Advanced Optimization

Lectures/Exercises 3 and 4: (Evolutionary) Multiobjective Optimmization

December 11, 2019 and December 16, 2019

Master AIC

Université Paris-Saclay, Orsay, France

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INRIA Saclay – Ile-de-France

INVENTORS FOR THE DIGITAL WORLD

Dimo Brockhoff
INRIA Saclay – Ile-de-France

Course Overview

	Date		Topic
1	Wed, 27.11.2019	Dimo	Randomized Algorithms for Discrete Problems
2	Wed, 4.12.2019	Dimo	Exercise: The Travelling Salesperson Problem
3	Wed, 11.12.2019	Dimo	Evolutionary Multiobjective Optimization I
4	Mon, 16.12.2019	Dimo	Evolutionary Multiobjective Optimization II
5	Wed, 18.12.2019	Dimo	Looking at Data
	Vacation		
6	Wed, 8.1.2020 (morning!)	Anne	Continuous Optimization I
7	Wed, 22.1.2020 (morning!)	Anne	Continuous Optimization II
	Wed, 5.2.2020		oral presentations (individual time slots)

Assignment of Papers

2) RM-MEDA: A regularity model-based multiobjective estimation of distribution algorithm. Gaetano, Francesco

3) A universal catalyst for first-order optimization. Simon, Wafa

5) Efficient optimization of many objectives by approximation-guided evolution. Gérémy

6) A Mean-Variance Optimization Algorithm. Ramine

8) Population Size Adaptation for the CMA-ES Based on the Estimation Accuracy of the Natural Gradient. Florian, Théo

9) CMA-ES with Optimal Covariance Update and Storage Complexity. Eric, Clément

11) A modified ABC algorithm approach for power system harmonic estimation problems Ansaar

Organization Oral Exams

	Wednesday, Feb 5, 2020	
1:30pm – 2pm		
2:00pm – 2:30pm		
2:30pm – 3pm		
3pm – 3:30pm		
3:30pm – 3pm		
4pm – 4:30pm		
4:30pm – 5pm		
5pm – 5:30pm		
5:30pm – 6pm		
6pm – 6:30pm		
6:30pm – 7pm		

to be assigned: Gaetano&Francesco, Simon&Wafa, Gérémy, Ramine, Florian&Théo, Eric&Clément, Ansaar

Overview of the Next Two Lectures

Introduction to multiobjective optimization

- difference to single-objective optimization, the basics
- algorithms and their design principles
- performance assessment and benchmarking
- integration of preferences
- a few aspects of visualization

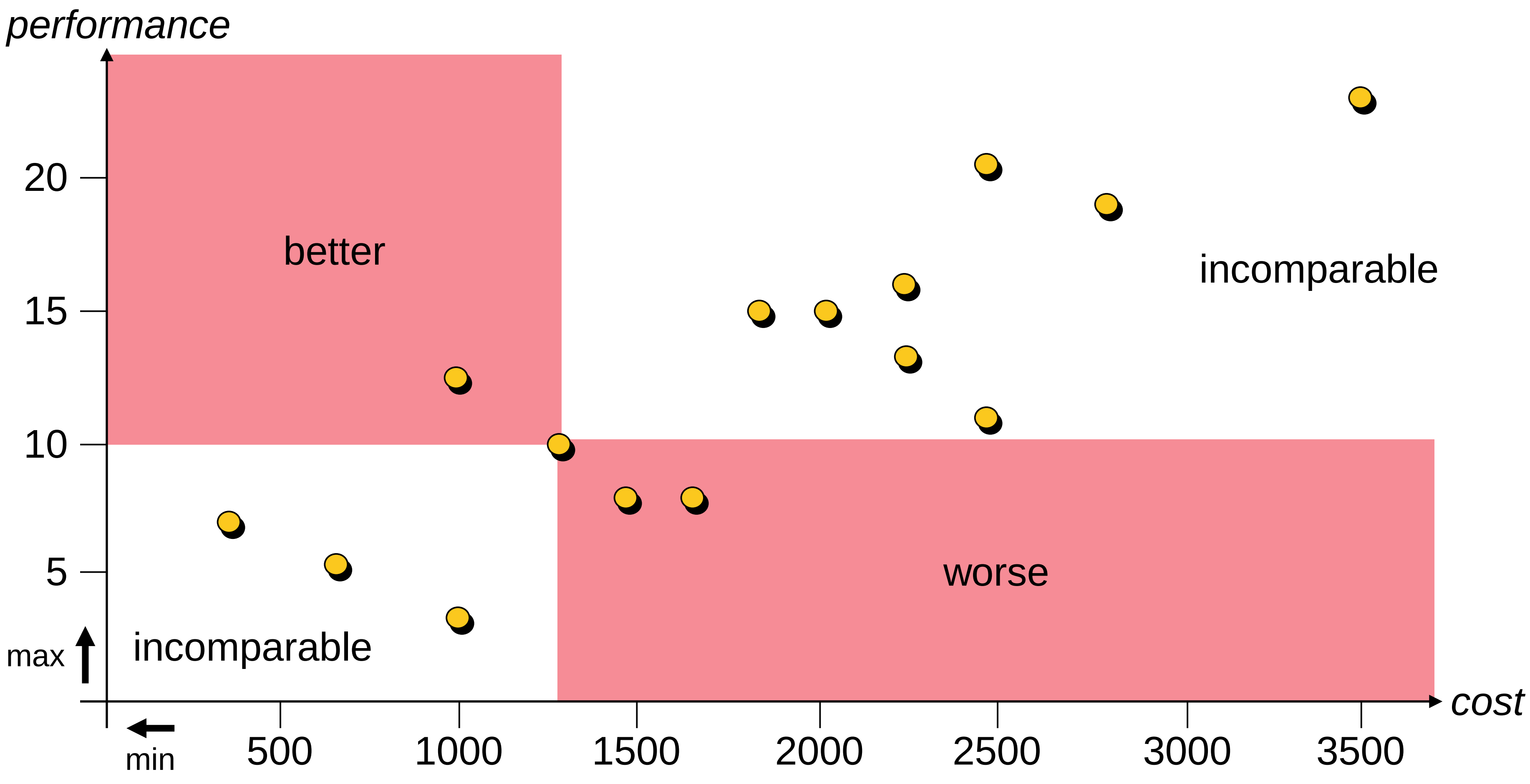
Exercise around COCO

- implement basic algorithm(s)
- benchmark on the COCO platform
  - two goals: testing your code and our software + gaining insights into what the algorithm can solve (and what not)

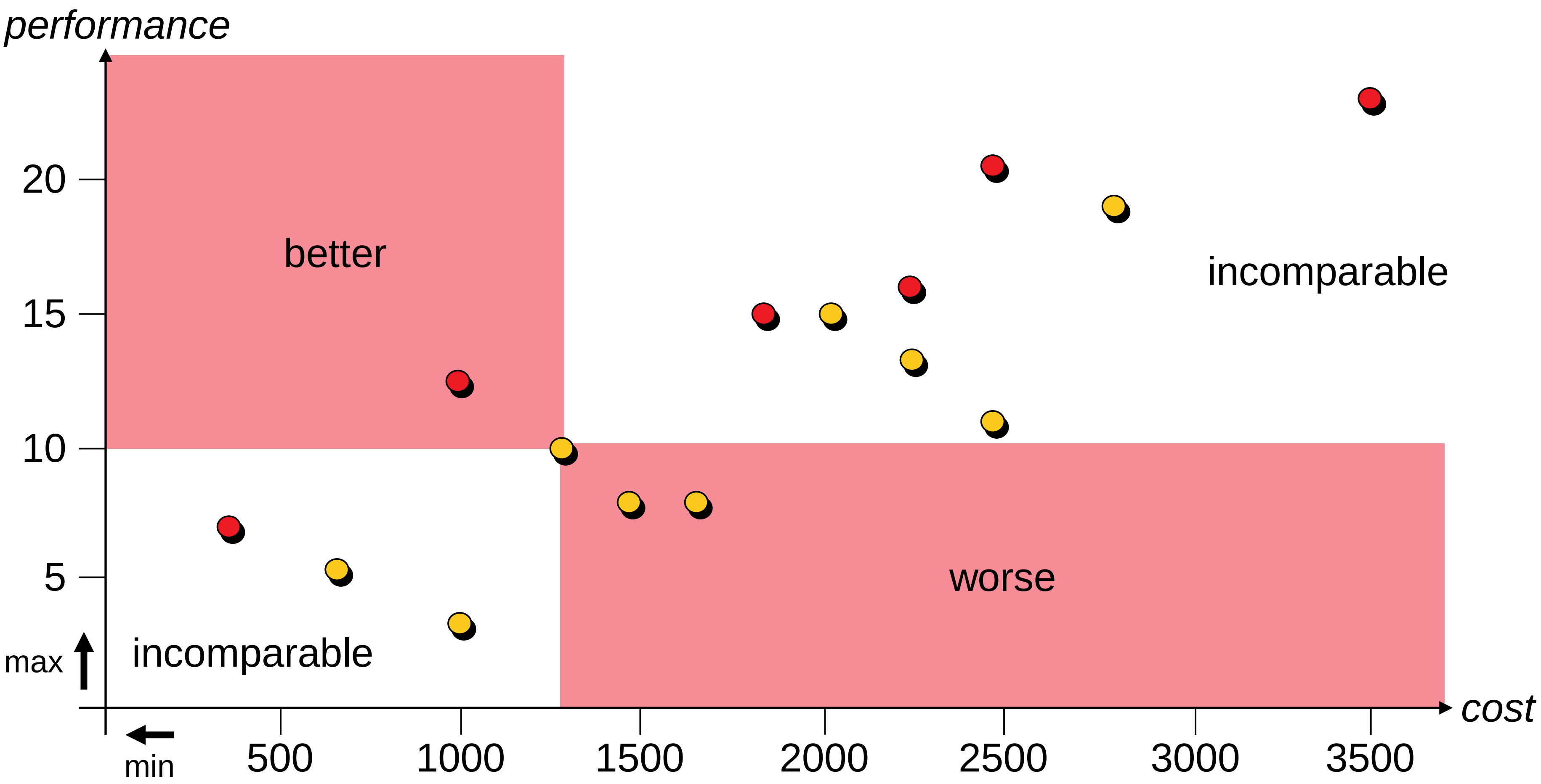
Multiobjective Optimization

Multiobjective Optimization

Multiple objectives that have to be optimized simultaneously

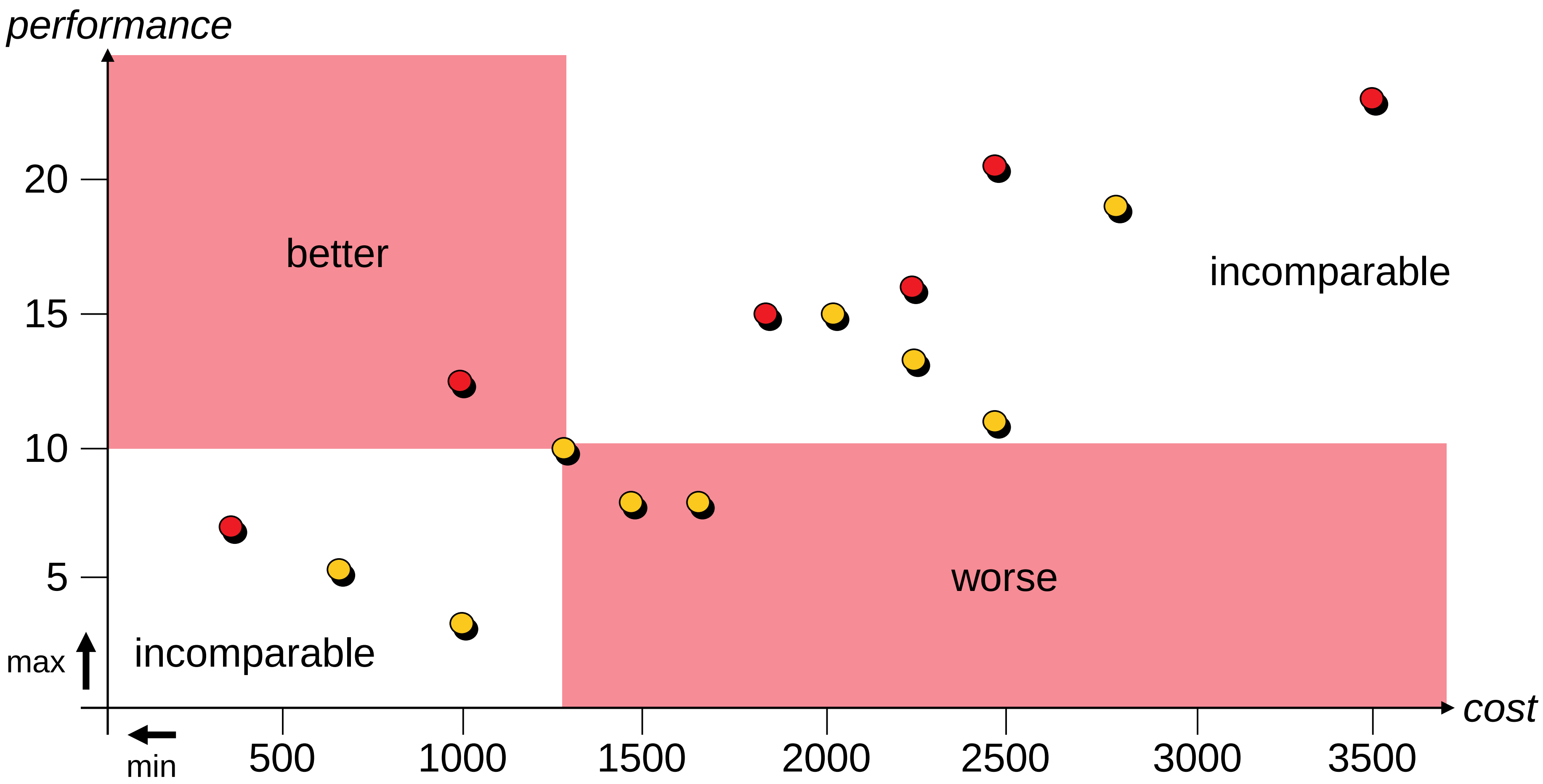


Observations: ❶ there is no single optimal solution, but
❷ some solutions (●) are better than others (●)



