Multi-criteria Optimization

Introduction

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

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

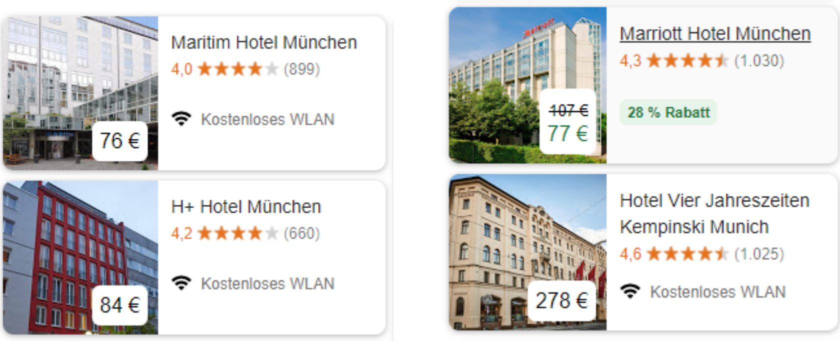
Example:
Choose the best hotel to stay at by maximizing ratings subject to a maximum price per night.

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 general approach to solving multi-criteria problems.

Introductory Example III



When booking a hotel: find the hotel with

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

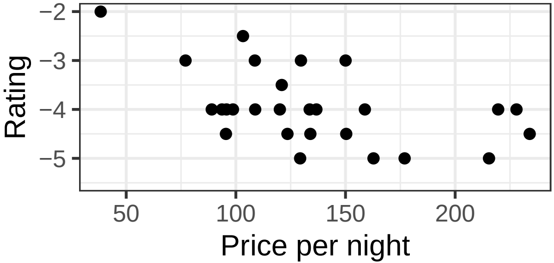
Since we limit ourselves to minimizing problems, we minimize negative ratings.

Introductory Example IV

The objectives often conflict with each other:

- Lower price → usually lower hotel rating.
- Better rating → usually higher price.

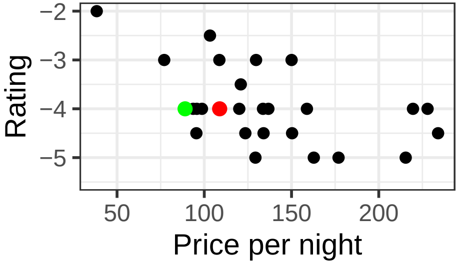
Example: (negative) average rating by hotel guests (1 - 5) vs. average price per night in USD from hotels (excerpt).

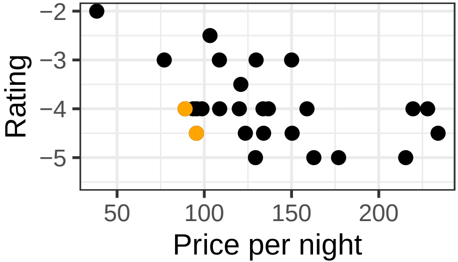


Introductory Example V

Oftentimes, objectives are not directly comparable as they are measured on different scales, for example:

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

- **Goal:** minimize multiple target functions simultaneously.
- $(c_1(\boldsymbol{\lambda}), ..., c_m(\boldsymbol{\lambda}))^\top \in \mathbb{R}^m$ is the objective function vector, which maps $\boldsymbol{\lambda}$ into the space $\mathbb{R}^m$.
- Often no clear best solution, but a set of solutions that are equally good.
- Objective functions are often conflicting.
- w.l.o.g. we look at minimization problems.
- Synonym terms: multi-criteria optimization, multi-objective optimization, Pareto optimization.

Pareto sets and Pareto optimality

Definition:
Given a multi-criteria optimization problem

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

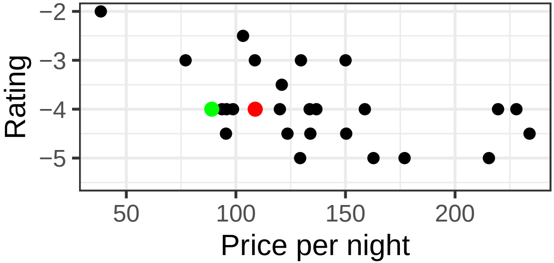
- A solution $\boldsymbol{\lambda}^{(1)}$ **(Pareto-) dominates** $\boldsymbol{\lambda}^{(2)}$, if $c(\boldsymbol{\lambda}^{(1)}) \prec c(\boldsymbol{\lambda}^{(2)})$, i.e.
  1. $c_i(\boldsymbol{\lambda}^{(1)}) \leq c_i(\boldsymbol{\lambda}^{(2)})$ for all $i \in \{1, 2, ..., m\}$ and
  2. $c_j(\boldsymbol{\lambda}^{(1)})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

