Derivative-Free Optimization

(Evolutionary) Multiobjective Optimization

January 10, 2025

Anne Auger
INRIA Saclay – Ile-de-France

Dimo Brockhoff
INRIA Saclay – Ile-de-France

Reminder Group Project

Tonight:

- deadline mini-report about progress
- please send it to
  dimo.brockhoff<at>inria.fr and
  anne.auger<at>inria.fr

24th of January (in 2 weeks):

- report (PDF) sent by email, 8 pages

31st of January (in 3 weeks):

- group presentations here in class
  (12’ presentation + ~10’ questions)

Reminder Group Project

A real science project with new results

Context: Noisy optimization / outliers

- How is the performance of algorithms "perturbed" if the objective function gets "perturbed"?
- code that wraps around deterministic test functions (from the bbob suite of the COCO platform) and an experiment script to do the benchmarking for varying levels of noise/outlier probability
- What I said last time about the type of noise/outlier choice was incorrect: by default, only additive noise is chosen (i.e. points can only get worse). Negative/good noise can be added via the parameters of the `noiser.py` code.

Now: quick hands-on tutorial about what we expect

Group Project Cheat Sheet

```
pip install --pre cocopp  # without the --pre, colors don't match values
```

```
import cocopp, glob
cocopp.main(glob.glob('FOLDER_WITH_EXPERIMENTDATA/*'))
```

Additionally, download (and rename with leading `0.0`) comparison algos from COCO data archive at https://coco-platform.org/testsuites/bbob/data-archive.html (this might help to find bugs in your experimental code if the algorithm performance without noise look significantly different for both algos)

The **?** is your friend in python to get the documentation of methods and modules ☺

Overview of the Today's Lecture

Introduction to multiobjective optimization

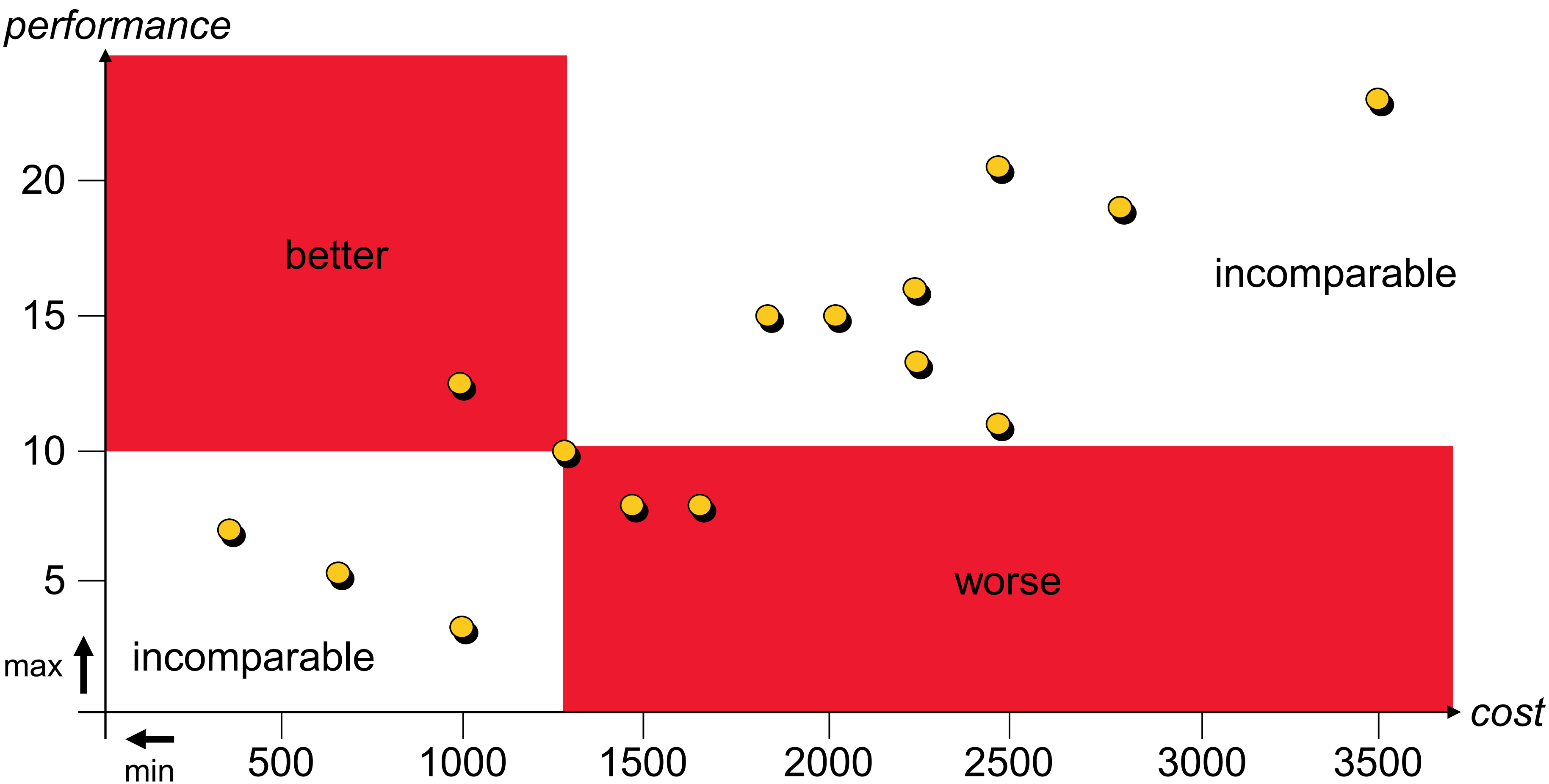
- difference to single-objective optimization, the basics
- algorithms and their design principles

introductory material (for example):

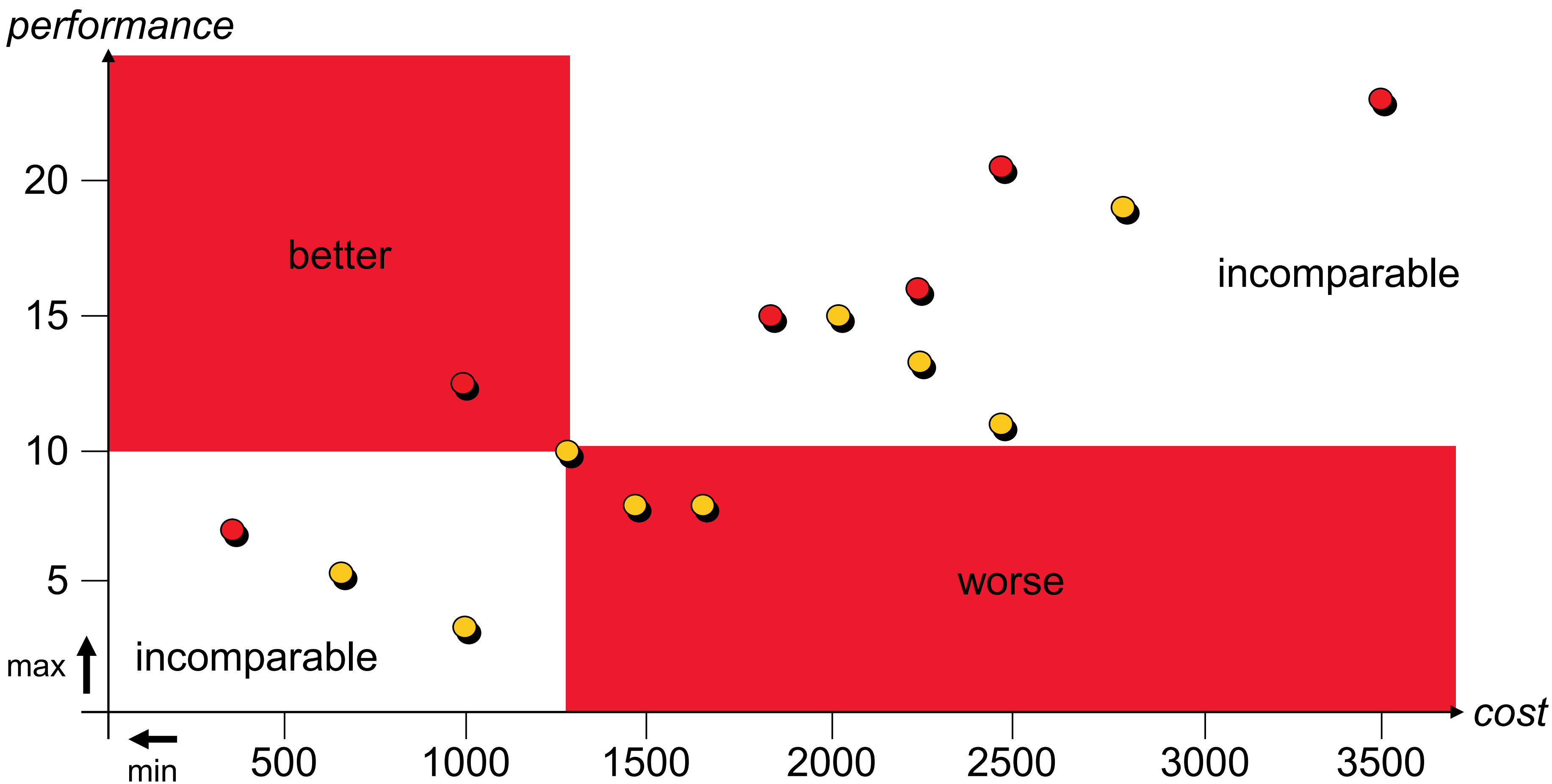
- P.J. Fleming*, R.C. Purshouse : Evolutionary algorithms in control systems engineering: a survey (sections 1&2 only)
- K. Deb: Introduction to Evolutionary Multiobjective Optimization, chapter 3 of J. Branke, K. Deb, K. Miettinen, R. Słowinski (Eds.): Multiobjective Optimization --- Interactive and Evolutionary Approaches

Multiobjective Optimization

Multiple objectives that have to be optimized simultaneously



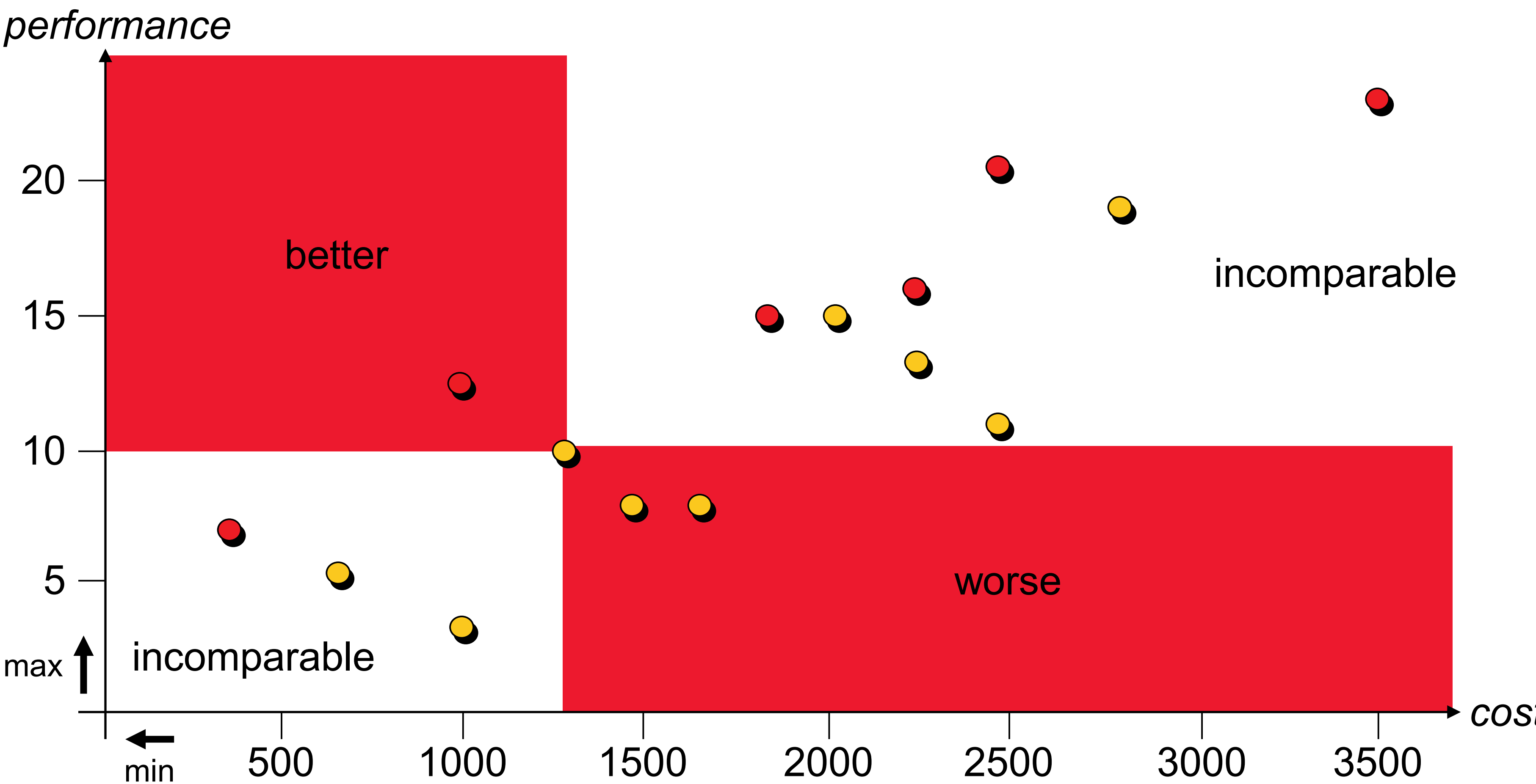
Observations: ❶ there is no single optimal solution, but
❷ some solutions (●) are better than others (●)



A Brief Introduction to Multiobjective Optimization

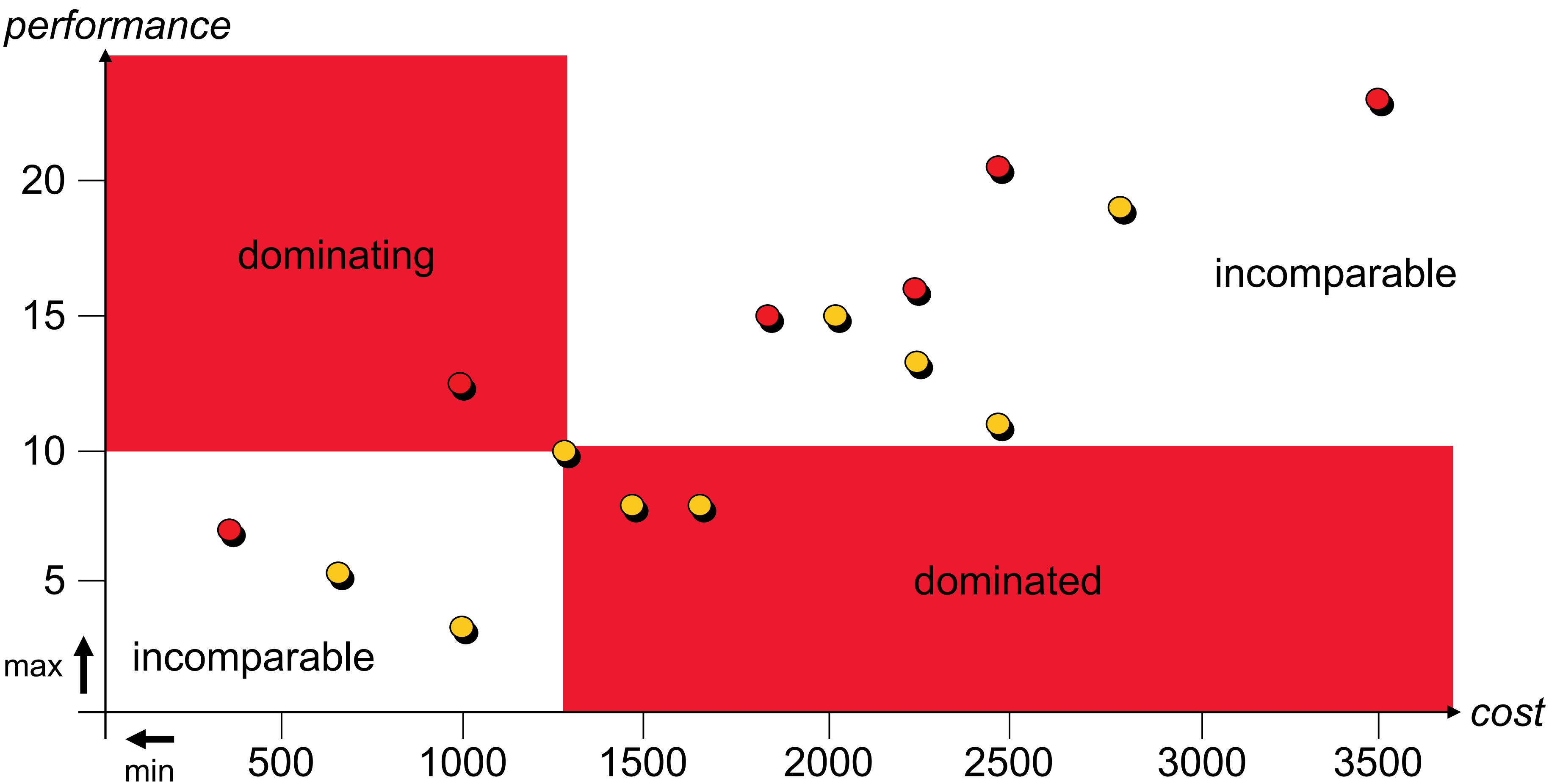
$$u \text{ weakly Pareto dominates } v \ (u \preccurlyeq_{par} v): \quad \forall 1 \leq i \leq k : f_i(u) \leq f_i(v)$$