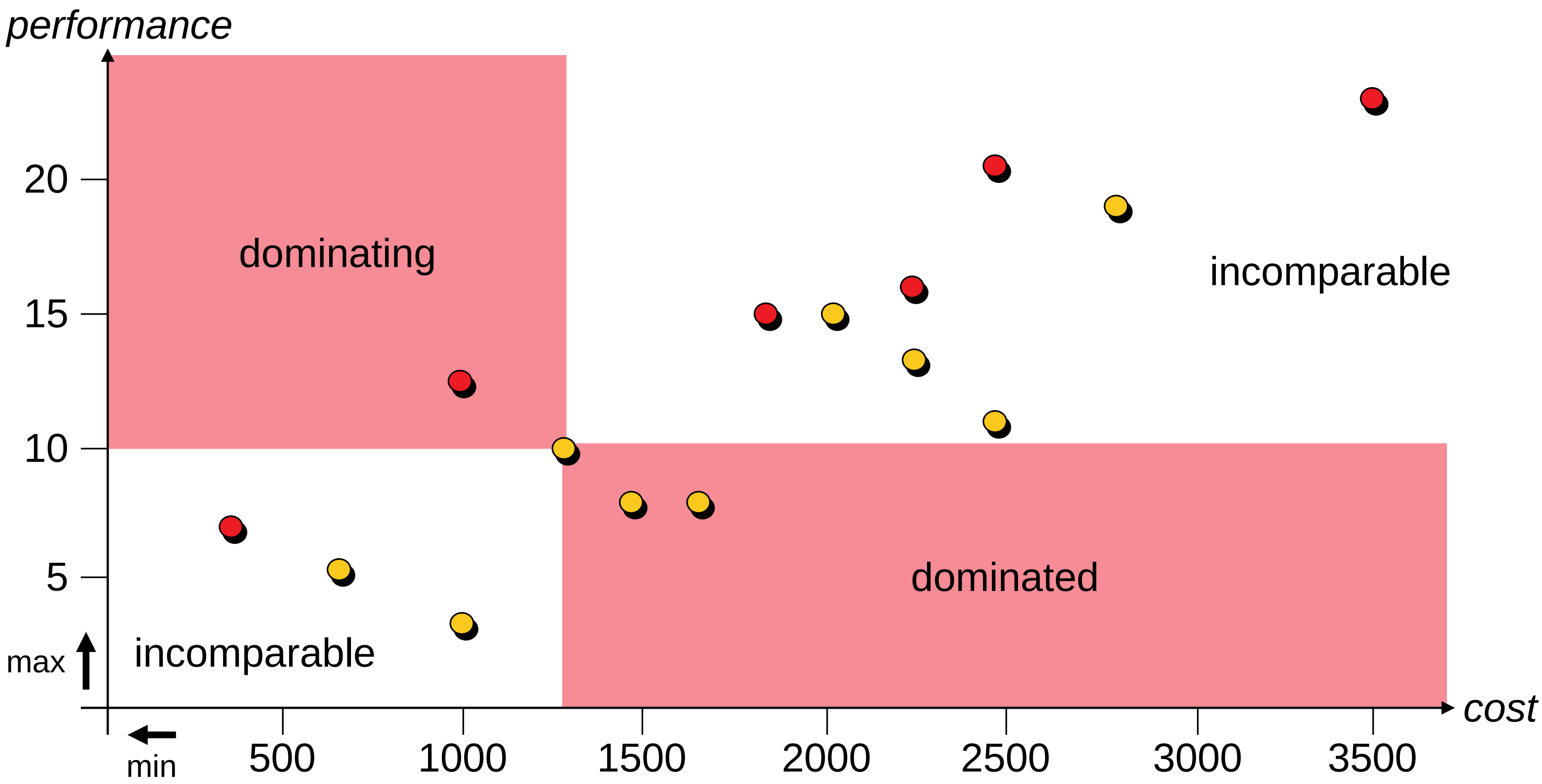
$$u \text{ weakly Pareto dominates } v \; (u \preceq_{par} v): \quad \forall 1 \leq i \leq k: f_i(u) \leq f_i(v)$$

$$u \text{ Pareto dominates } v \; (u \prec_{par} v): \quad u \preceq_{par} v \;\wedge\; v \not\preceq_{par} u$$



$$u \ \textit{weakly Pareto dominates} \ v \ (u \leqslant_{par} v): \quad \forall 1 \leq i \leq k : f_i(u) \leq f_i(v)$$

$$u \ \textit{Pareto dominates} \ v \ (u <_{par} v): \quad u \leqslant_{par} v \ \wedge \ v \not\leqslant_{par} u$$



Exercise 1

Show the equivalence between

$$u <_{par} v: \quad u \leq_{par} v \wedge v \nleq_{par} u$$

and

$$\forall 1 \leq i \leq k: f_i(u) \leq f_i(v) \text{ and } \exists 1 \leq j \leq k: f_j(u) < f_j(v)$$

Exercise 2: Understanding Pareto Dominance

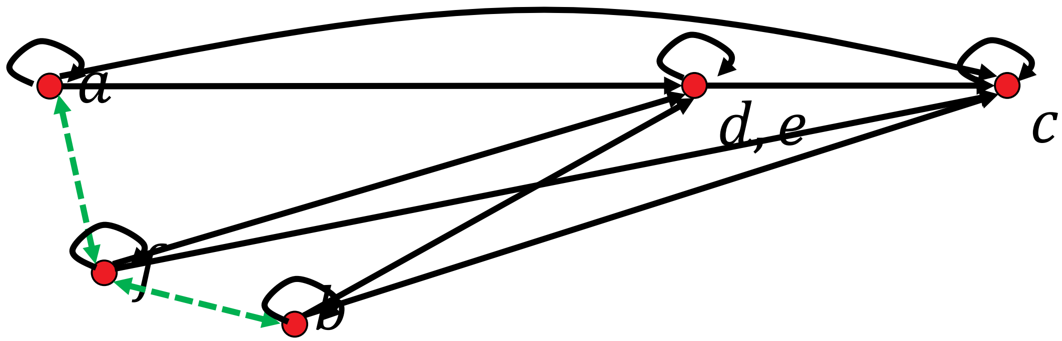
Given the following solutions, tell which ones dominate each other and which don't for the double sphere (minimization) problem

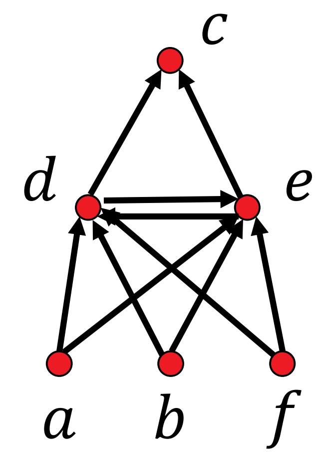
$$f_{\text{doublesphere}}: x \mapsto \left(\sum_{i=1}^{n} x_i^2 \,,\, \sum_{i=1}^{n} (x_i - 1)^2\right).$$

- $a = (0, 0, 0)$
- $b = (1, 1, 1)$
- $c = (2, 2, 2)$
- $d = (2, 2, 0)$
- $e = (0, 2, 2)$
- $f = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$

Visualizing Dominance Relations as Graphs

We can simplify the visualization of the (weak) Pareto dominance relation by *transitive reduction:*



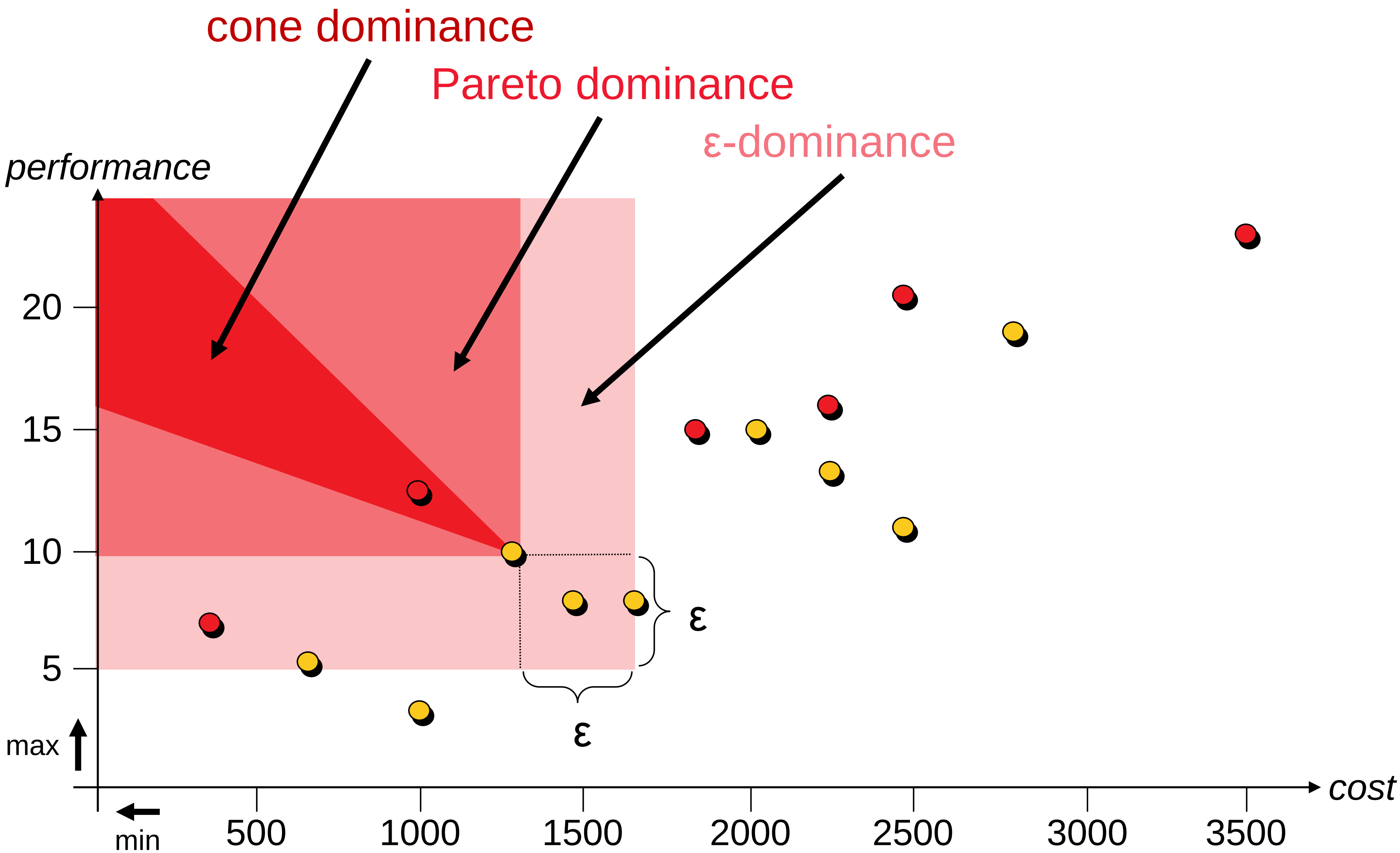


The weak Pareto dominance is a preorder, i.e. a relation that is

- reflexive and transitive
- minimal elements = Pareto-optimal solutions

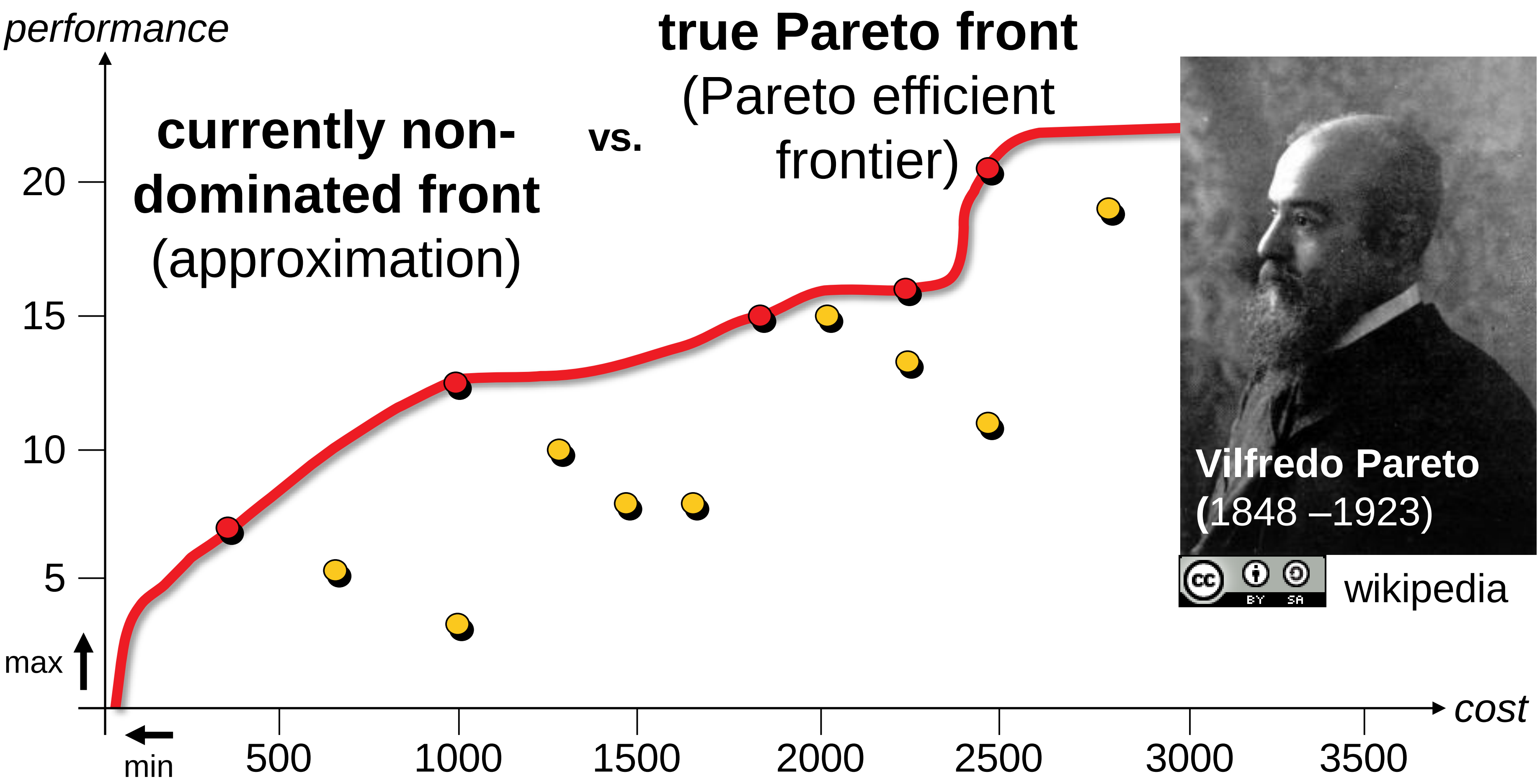
If no *indifferent* solutions $x \neq y$ with $f(x) = f(y)$ exist, we have antisymmetry and a partial order ("poset")---visualizable as Hasse diagram.

