Derivative-Free Optimization

(Evolutionary) Multiobjective Optimization

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Overview of the Today's Lecture

Introduction to multiobjective optimization

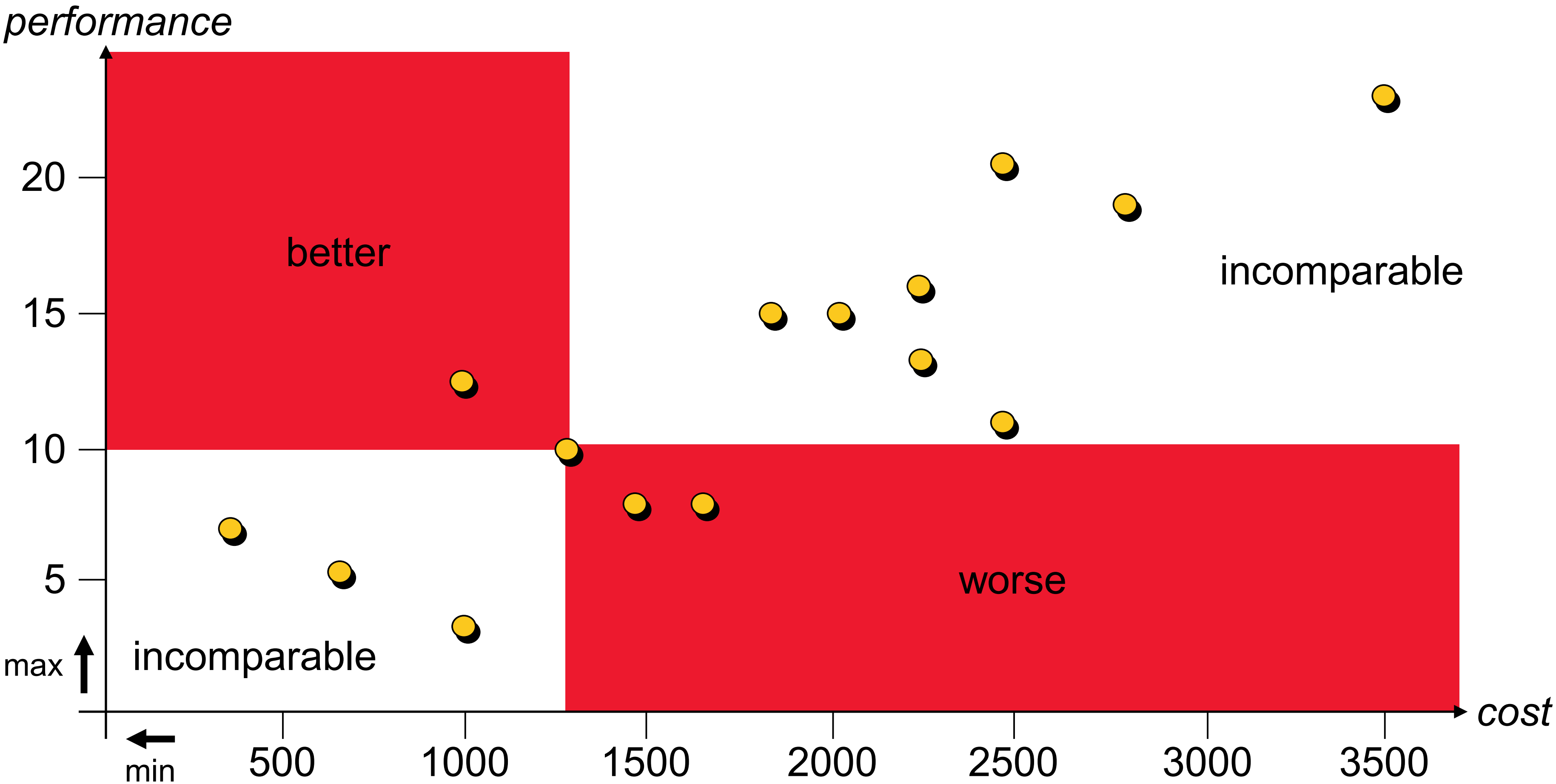
- difference to single-objective optimization, the basics
- algorithms and their design principles

introductory material (for example):

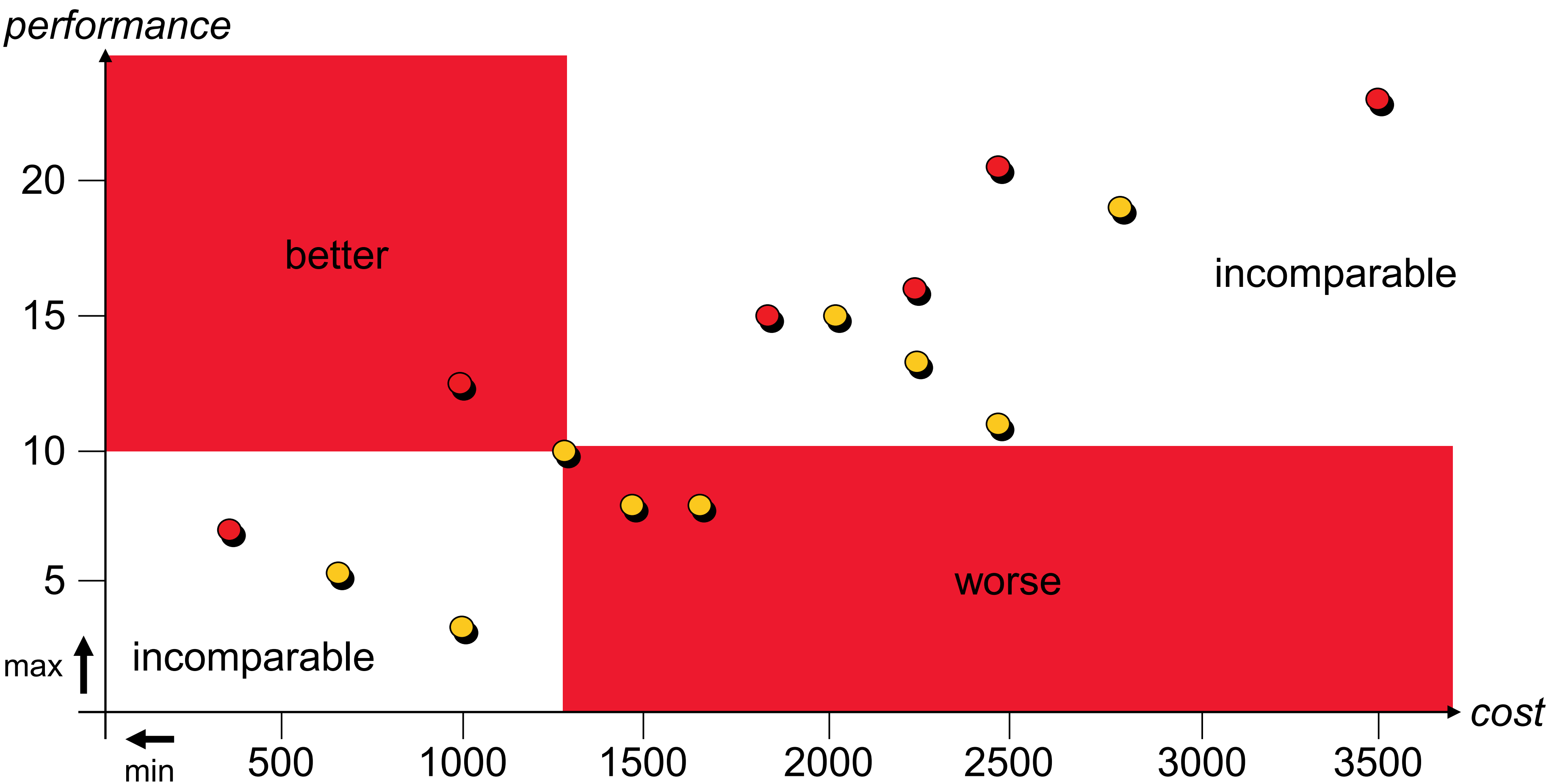
- P.J. Fleming*, R.C. Purshouse : Evolutionary algorithms in control systems engineering: a survey (sections 1&2 only)
- K. Deb: Introduction to Evolutionary Multiobjective Optimization, chapter 3 of J. Branke, K. Deb, K. Miettinen, R. Słowinski (Eds.): Multiobjective Optimization --- Interactive and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

Multiobjective Optimization

Multiple objectives that have to be optimized simultaneously



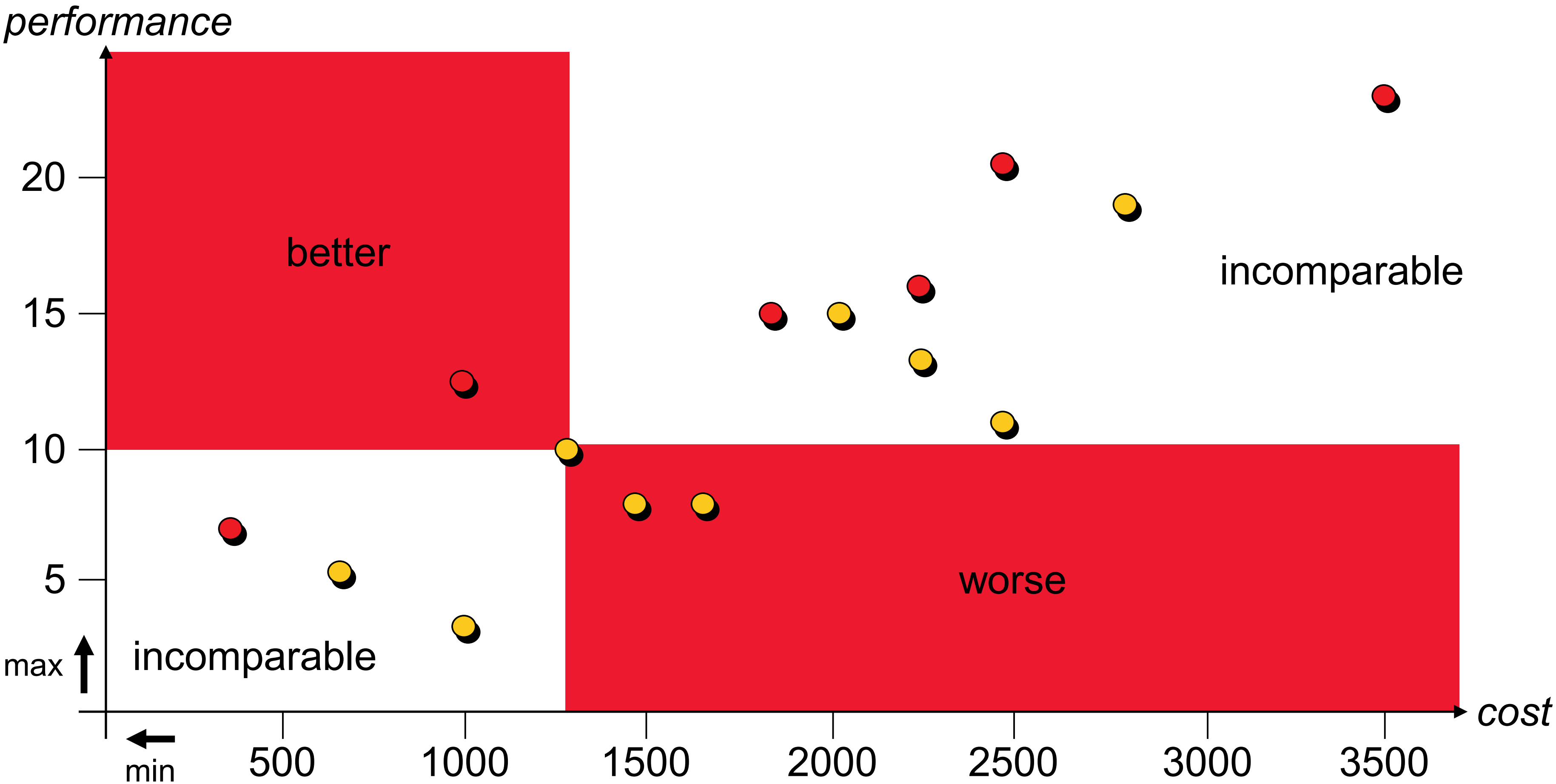
Observations: ❶ there is no single optimal solution, but
❷ some solutions (●) are better than others (●)