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



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

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



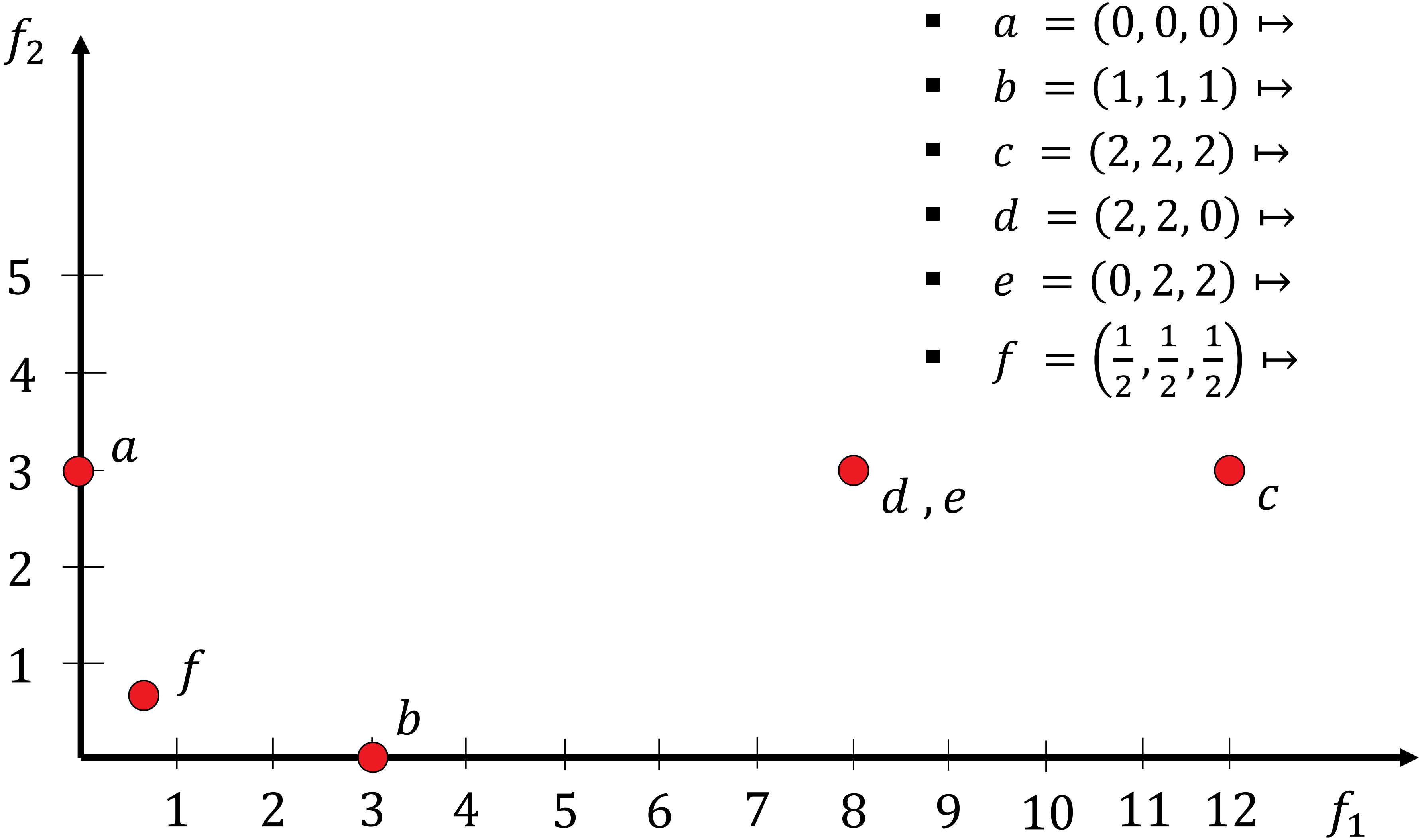
Example: Understanding Pareto Dominance

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

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

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

Example: Understanding Pareto Dominance



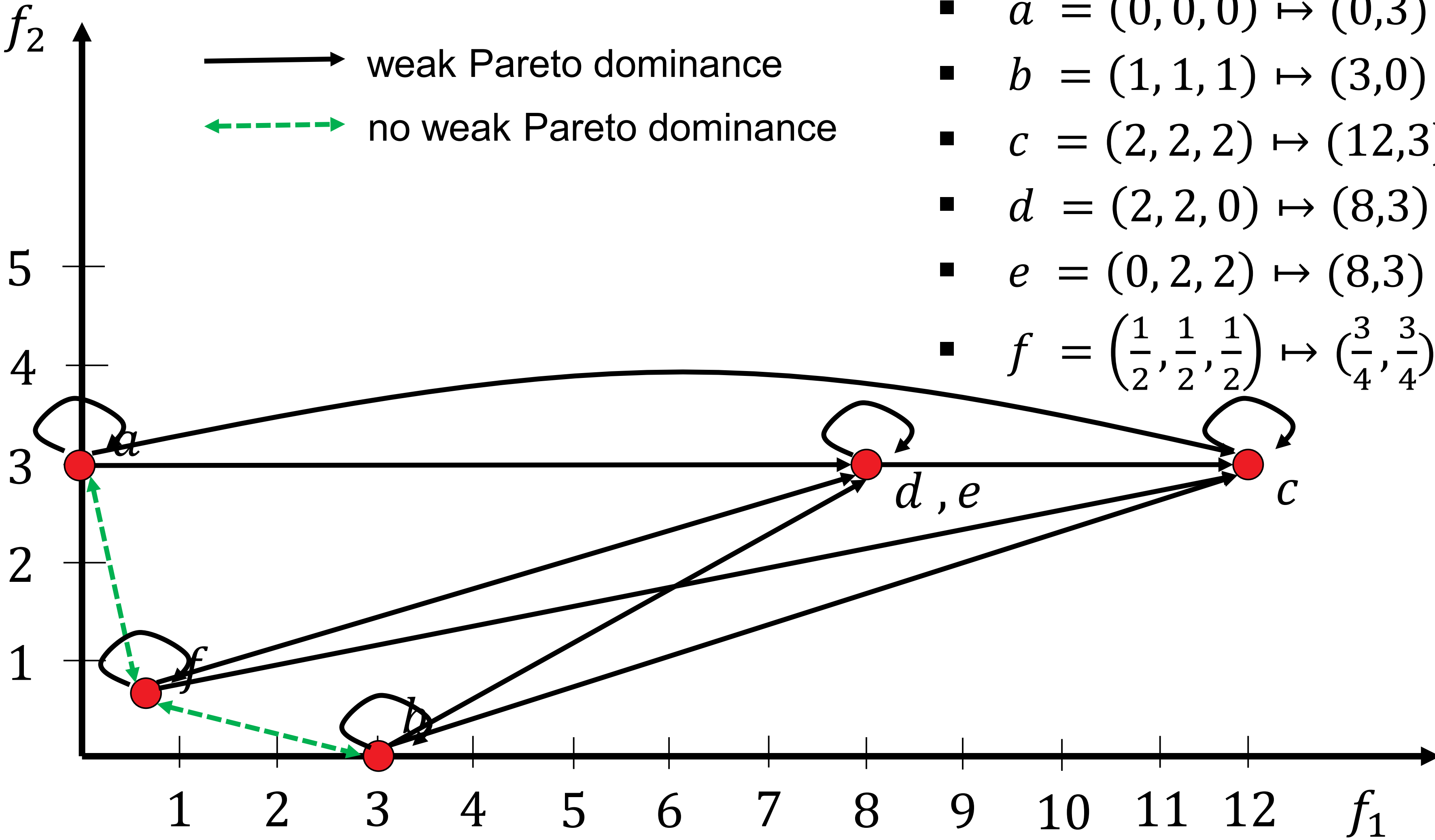
$f_{\text{doublesphere}}: x \mapsto$
$\left(\sum_{i=1}^{n} x_i^2\ ,\ \sum_{i=1}^{n}(x_i - 1)^2\ \right).$

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

Example: Understanding Pareto Dominance

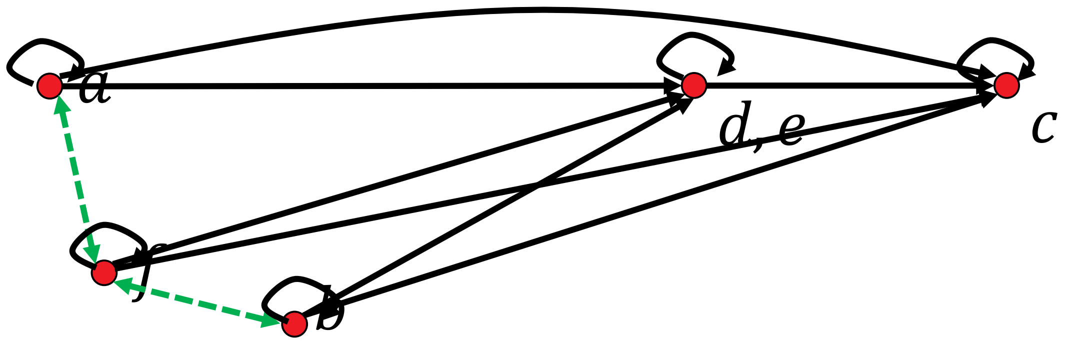
$f_{\text{doublesphere}}: x \mapsto \left(\sum_{i=1}^{n} x_i^2 \,,\, \sum_{i=1}^{n}(x_i - 1)^2\right).$

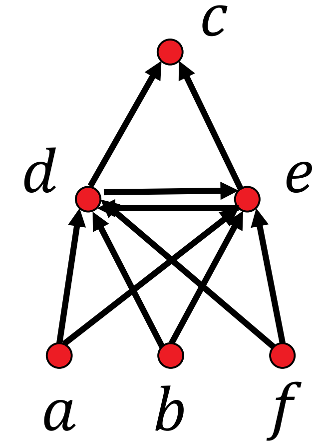
- $a \;= (0,0,0) \mapsto (0{,}3)$
- $b \;= (1,1,1) \mapsto (3{,}0)$
- $c \;= (2,2,2) \mapsto (12{,}3)$
- $d \;= (2,2,0) \mapsto (8{,}3)$
- $e \;= (0,2,2) \mapsto (8{,}3)$
- $f \;= \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right) \mapsto \left(\frac{3}{4},\frac{3}{4}\right)$



Visualizing Dominance Relations as Graphs

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





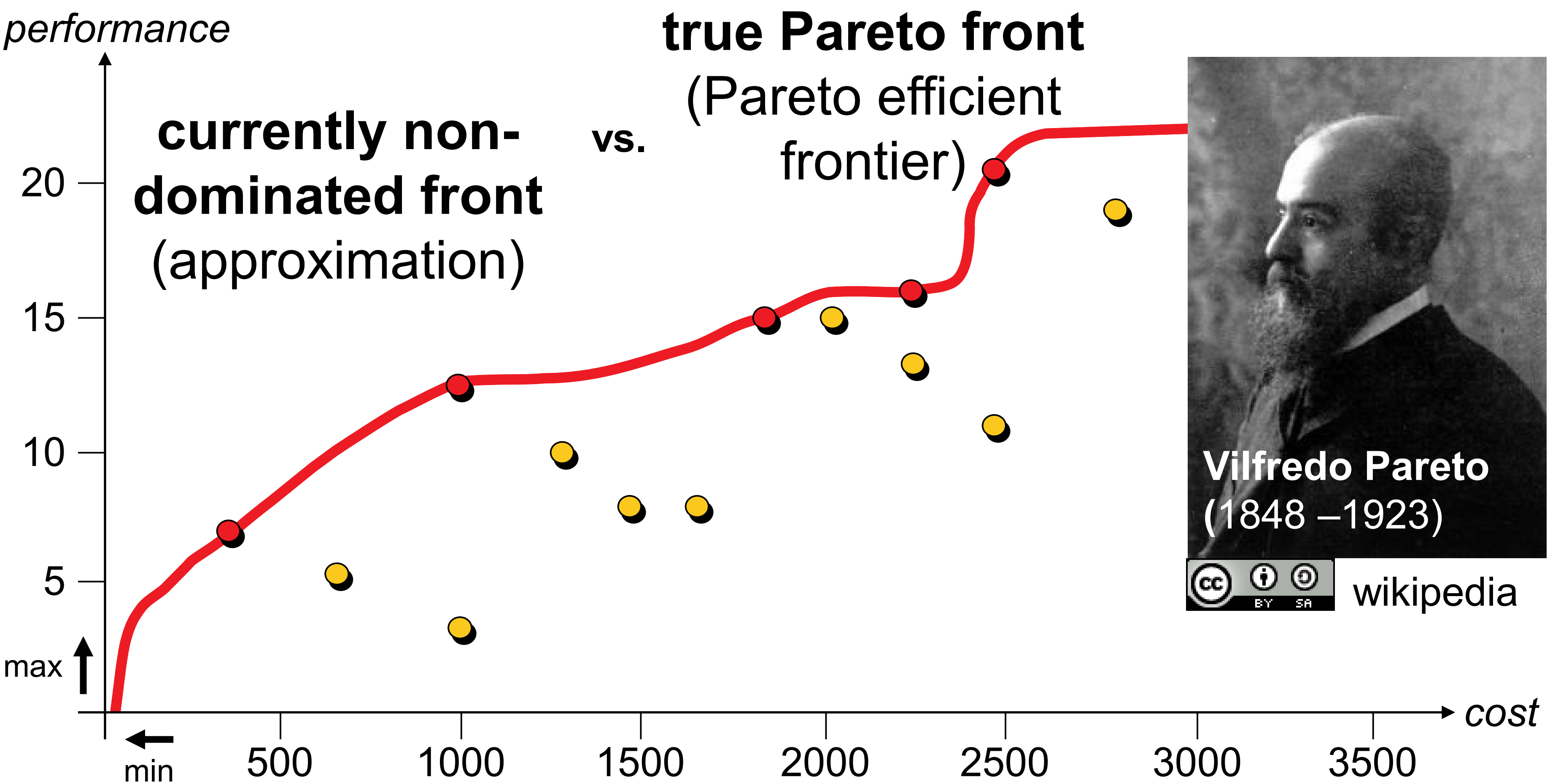
The weak Pareto dominance is a preorder, i.e. a relation that is

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

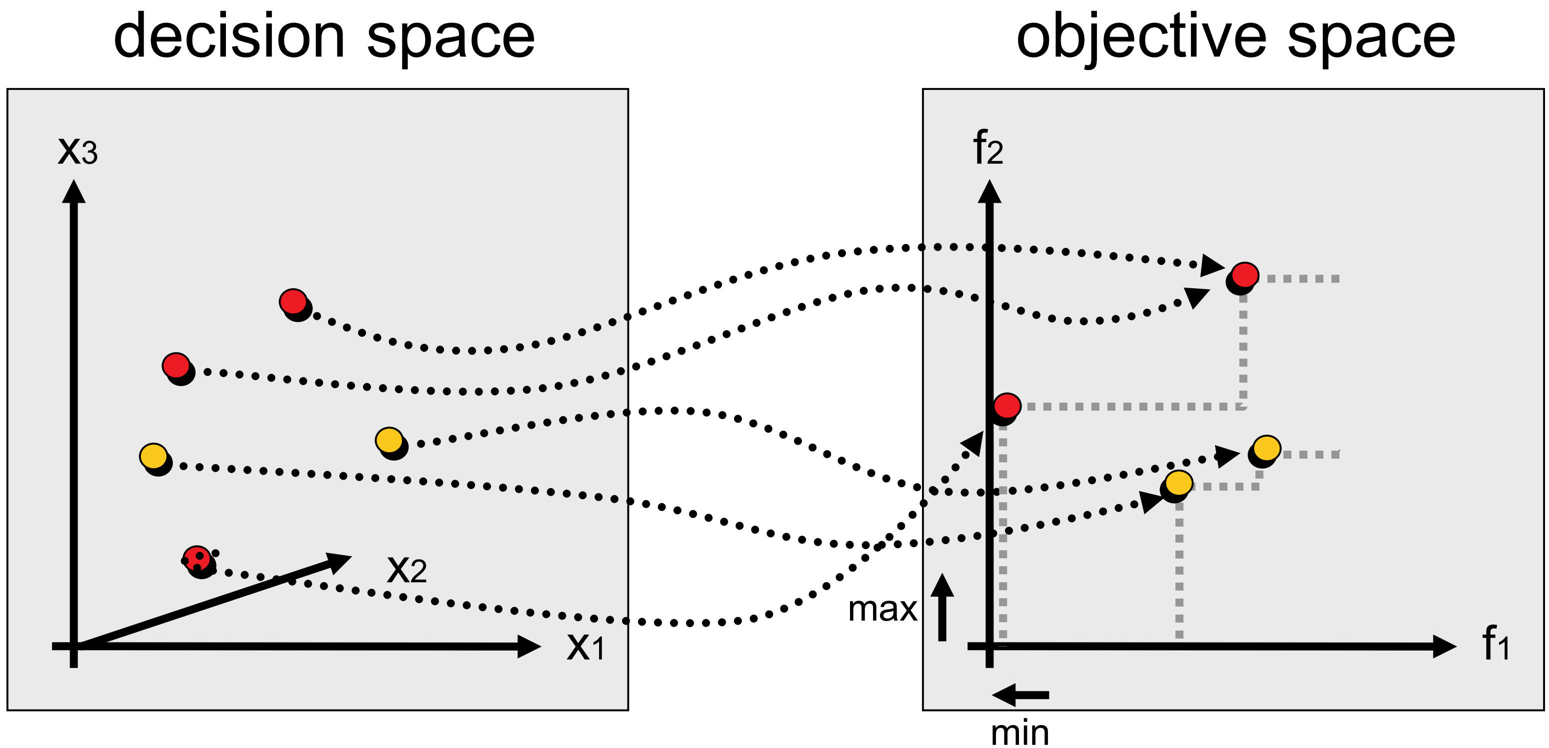
If no *indifferent* solutions $x \neq y$ with $f(x) = f(y)$ exist, we have antisymmetry and a partial order ("poset")---visualizable as Hasse diagram.

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

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



A Brief Introduction to Multiobjective Optimization



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

non-optimal decision vector ● non-optimal objective vector

Exercise: Pareto Front of Double Sphere

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

a) what is the Pareto set?

b) what is the associated Pareto front?