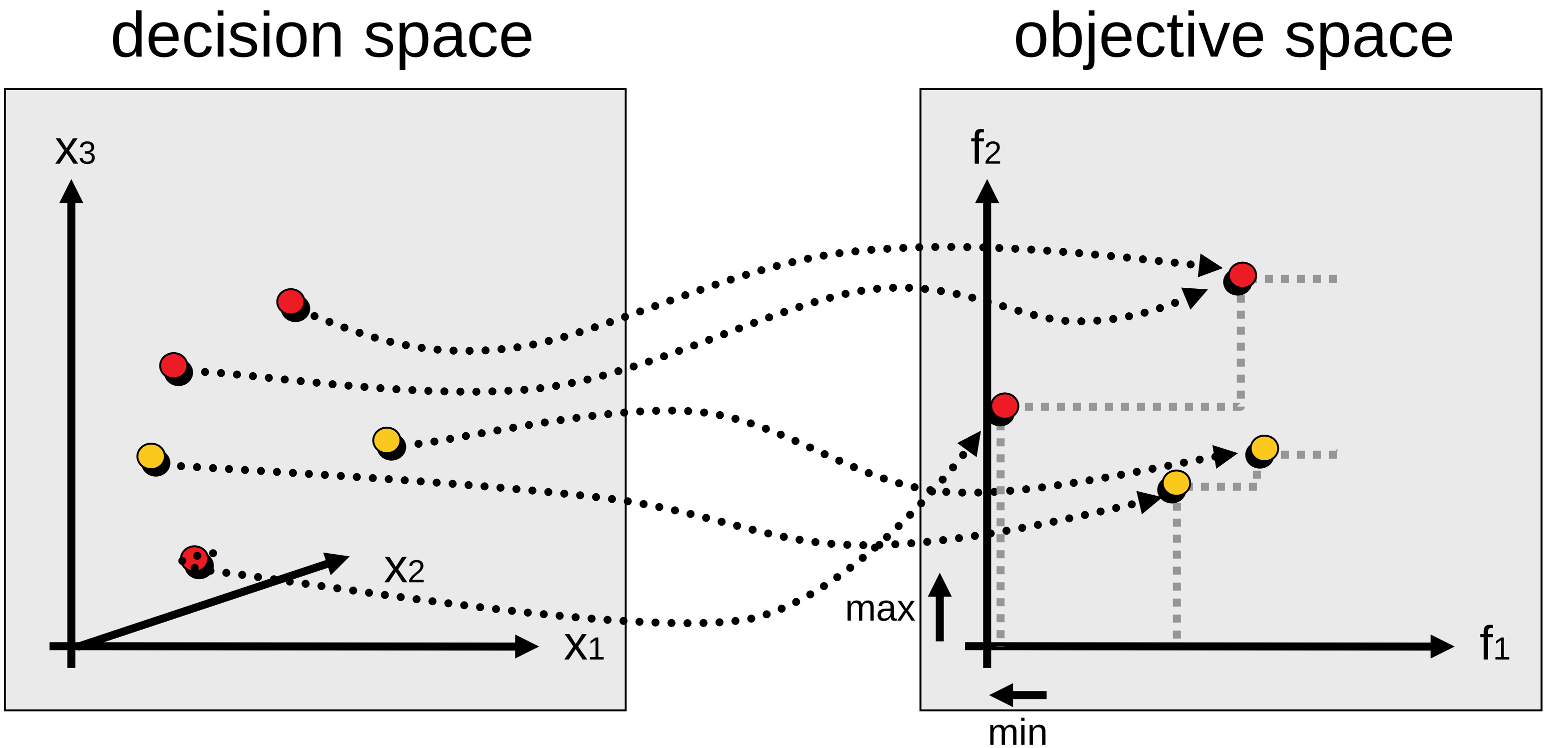
! The Pareto dominance itself is not reflexive and thus, never a poset!



cone dominance
Pareto dominance
ε-dominance
performance
20
15
10
5
max
ε
ε
cost
min
500
1000
1500
2000
2500
3000
3500

Pareto set: set of all non-dominated solutions (decision space)
Pareto front: its image in the objective space





solution of Pareto-optimal set ● vector of Pareto-optimal front

non-optimal decision vector ● non-optimal objective vector

Exercise 3: Pareto Front of Double Sphere

What is the Pareto set/front of the double sphere problem
$f_{\text{doublesphere}}: x \mapsto \left(\sum_{i=1}^{n} x_i^2 \,,\, \sum_{i=1}^{n}(x_i - 1)^2\right)$?

a) what is the Pareto set?

b) what is the associated Pareto front?

Tips for a)

- display some solutions in the search space (let's say in 2-D)
- investigate where dominating solutions lie
- investigate where dominated solutions lie
- finally, show graphically that what you think is the Pareto set is actually the Pareto set (take a point anywhere within your guessed set and show in which direction you can improve and where you cannot improve anymore)

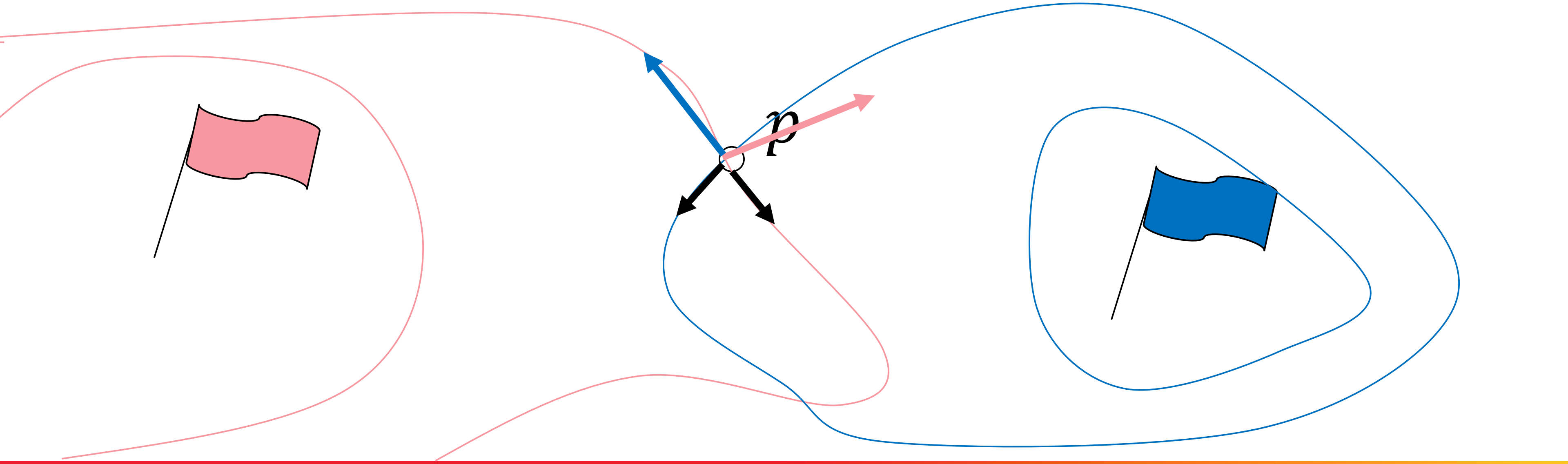
Necessary Condition:

For a Pareto-optimal solution p, the gradients of all objective functions in p must be collinear.

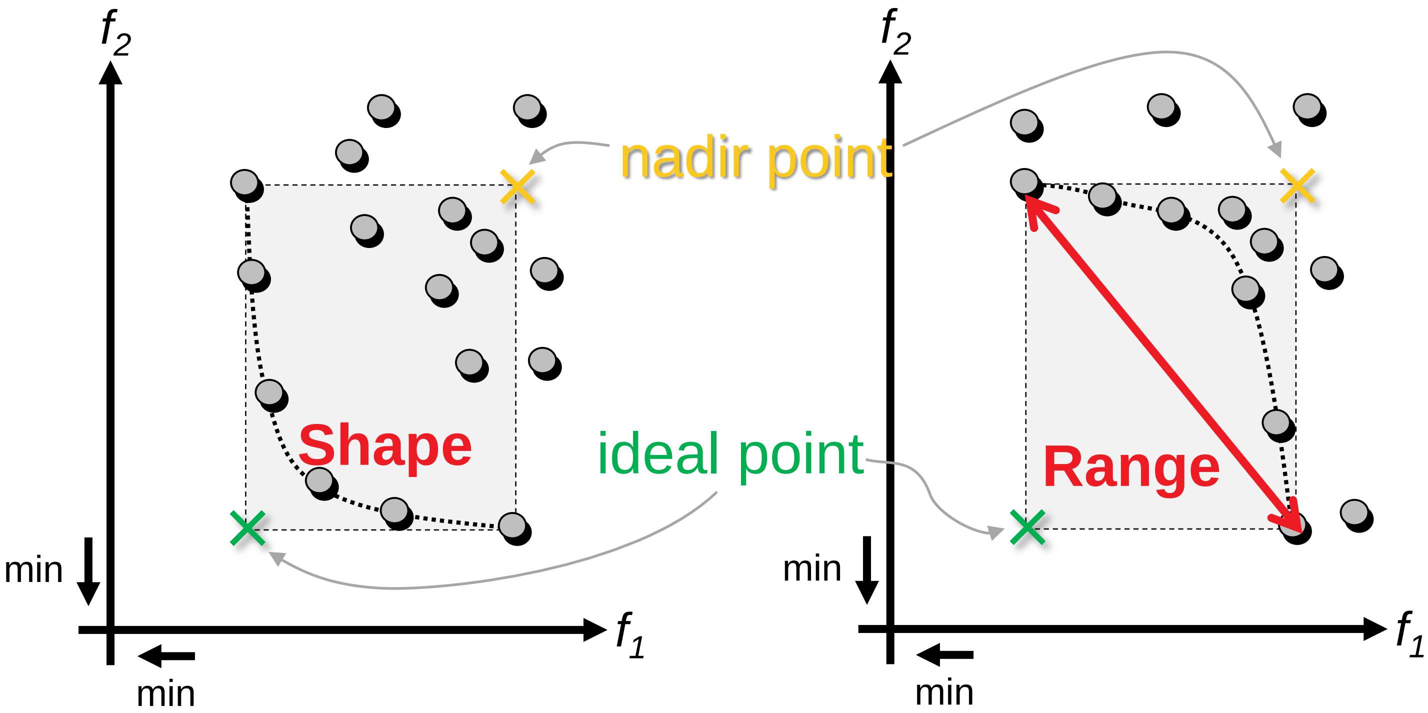
(Visual) Reasoning:

If this is not the case, we can move along one level set and improve on the other objective.