A Brief Introduction to Multiobjective Optimization

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

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



A Brief Introduction to Multiobjective Optimization

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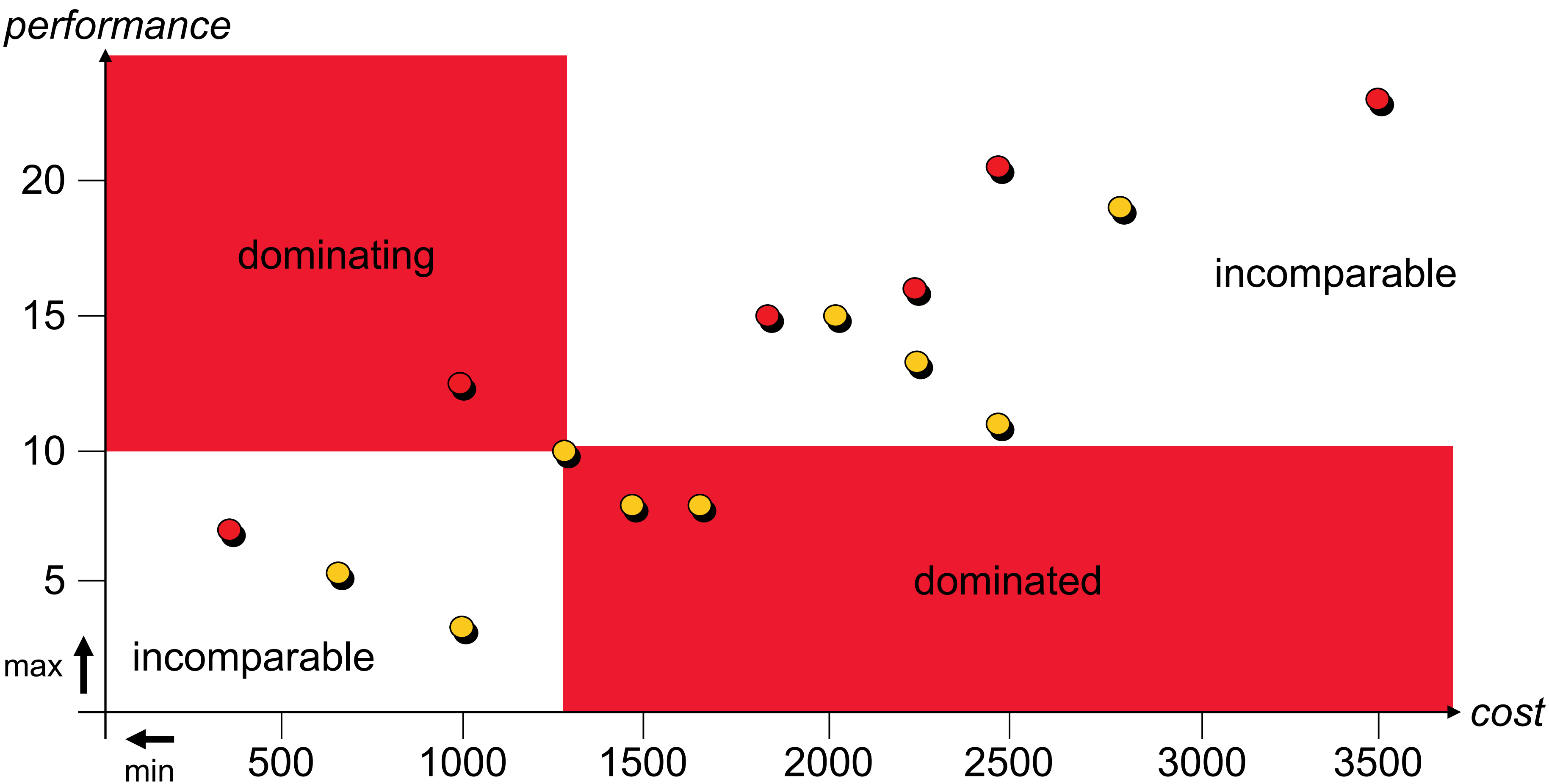


Exercise: Understanding Pareto Dominance

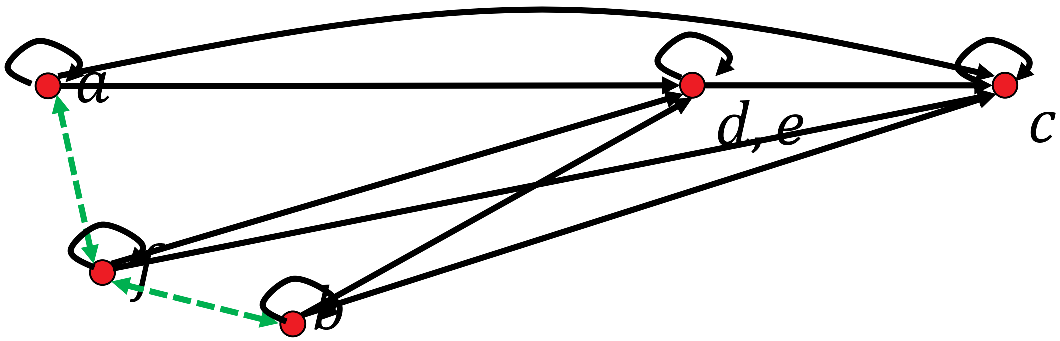
Given the following solutions, tell which ones dominate each other and which don't for the double sphere (minimization) problem

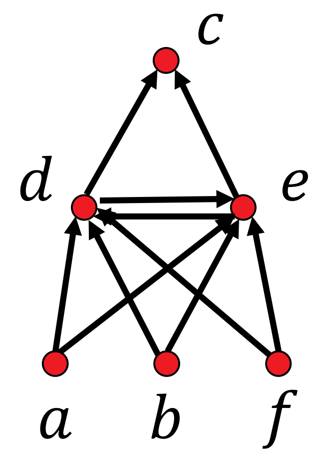
$$f_{\text{doublesphere}}: x \mapsto \left(\sum_{i=1}^{n} x_i^2 \,,\, \sum_{i=1}^{n} (x_i - 1)^2\right).$$

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

Visualizing Dominance Relations as Graphs

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





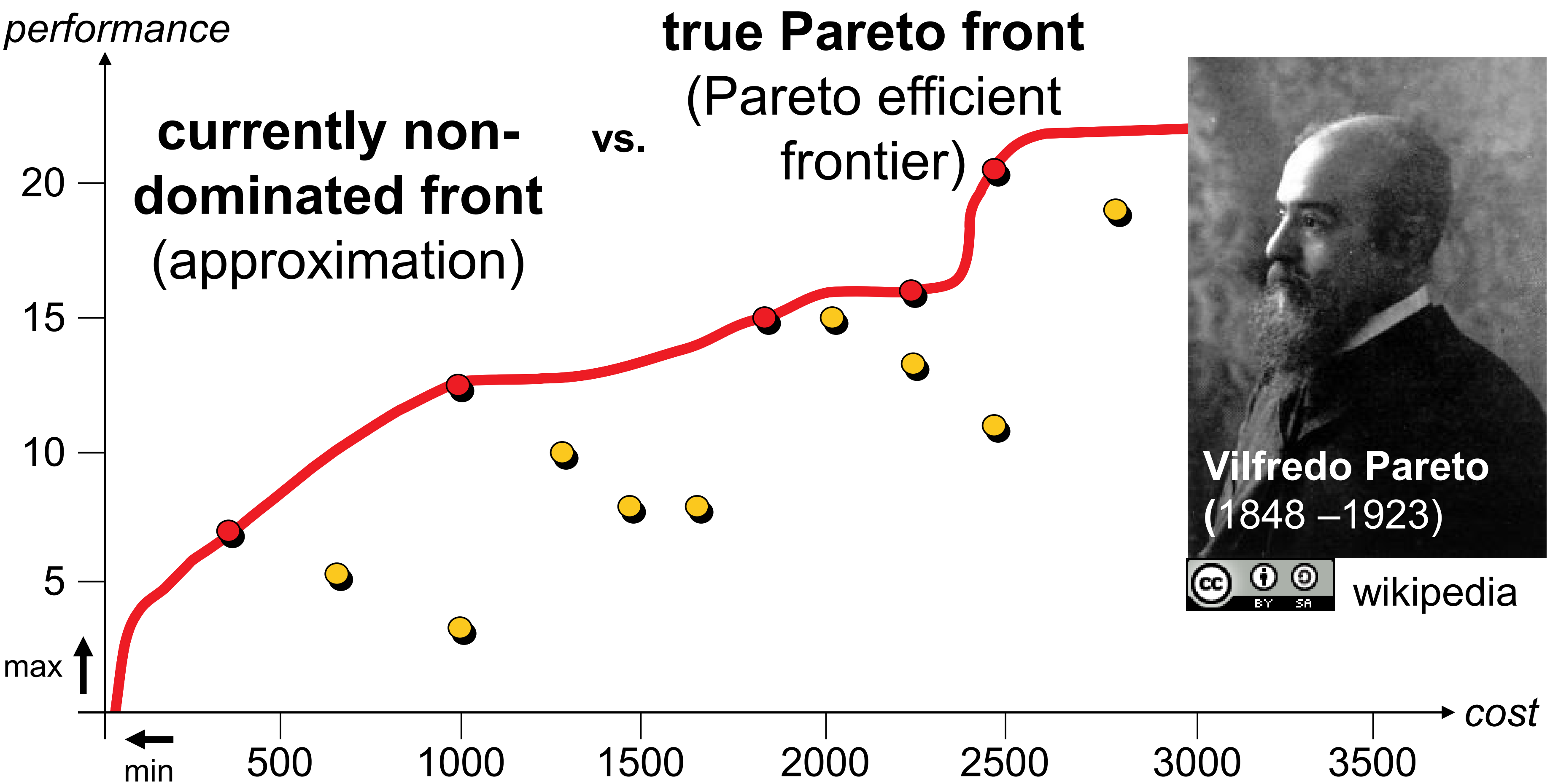
The weak Pareto dominance is a preorder, i.e. a relation that is