Tips:

- where are the single-objective optima?
- display some solutions in the search space (let's say in 2-D)
- investigate where dominating/dominated/incomparable 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)

A Necessary Condition On the Pareto Set

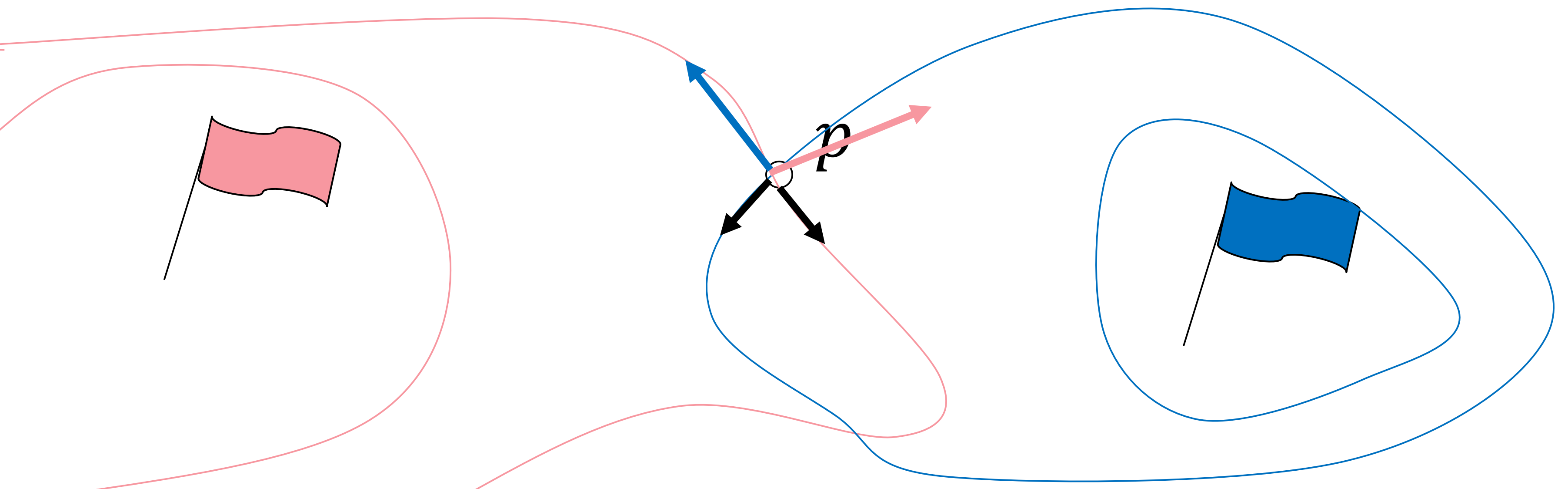
Necessary Condition:

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

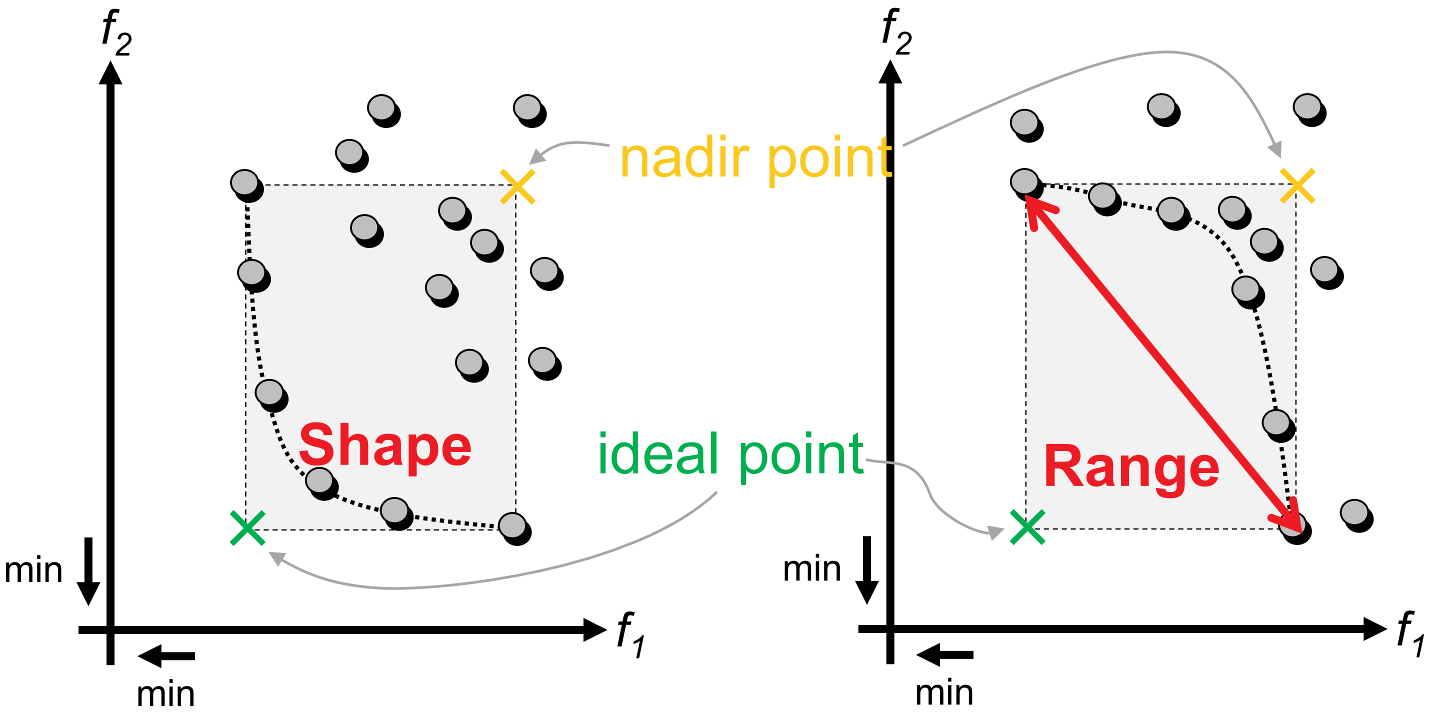
(Visual) Reasoning:

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

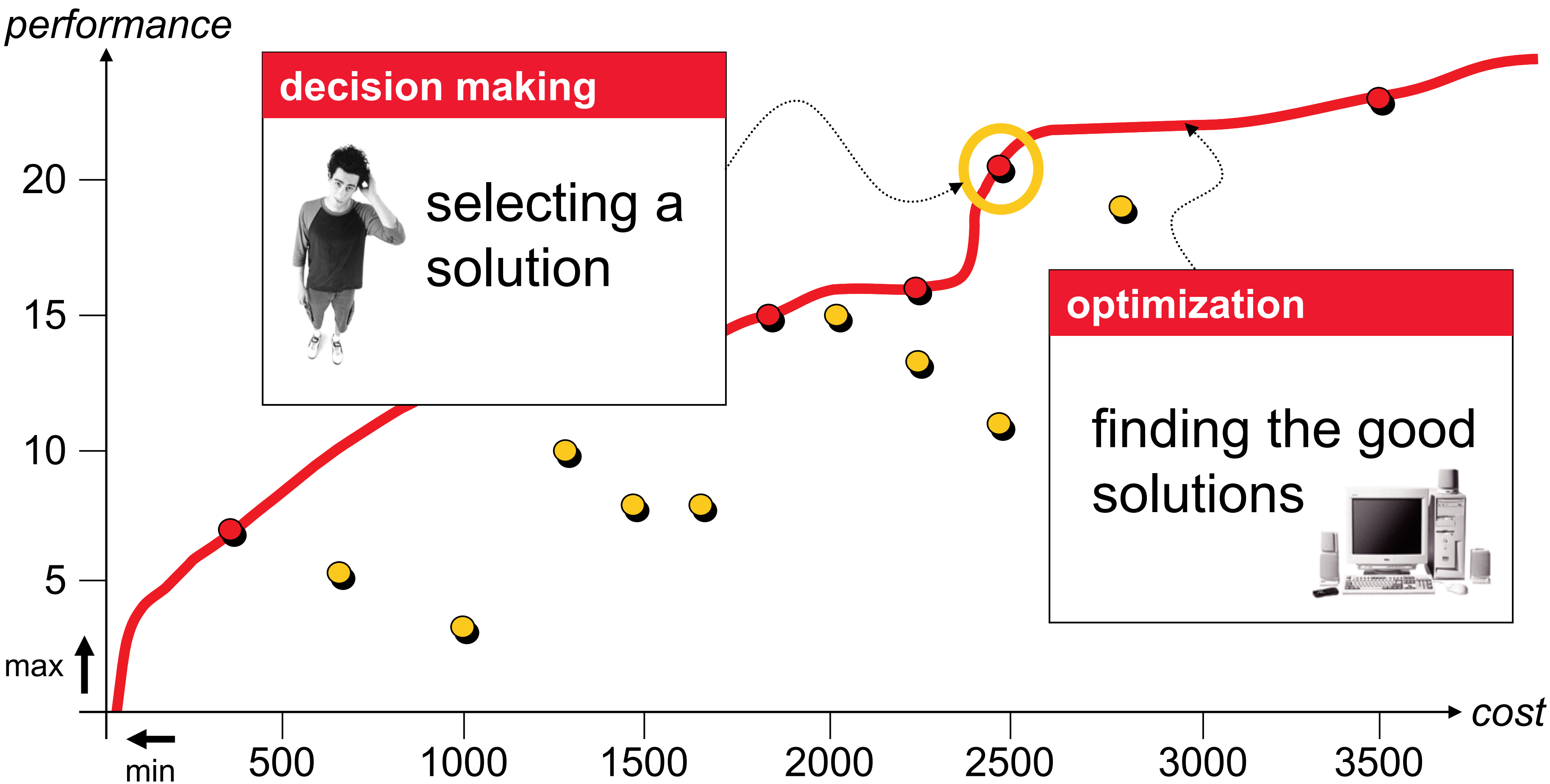


ideal point: best values
nadir point: worst values
} obtained for *Pareto-optimal* points

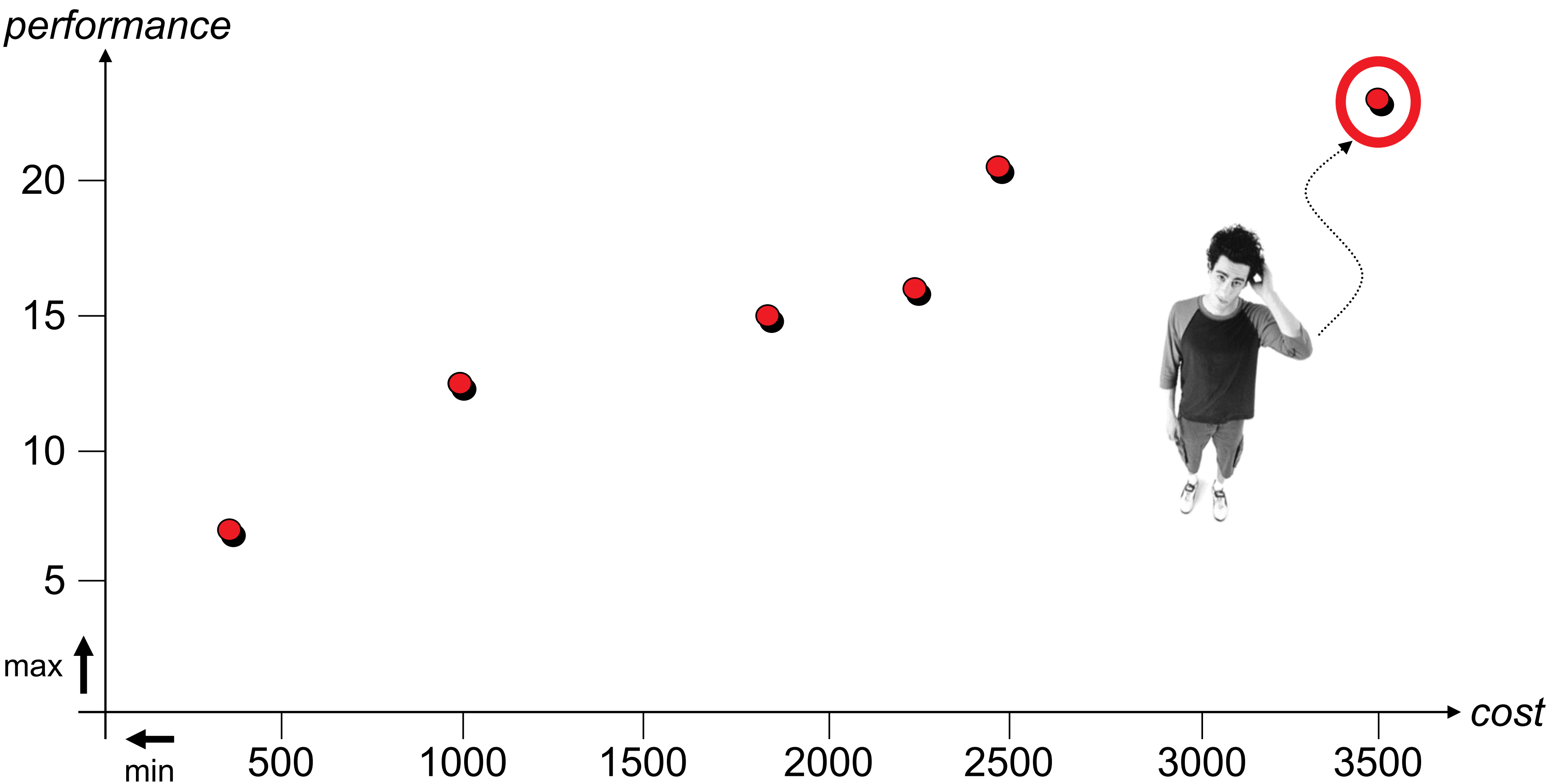
Optimization vs. Decision Making

Multiobjective Optimization

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

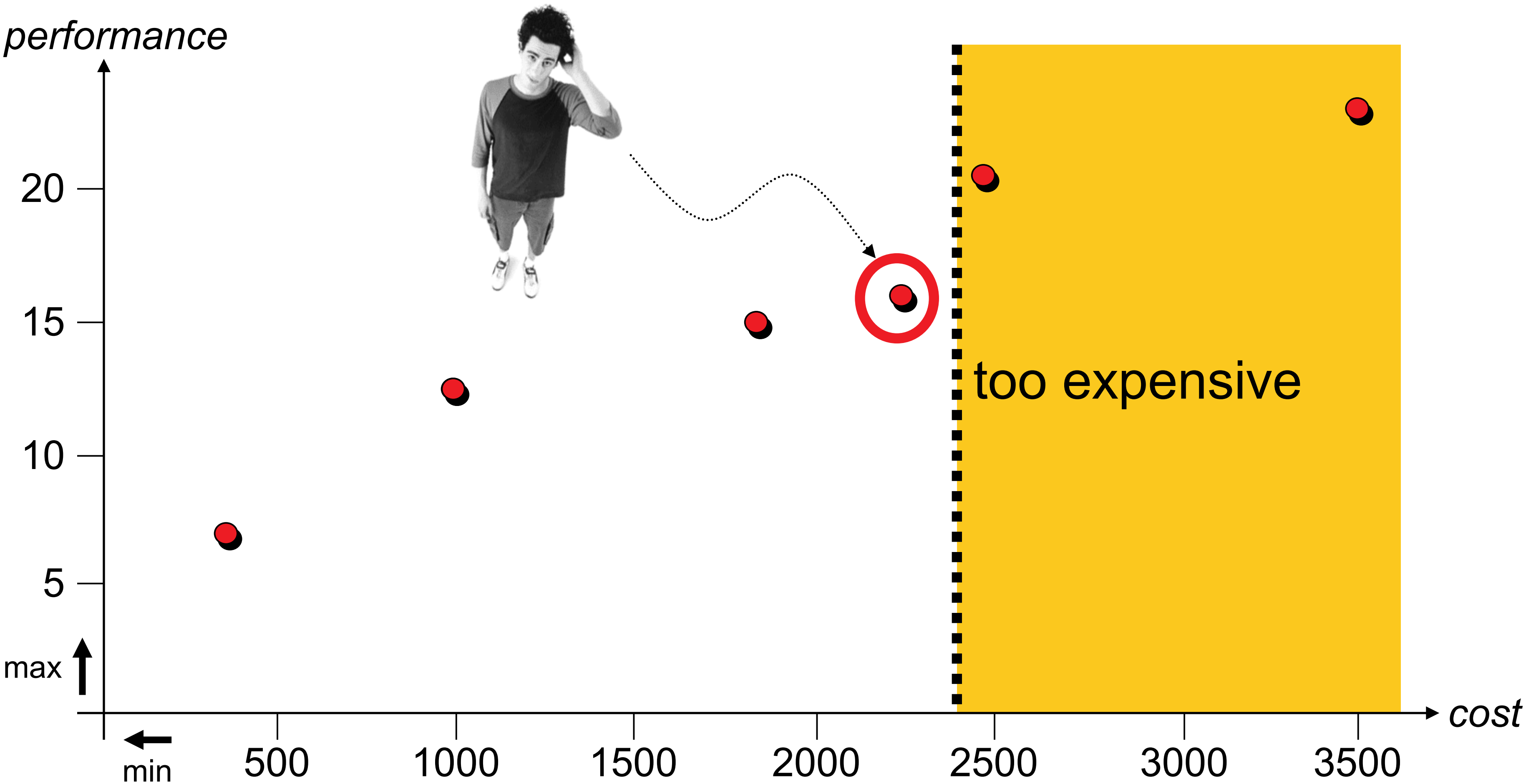


Possible Approaches: ❶ **ranking:** performance more important than cost



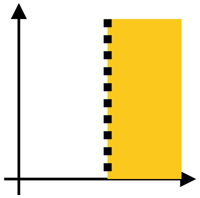
Selecting a Solution: Examples

Possible Approaches:
❶ ranking: performance more important than cost
❷ **constraints:** cost must not exceed 2400

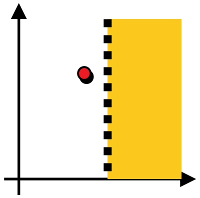


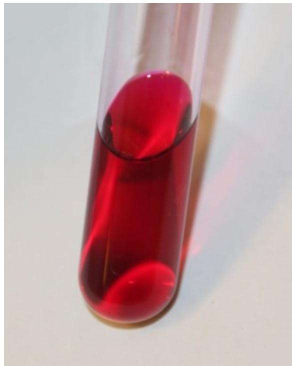
Before Optimization:

rank objectives,
define constraints,…



search for one
(good) solution

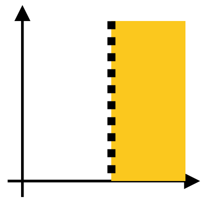




When to Make the Decision

Before Optimization:

rank objectives,
define constraints,…



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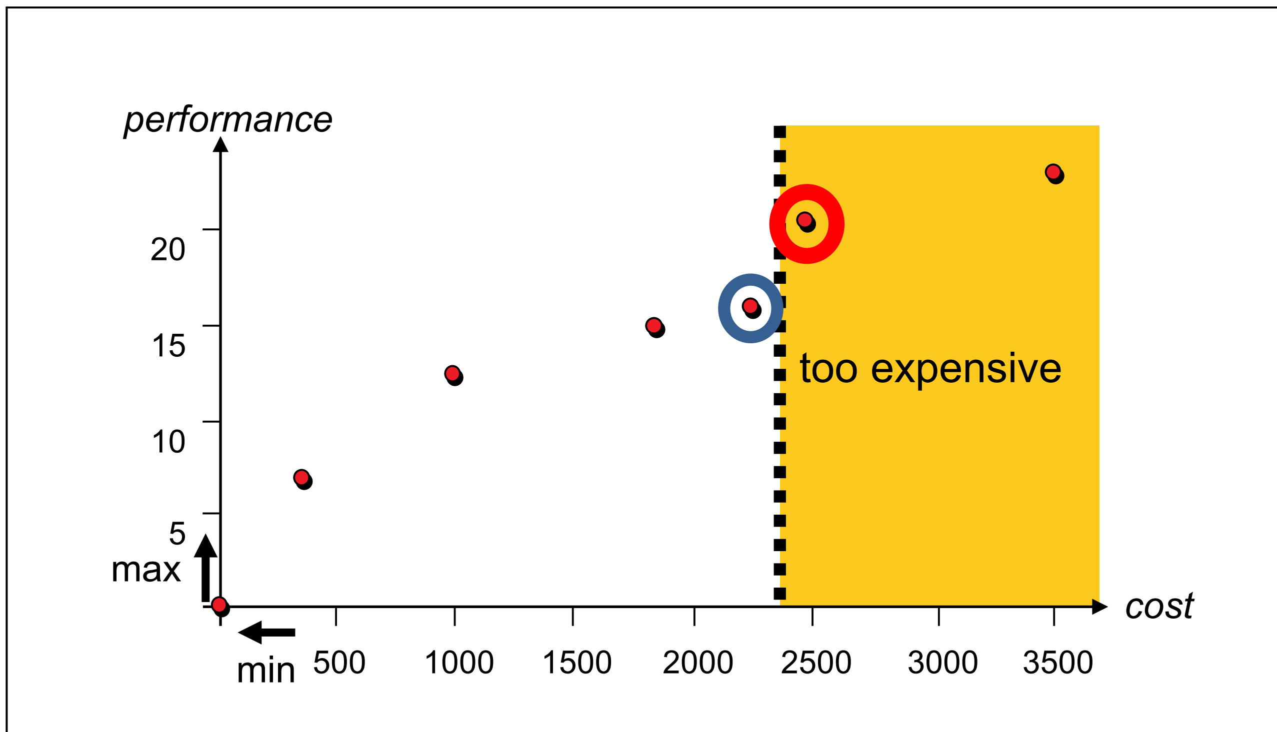

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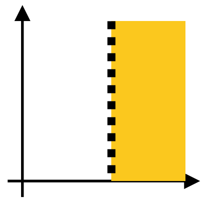

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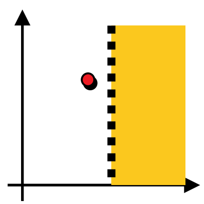
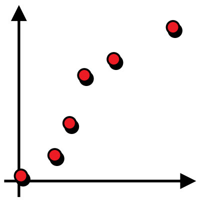
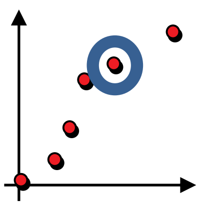


After Optimization:

search for a set of
(good) solutions



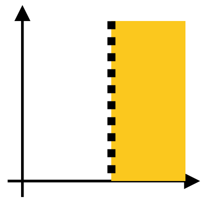
select one solution
considering
constraints, etc.