[remember the KKT conditions for constrained optimization]



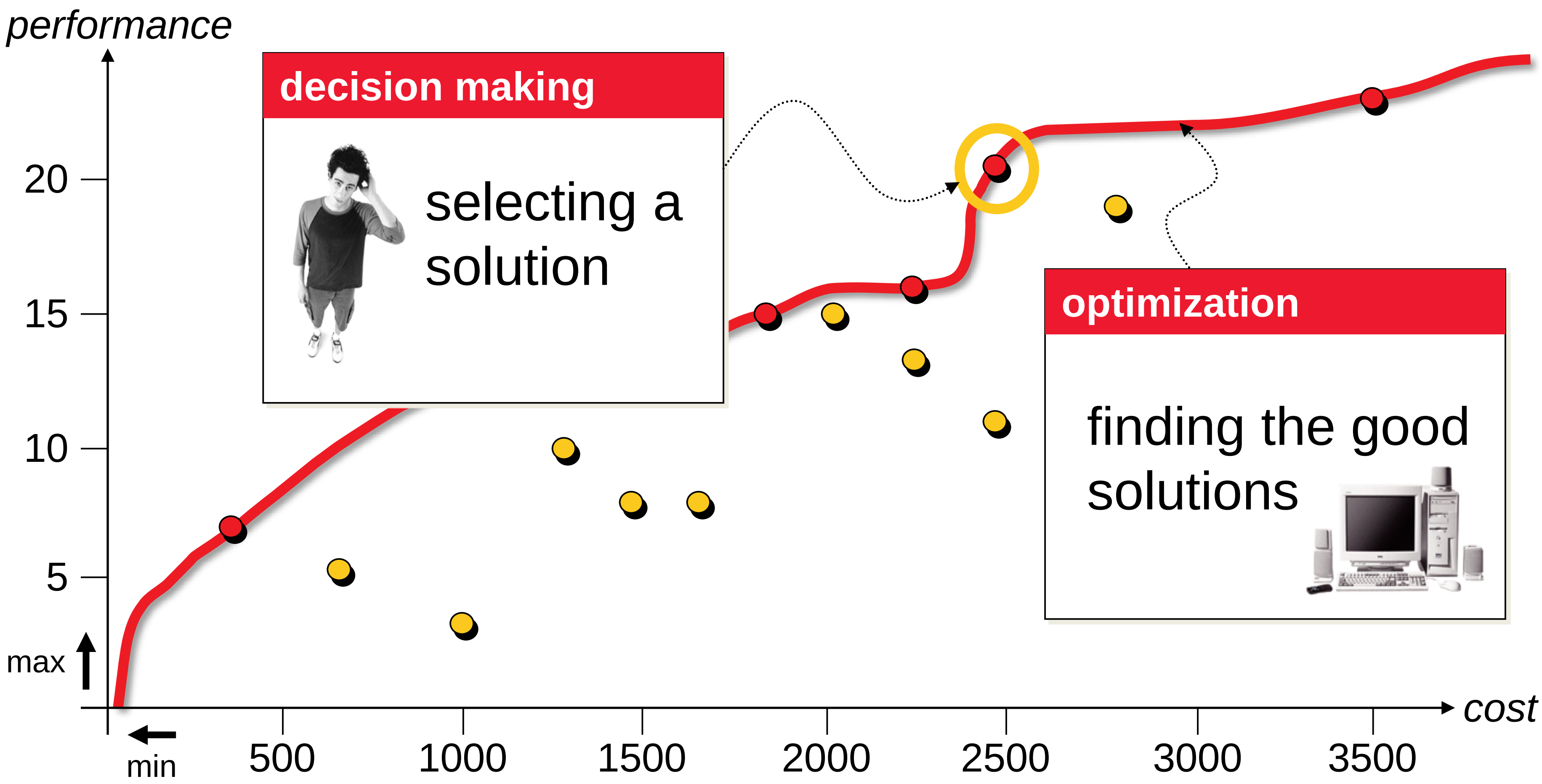
Ideal and Nadir Point



ideal point: best values
nadir point: worst values
} obtained for *Pareto-optimal* points

Multiobjective Optimization

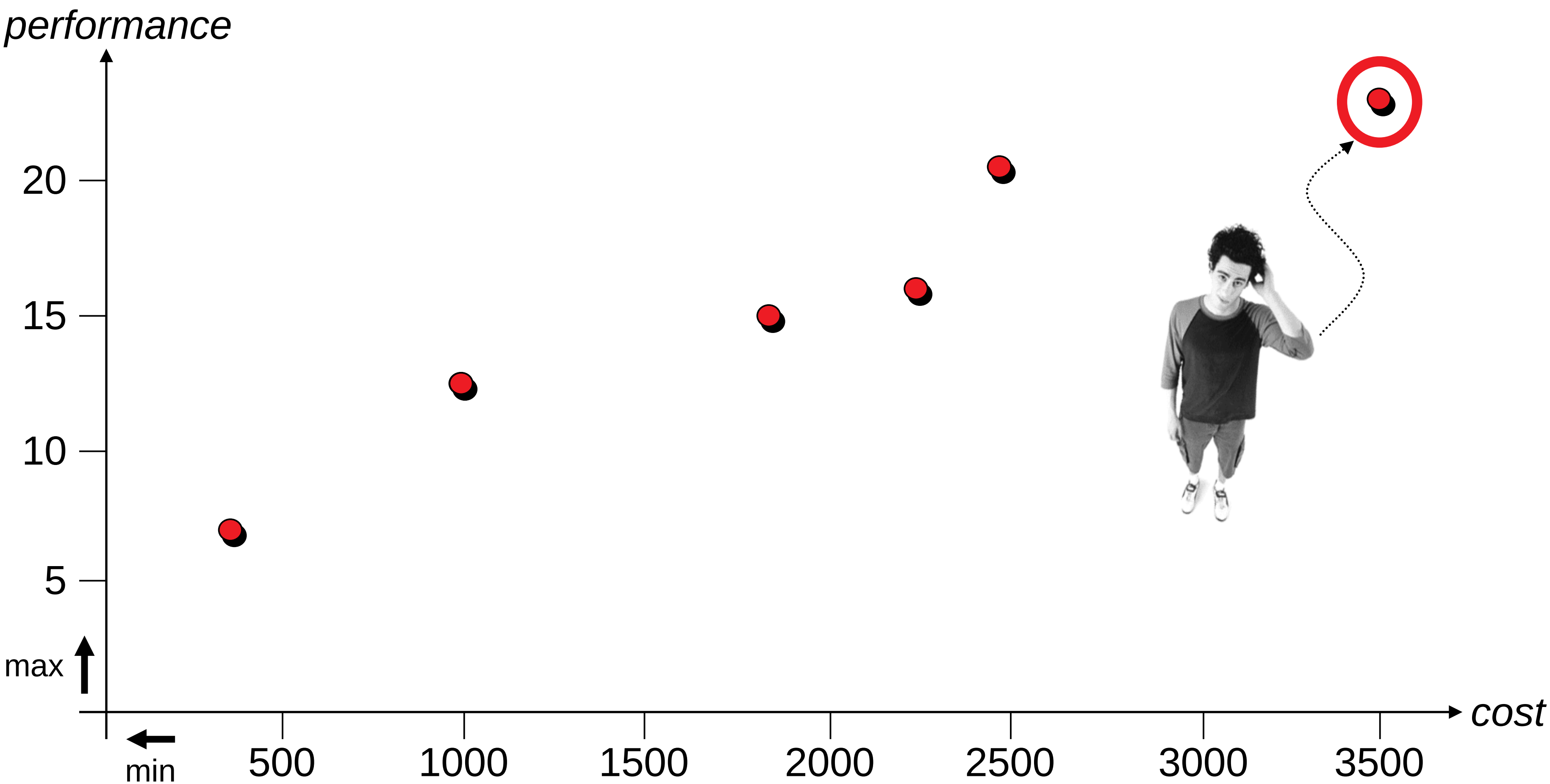
combination of optimization of a set and a decision for a solution



Selecting a Solution: Examples

Possible Approaches:

➊ **ranking:** performance more important than cost

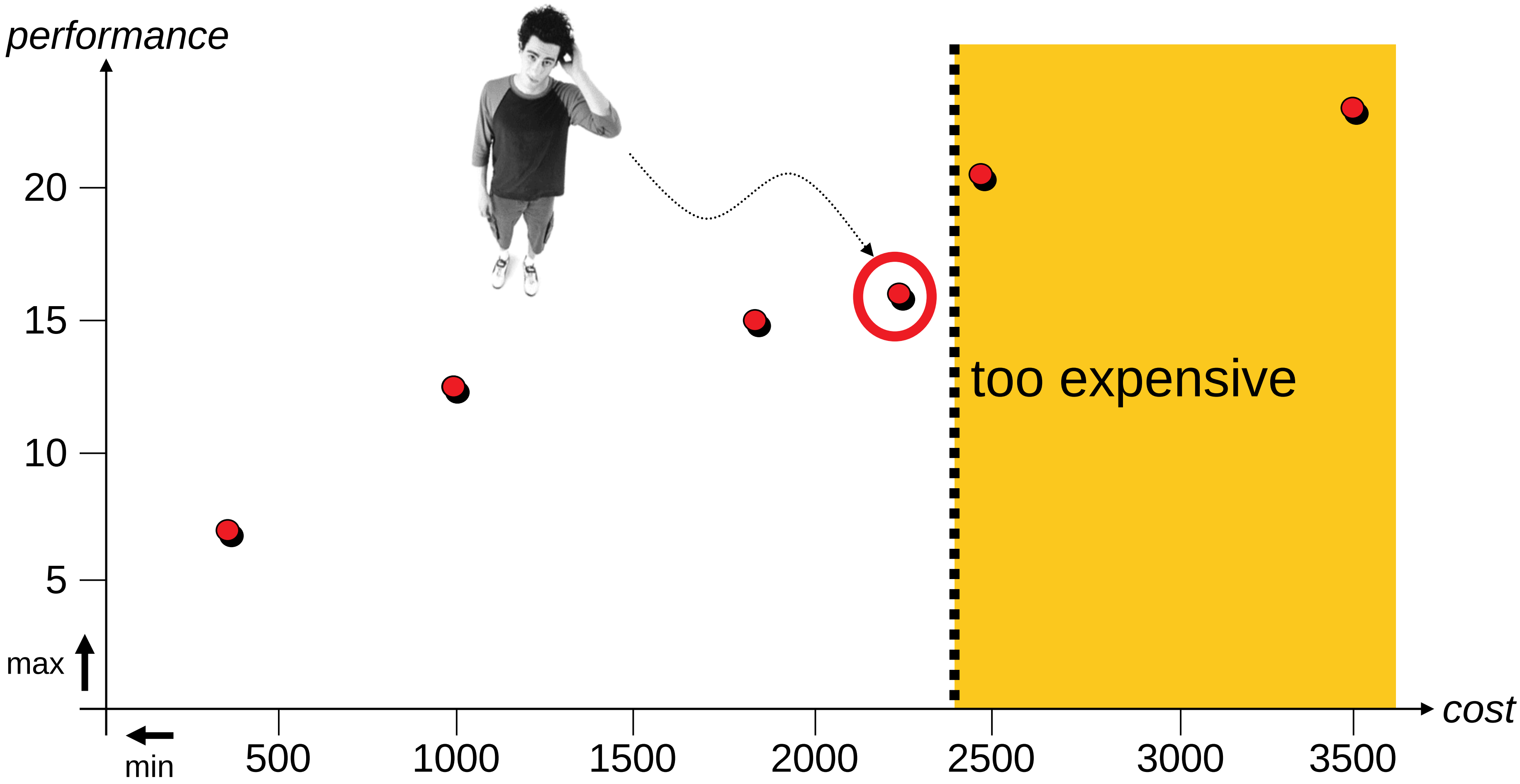


Selecting a Solution: Examples

Possible Approaches:

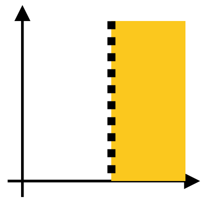
❶ ranking: performance more important than cost

❷ **constraints:** cost must not exceed 2400

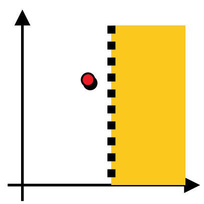


Before Optimization:

rank objectives,
define constraints,…

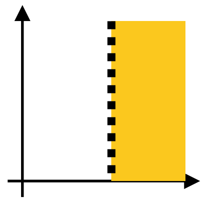


search for one
(good) solution



When to Make the Decision

Before Optimization:



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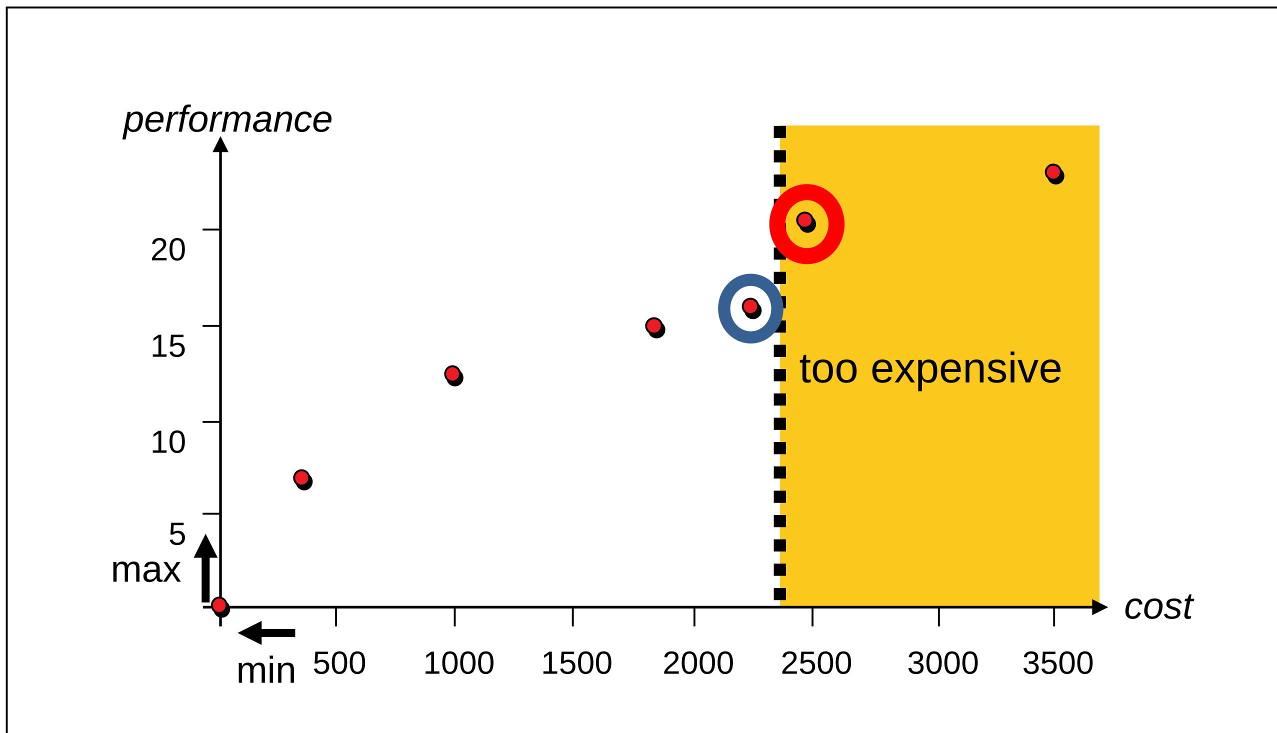

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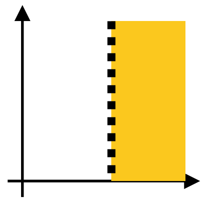

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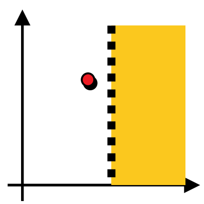
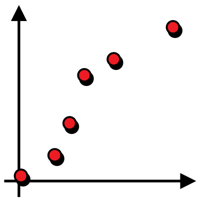
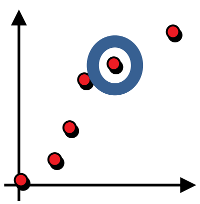


After Optimization:

search for a set of
(good) solutions



select one solution
considering
constraints, etc.