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

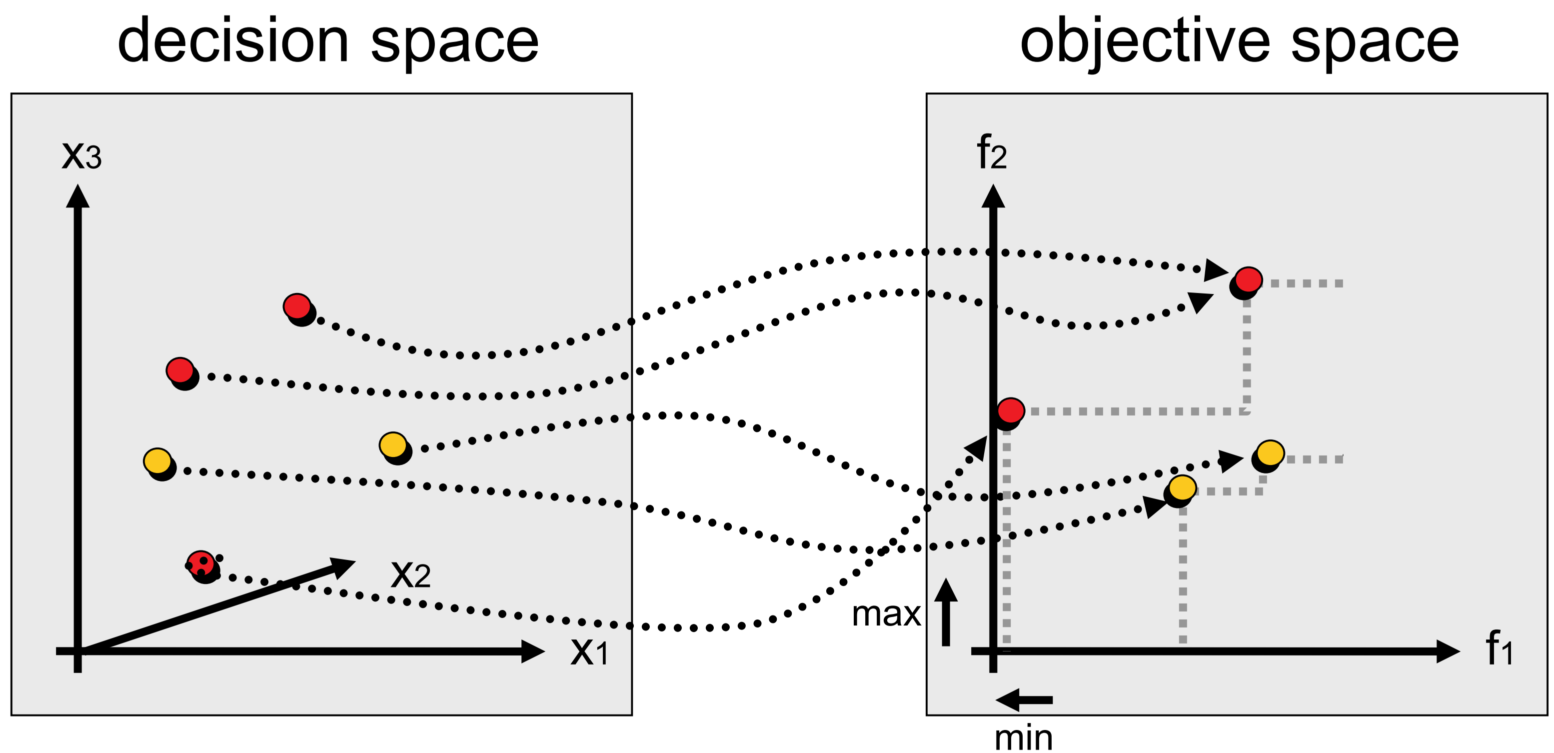
If no *indifferent* solutions $x \neq y$ with $f(x) = f(y)$ exist, we have antisymmetry and a partial order ("poset")---visualizable as Hasse diagram.

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

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

a) what is the Pareto set?

b) what is the associated Pareto front?

Tips:

- 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)

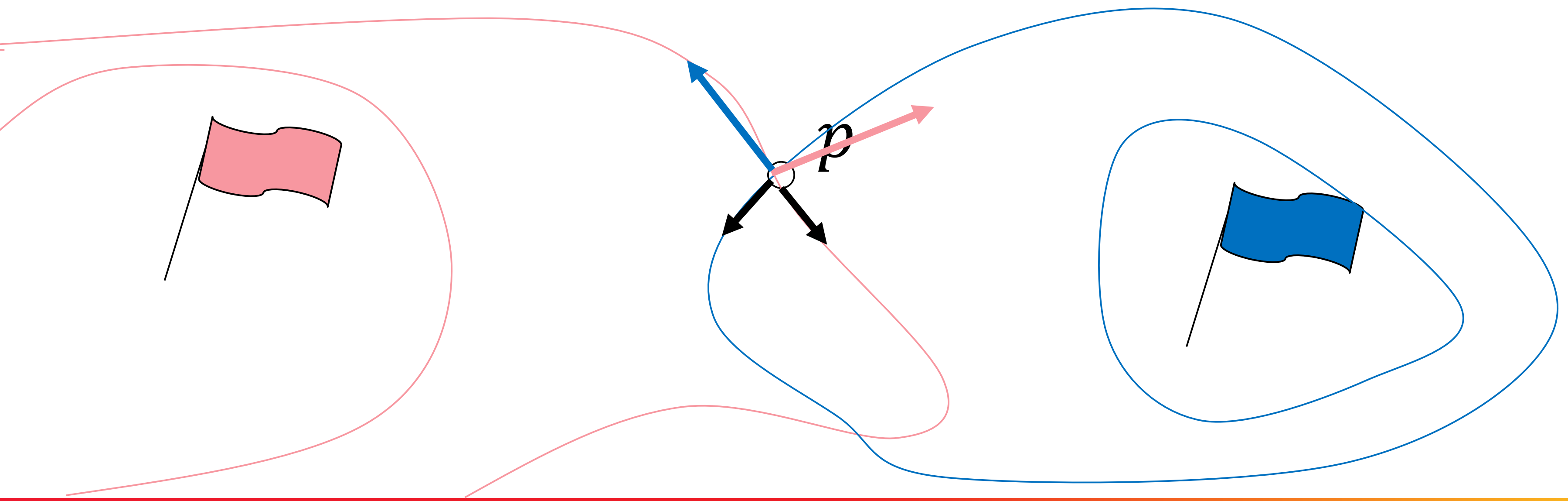
Necessary Condition:

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

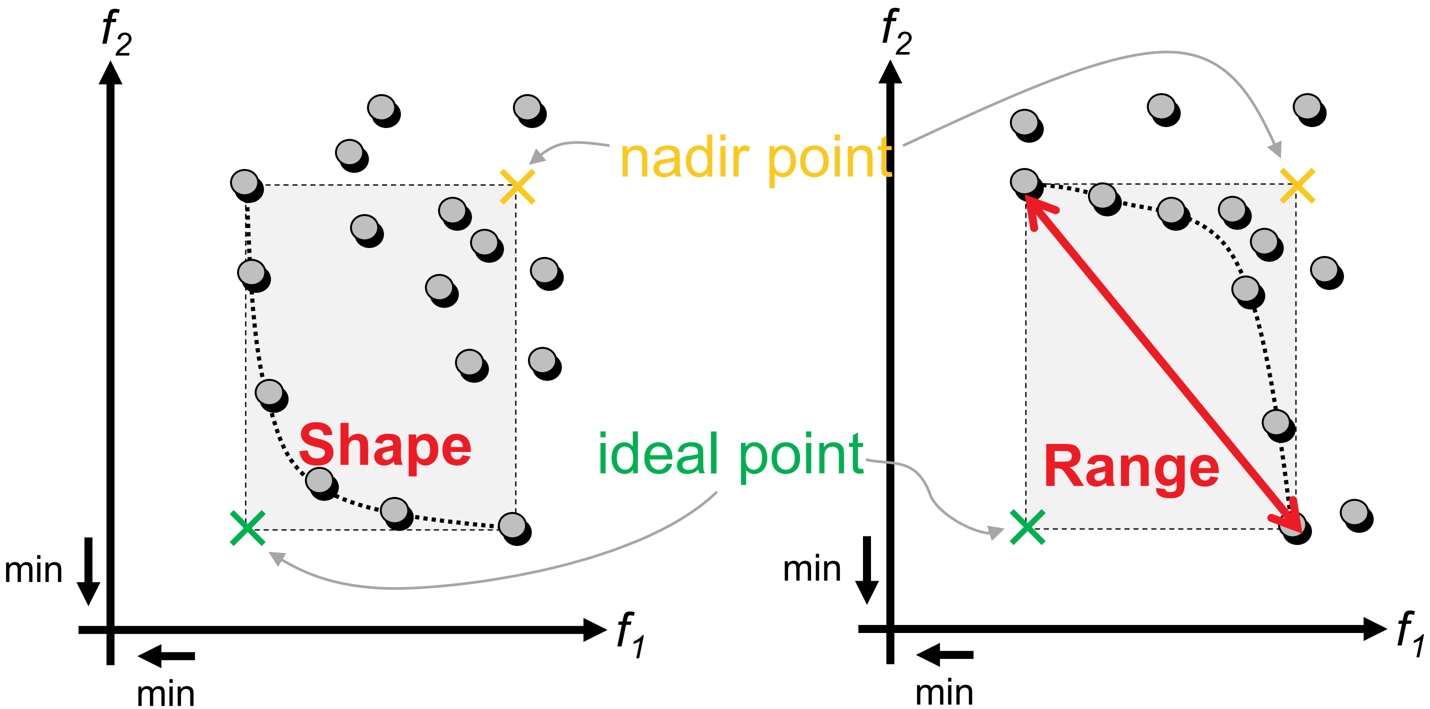
(Visual) Reasoning:

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



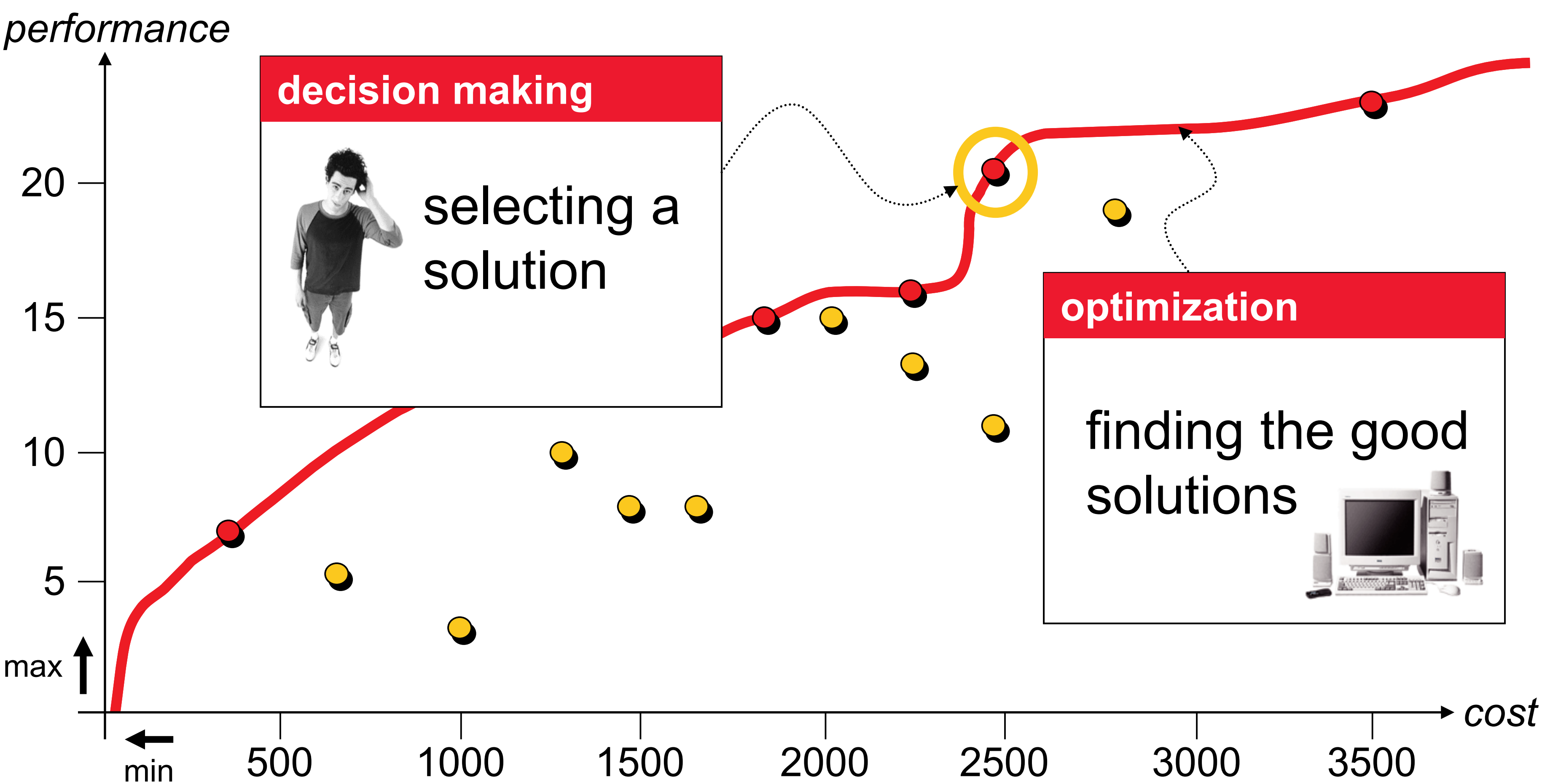
ideal point: best values
nadir point: worst values

