Multi-criteria Optimization Introduction

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Introductory example I

Often we want to solve optimization problems concerning several goals.

General applications:

- Medicine: maximum effect, but minimum side effect of a drug.
- Finances: maximum return, but minimum risk of an equity portfolio.
- Production planning: maximum revenue, but minimum costs.
- Booking a hotel: maximum rating, but minimum costs.

In machine learning:

- Sparse models: maximum predictive performance, but minimal number of features.
- Fast models: maximum predictive performance, but short prediction time.
- ...

Introductory example II

Example:

Choose the best hotel to stay at by maximizing ratings subject to a maximum price per night.

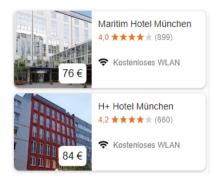
Problems:

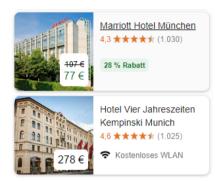
- The result depends on how we select the maximum price and usually returns different solutions for different maximum price values.
- We could also choose a minimum rating and optimize the price per night.
- The more objectives we optimize, the more difficult such a definition becomes.

Goal:

Find a more general approach to solve multi-criteria problems.

Introductory example III





When booking a hotel: find the hotel with

- minimum price per night (costs) and
- maximum user rating (performance).

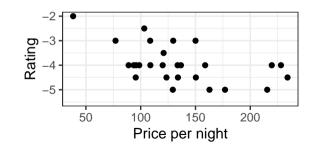
Since our standard is to minimize objectives, we minimize negative ratings.

Introductory example IV

The objectives often conflict with each other:

- ullet Lower price o usually lower hotel rating.
- ullet Better rating o usually higher price.

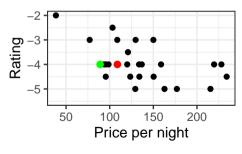
Example: (negative) average rating by hotel guests (1 - 5) vs. average price per night (excerpt).

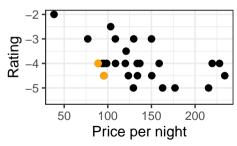


Introductory example V

Often, objectives are not directly comparable as they are measured on different scales:

- Left: A hotel with rating 4 for 89 Euro ($c^{(1)} = (89, -4.0)$) would be preferred to a hotel for 108 Euro with the same rating ($c^{(2)} = (108, -4.0)$).
- Right: How to decide if $c^{(1)} = (89, -4.0)$ or $c^{(1)} = (95, -4.5)$ is preferred?
- How much is one rating point worth?





Definition: multi-criteria optimization problem

A multi-criteria optimization problem is defined by

$$\min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} c(\boldsymbol{\lambda}) \Leftrightarrow \min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} \left(c_1(\boldsymbol{\lambda}), c_2(\boldsymbol{\lambda}), ..., c_m(\boldsymbol{\lambda}) \right),$$

with $\Lambda \subset \mathbb{R}^n$ and multi-criteria objective function $c: \Lambda \to \mathbb{R}^m$, $m \geq 2$.

- **Goal:** minimize multiple target functions simultaneously.
- $(c_1(\lambda),...,c_m(\lambda))^{\top}$ maps each candidate λ into the objective space \mathbb{R}^m .
- Often no clear best solution, as objective are usually conflicting and we cannot totally order in \mathbb{R}^m .
- W.I.o.g. we always minimize.
- Alternative names: multi-criteria optimization, multi-objective optimization, Pareto optimization.