When to Make the Decision

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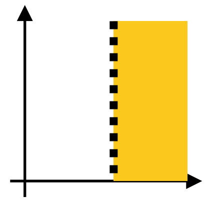

search for one
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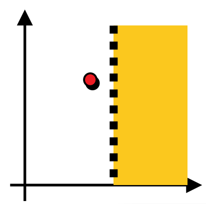

After Optimization:

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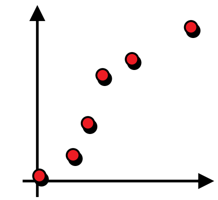

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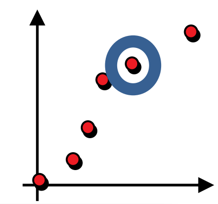


Focus: learning about a problem

- trade-off surface
- interactions among criteria
- structural information
- also: interactive optimization

Two Communities...

MCDM International Society on Multiple Criteria Decision Making

EMO

- established field (beginning in 1950s/1960s)
- bi-annual conferences since 1975
- background in economics, math, management and social sciences
- focus on optimization and decision making

- quite young field (first papers in mid 1980s)
- bi-annual conference since 2001
- background in computer science, applied math and engineering
- focus on optimization algorithms

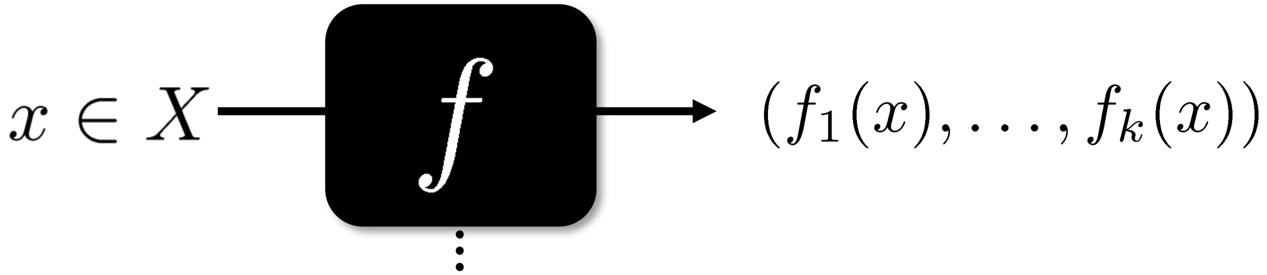
...Slowly Merge Into One

MCDM International Society on Multiple Criteria Decision Making

emo

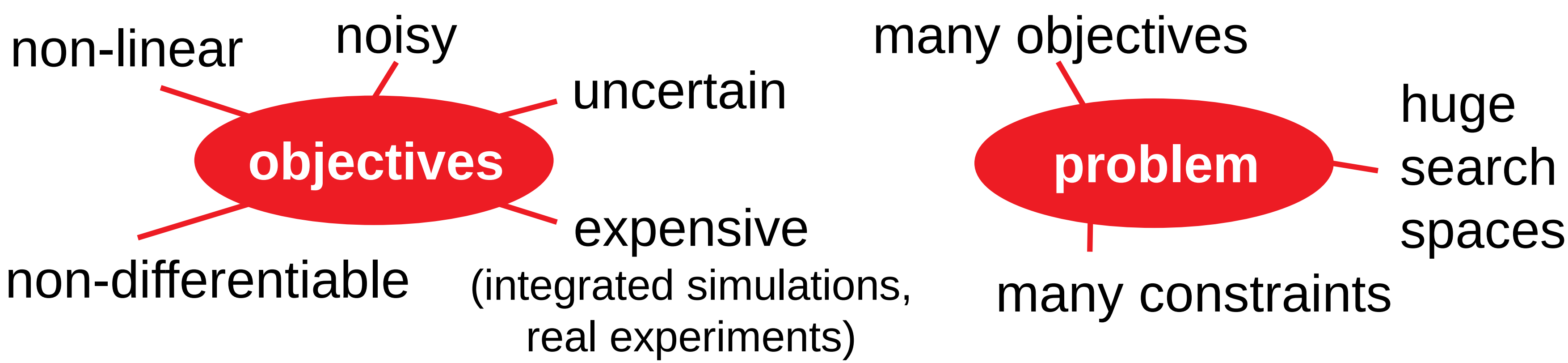
- MCDM track at EMO conference since 2009
- special sessions on EMO at the MCDM conference since 2008
- joint Dagstuhl seminars since 2004

Blackbox optimization



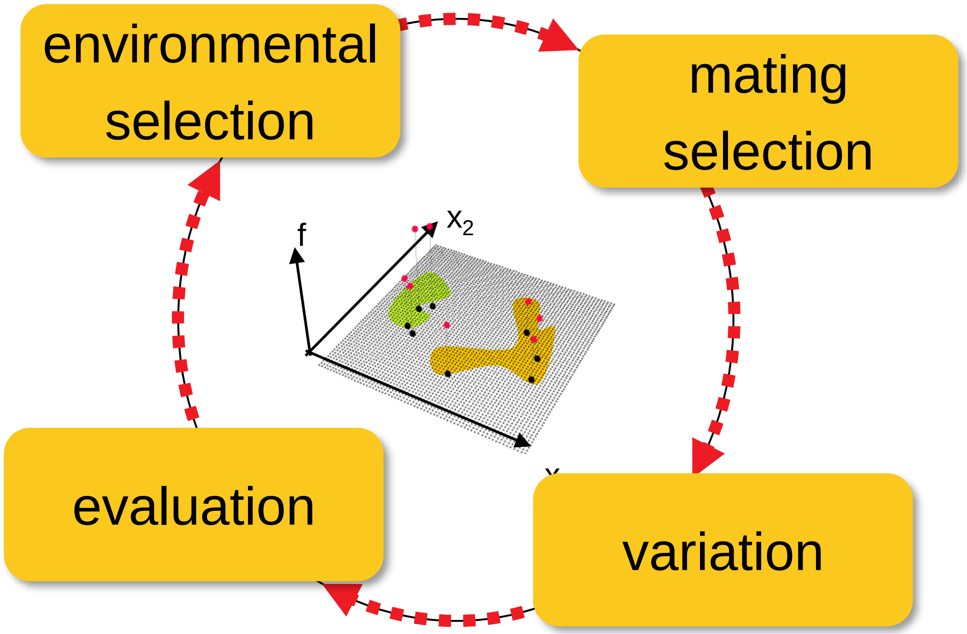
only mild assumptions

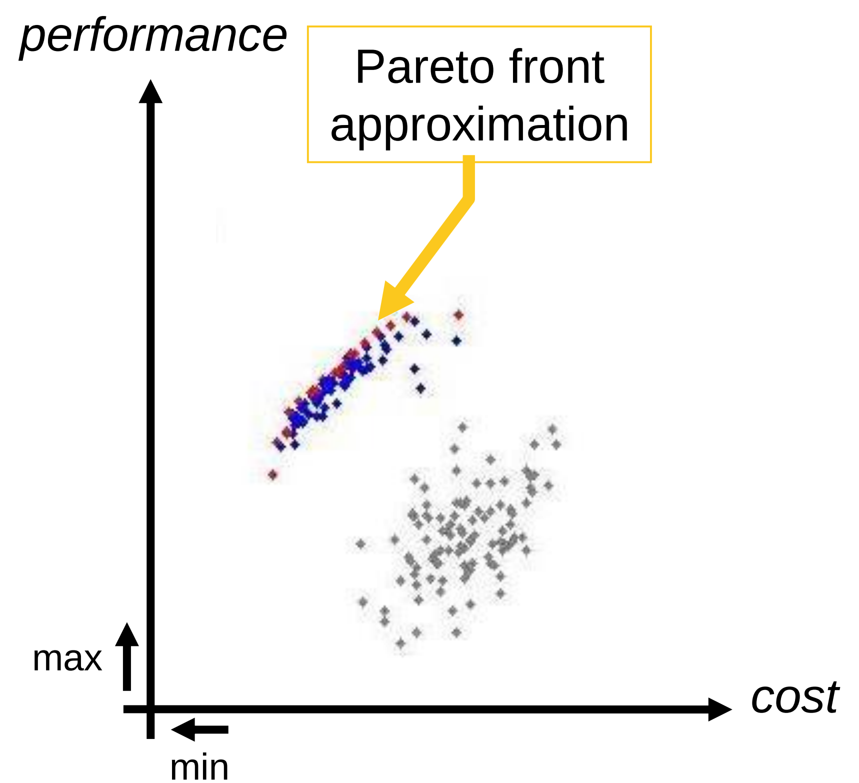
→ EMO therefore well-suited for real-world engineering problems



Evolutionary Multiobjective Optimization

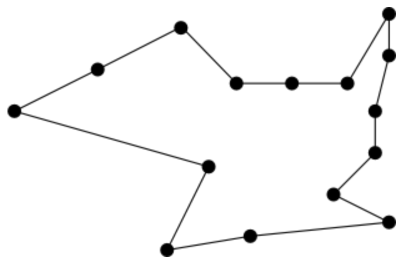
- set-based algorithms
- therefore possible to approximate the Pareto front in one run



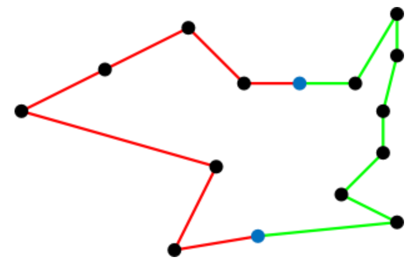


Some problems are easier to solve in a multiobjective scenario

example: TSP
[Knowles et al. 2001]



$\pi \in S_n \rightarrow f(\pi)$



$\pi \in S_n \rightarrow (f_1(\pi, a, b), f_2(\pi, a, b))$

Multiobjectivization

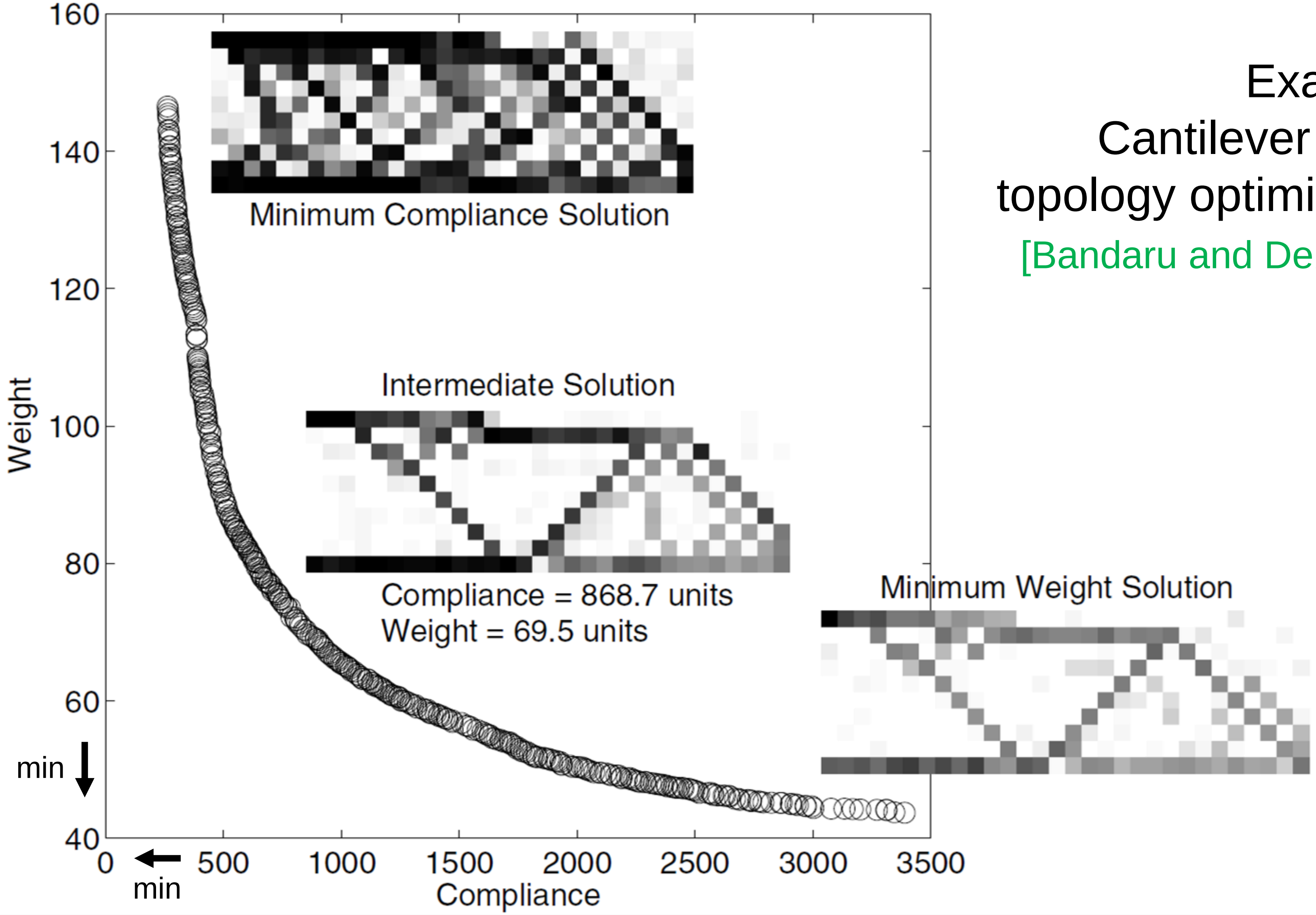
- by addition of new "helper objectives" [Jensen 2004]
  - job-shop scheduling [Jensen 2004], frame structural design [Greiner et al. 2007], VRP [Watanabe and Sakakibara 2007], ...
- by decomposition of the single objective
  - TSP [Knowles et al. 2001], minimum spanning trees [Neumann and Wegener 2006], protein structure prediction [Handl et al. 2008a], ...