} obtained for *Pareto-optimal* points

Optimization vs. Decision Making

Multiobjective Optimization

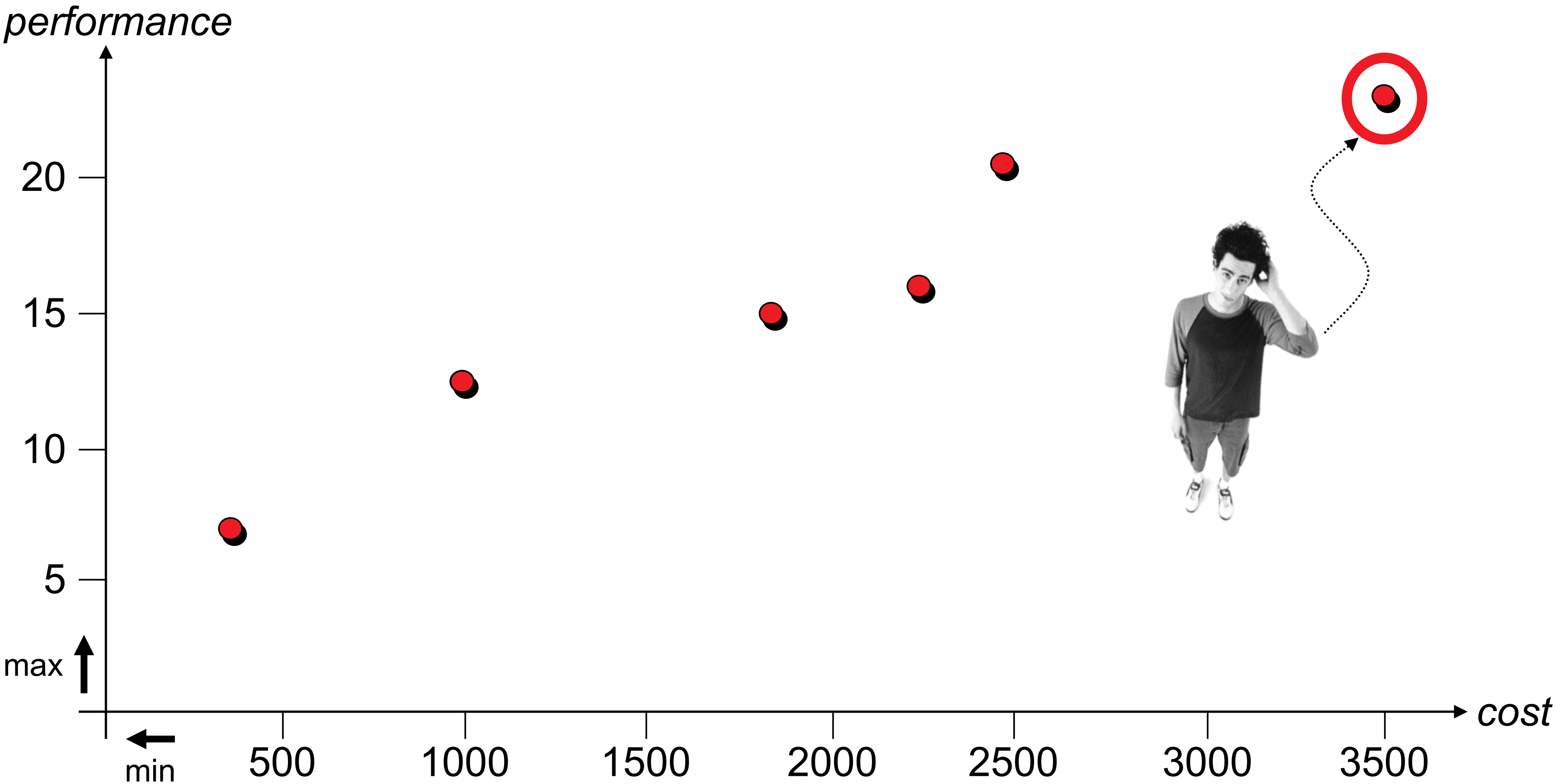
combination of optimization of a set and a decision for a solution



Selecting a Solution: Examples

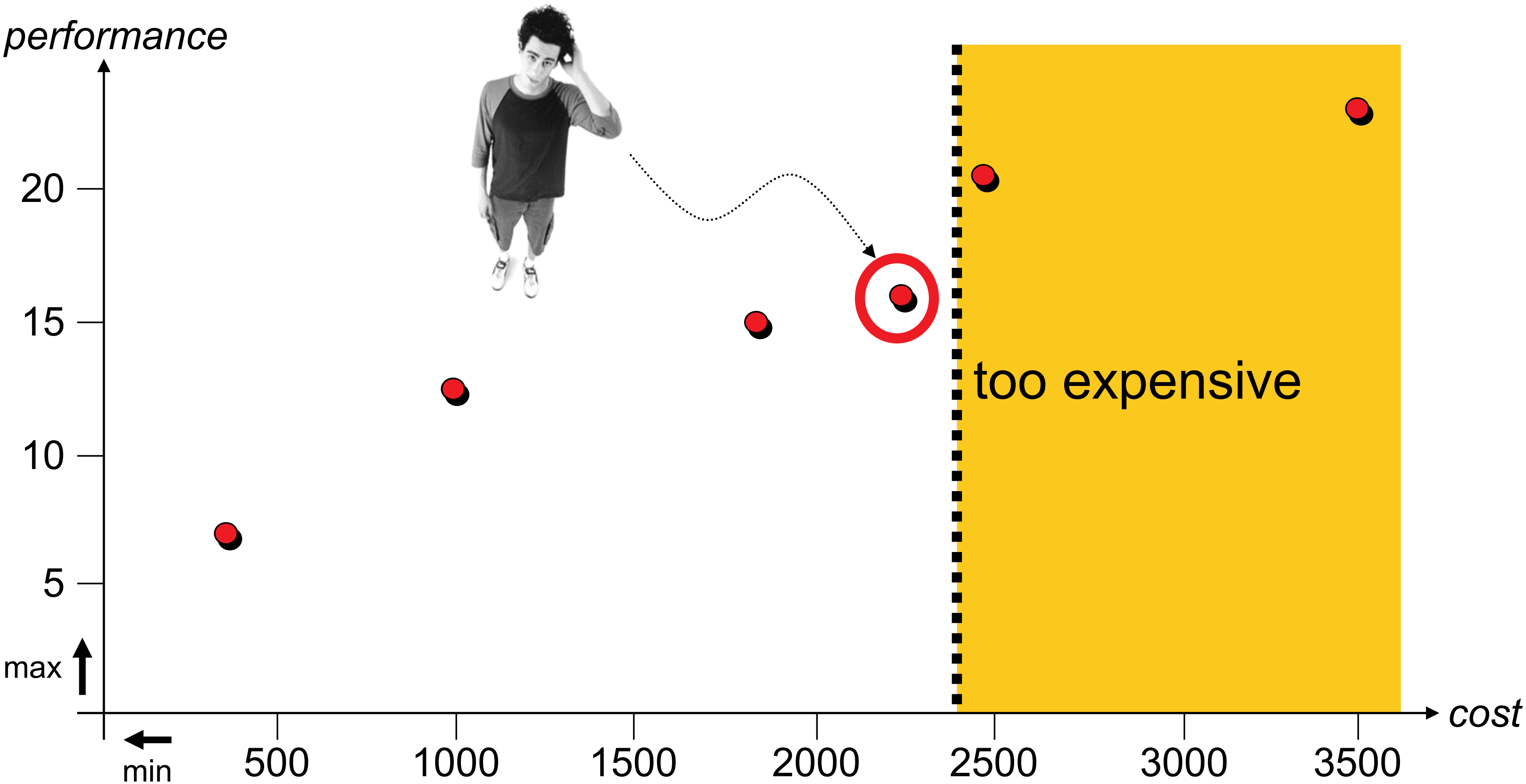
Possible Approaches:

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



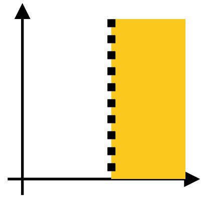
Selecting a Solution: Examples

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



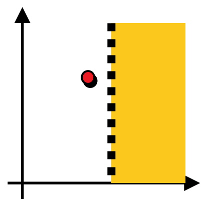
When to Make the Decision

Before Optimization:



rank objectives,
define constraints,…

search for one
(good) solution



When to Make the Decision

Before Optimization:

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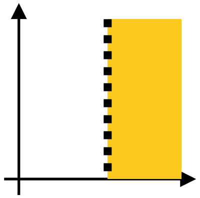

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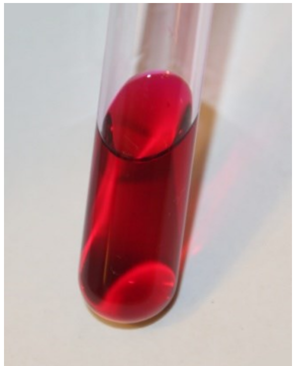