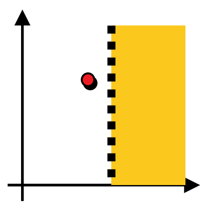
When to Make the Decision

Before Optimization:

rank objectives,
define constraints,…

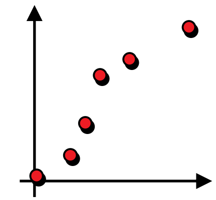


search for one
(good) solution



After Optimization:

search for a set of
(good) solutions



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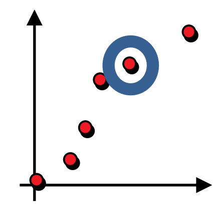


Focus: learning about a problem

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

All slides with blue background have not been discussed in class and are thus also not considered for the exam.

Two Communities...

MCDM International Society on Multiple Criteria Decision Making

- 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

EMO

- relatively 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

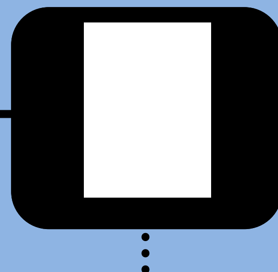
MCDM International Society on Multiple Criteria Decision Making

emo

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

One of the Main Differences

Blackbox optimization

$x \in \mathbb{R}^n$  $(f_1(x), \ldots, f_k(x))$

only mild assumptions

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

objectives

- non-linear
- noisy
- uncertain
- expensive (integrated simulations, real experiments)
- non-differentiable

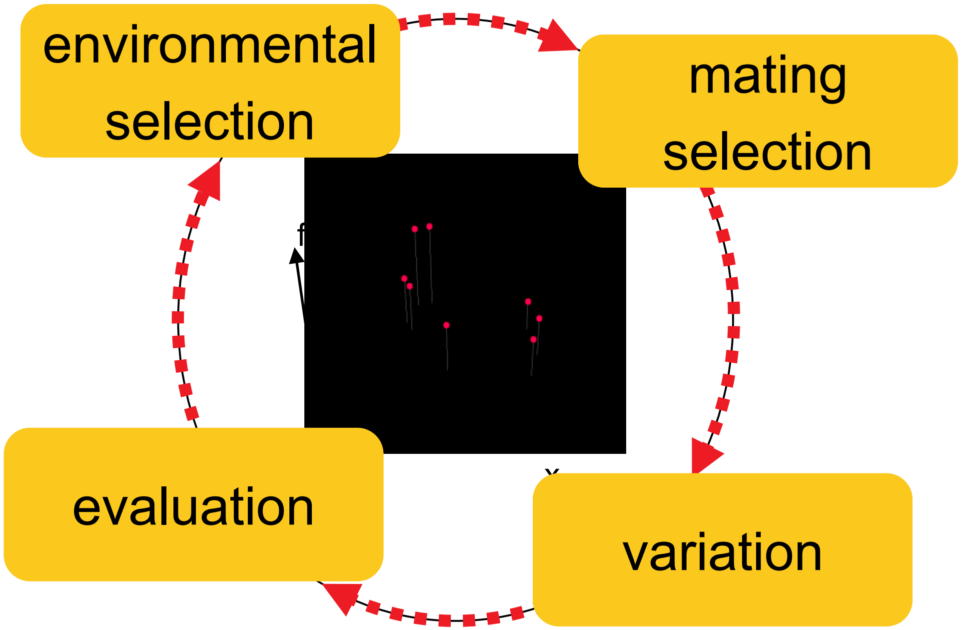
problem

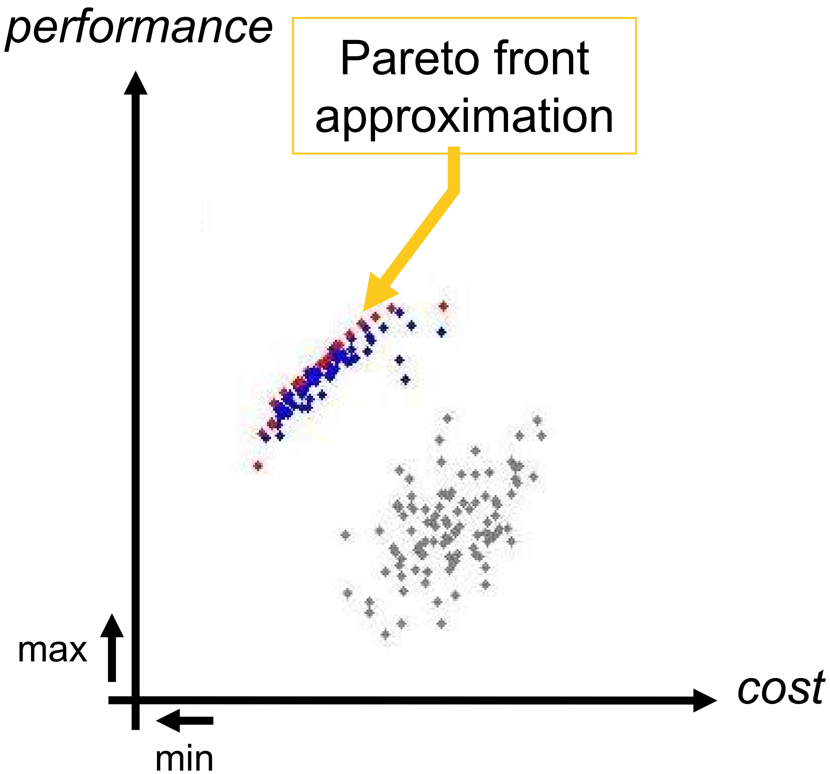
- many objectives
- huge search spaces
- many constraints

The Other Main Difference

Evolutionary Multiobjective Optimization

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

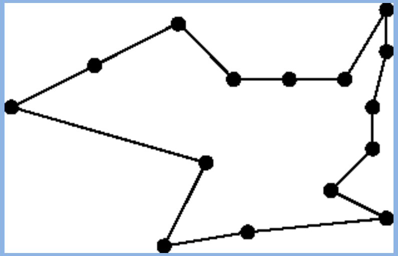




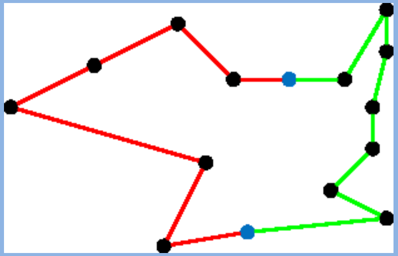
Multiobjectivization

Some problems are easier to solve in a multiobjective scenario

example: TSP
[Knowles et al. 2001]



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



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

Multiobjectivization

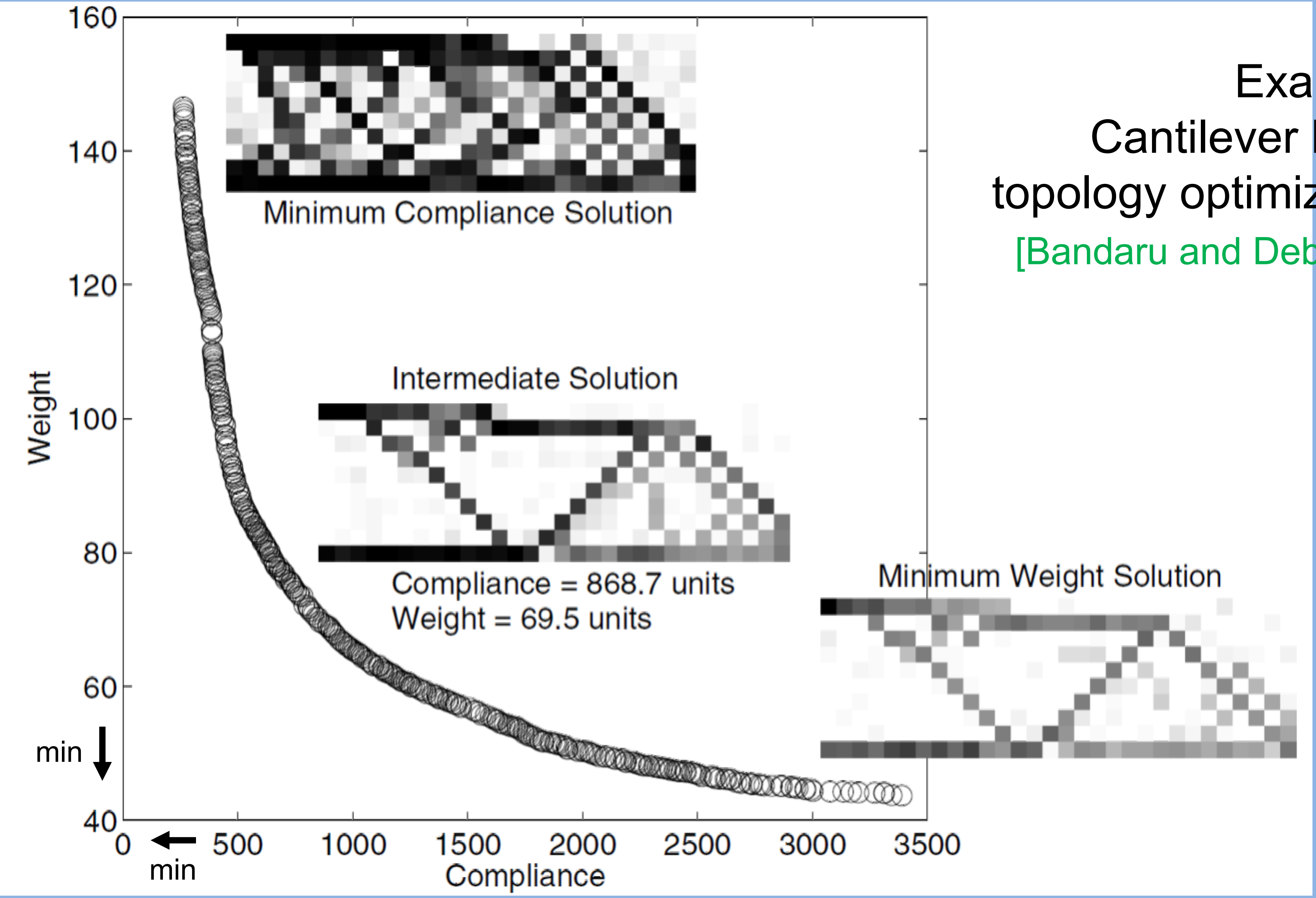
- by addition of new "helper objectives" [Jensen 2004]
  - job-shop scheduling [Jensen 2004], frame structural design [Greiner et al. 2007], VRP [Watanabe and Sakakibara 2007], ...
- by decomposition of the single objective
  - TSP [Knowles et al. 2001], minimum spanning trees [Neumann and Wegener 2006], 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 overview: [Segura et al. 2013]

Often innovative design principles among solutions are found



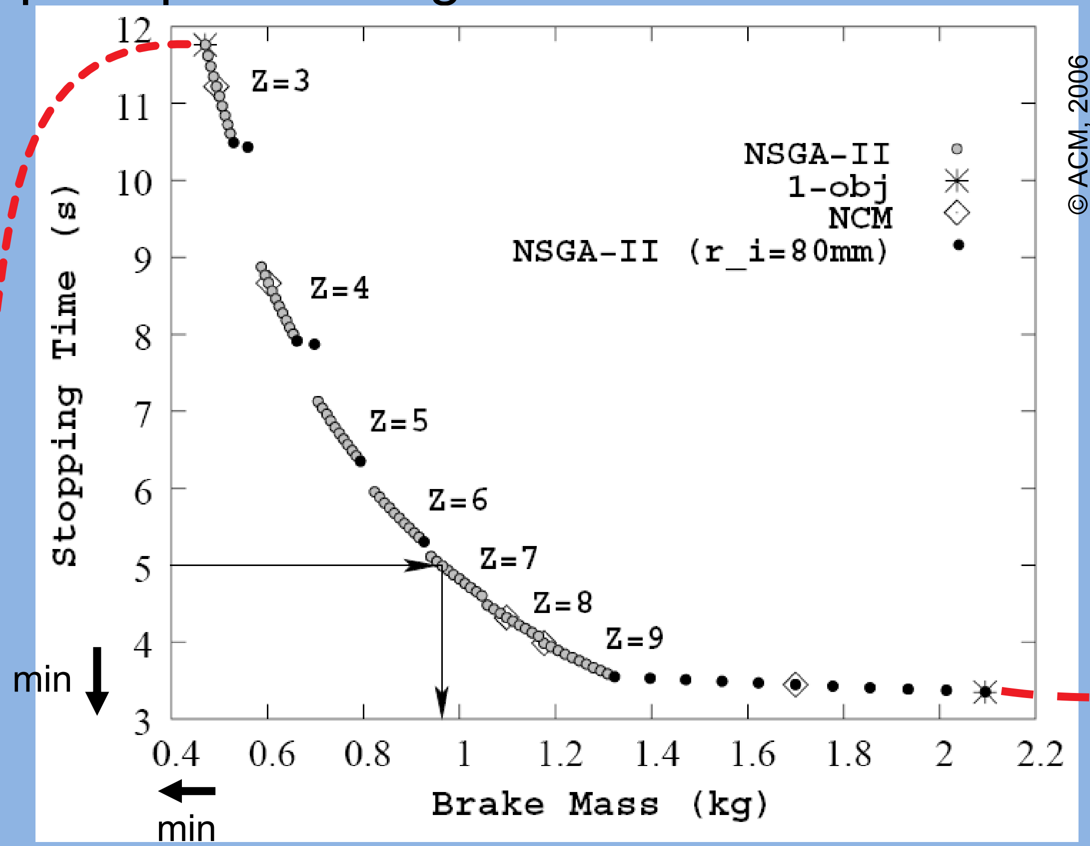
Example:
Cantilever beam
topology optimization
[Bandaru and Deb 2015]

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]

Approaches to Multiobjective Optimization

aggregation-based

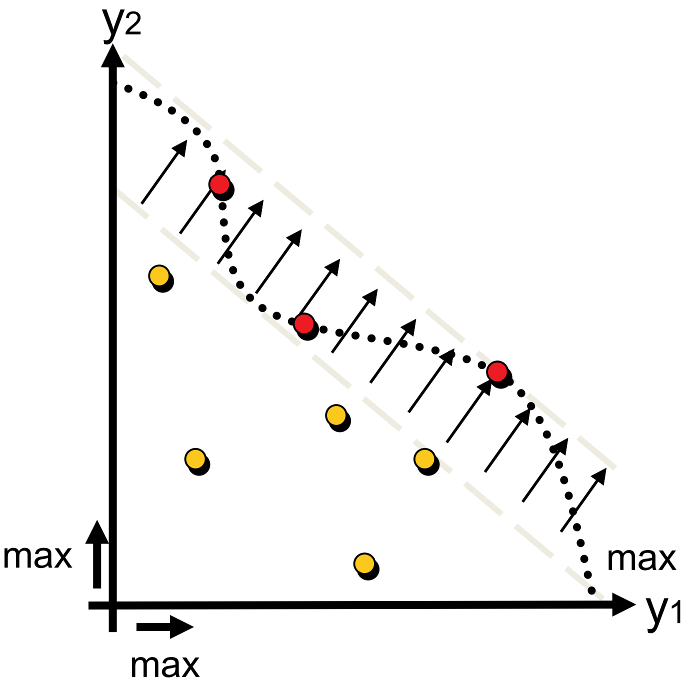
problem decomposition (multiple single-objective optimization problems)

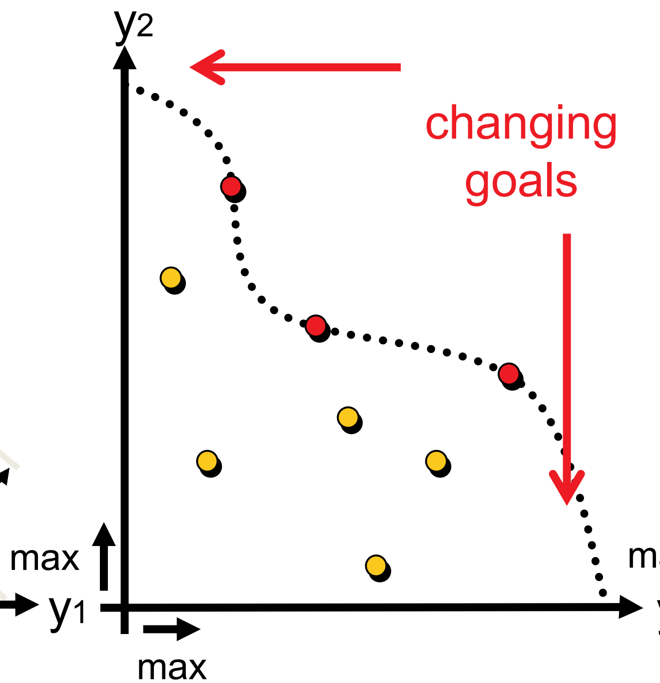
criterion-based

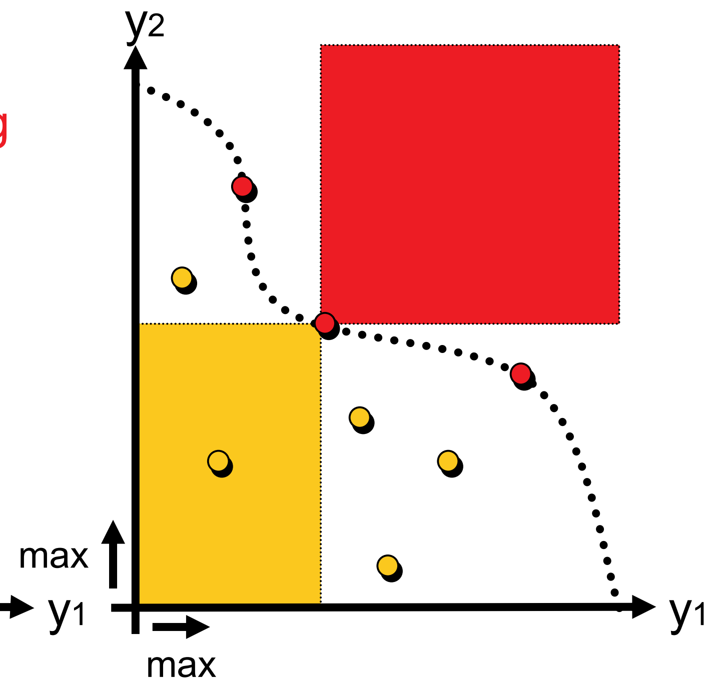
VEGA

dominance-based

SPEA2, NSGA-II
“modern” EMOA







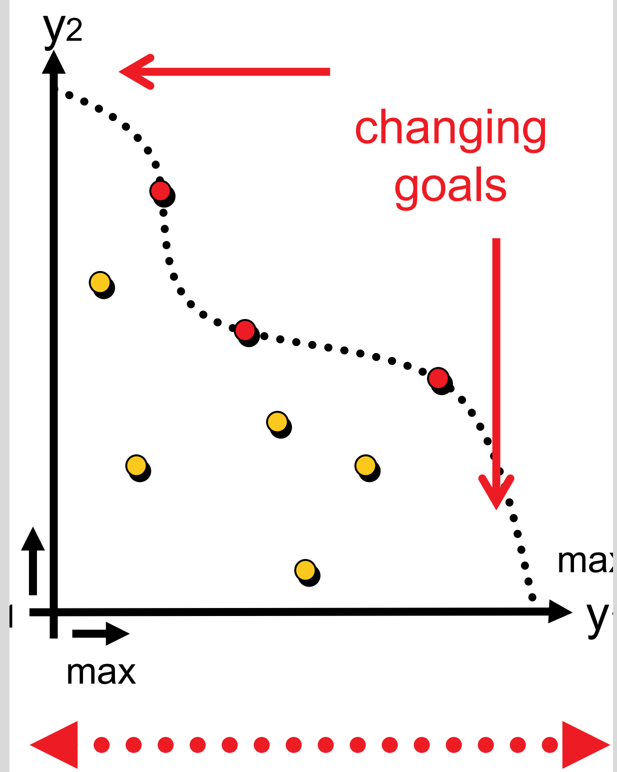
solution-oriented
scaling-dependent

set-oriented
less scaling-independent

Approaches to Multiobjective Optimization

criterion-based

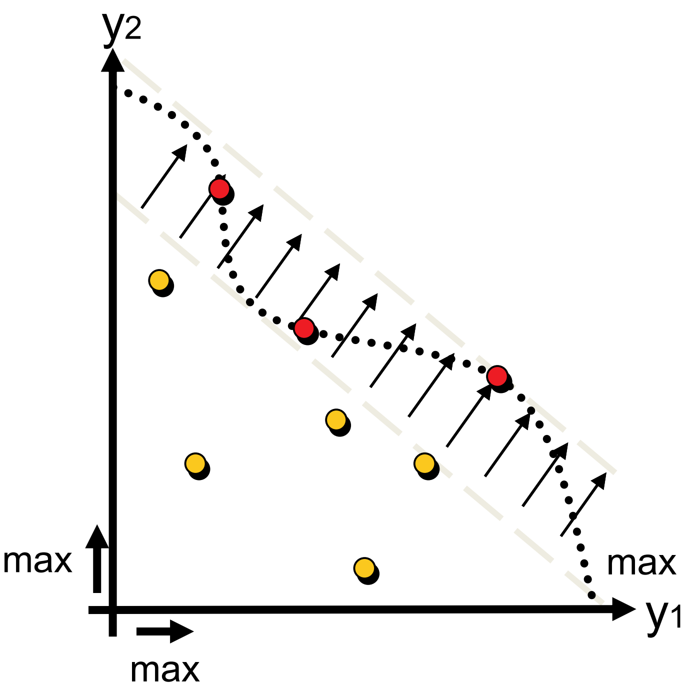
VEGA



less

aggregation-based

problem decomposition (multiple single-objective optimization problems)