also backed up by theory e.g. [Brockhoff et al. 2009, Handl et al. 2008b]

related to *constrained* and *multimodal* single-objective optimization

see also this recent overview: [Segura et al. 2013]

Often innovative design principles among solutions are found



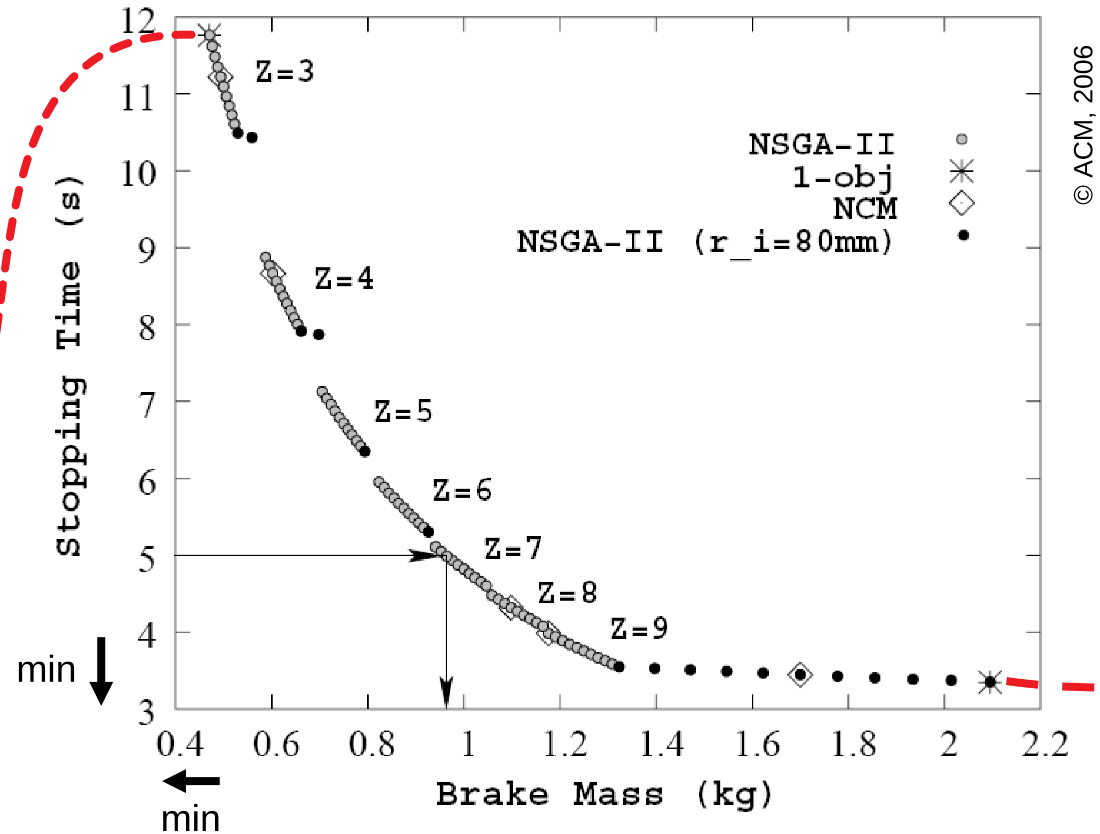
Example:
Cantilever beam
topology optimization
[Bandaru and Deb 2015]

Often innovative design principles among solutions are found

Example:

Clutch brake design

[Deb and Srinivasan 2006]



Solution	x_1	x_2	x_3	x_4	x_5	f_1	f_2
Min. f_1	70	90	1.5	1000	3	0.4704	11.7617
Min. f_2	80	110	1.5	1000	9	2.0948	3.3505

Innovization

Often innovative design principles among solutions are found

Innovization [Deb and Srinivasan 2006]

= using machine learning techniques to find new and innovative design principles among solution sets

= learning from/about a multiobjective optimization problem

Other examples:

- Self-Organizing Maps for supersonic wing design [Obayashi and Sasaki 2003]
- Biclustering for processor design and knapsack [Ulrich et al. 2007]
- Successful case studies in engineering
  (noise barrier design, polymer extrusion, friction stir welding)
  [Deb et al. 2014]

Overview

The Big Picture

Basic Principles of Multiobjective Optimization

- algorithm design principles and concepts
- performance assessment

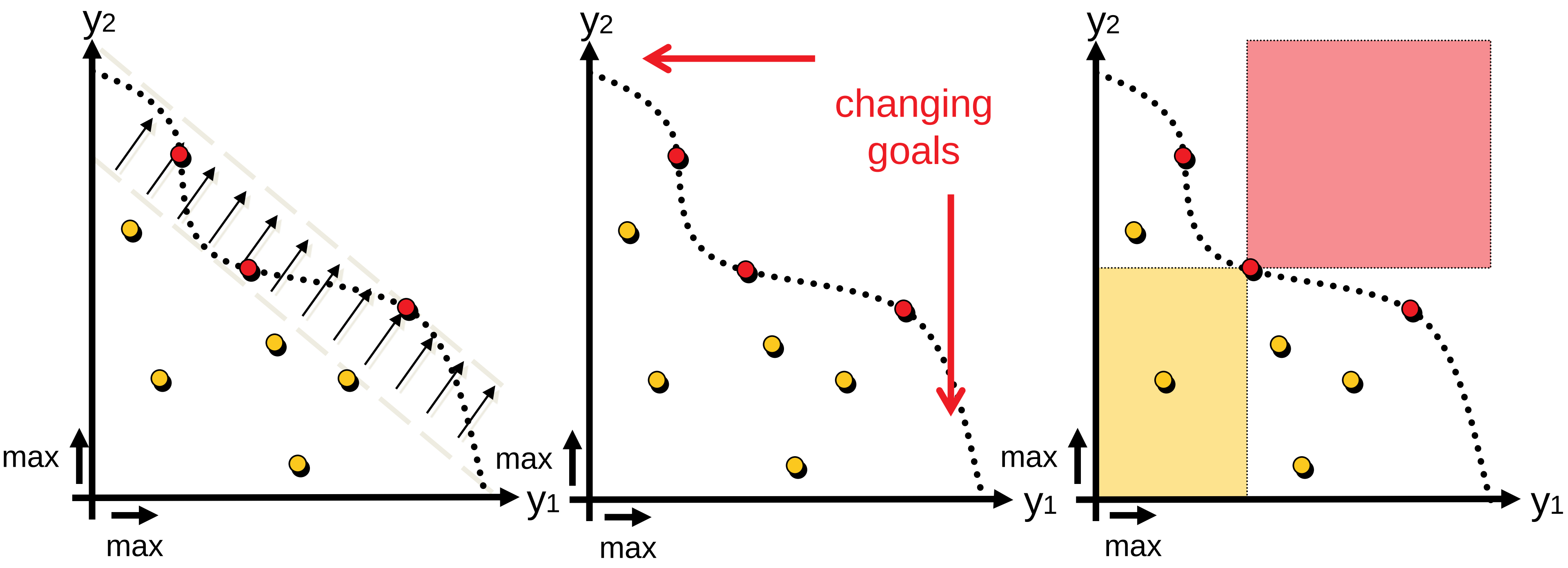
Selected Advanced Concepts

- preference articulation
- visualization aspects

aggregation-based
problem decomposition (multiple single-objective optimization problems)

criterion-based
VEGA

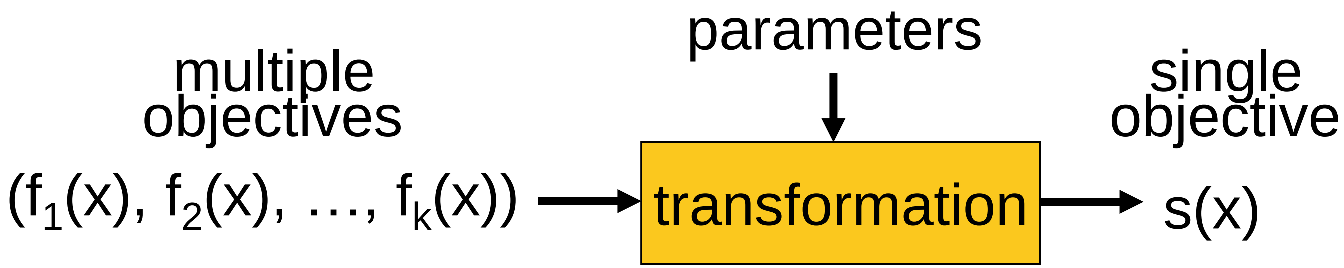
dominance-based
SPEA2, NSGA-II “modern” EMOA



solution-oriented
scaling-dependent

set-oriented
less scaling-independent

Solution-Oriented Problem Transformations



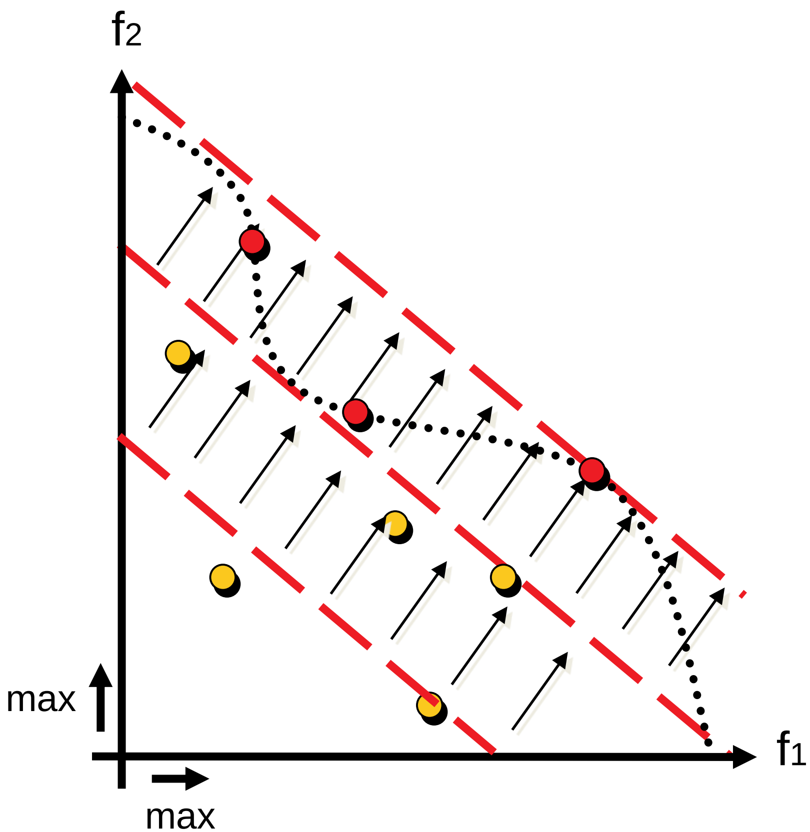
A scalarizing function s is a function $s: Z \to \mathbb{R}$ that maps each objective vector $u = (u_1, \ldots, u_n) \in Z$ to a real value $s(u) \in \mathbb{R}$