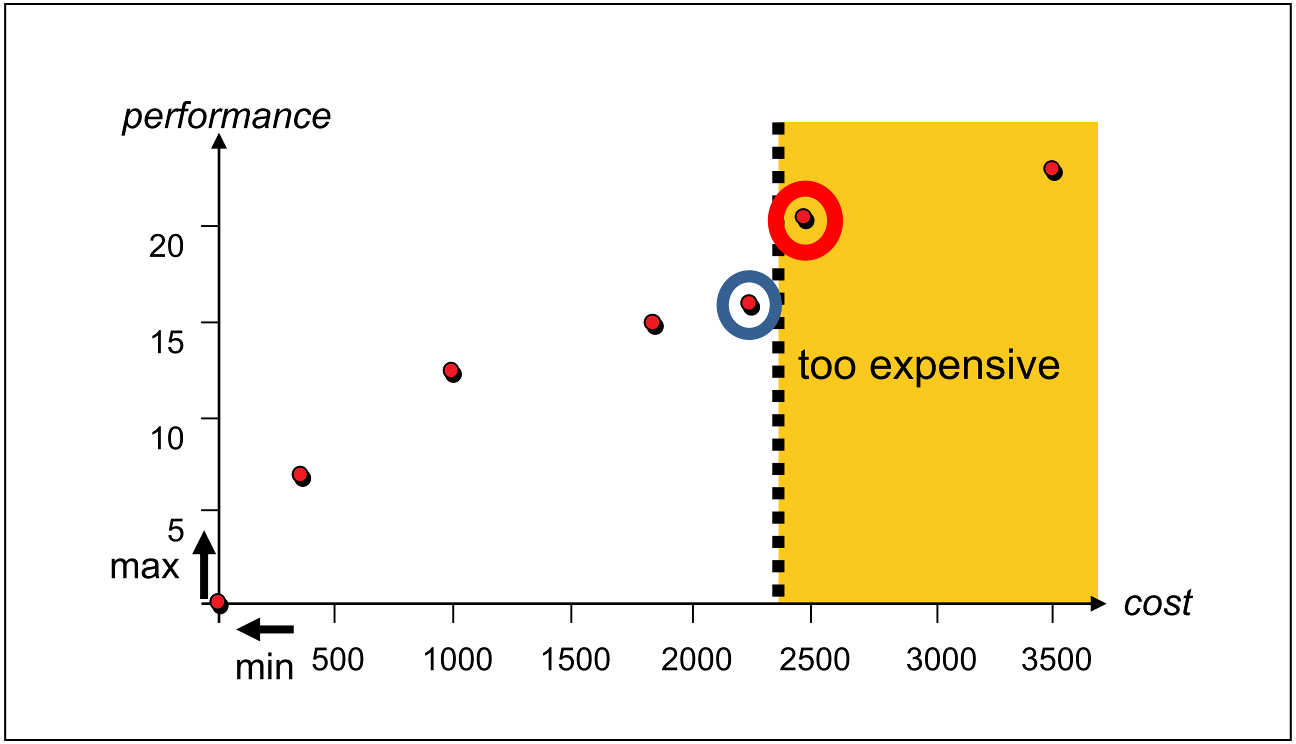

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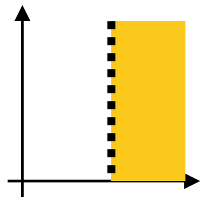

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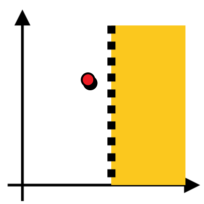
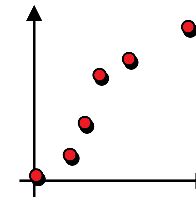
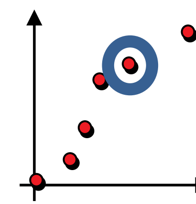


After Optimization:

search for a set of
(good) solutions



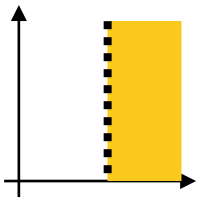
select one solution
considering
constraints, etc.



When to Make the Decision

Before Optimization:

rank objectives,
define constraints,…



search for one
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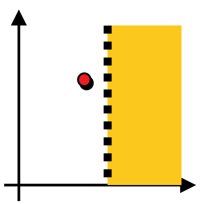

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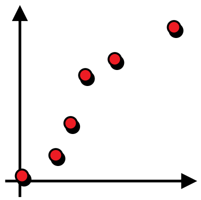

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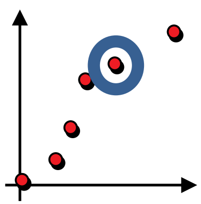


Focus: learning about a problem

- 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

- 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

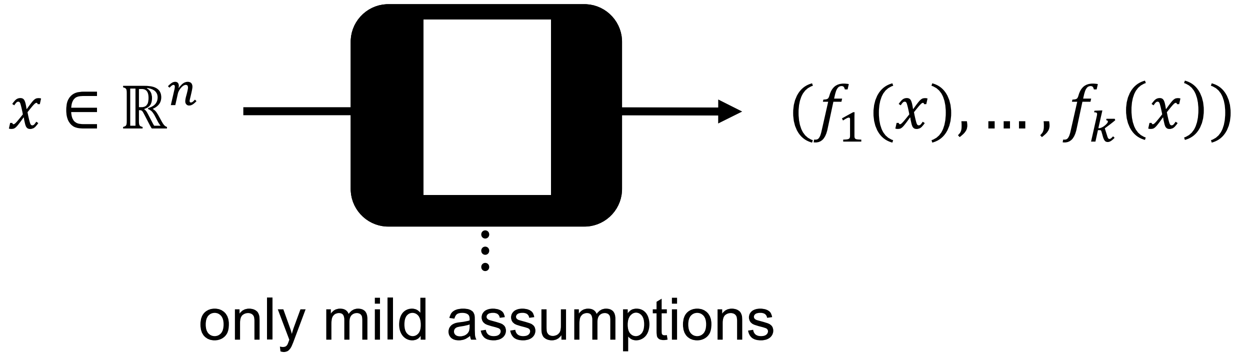
...Slowly Merge Into One

MCDM International Society on Multiple Criteria Decision Making

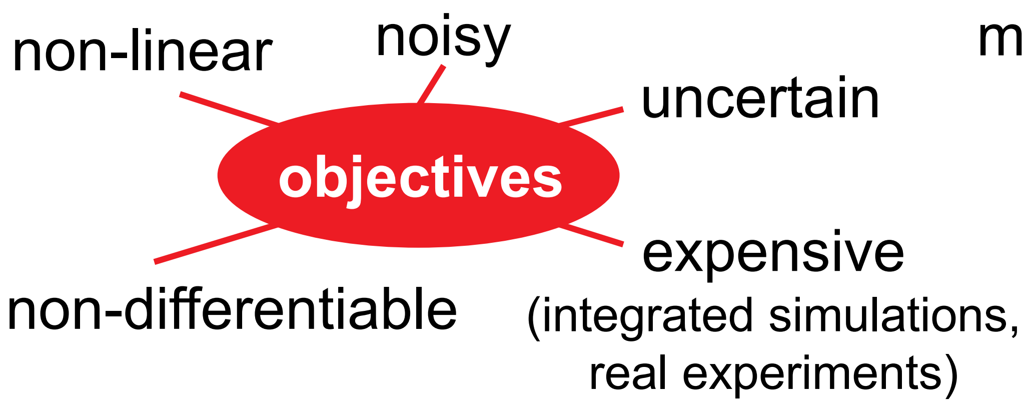
emo

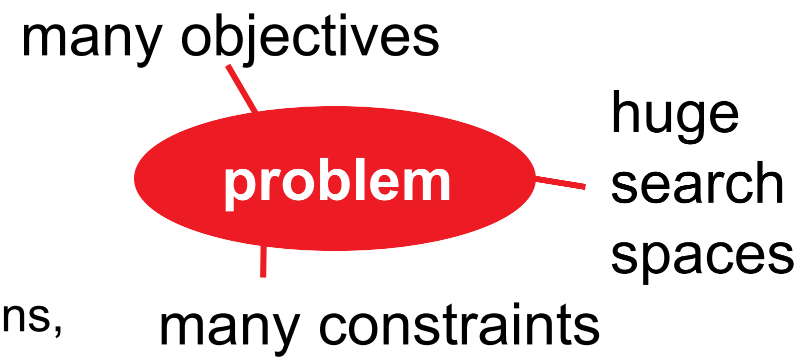
- MCDM track at EMO conference since 2009
- special sessions on EMO at the MCDM conference since 2008
- joint Dagstuhl seminars since 2004

Blackbox optimization



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

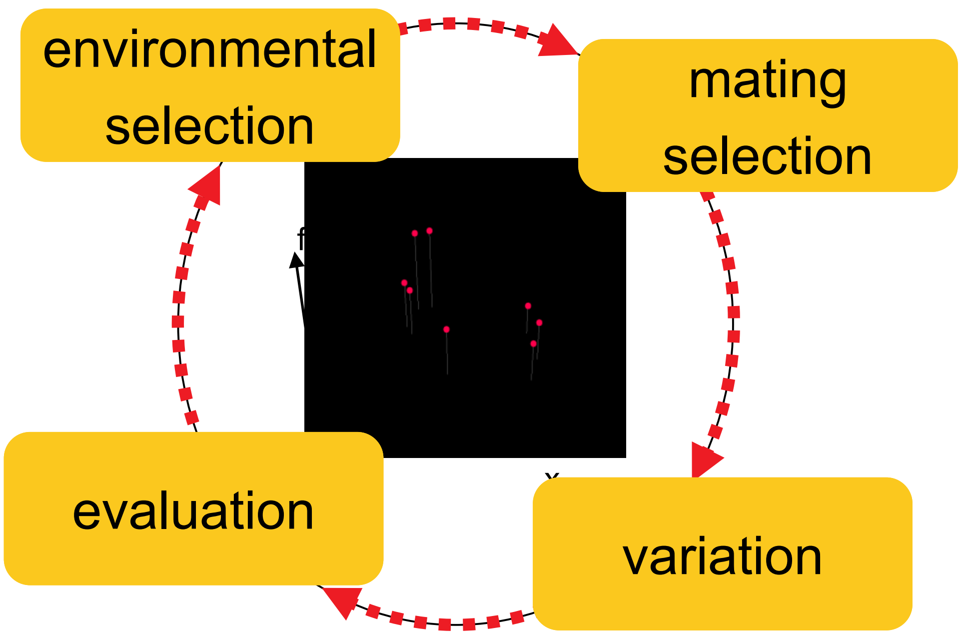


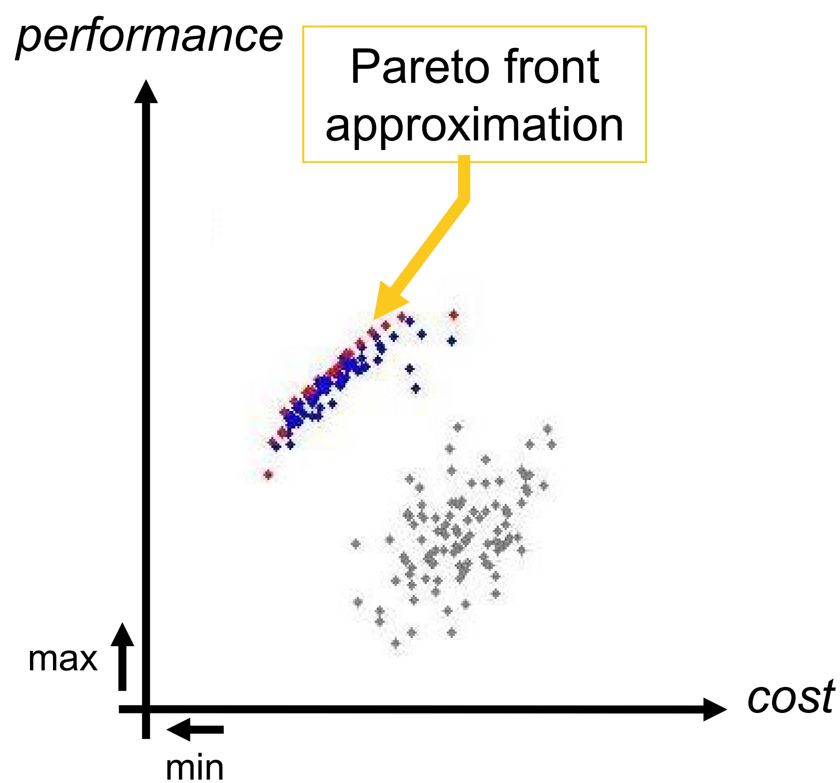


The Other Main Difference

Evolutionary Multiobjective Optimization

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

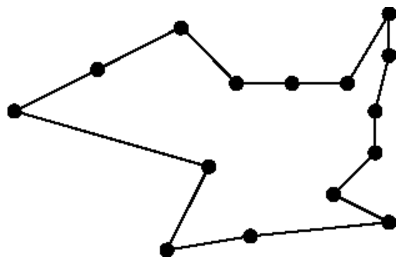


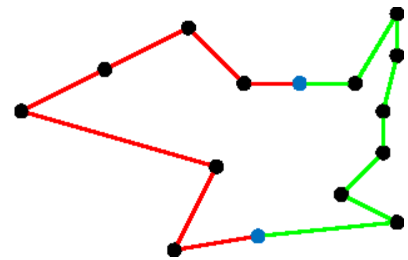


Multiobjectivization

Some problems are easier to solve in a multiobjective scenario

example: TSP
[Knowles et al. 2001]





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

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], ...