solution-oriented
scaling-dependent

Solution-Oriented Problem Transformations

parameters

multiple objectives

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

single objective

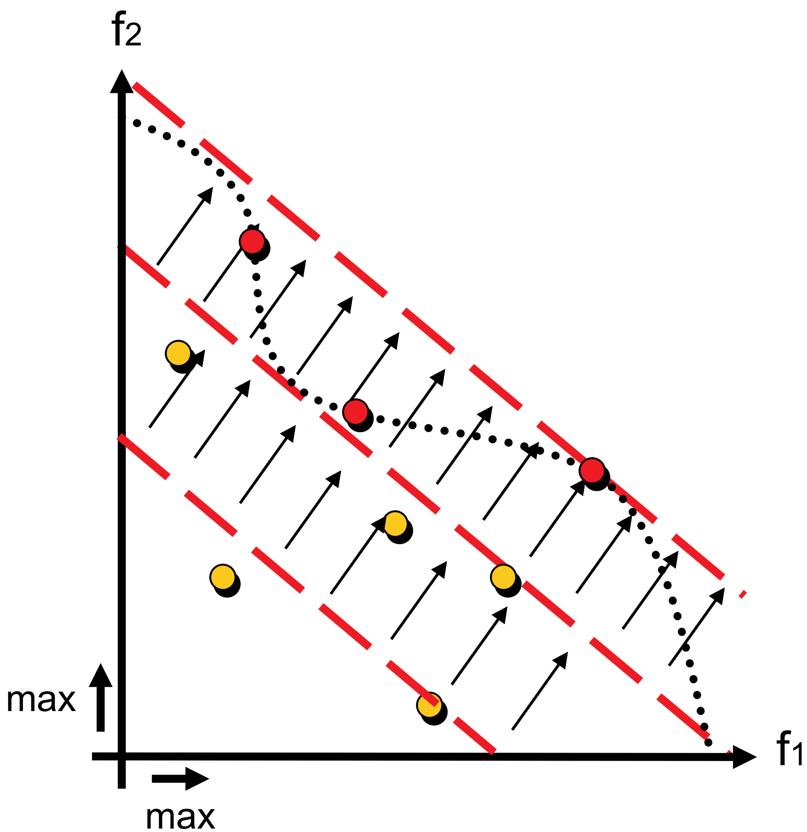
A scalarizing function s is a function $s: Z \rightarrow \mathbb{R}$ that maps each objective vector $u = (u_1, \ldots, u_n) \in Z$ to a real value $s(u) \in \mathbb{R}$

Solution-Oriented Problem Transformations

multiple objectives

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

single objective

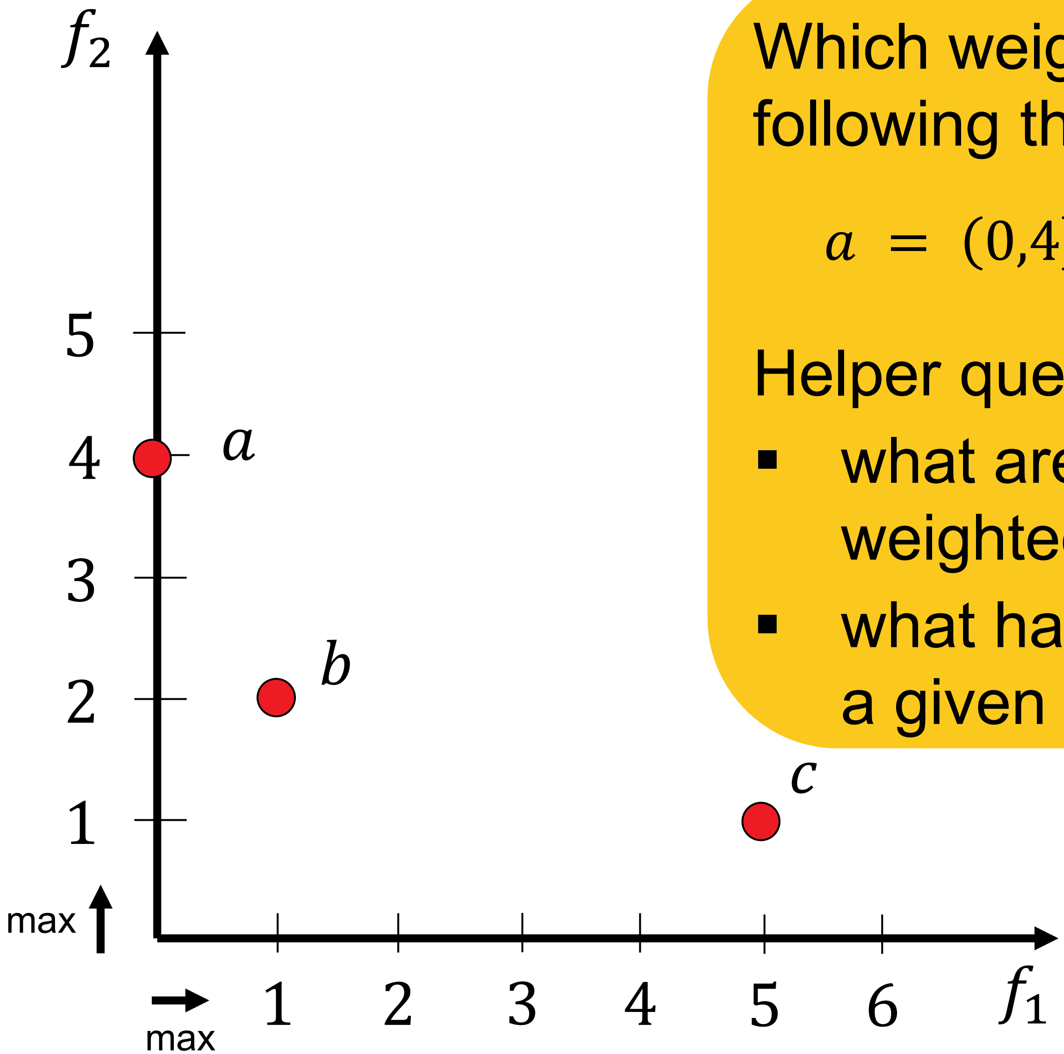


Example 1: weighted sum approach

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

→ $y = w_1 y_1 + \ldots + w_k y_k$ →

Exercise: Weighted Sum



Which weights are optimal for the following three points?

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

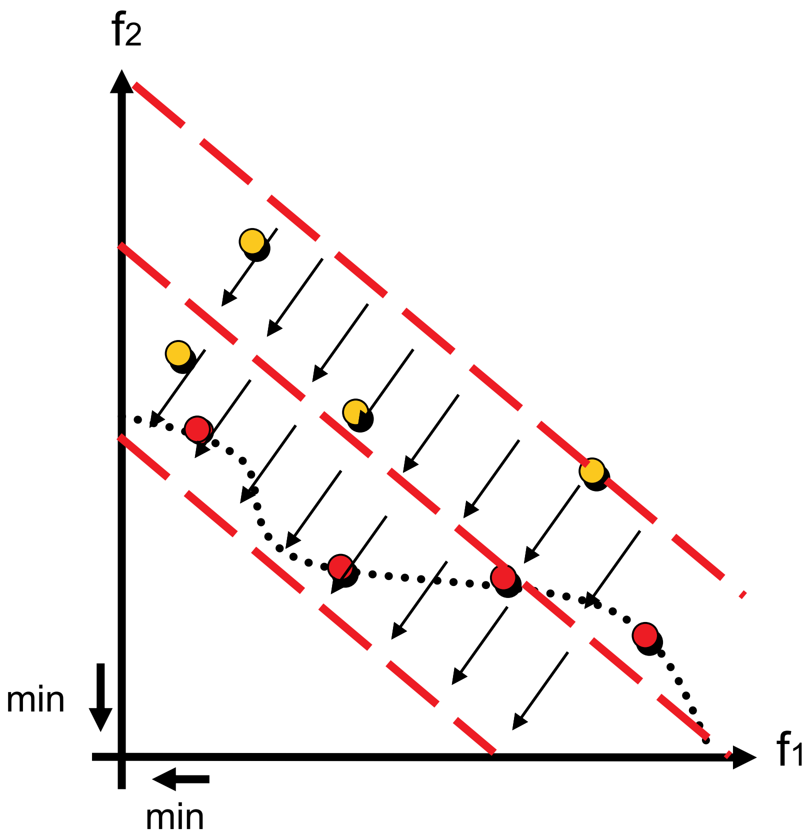
Helper questions:

- 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

parameters

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



Example 1: weighted sum approach

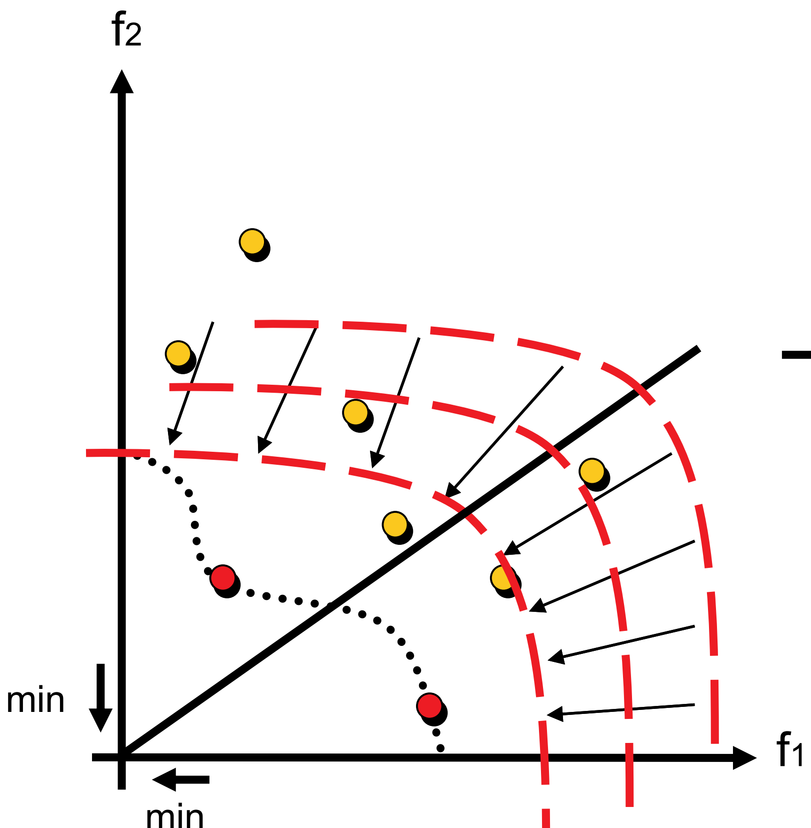
$(w_1, w_2, \ldots, w_k)$

→ $y = w_1 y_1 + \ldots + w_k y_k$ →

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

Solution-Oriented Problem Transformations

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



Example 2: weighted p-norm

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

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

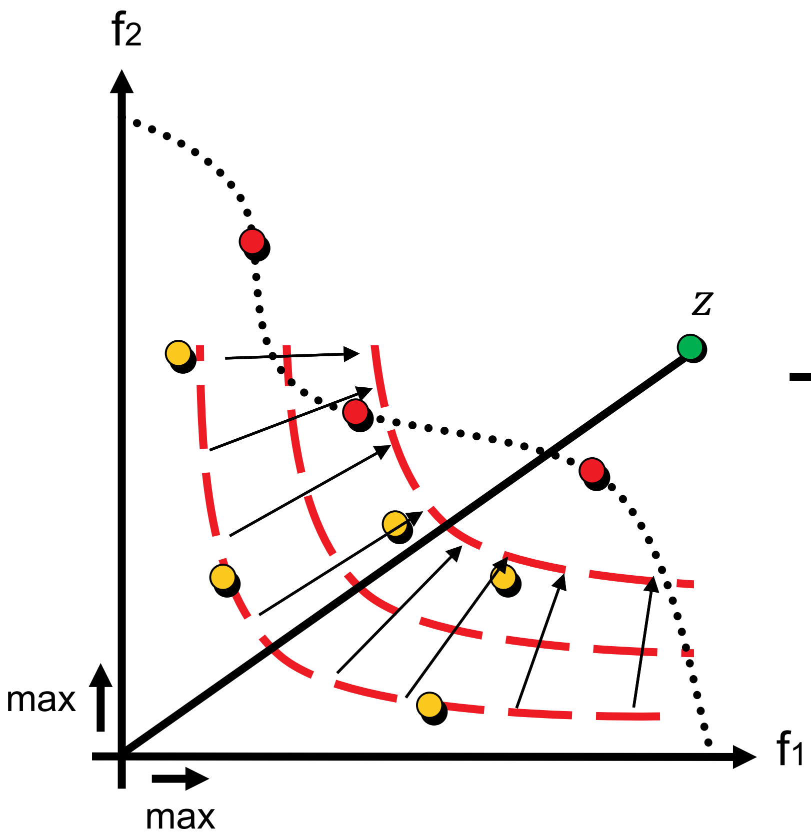
$p = 1$: weighted sum

$p = \infty$: weighted Tchebycheff

Solution-Oriented Problem Transformations

parameters

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



Example 2: weighted p-norm

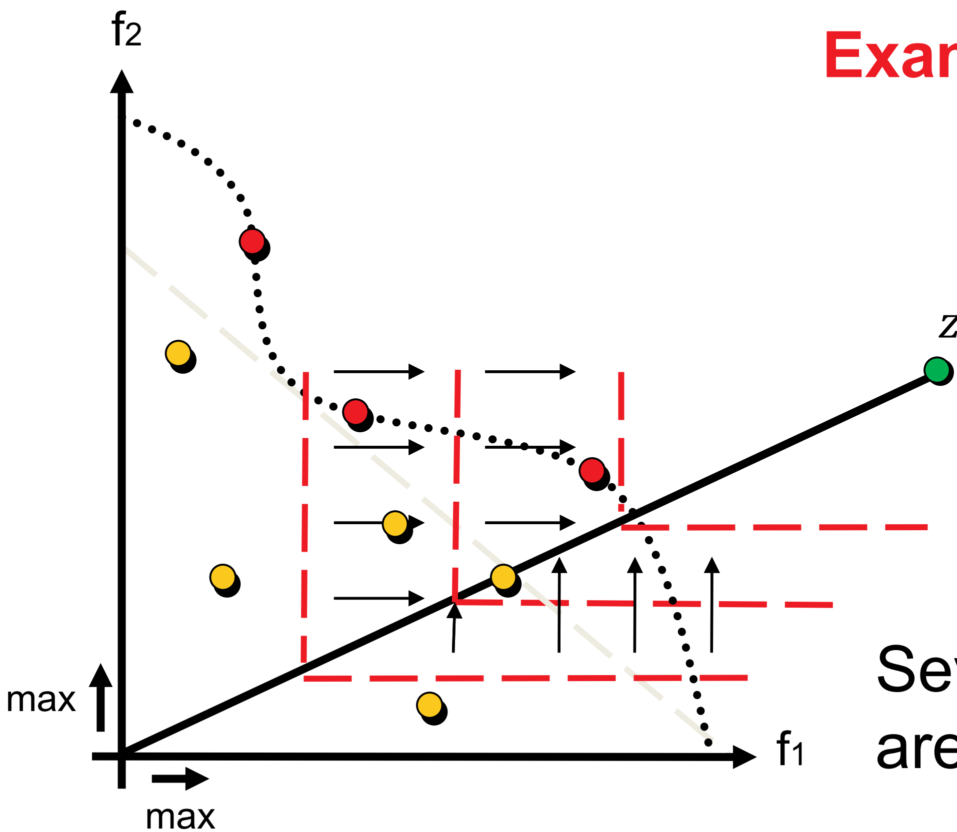
$(w_1, w_2, \ldots, w_k)$

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

$p = 1$: weighted sum

$p = \infty$: weighted Tchebycheff

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



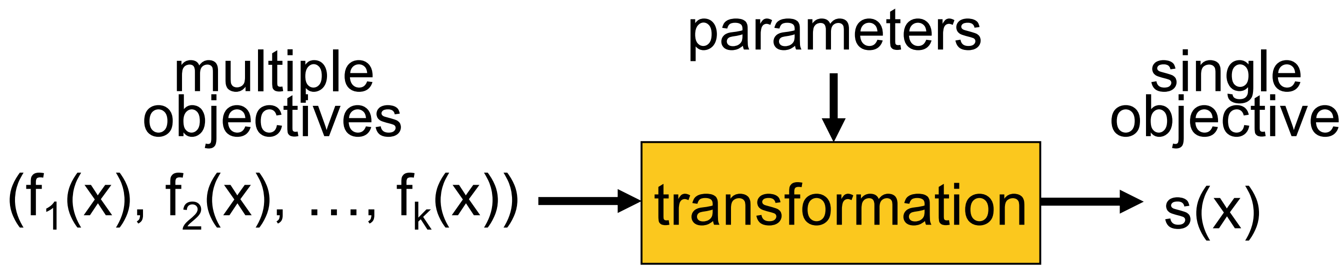
Example 2: weighted Tchebycheff

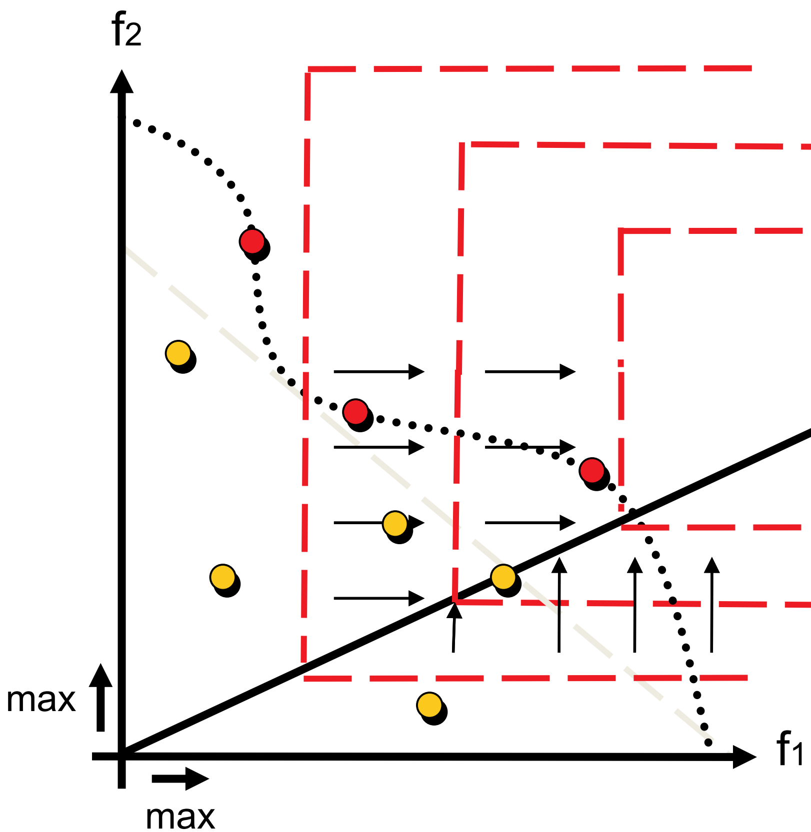
$(\lambda_1, \lambda_2, \ldots, \lambda_k)$