Solution-Oriented Problem Transformations

parameters

multiple objectives → **transformation** → single objective

$(f_1(x), f_2(x), \ldots, f_k(x))$ → transformation → $s(x)$

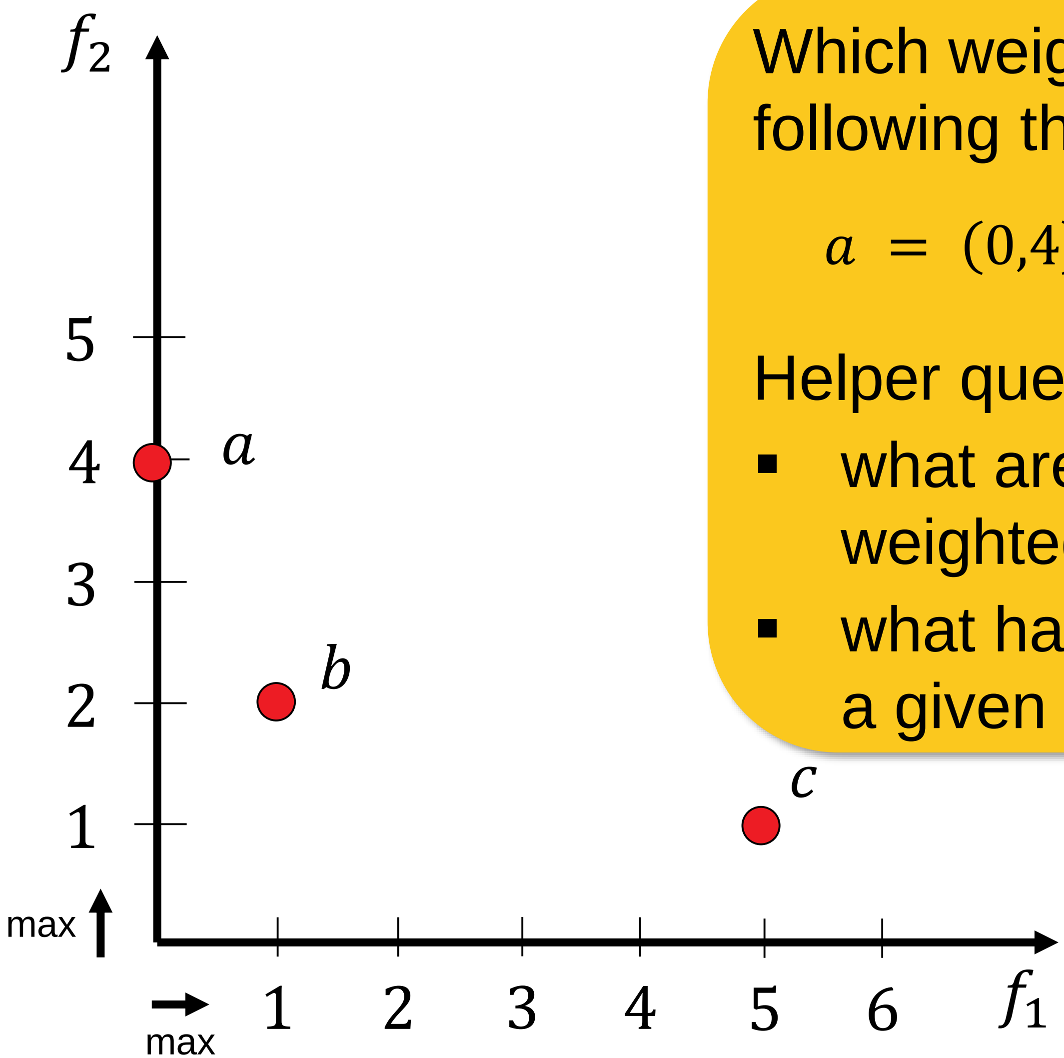


Example 1: weighted sum approach

$(w_1, w_2, \ldots, w_k)$

→ $y = w_1 y_1 + \ldots + w_k y_k$ →

Exercise 4: Weighted Sum



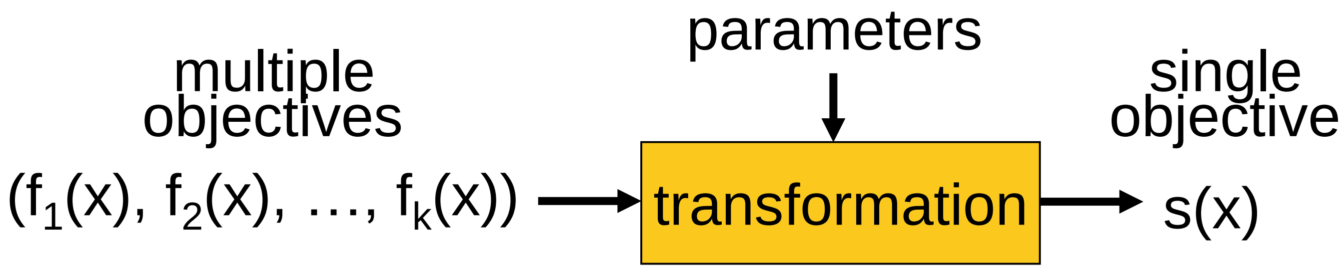
Which weights are optimal for the following three points?

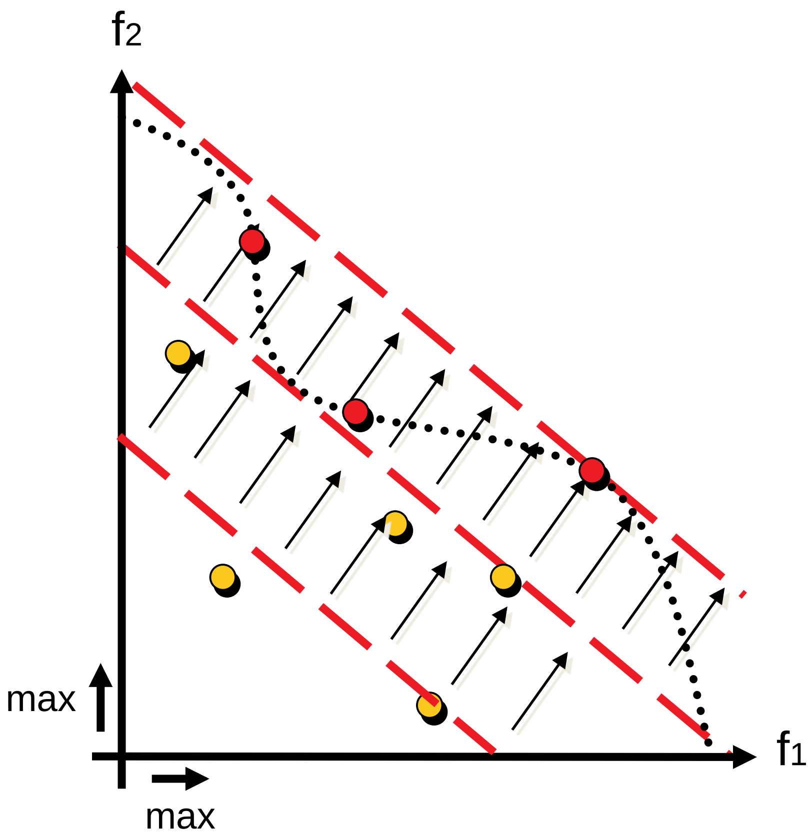
$$a = (0,4) \quad b = (1,2) \quad c = (5,1)$$

Helper questions:

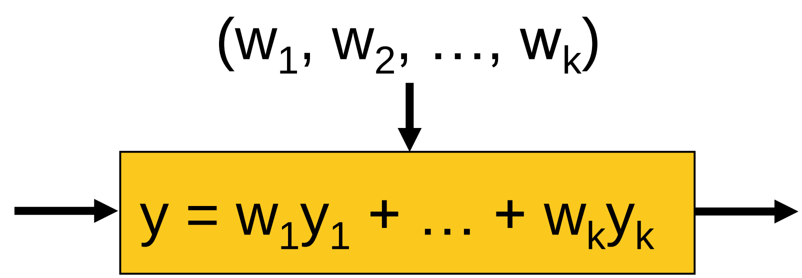
- what are the lines of equal weighted sum for a given weight?
- what happens if you optimize wrt. a given weighted sum?

Solution-Oriented Problem Transformations





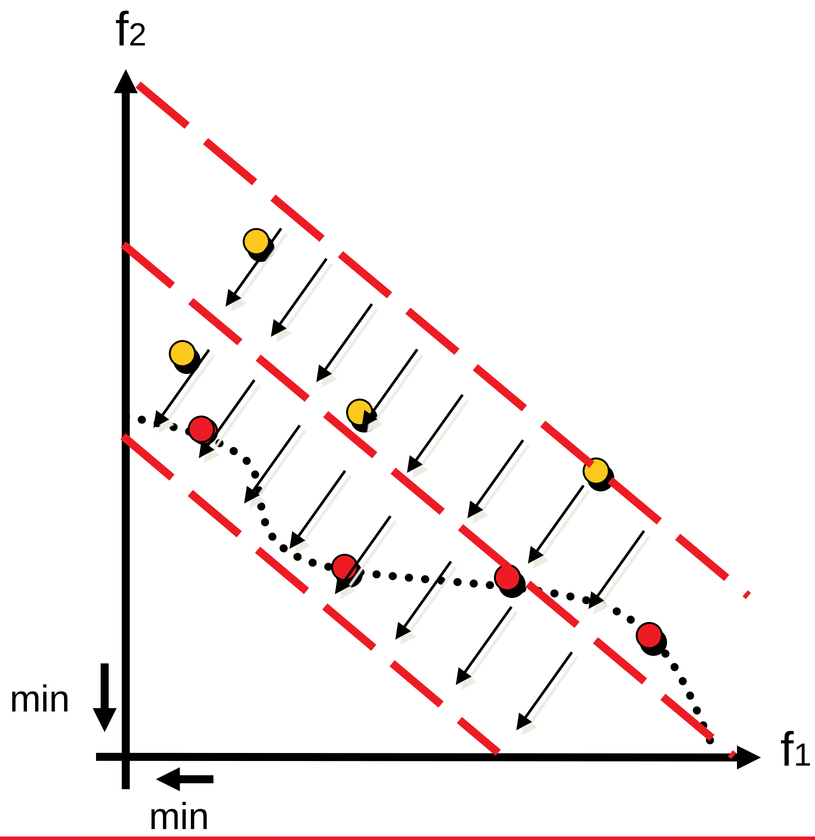
Example 1: weighted sum approach



Disadvantage: not all Pareto-optimal solutions can be found if the front is not concave (for maximization)

Solution-Oriented Problem Transformations

multiple objectives $(f_1(x), f_2(x), \ldots, f_k(x))$ → transformation (parameters) → single objective $s(x)$



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$(w_1, w_2, \ldots, w_k)$

$$y = w_1y_1 + \ldots + w_ky_k$$

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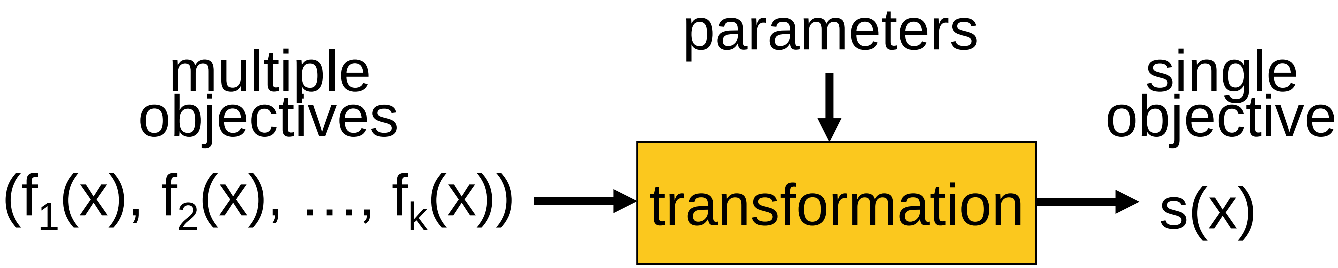
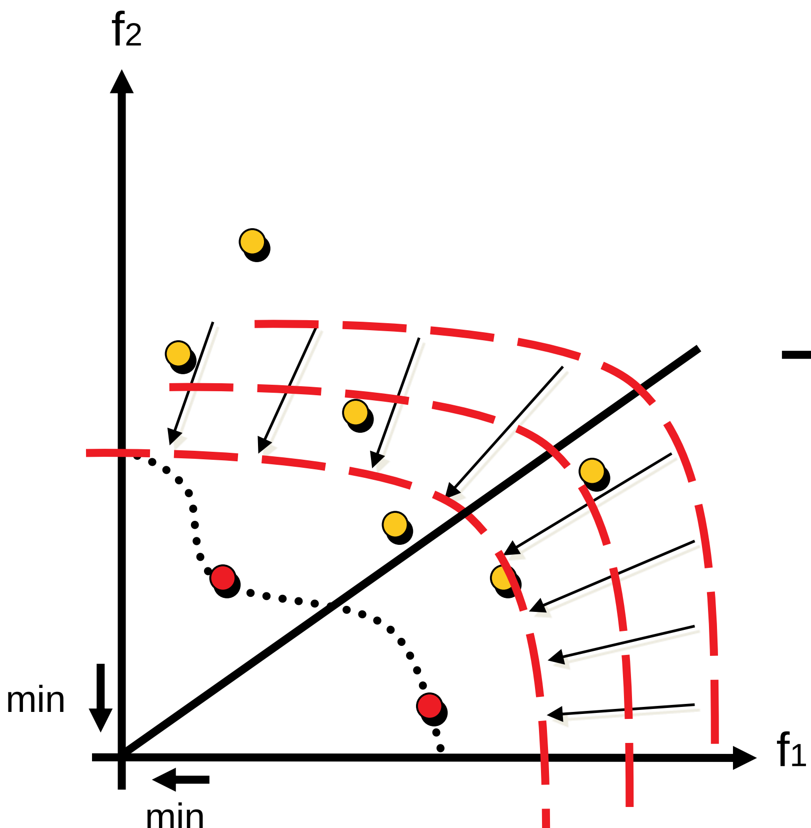




Example 2: weighted p-norm

$(w_1, w_2, \dots, w_k)$

$$y = \sqrt[p]{(w_1 y_1)^p + \dots + (w_k y_k)^p}$$

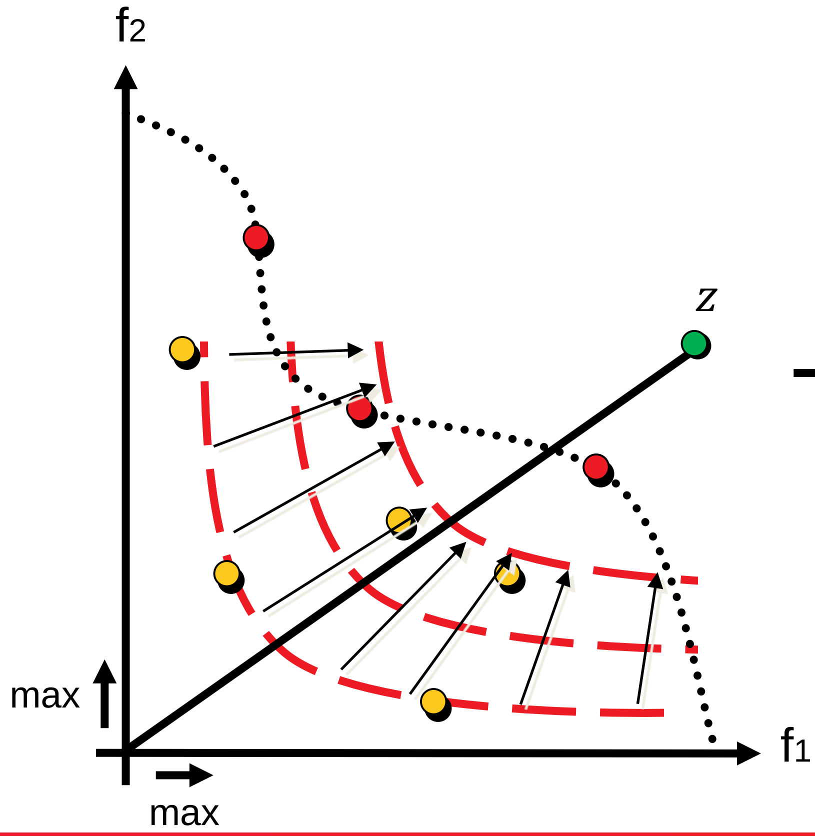
$p = 1$: weighted sum

$p = \infty$: weighted Tchebycheff

Solution-Oriented Problem Transformations

multiple objectives

$(f_1(x), f_2(x), \ldots, f_k(x))$ → **transformation** (parameters) → single objective $s(x)$