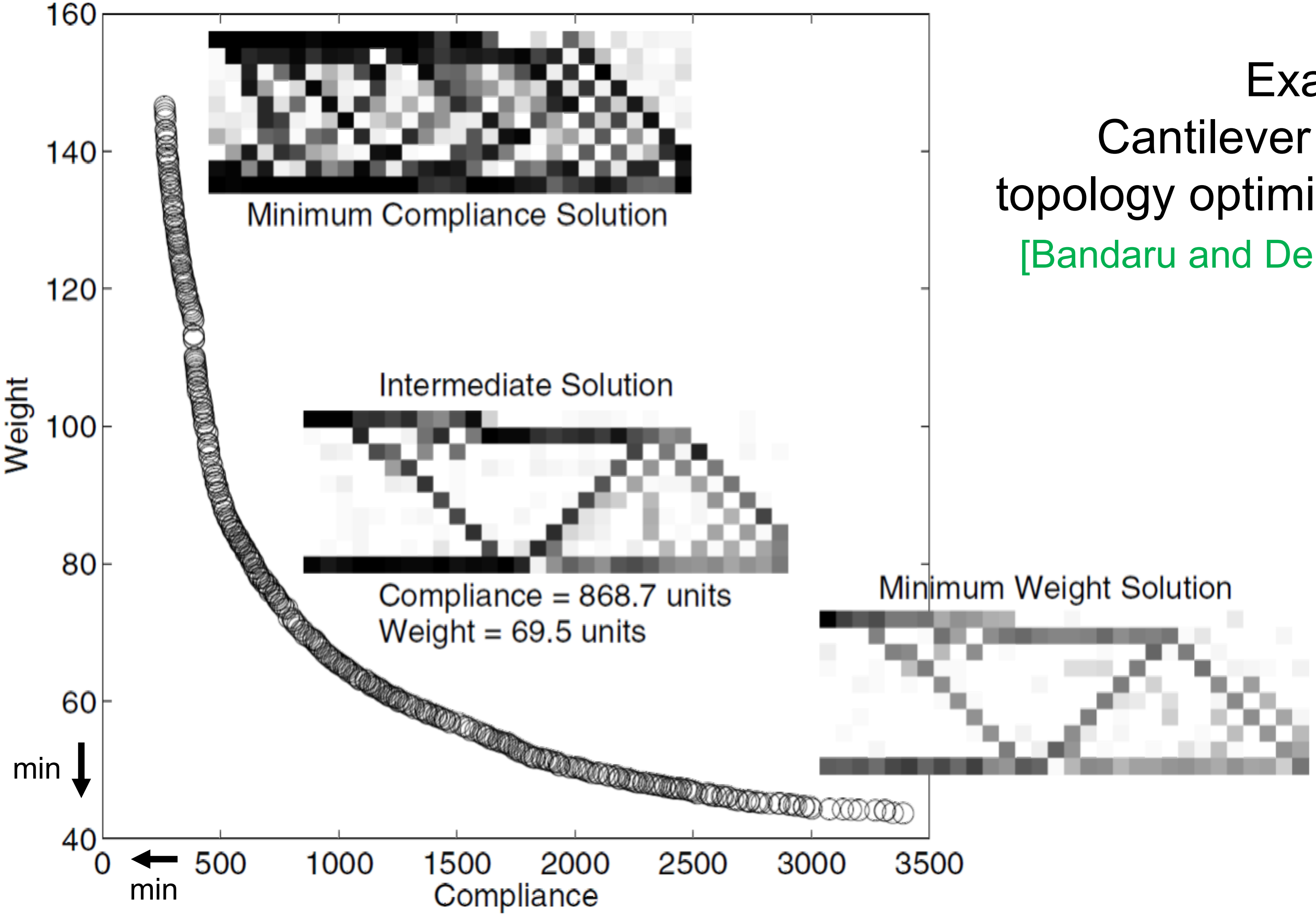
also backed up by theory e.g. [Brockhoff et al. 2009, Handl et al. 2008b]

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

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

Innovization

Often innovative design principles among solutions are found



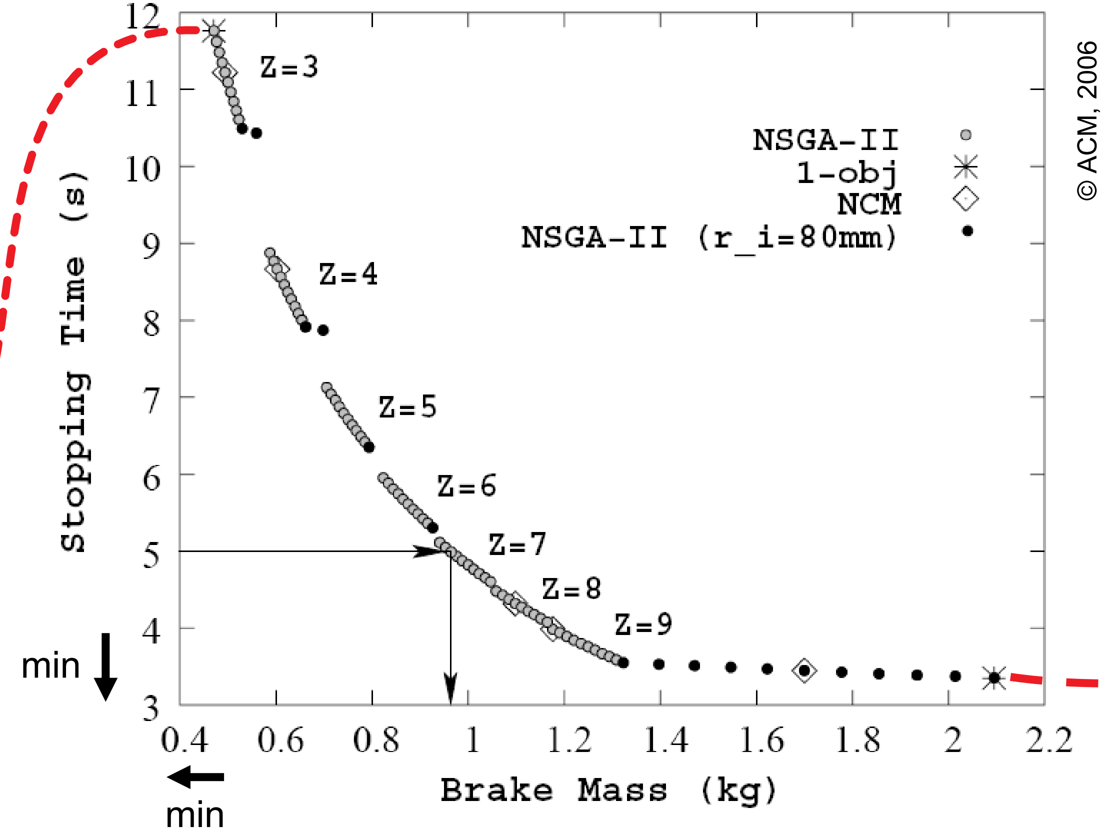
Example:
Cantilever beam
topology optimization
[Bandaru and Deb 2015]

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]

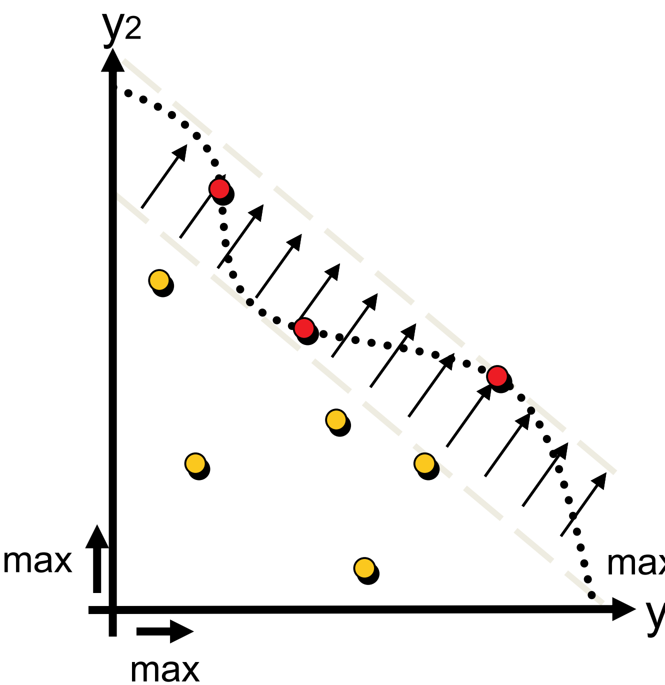
= using machine learning techniques to find new and innovative design principles among solution sets

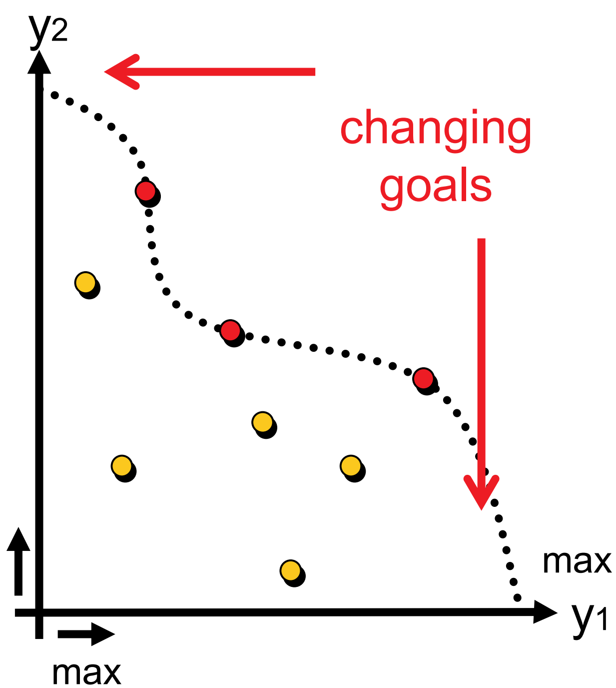
= learning from/about a multiobjective optimization problem

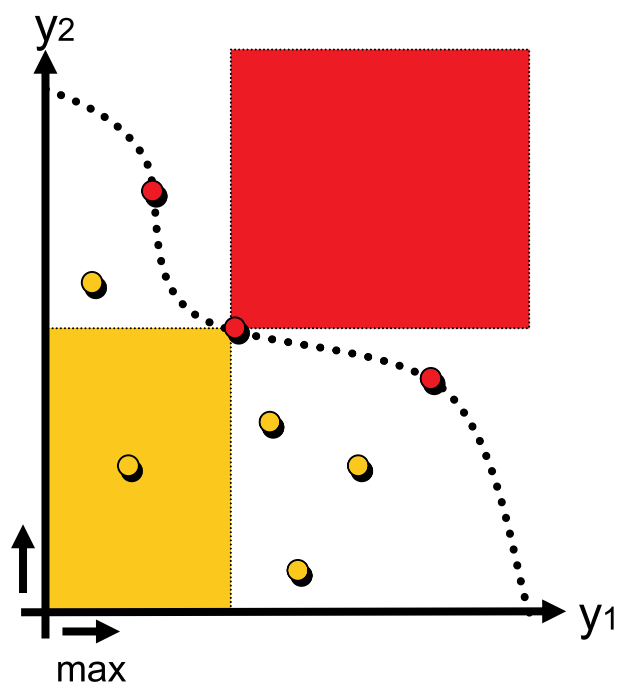
Other examples:

- 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]

aggregation-based	criterion-based	dominance-based
problem decomposition (multiple single-objective optimization problems)	*VEGA*	*SPEA2, NSGA-II "modern" EMOA*







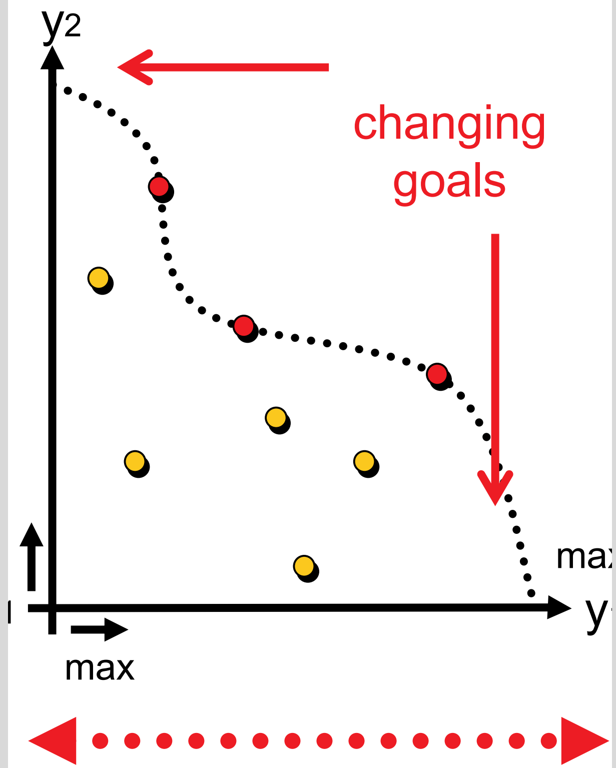
solution-oriented
scaling-dependent

set-oriented
less scaling-independent

Approaches to Multiobjective Optimization

criterion-based

VEGA

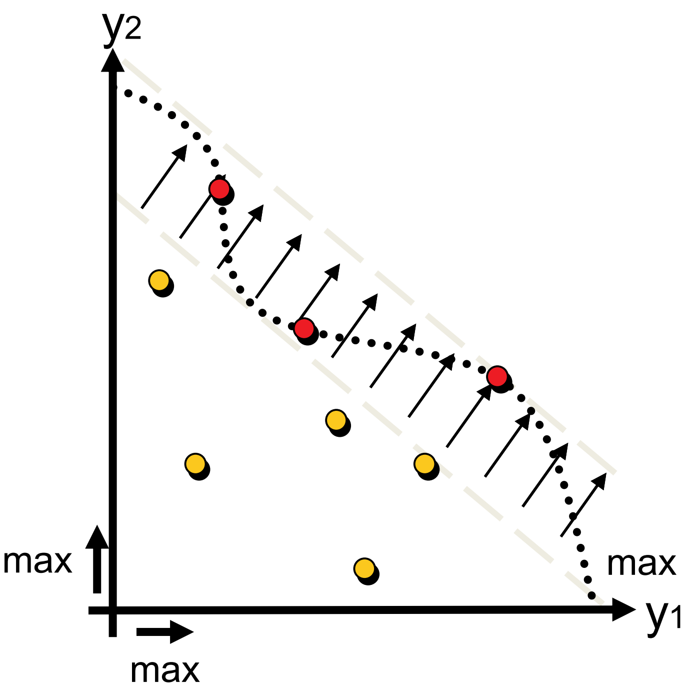


less

Approaches to Multiobjective Optimization

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 → single objective $s(x)$

A scalarizing function s is a function $s\colon Z \to \mathbb{R}$ 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

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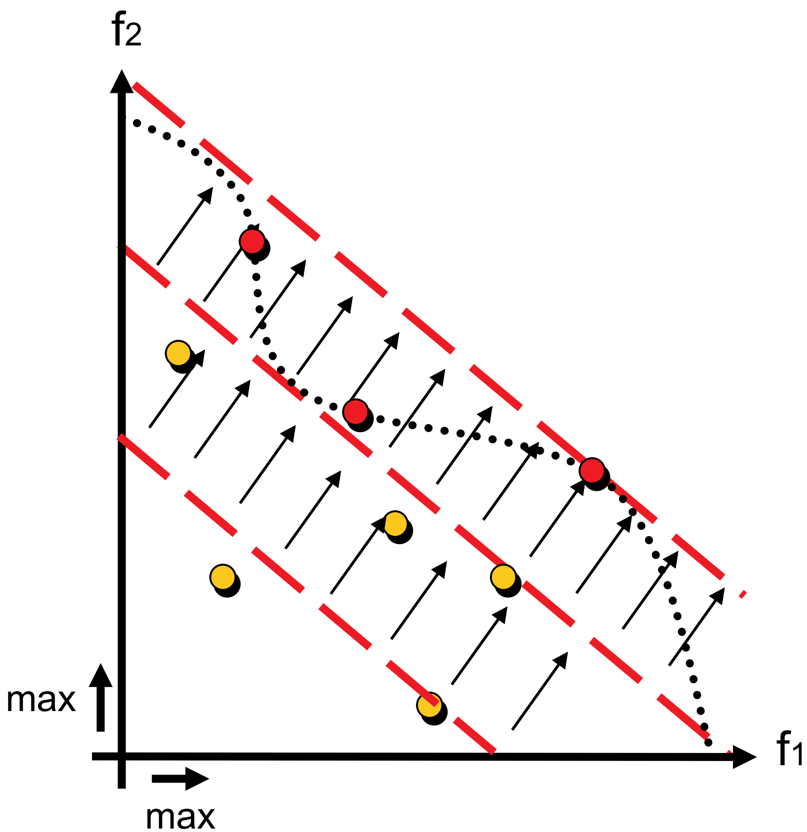
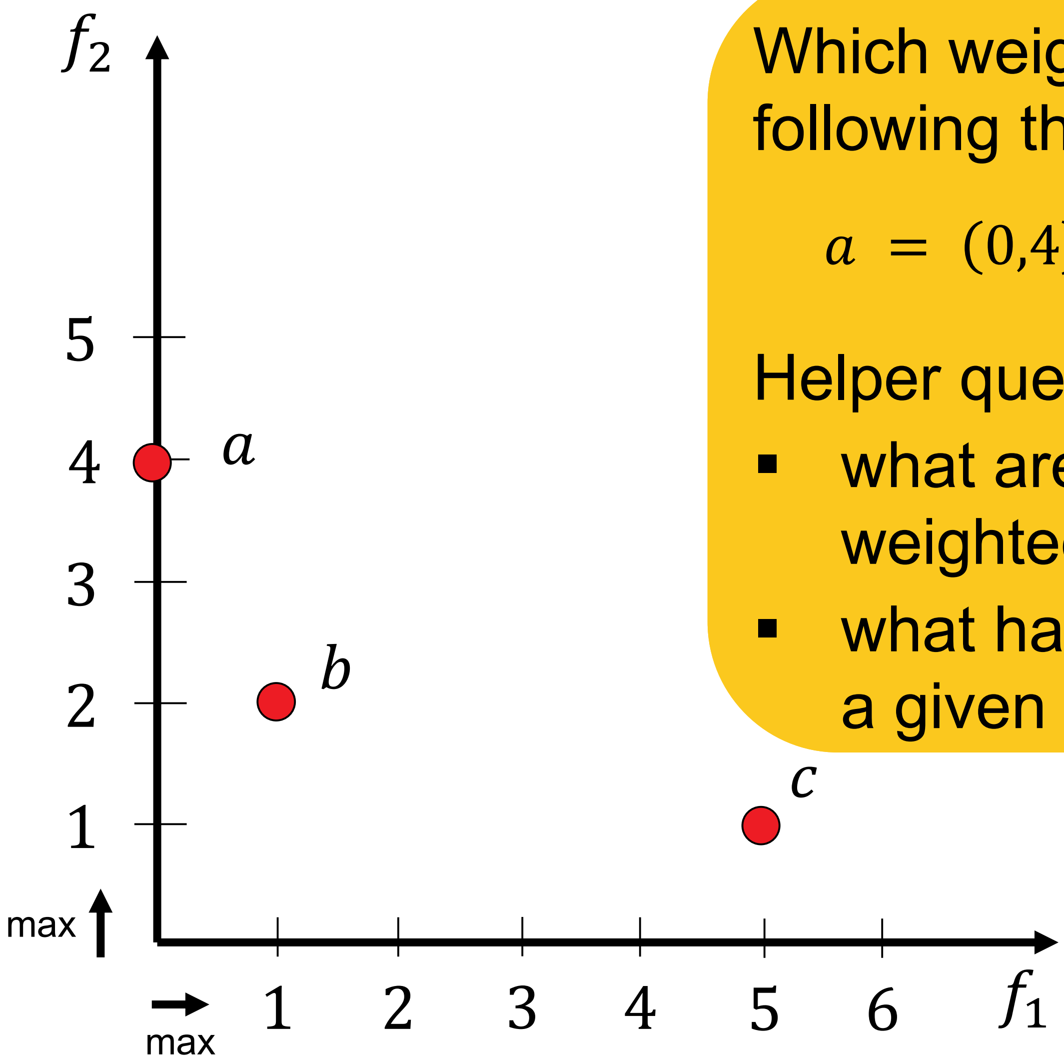


Example 1: weighted sum approach

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

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

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

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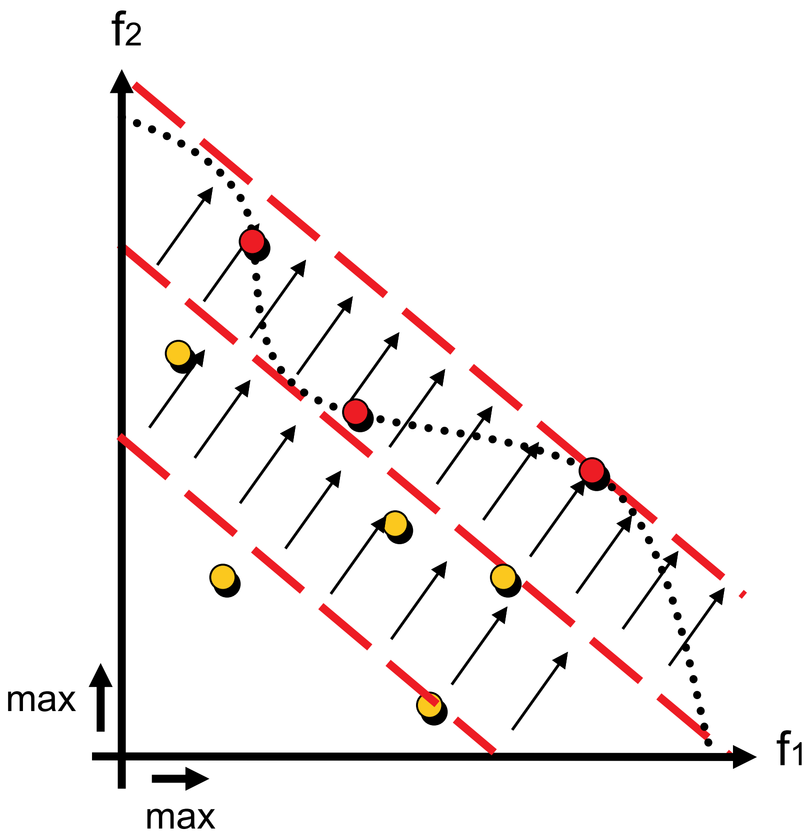