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

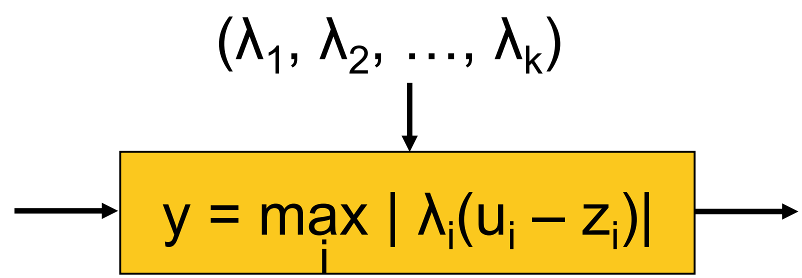
Several other scalarizing functions are known, see e.g. [Miettinen 1999]

Solution-Oriented Problem Transformations





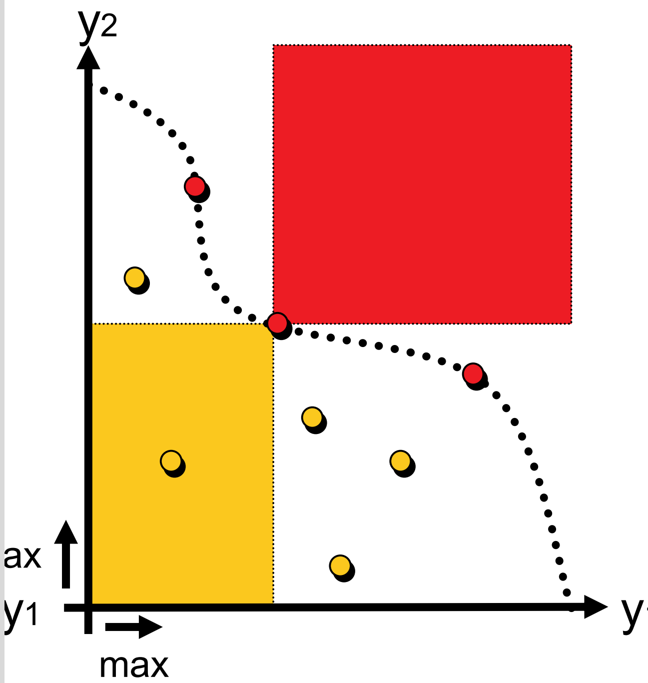
Example 2: weighted Tchebycheff



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

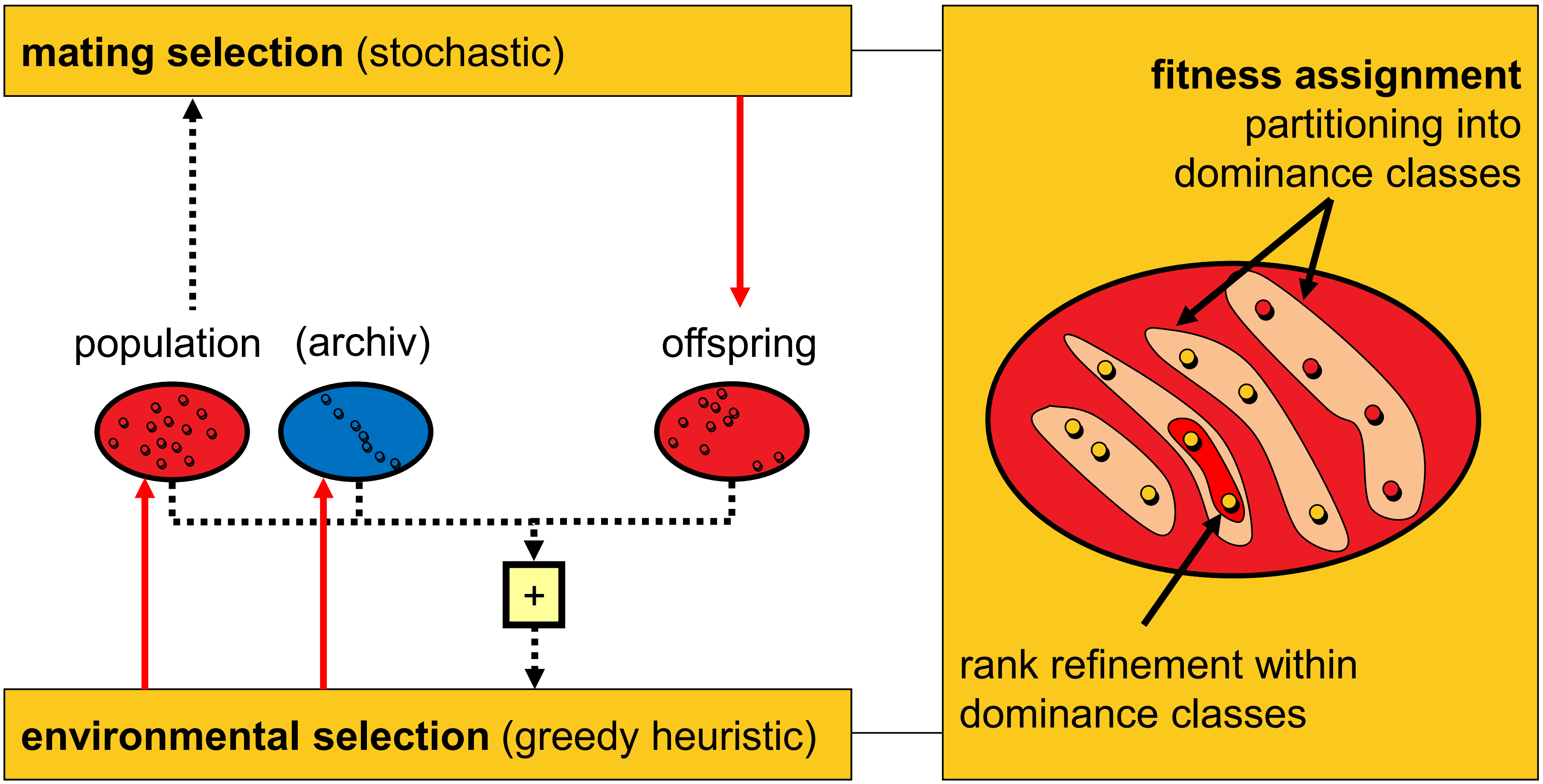
dominance-based

SPEA2, NSGA-II
"modern" EMOA



set-oriented
s scaling-independent

General Scheme of Most Set-Oriented EMO

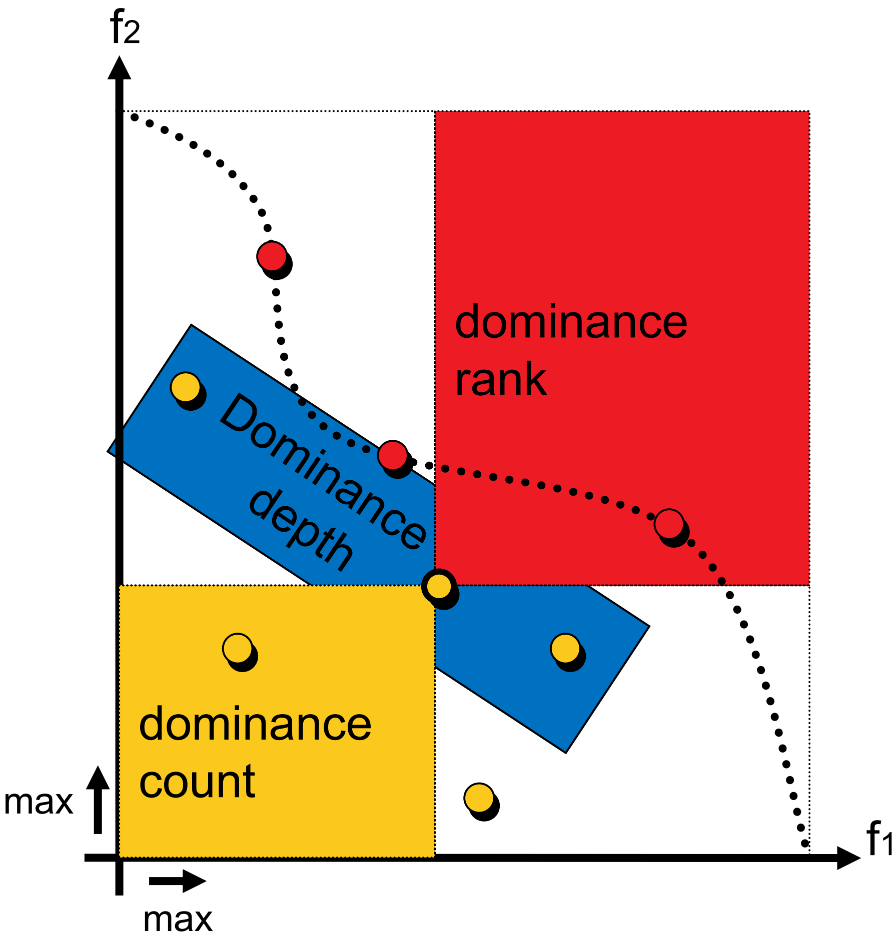


Ranking of the Population Using Dominance

... goes back to a proposal by David Goldberg in 1989.

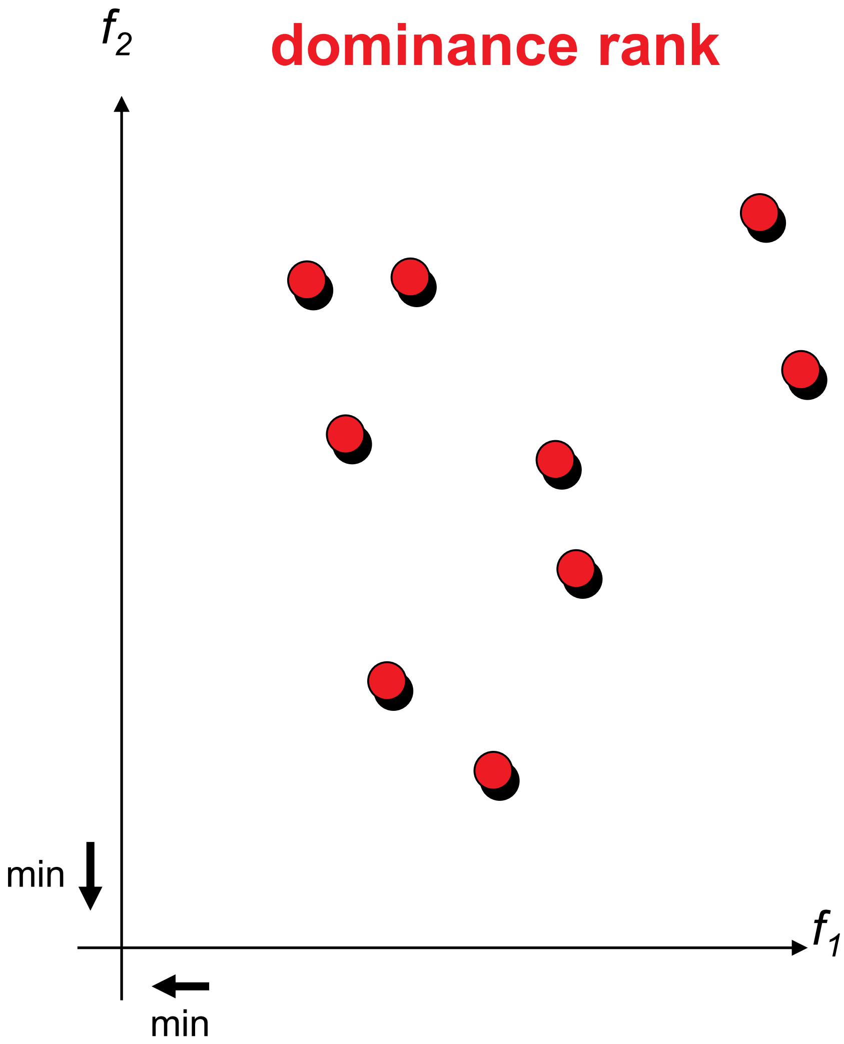
... is based on pairwise comparisons of the individuals only.

- **dominance rank:** by how many individuals is an individual dominated?
  MOGA, NPGA
- **dominance count:** how many individuals does an individual dominate?
  SPEA, SPEA2
- **dominance depth:** at which front is an individual located?
  NSGA, NSGA-II, most of the recently proposed algorithms



Exercise: Dominance-Based Partitioning

dominance rank



dominance depth

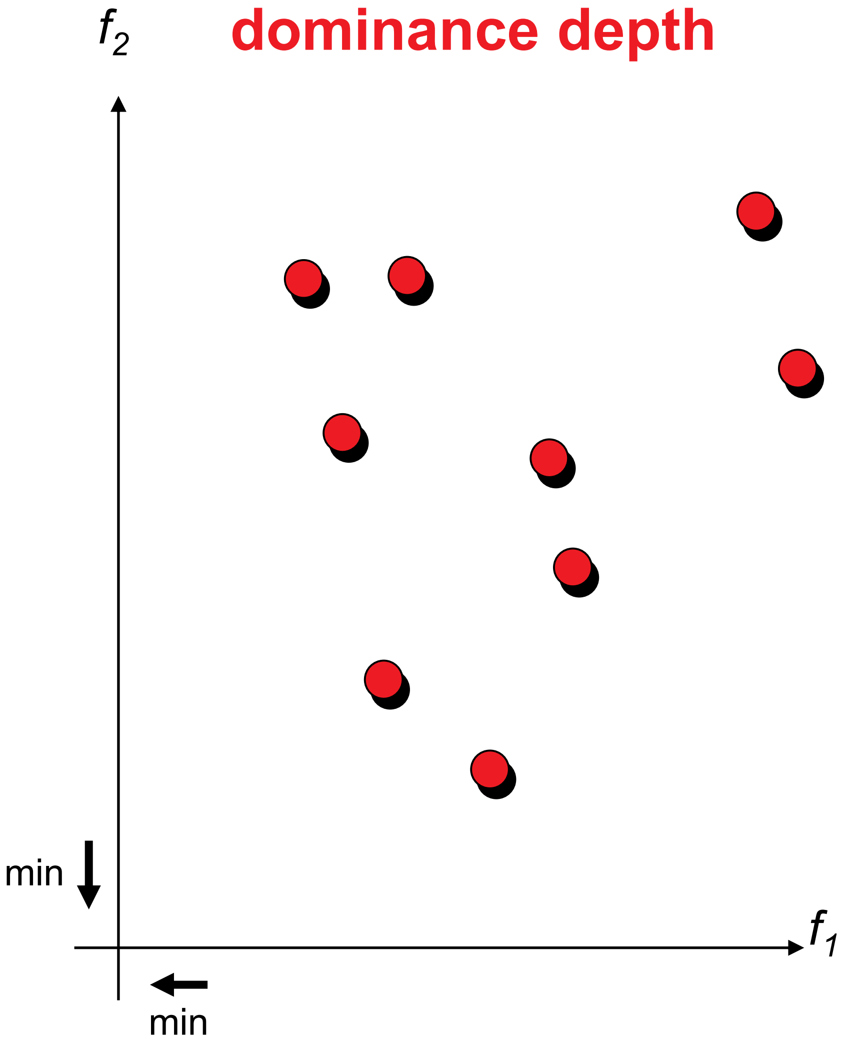
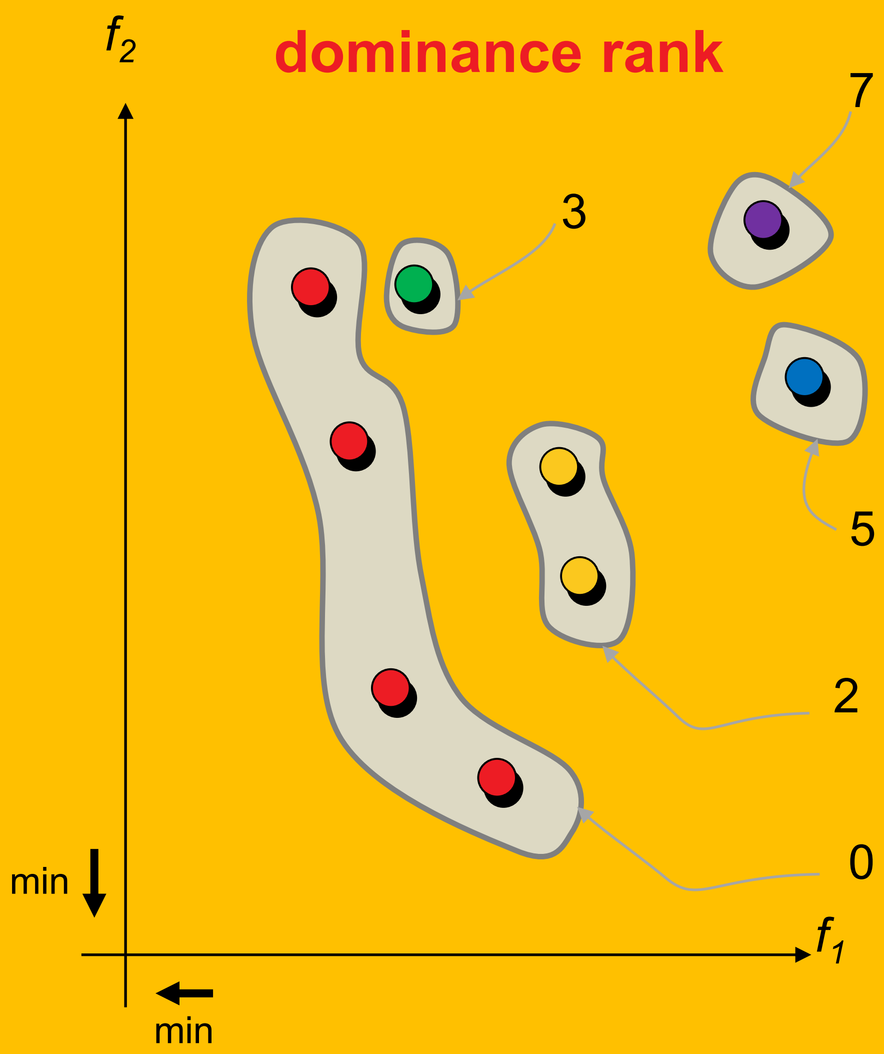
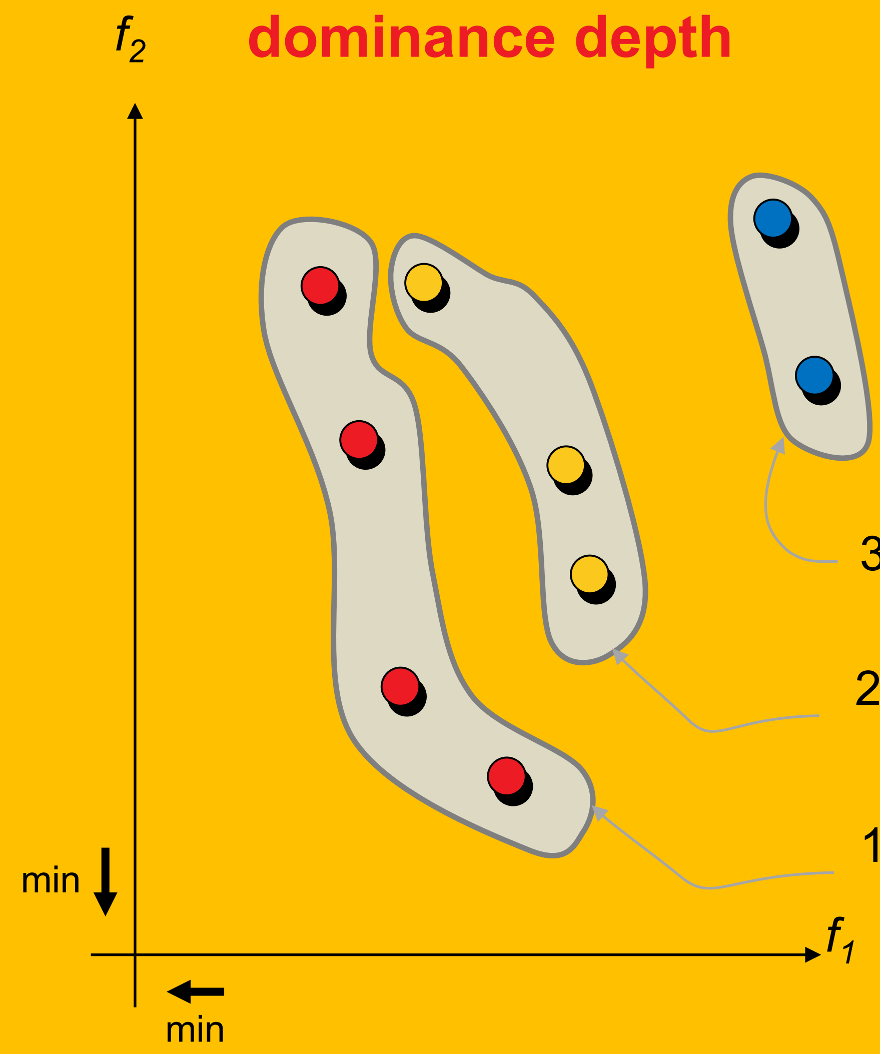