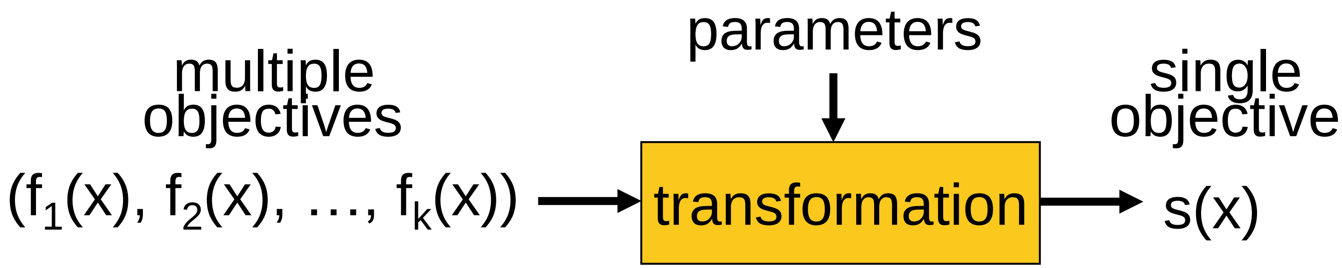
Example 2: weighted p-norm

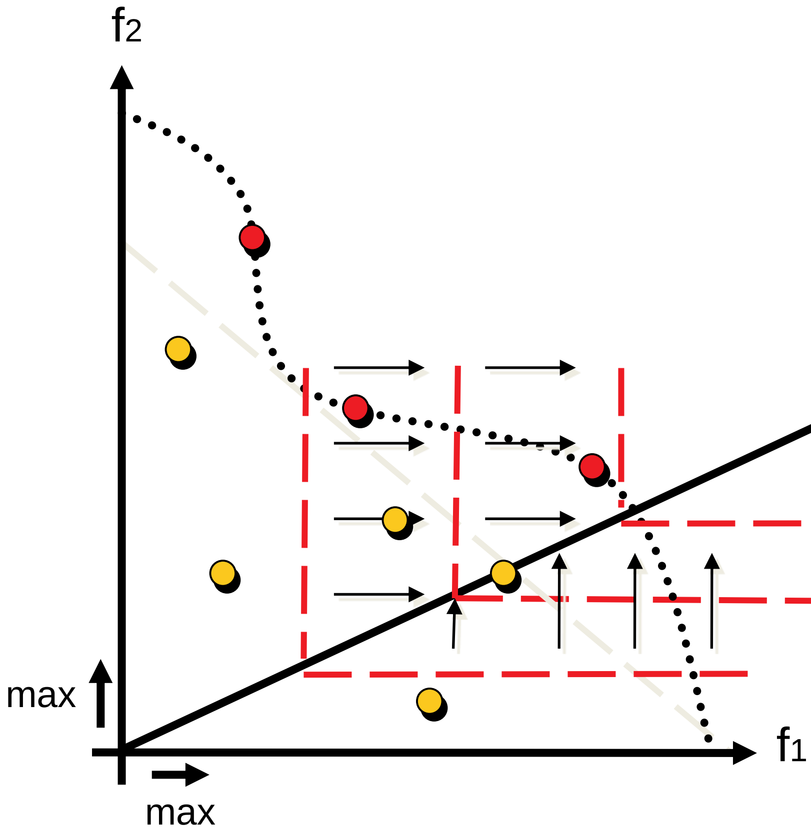
$(w_1, w_2, \ldots, w_k)$

$$y = \sqrt[p]{\sum_{i=1}^{k} (|w_1(y_1 - z_i)|)^p}$$

$p = 1$: weighted sum

$p = \infty$: weighted Tchebycheff





Example 2: weighted Tchebycheff

$(\lambda_1, \lambda_2, \ldots, \lambda_k)$

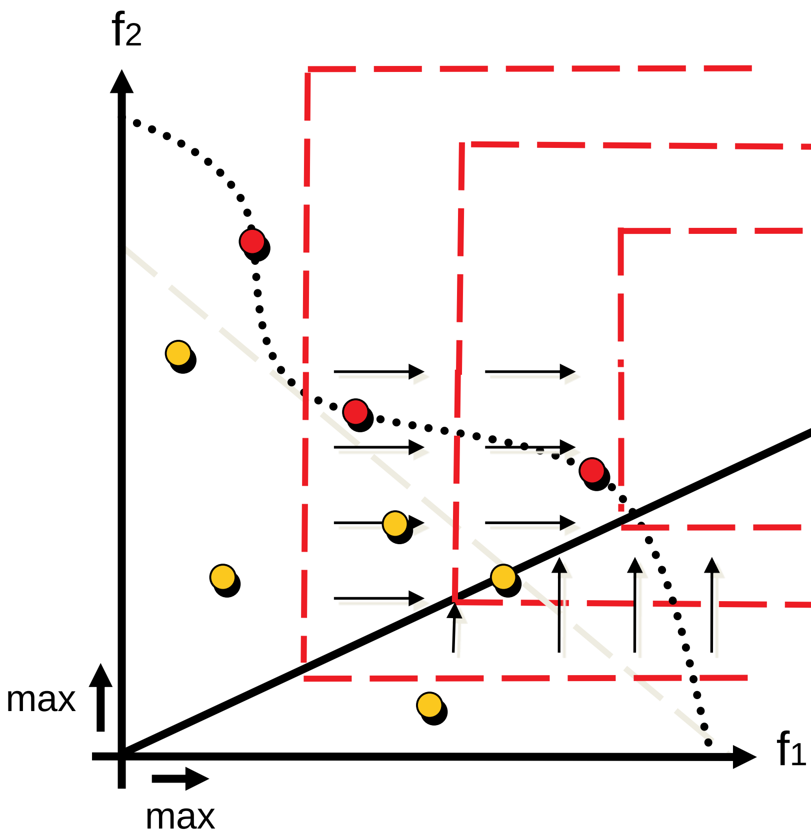
$$y = \max_i | \lambda_i (u_i - z_i) |$$

Several other scalarizing functions are known, see e.g. [Miettinen 1999] multiple objectives

$(f_1(x), f_2(x), \ldots, f_k(x))$ → transformation → single objective $s(x)$

parameters ↓ (transformation)

Example 2: weighted Tchebycheff



$(\lambda_1, \lambda_2, \ldots, \lambda_k)$ ↓

→ $y = \max_i |\lambda_i(u_i - z_i)|$ →

Several other scalarizing functions are known, see e.g. [Miettinen 1999]

Exercise: Benchmarking a Weighted Sum Approach on COCO

Exercise

Goal: Implement a Simple Weighted Sum Approach:

- N scalarizing functions, optimized with CMA-ES
- Python: use CMA-ES after **`pip install cma`** (more details here: **`https://pypi.python.org/pypi/cma`**)
- use ask and tell interface (next slide)
- CMA-ES parameters as default (with $\sigma_{init} = 3$ and initialized in [-5,5]
- no details given about:
  - how to normalize the objectives and estimate z
  - the order in which the N scalarizing functions are optimized
  - how to do restarts and how to distribute the budget

2nd Goal:

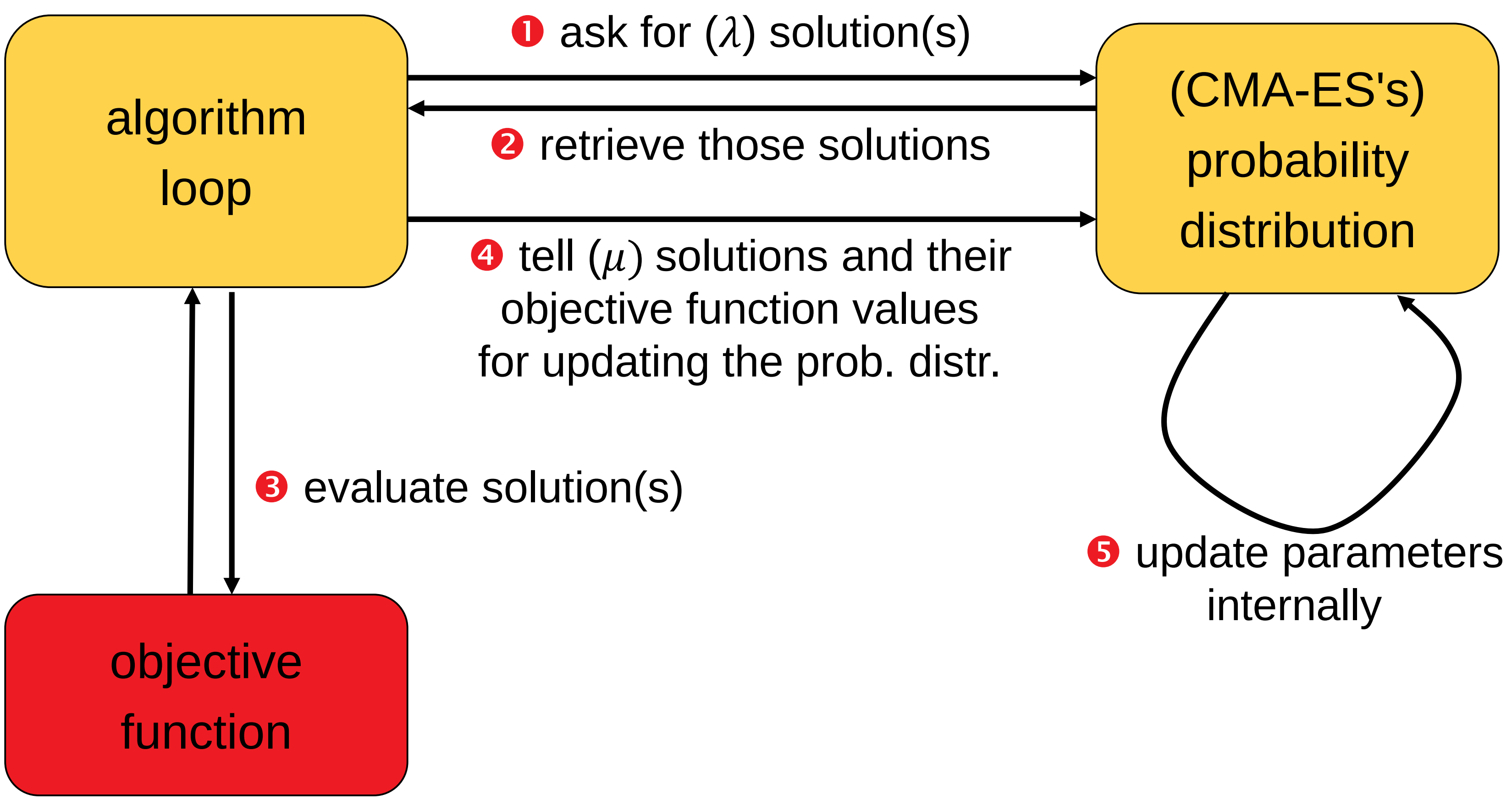
- produce data for the new **`bbob-biobj-ext`** suite
- hence, interested in your evaluations

The Idea of the Ask&Tell Interface to Optimization

example from the CMA-ES web page:

```
>>> import cma
>>> es = cma.CMAEvolutionStrategy(12 * [0], 0.5)
>>> while not es.stop():
...     solutions = es.ask()
...     es.tell(solutions,
                [cma.ff.rosen(x) for x in solutions])
...     es.logger.add() # write data to disc
                          to be plotted
...     es.disp()
<output omitted>
>>> es.result_pretty()
<output omitted>
>>> cma.plot() # shortcut for es.logger.plot()
```

Ask&Tell with CMA-ES (Visually)



Exercise: concrete

a) download COCO (release 2.2.1) from **`https://github.com/numbbo/coco/`**

b) install and test it via **`python do.py run-python`**

c) run the previous example code of CMA-ES (e.g. in ipython shell) to get an idea how it works

d) start your implementation of a weighted sum optimizer from [**`http://www.cmap.polytechnique.fr/~dimo.brockhoff/advancedOptSaclay/2019/exercises/example_experiment_WS.py`**](http://www.cmap.polytechnique.fr/~dimo.brockhoff/advancedOptSaclay/2019/exercises/example_experiment_WS.py) within the function **`def weighted_sum(fun, budget)`**

tip: start simple and extend!

Exercise: concrete

e) run the experiments by typing
`python example_experiment_WS.py bbob-biobj-ext BUDGET`
with **`BUDGET`** any integer (start small and then increase)

f) post-process/investigate the data:
- **`python do.py install-postprocessing`**
  [in the COCO-repo folder once]
- **`python -m cocopp YOURDATAFOLDER`**
  [YOURDATAFOLDER is typically something in **`exdata/`**]

g) iterate with larger budget, more functions, more instances, different parameters, …

h) send final data to me by email if you wish ☺

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