Pareto sets and Pareto optimality

Definition:

Given a multi-criteria optimization problem

$$\min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} \left(c_1(\boldsymbol{\lambda}), ..., c_m(\boldsymbol{\lambda}) \right), \quad c_i : \boldsymbol{\Lambda} \to \mathbb{R}.$$

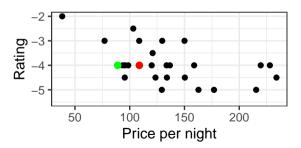
- A candidate $\lambda^{(1)}$ (Pareto-) dominates $\lambda^{(2)}$, if $c(\lambda^{(1)}) \prec c(\lambda^{(2)})$, i.e.
 - $\mathbf{0} \ c_i(\boldsymbol{\lambda}^{(1)}) \leq c_i(\boldsymbol{\lambda}^{(2)})$ for all $i \in \{1,2,...,m\}$ and
 - ② $c_j(\pmb{\lambda}^{(1)}) < c_j(\pmb{\lambda}^{(2)})$ for at least one $j \in \{1,2,...,m\}$
- ullet A candidate λ^* that is not dominated by any other candidate is called **Pareto optimal**.
- The set of all Pareto optimal candidates is called **Pareto set** $\mathcal{P} := \{ \boldsymbol{\lambda} \in \boldsymbol{\Lambda} | \not\exists \tilde{\boldsymbol{\lambda}} \text{ with } c(\tilde{\boldsymbol{\lambda}}) \prec c(\boldsymbol{\lambda}) \}$
- $\mathcal{F} = c(\mathcal{P}) = \{c(\lambda) | \lambda \in \mathcal{P}\}$ is called **Pareto front**.

How to define optimality? I

Let c = (price, -rating). For some cases it is *clear* which point is the better one:

• The candidate $c^{(1)}=(89,-4.0)$ dominates $c^{(2)}=(108,-4.0)$: $c^{(1)}$ is not worse in any dimension and is better in one dimension. Therefore, $c^{(2)}$ gets **dominated** by $c^{(1)}$

$$c^{(2)} \prec c^{(1)}.$$



How to define optimality? II

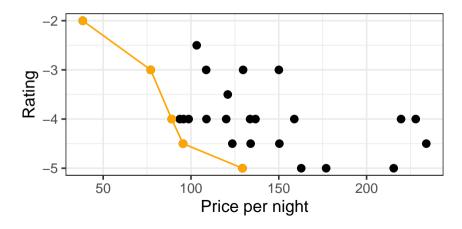
For the points $c^{(1)}=(89,-4.0)$ and $c^{(2)}=(95,-4.5)$ we cannot say which one is better.

• We define the points as equivalent and write

$$c^{(1)} \not\prec c^{(2)}$$
 and $c^{(2)} \not\prec c^{(1)}$.

How to define optimality? III

• The set of all equivalent points that are not dominated by another point is called the **Pareto front**.

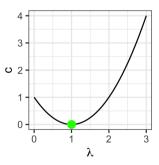


Example: One objective function

We consider the minimization problem

$$\min_{\lambda} c(\lambda) = (\lambda - 1)^2, \qquad 0 \le \lambda \le 3.$$

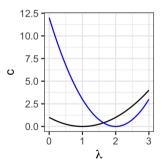
The optimum is at $\lambda^* = 1$.



Example: Two target functions I

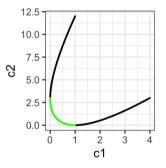
We extend the above problem to two objective functions $c_1(\lambda)=(\lambda-1)^2$ and $c_2(\lambda)=3(\lambda-2)^2$, thus

$$\min_{\boldsymbol{\lambda}} c(\boldsymbol{\lambda}) = (c_1(\boldsymbol{\lambda}), c_2(\boldsymbol{\lambda})), \qquad 0 \leq \boldsymbol{\lambda} \leq 3.$$



Example: Two target functions II

We consider the functions in the objective function space $c(\Lambda)$ by drawing the objective function values $(c_1(\lambda), c_2(\lambda))$ for all $0 \le \lambda \le 3$.



The Pareto front is shown in green. The Pareto front cannot be *left* without getting worse in at least one objective function.

A-priori vs. A-posteriori

- The Pareto set is a set of equally optimal solutions.
- In many applications one is often interested in a **single** optimal solution.
- Without further information no unambiguous optimal solution can be determined.
 - ightarrow The decision must be based on other criteria.

There are two possible approaches:

- **A-priori approach**: User preferences are considered **before** the optimization process
- A-posteriori approach: User preferences are considered after the optimization process

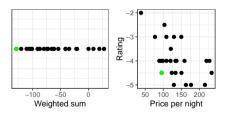
A-priori procedure I

Example: Weighted total

Prior knowledge: One rating point is worth 50 Euro to a customer.