How to define optimality? I

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

- The solution $c^{(1)} = (89, -4.0)$ 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 $c^{(1)}$

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

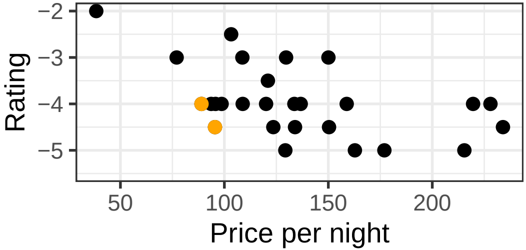


How to define optimality? II

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

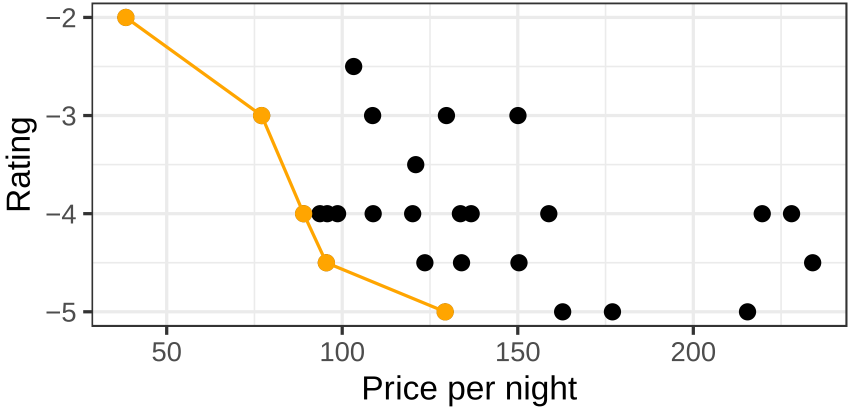
- We define the points as **equivalent** and write

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



How to define optimality? III

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

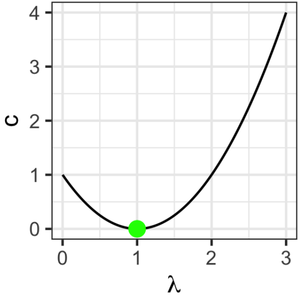


Example: One objective function

We consider the minimization problem

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

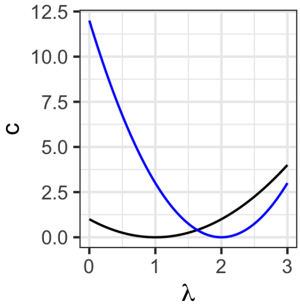
The optimum is at $\boldsymbol{\lambda}^* = 1$.



Example: Two target functions I

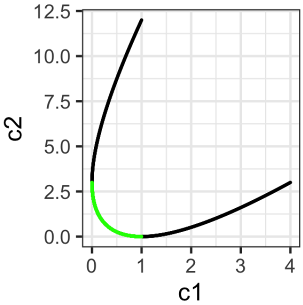
We extend the above problem to two objective functions $c_1(\boldsymbol{\lambda}) = (\boldsymbol{\lambda} - 1)^2$ and $c_2(\boldsymbol{\lambda}) = 3(\boldsymbol{\lambda} - 2)^2$, thus

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



Example: Two target functions II

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



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

Two solutions

- 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.
  $\rightarrow$ The decision must be based on other criteria.

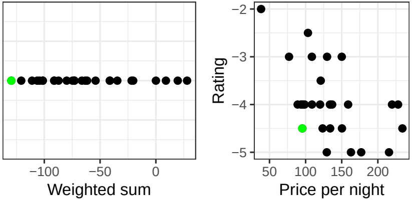
There are two possible approaches:

- **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:

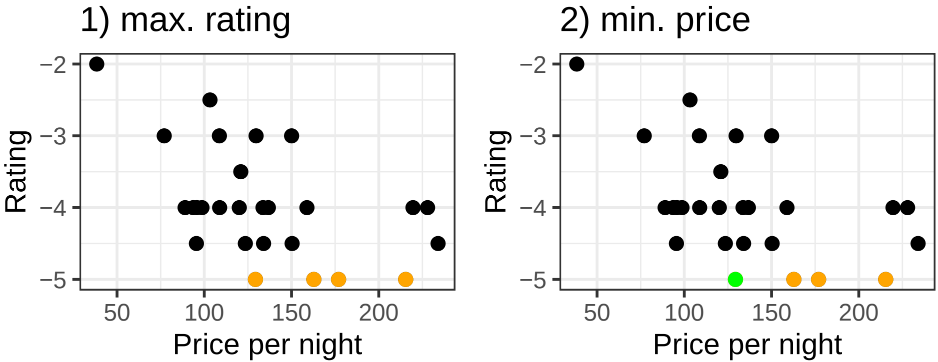
$$\min_{\text{Hotel}} (\text{Price / Night}) - 50 \cdot \text{Rating}$$



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

$$
\begin{aligned}
c_1^* &= \min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} c_1(\boldsymbol{\lambda}) \\
c_2^* &= \min_{\boldsymbol{\lambda} \in \{\boldsymbol{\lambda} \mid c_1(\boldsymbol{\lambda}) = c_1^*\}} c_2(\boldsymbol{\lambda}) \\
c_3^* &= \min_{\boldsymbol{\lambda} \in \{\boldsymbol{\lambda} \mid c_1(\boldsymbol{\lambda}) = c_1^* \wedge c_2(\boldsymbol{\lambda}) = c_2^*\}} c_3(\boldsymbol{\lambda}) \\
&\vdots
\end{aligned}
$$

But: Different sequences provide different solutions.

A-priori procedure IV

Summary a-priori approach:

- Only one solution is obtained, which depends on the a-priori selection of weights, order, etc.
- Several solutions can be obtained if weights, order, etc. are systematically varied.
- Usually there are solutions that cannot be found by these methods.
- Implicit assumption: Single-objective optimization is *easy*.

A-posteriori procedure I

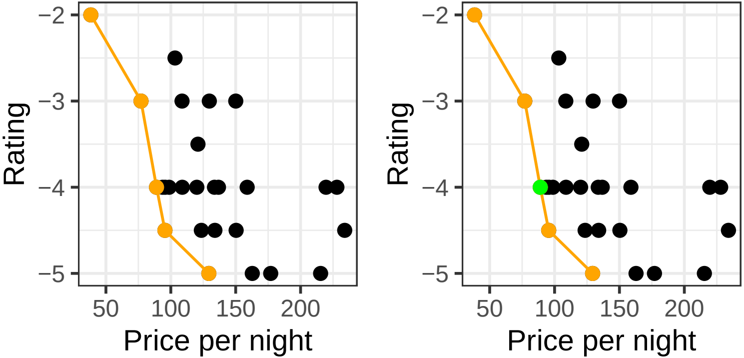
A-posteriori methods try to

- find the set of **all** optimal solutions (the Pareto set),
- select (if necessary) an optimal solution based on prior knowledge or individual preferences.

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

A-posteriori procedure II

Example: A user gets more detailed information about all Pareto optimal hotels (left) and chooses an optimal solution (right) based on previous knowledge or additional criteria (e.g. location of the hotel).



Evaluation of solutions I

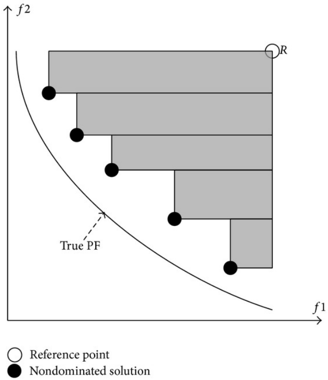
A common metric for evaluating the performance of a set of solutions $\mathcal{P} \subset \mathbf{\Lambda}$ is the **dominated hypervolume**

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

where Λ is the Lebuesge measure.

- The dominated hypervolume is calculated respective to the reference point R, that can be chosen arbitrarily.
- The dominated hypervolume is also often called **S-Metric**.
- Computation of the dominated hypervolume scales exponentially in the number of objective functions $\mathcal{O}(n^{m-1})$.
- Fast approximations exist for small values of m and especially for machine learning applications we rarely optimize $m > 3$ objectives.

Evaluation of solutions II



The dominated hypervolume of $\mathcal{P}$ (5 black points) is the area in the target function space (in respect to the reference point R) which is dominated by points $\mathcal{P}$.