal with integer variables, ...).
- Tunable.

Cons

- Tunable.
- Not really efficient.
- Are really bad to deal with constraints.
- Difficult to scale with a huge number of variables.
- The population size parameter limits the number of potential solutions.

Exact black-box/derivative-free optimization methods

Algorithms

- Direct Multi Search (DMS) [Custódio et al., 2011].
- Multiobjective Implicit Filtering Optimization (MOIF) [Cocchi et al., 2018].
- Derivative-Free Multiobjective Optimization (DFMO) [Liuzzi et al., 2016].

Advantages

- Very similar to heuristics
  1. Start from an initial population of points.
  2. Update the population towards iterations.
- Do not make any restrictions on the size of the population.
- Deterministic convergence analysis.
- Efficient.

Conclusion

At the end of this tutorial, you are now able to:

- Describe what a solution in multiobjective optimization is; the principal properties of a Pareto front.
- List some general multiobjective resolution methods.

Conclusion

What I did not mention

- The construction of efficient data structures for Pareto fronts [Bentley et al., 1993, Chen et al., 2012, De et al., 2017, Jaszkiewicz and Lust, 2018]:
  see `https://alandefreitas.github.io/pareto/` for an implementation.
- The evaluation of the performance of multiobjective optimization algorithms [Audet et al., 2021, Li and Yao, 2019].
- Discrete multiobjective optimization
  ([Ehrgott, 2005, Holzmann and Smith, 2018, Kirlik and Sayın, 2014] for example).

Conclusion

Multiobjective optimization algorithms

- are a tool to **better model** engineering problems.
- are **more difficult to solve** than single-objective optimization problems.
- traditionally are dealt using single-objective optimization methods and scalarization techniques.

But

- **difficult** to implement;
- there are a **limited number** of bullet-proof available algorithms;
- hence the predominance of heuristics.
- To follow...

Thank you for your attention !
Do you have any questions ?

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