 \rightarrow We optimize the weighted sum:

$$\min_{\mathsf{Hotel}} \big(\mathsf{Price} \ / \ \mathsf{Night}\big) - 50 \cdot \mathsf{Rating}$$



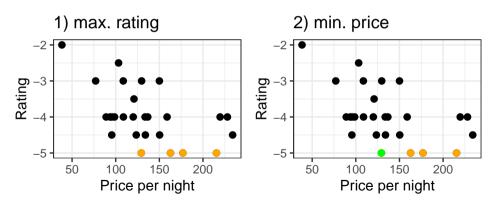
Alternative a weighted sum: $\min_{\lambda \in \Lambda} \sum_{i=1}^m w_i c_i(\lambda)$ with $w_i \geq 0$

A-priori procedure II

Example: Lexicographic method

Prior knowledge: Customer prioritizes rating over price.

 \rightarrow Optimize target functions one after the other.



A-priori procedure III

A-priori approach: Lexicographic method

$$c_1^* = \min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} c_1(\boldsymbol{\lambda})$$

$$c_2^* = \min_{\boldsymbol{\lambda} \in \{\boldsymbol{\lambda} \mid c_1(\boldsymbol{\lambda}) = c_1^*\}} c_2(\boldsymbol{\lambda})$$

$$c_3^* = \min_{\boldsymbol{\lambda} \in \{\boldsymbol{\lambda} \mid c_1(\boldsymbol{\lambda}) = c_1^* \land c_2(\boldsymbol{\lambda}) = c_2^*\}} c_3(\boldsymbol{\lambda})$$

$$\vdots$$

But: Different sequences provide different solutions.

A-priori procedure IV

Summary a-priori approach:

- Implicit assumption: Single-objective optimization is *easy*.
- Only one solution is obtained, which depends on a-priori weights, order, etc.
- Several solutions can be obtained if weights, order, etc. are systematically varied.
- Usually not all non-dominated candidates can be found by these methods.

A-posteriori procedure I

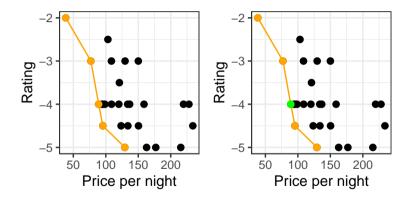
A-posteriori methods try to

- find the set of **all** optimal candidates (the Pareto set),
- select (if necessary) an optimal candidate based on prior knowledge or individual preferences.
- Implicit assumption: Specifying your hidden preferences / making a selection from a pool of candidates is easier, if you see the non-dominated solutions.

A-posteriori methods are therefore the more generic approach to solving a multi-criteria optimization problem.

A-posteriori procedure II

Example: A user is displayed all Pareto optimal hotels (left) and chooses an optimal candidate (right) based on his hidden preferences or additional criteria (e.g. location of the hotel).

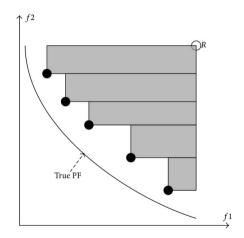


Evaluation of solutions I

A common metric for evaluating the performance of a set of candidates $\mathcal{P}\subset \Lambda$ is the dominated hypervolume

$$S(\mathcal{P}, R) = \Lambda \left(\bigcup_{\tilde{\lambda} \in \mathcal{P}} \left\{ \lambda | \tilde{\lambda} \prec \lambda \prec R \right\} \right),$$

where Λ is the Lebuesge measure.





Evaluation of solutions II

- HV is calculated w.r.t the reference point R, which often reflects in each component the natural maximum of the respective objective if possible
- The dominated hypervolume is also often called S-Metric.
- Computation of HV scales exponentially in the number of objective functions $\mathcal{O}(n^{m-1})$.
- ullet Fast approximations exist for small values of m and especially for machine learning applications we rarely optimize m>3 objectives.