Illustration of Dominance-Based Partitioning





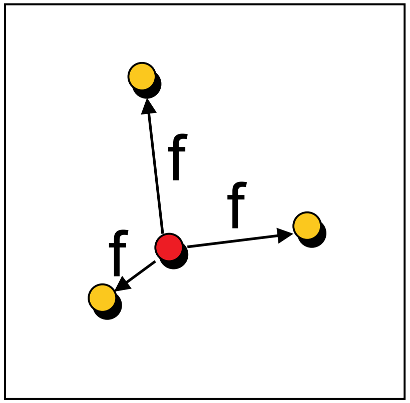
Refinement of Dominance Rankings

Goal: rank incomparable solutions within a dominance class

❶ Diversity information

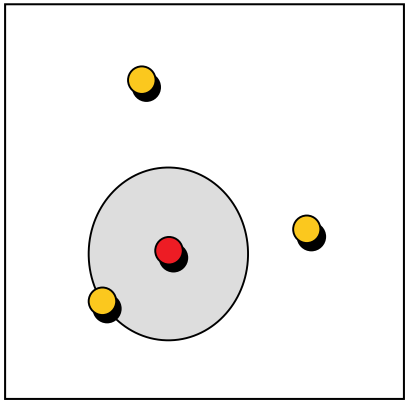
Kernel method

diversity =
function of the
distances



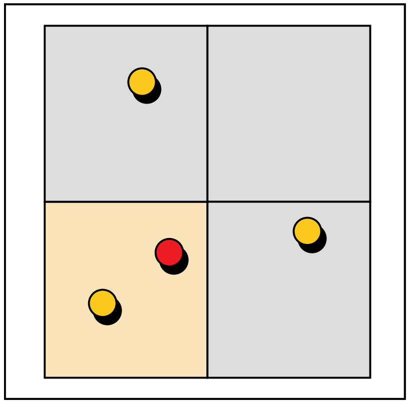
k-th nearest neighbor

diversity =
function of distance
to k-th nearest neighbor



Histogram method

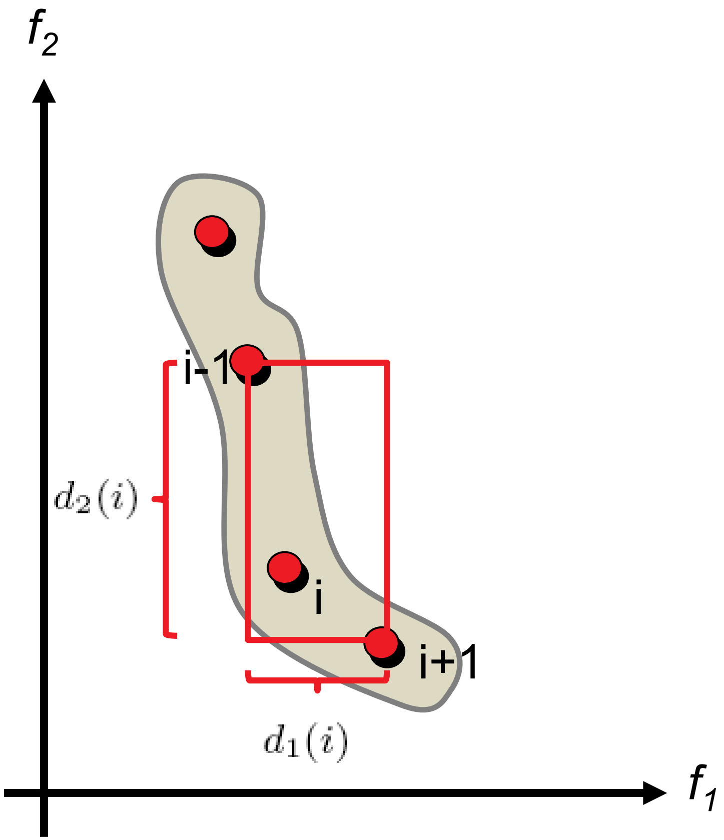
diversity =
number of elements
within box(es)



❷ (Contribution to a) quality indicator

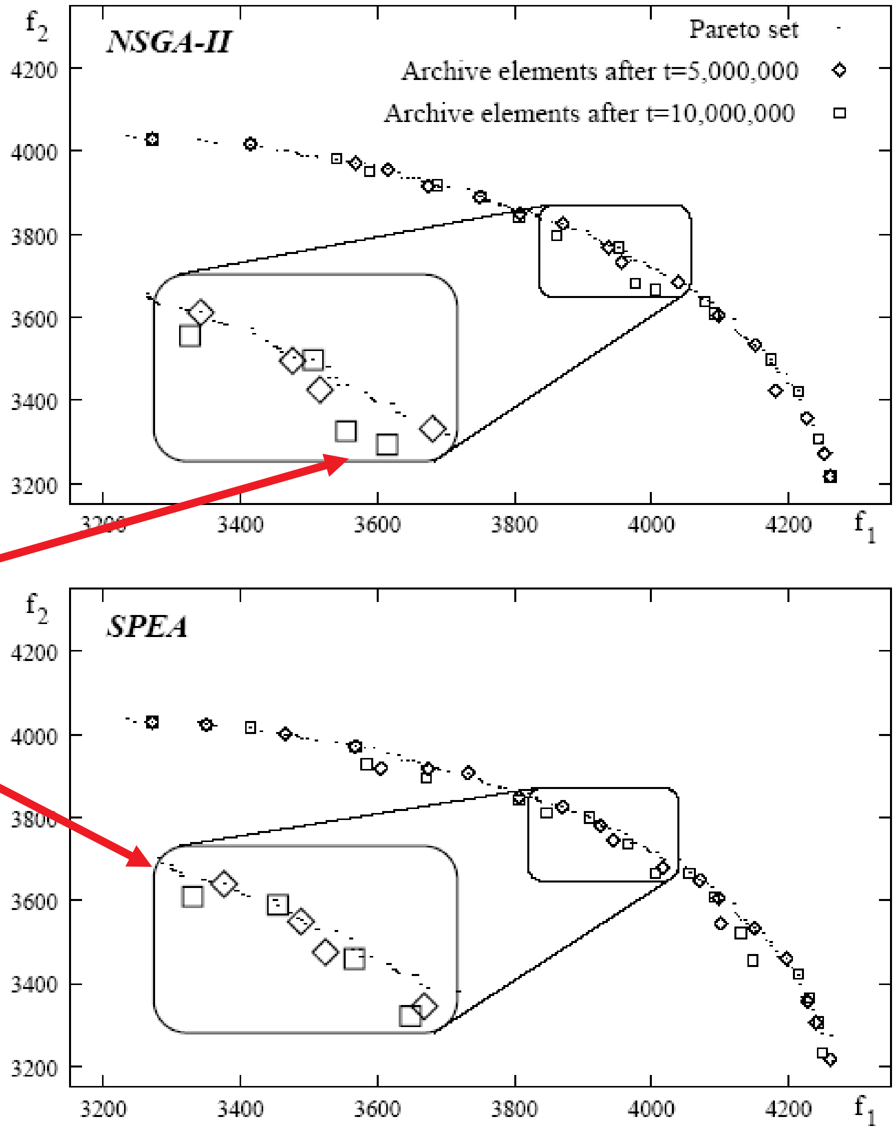
Crowding Distance (CD)

- sort solutions with regard to each objective
- assign CD maximum value to extremal objective vectors
- compute CD based on the distance to the neighbors in each objective



$$\mathrm{CD}(i) = \frac{d_1(i)}{f_{1,\max} - f_{1,\min}} + \cdots + \frac{d_m(i)}{f_{m,\max} - f_{m,\min}}$$

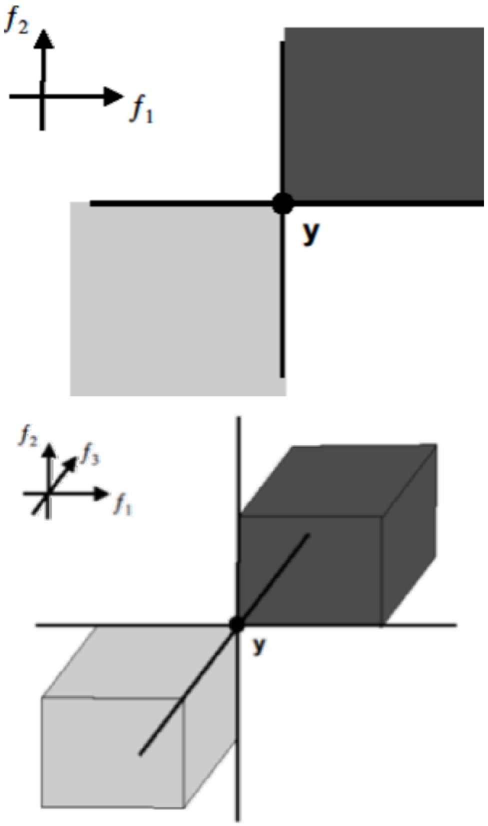
Selection in SPEA2 and NSGA-II can result in *deteriorative* cycles

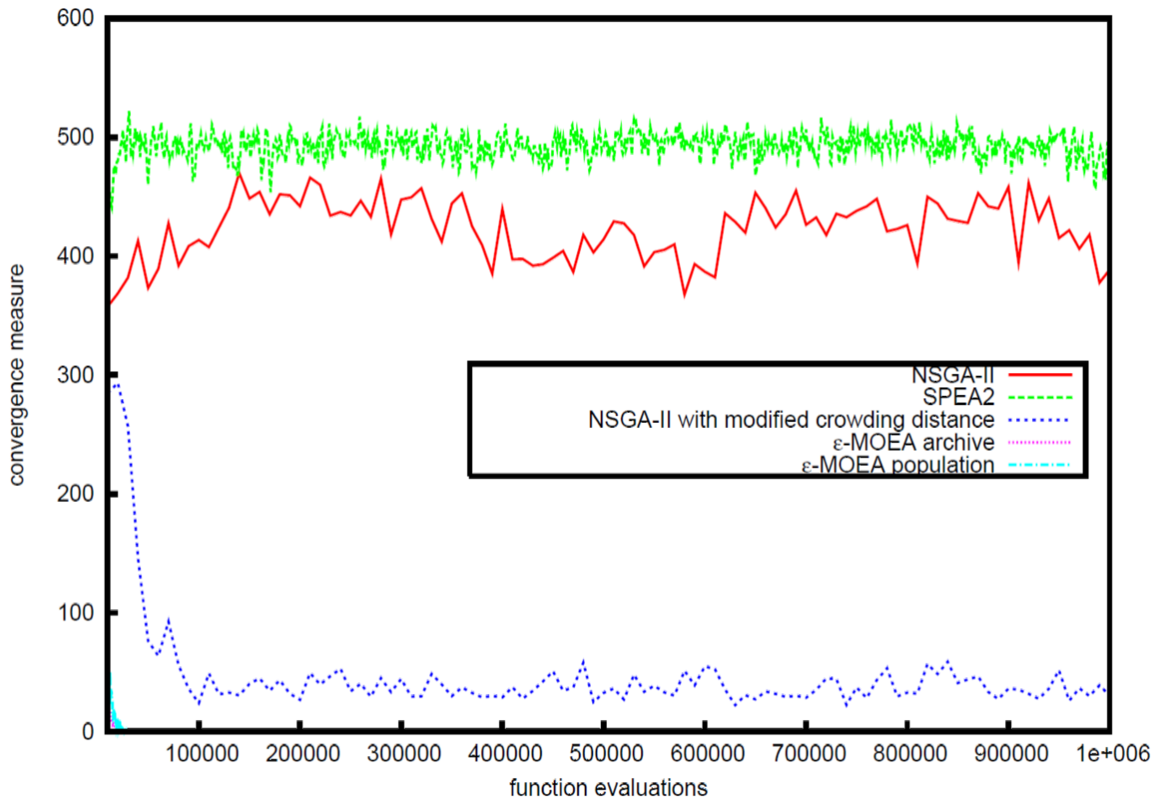


non-dominated solutions already found can be lost

Remark: Many-Objective Optimization

- high number of objectives
  → percentage of non-dominated solutions within a random sample quickly approaches 100 %
  → optimization is mainly guided by diversity criterion
  → apply secondary criterion compliant with dominance relation





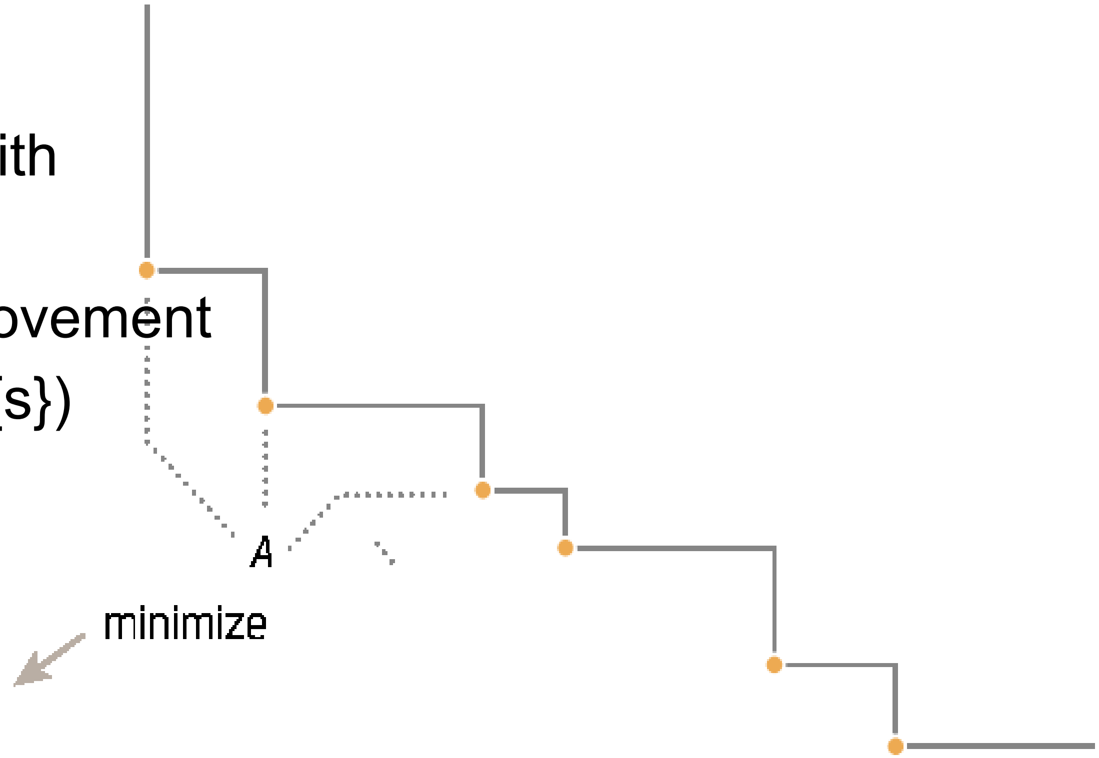
Hypervolume-Based Selection

Latest Approach (SMS-EMOA, MO-CMA-ES, HypE, …)

use hypervolume indicator to guide the search: refines dominance

Main idea

Delete solutions with the smallest hypervolume improvement $d(s) = I_H(P)-I_H(P / \{s\})$ iteratively



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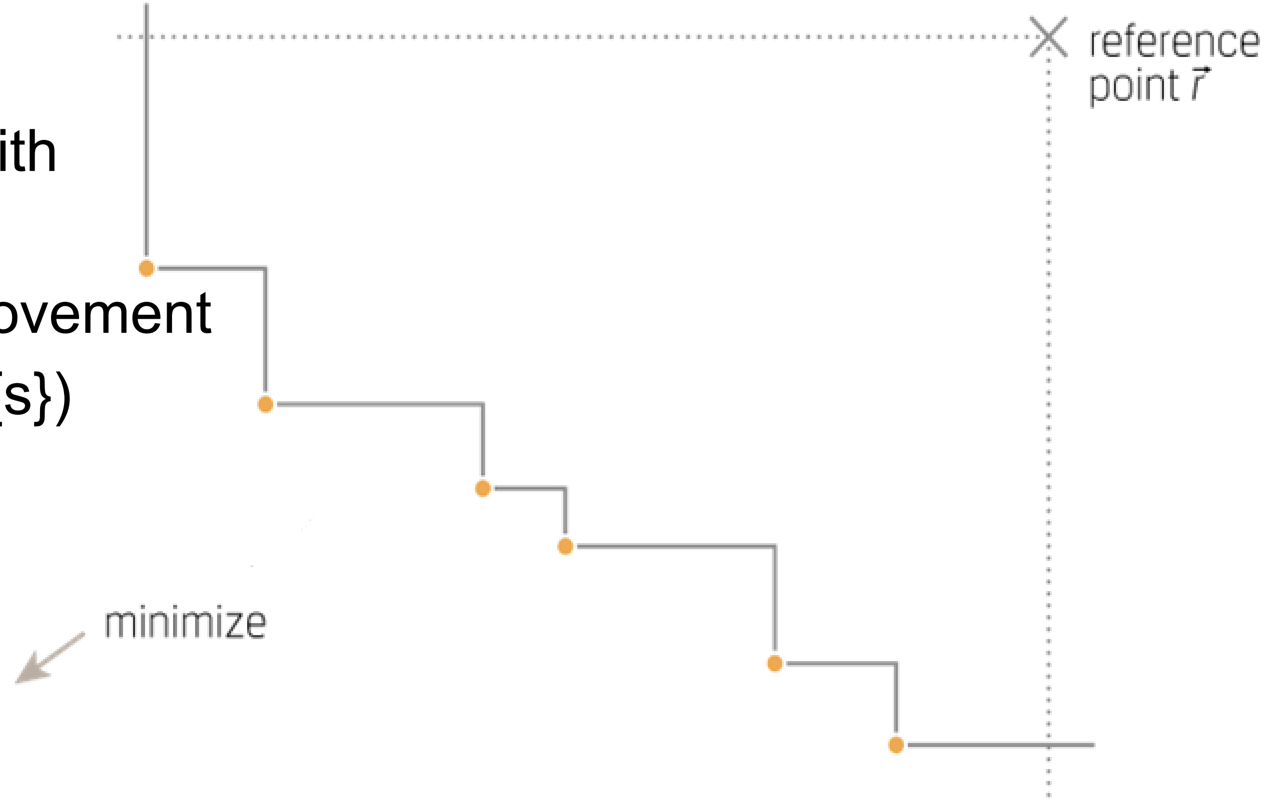

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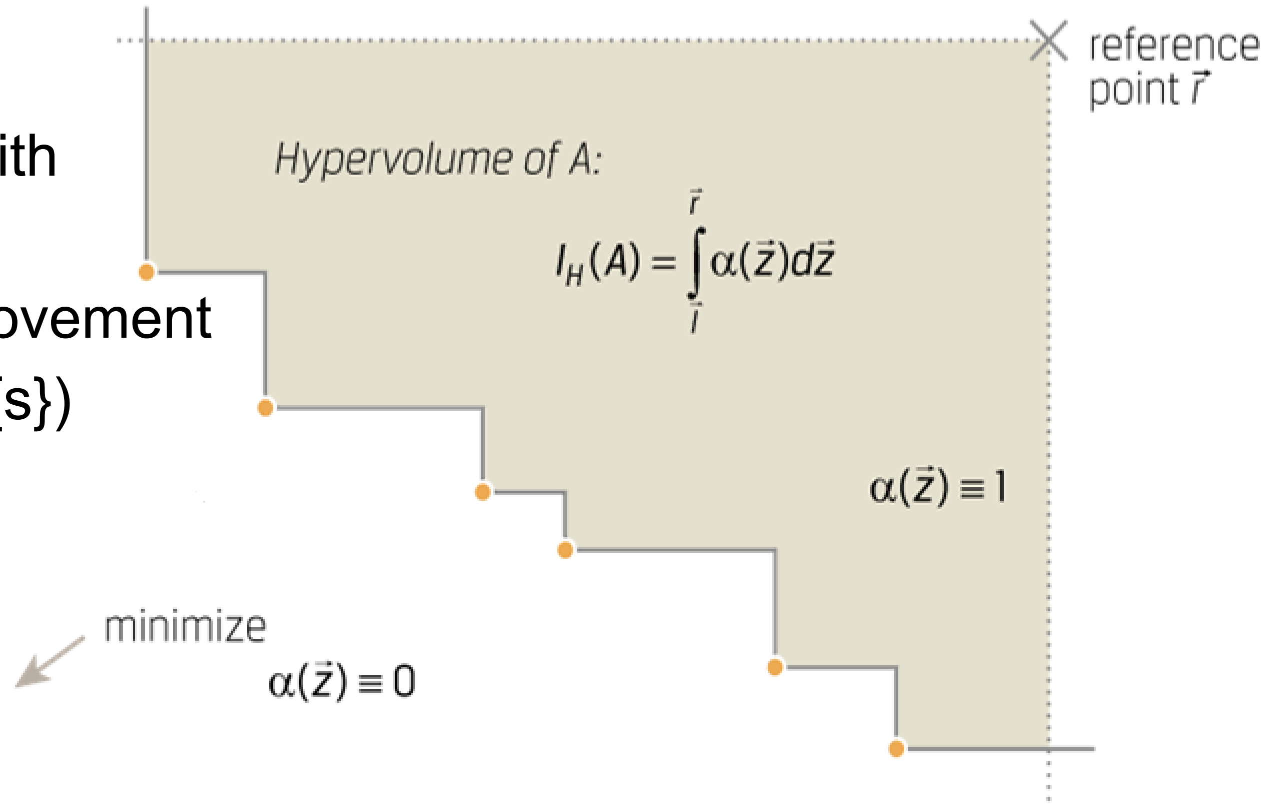

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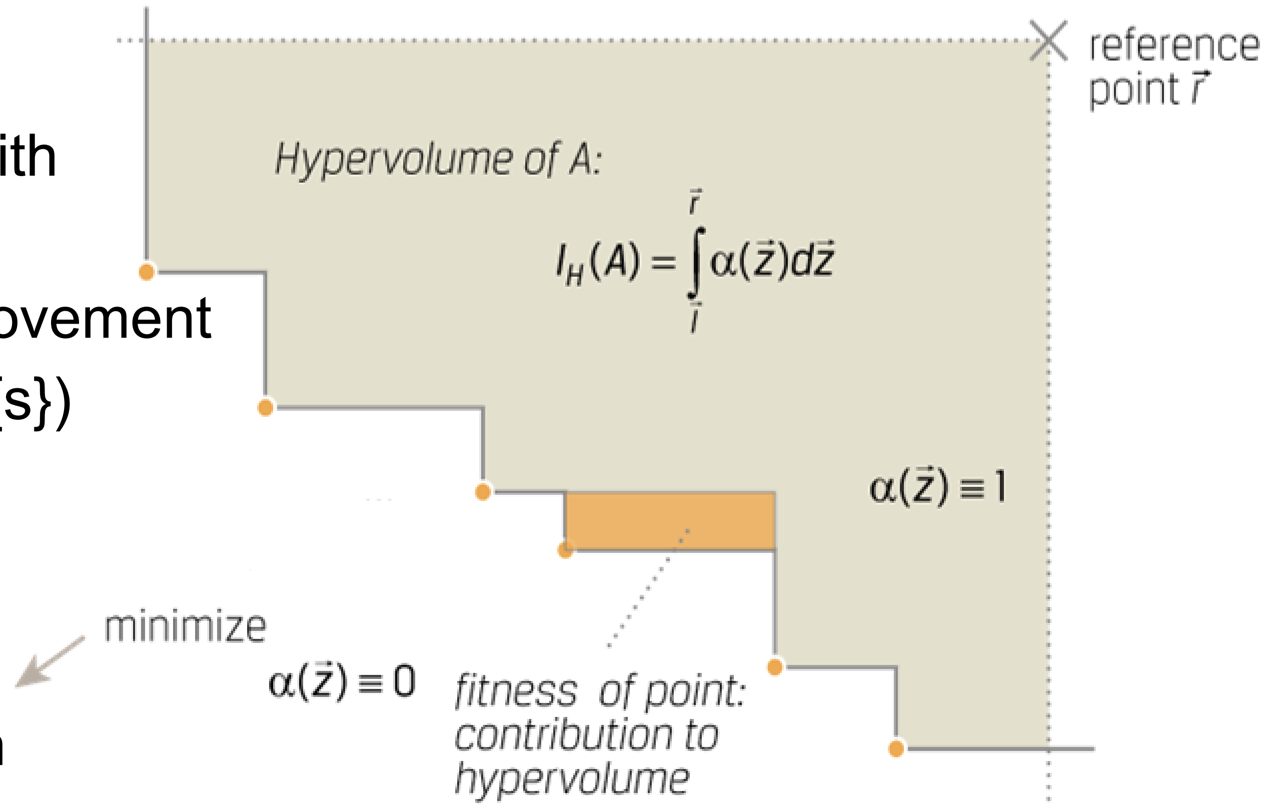
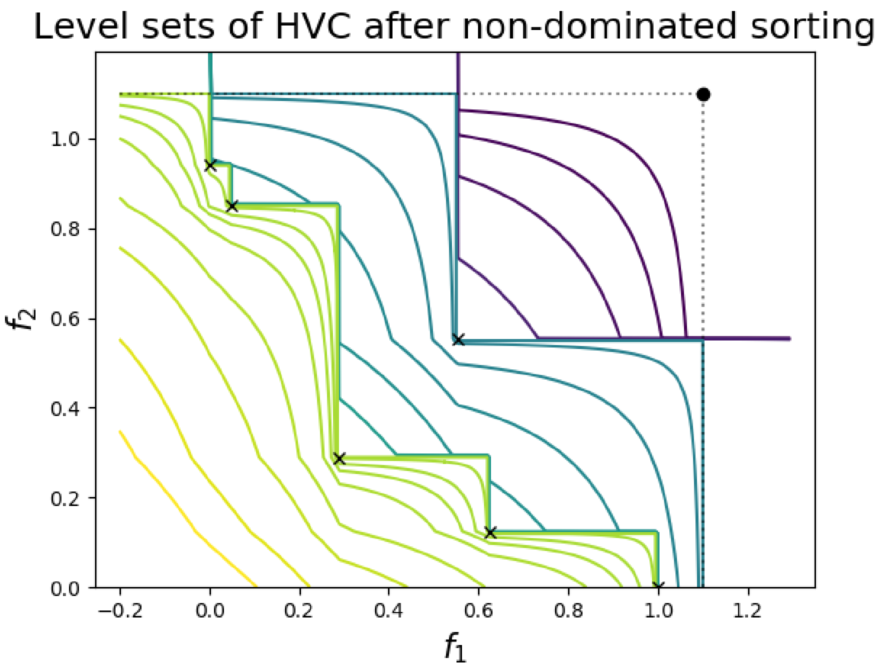
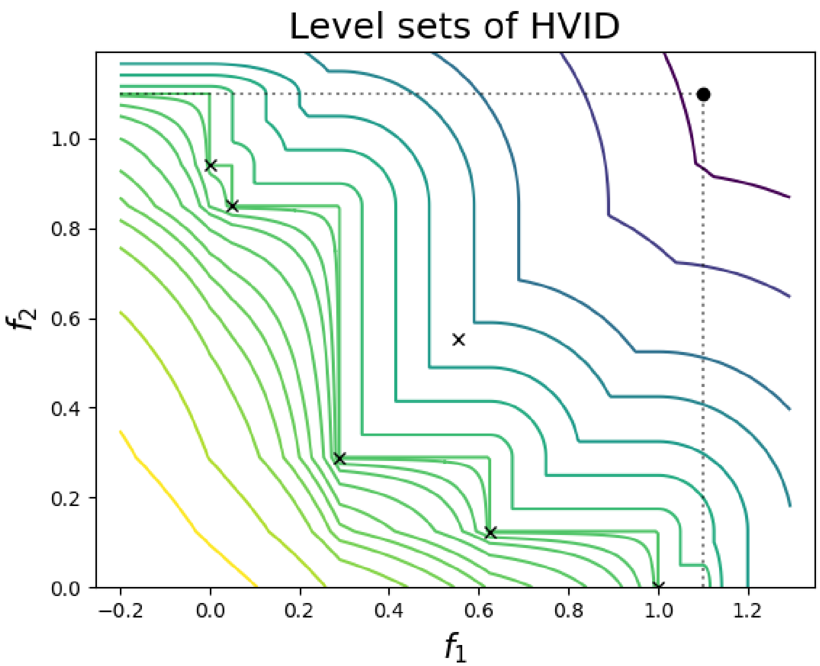


But: can also result in cycles if reference point is not constant [Judt et al. 2011] and is expensive to compute exactly [Bringmann and Friedrich 2009]

COMO-CMA-ES: latest multiobjective CMA-ES version

- p single-objective CMA-ESs optimize their hypervolume improvement to the other p-1 CMA-ES means
- for this to work, a slightly modified hypervolume improvement, the UHVI has been introduced





- Source code available at https://github.com/CMA-ES/pycomocma

Indicator-Based Selection

- Concept can be generalized to any quality indicator

A (unary) quality indicator I is a function $I : \Psi = 2^X \mapsto \mathbb{R}$ that assigns a Pareto set approximation a real value.

$$\text{Multiobjective Problem} \xrightarrow{\text{Indicator}} \text{Single-objective Problem}$$

- for example: R2-indicator [Brockhoff et al. 2012], [Trautmann et al. 2013], [Díaz-Manríquez et al. 2013]

- Generalizable also to contribution to larger sets

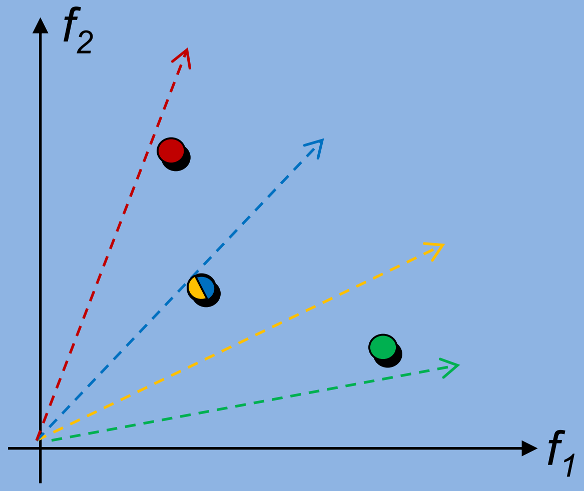
  HypE [Bader and Zitzler 2011]: Hypervolume sampling + contribution if more than 1 (random) solution deleted

Decomposition-Based Selection: MOEA/D

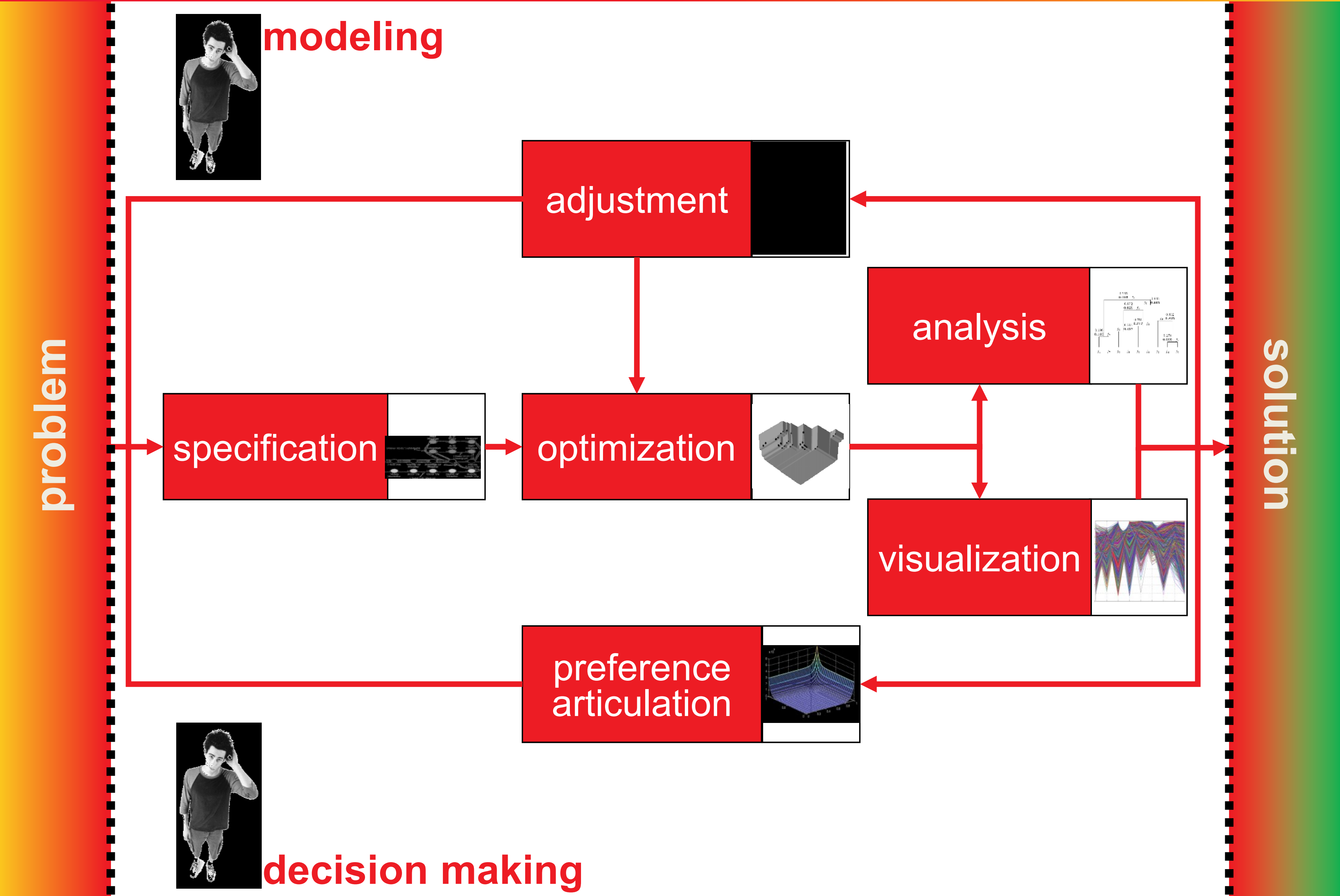
MOEA/D: Multiobjective Evolutionary Algorithm Based on Decomposition [Zhang and Li 2007]

Ideas:

- optimize N scalarizing functions in parallel
- use best solutions of neighbor subproblems for mating
- keep the best solution for each scalarizing function
- update neighbors
- use external archive for non-dominated solutions
- several variants and enhancements



Conclusions: EMO as Interactive Decision Support



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