Example 1: weighted sum approach

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

→ $y = w_1 y_1 + \ldots + w_k y_k$ →

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

Solution-Oriented Problem Transformations

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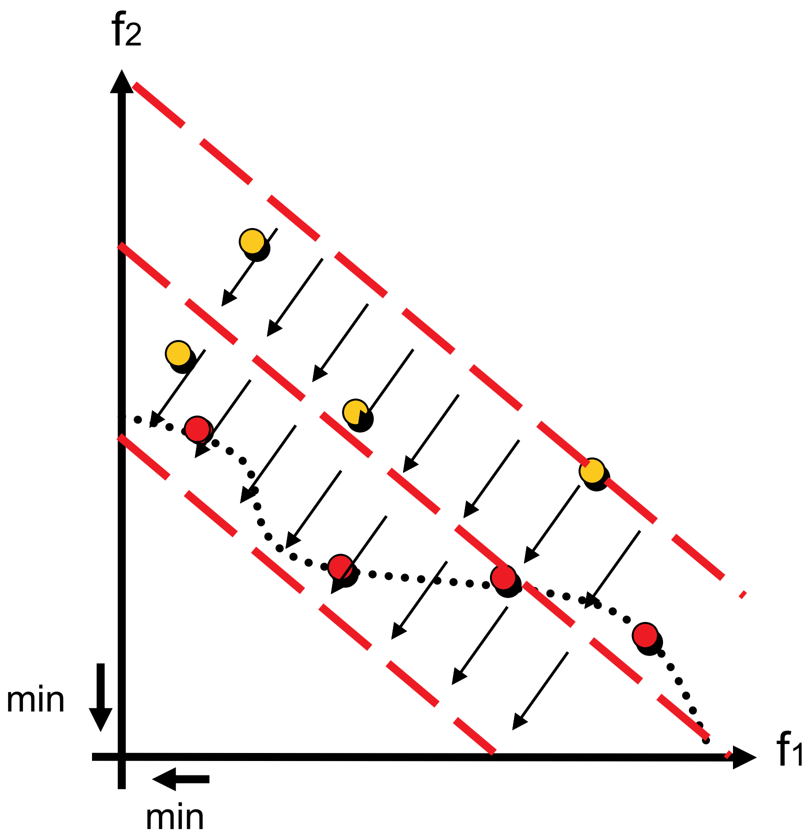

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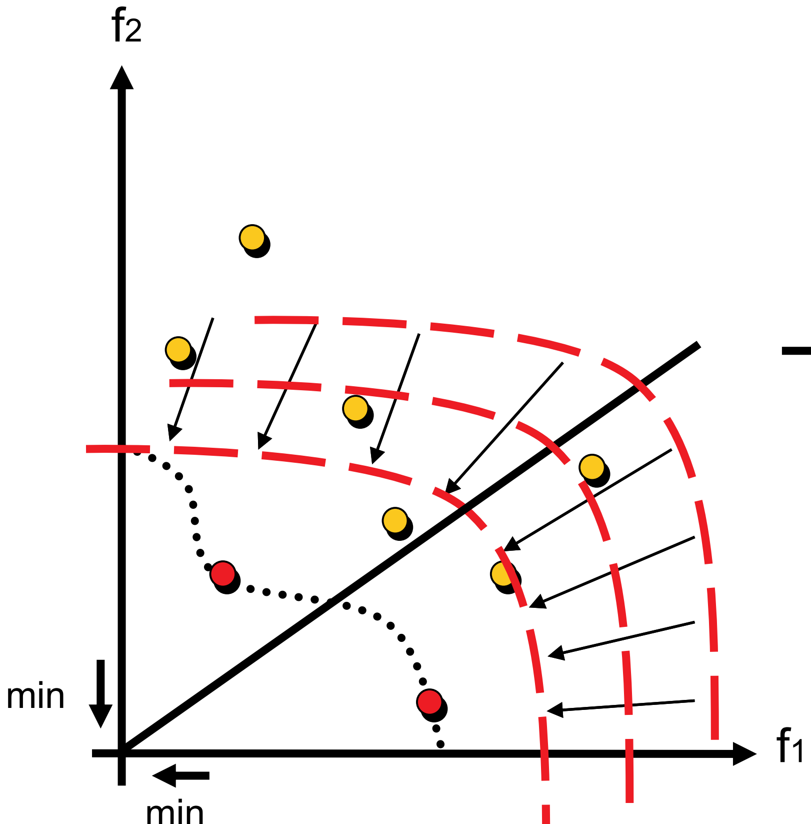
multiple objectives $(f_1(x), f_2(x), \dots, f_k(x))$ → **transformation** → single objective $s(x)$



Example 2: weighted p-norm

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

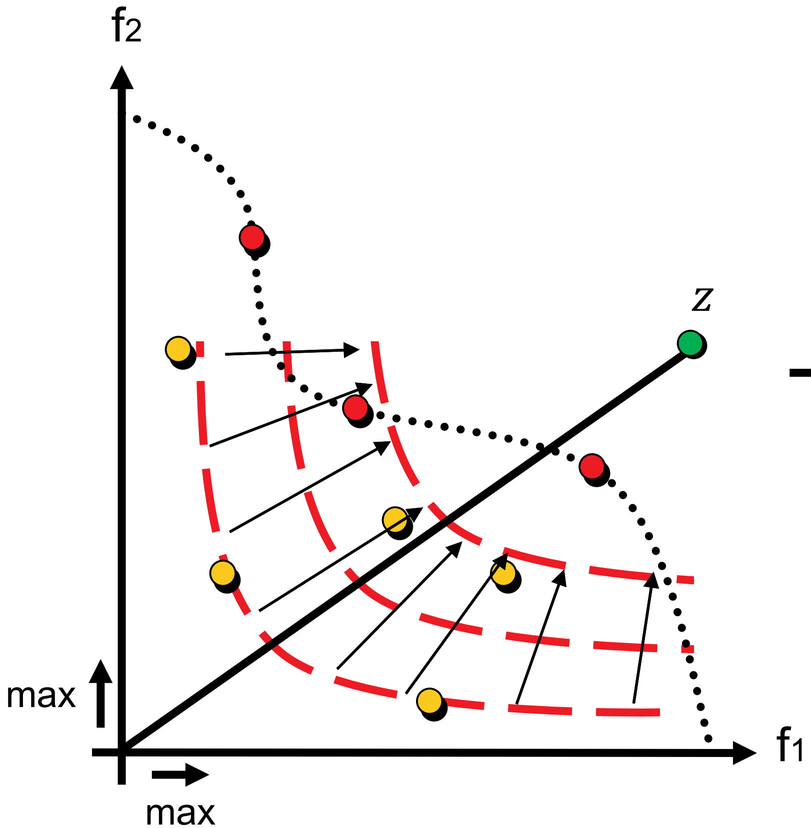
$$y = \sqrt[p]{(w_1 y_1)^p + \ldots + (w_k y_k)^p}$$

$p = 1$: weighted sum

$p = \infty$: weighted Tchebycheff

parameters

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



Example 2: weighted p-norm

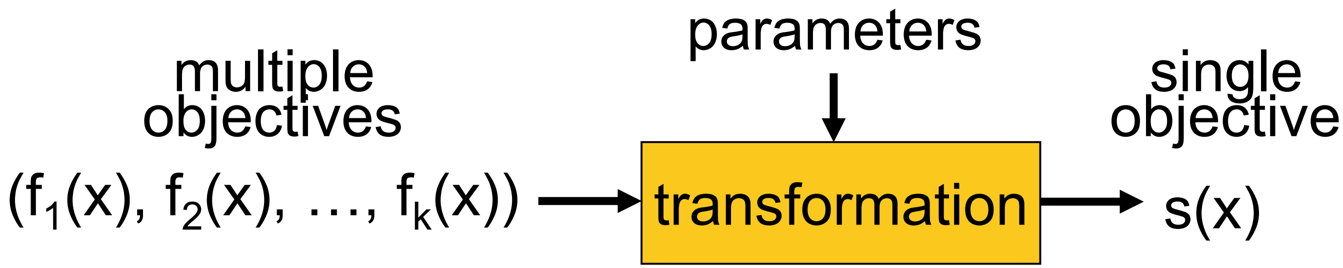
$(w_1, w_2, \ldots, w_k)$

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

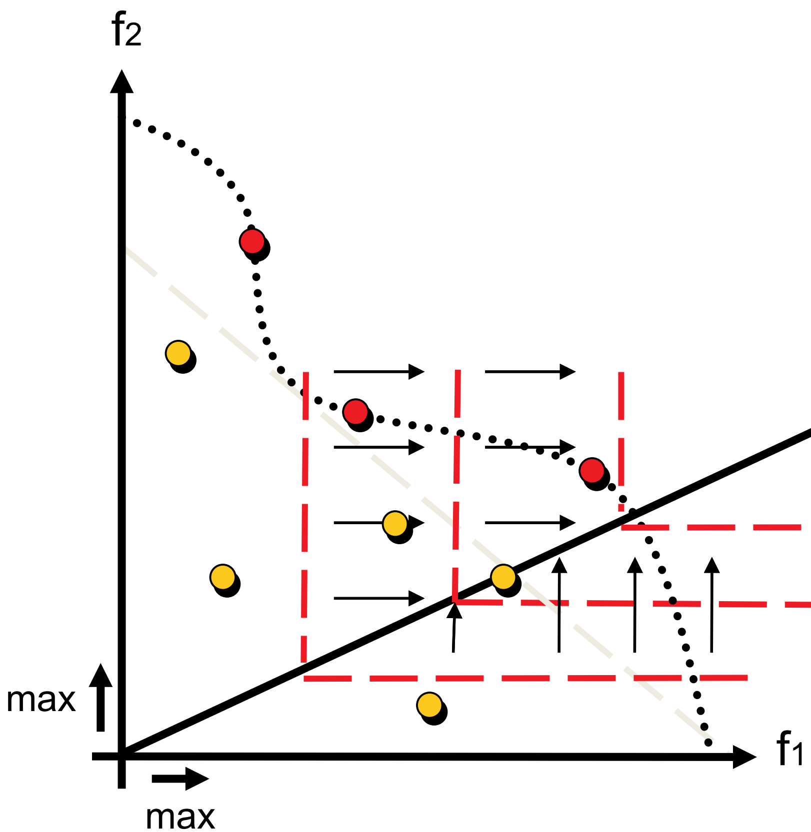
$p = 1$: weighted sum

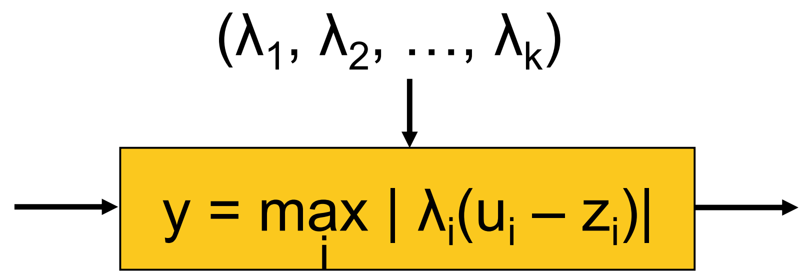
$p = \infty$: weighted Tchebycheff

Solution-Oriented Problem Transformations



Example 2: weighted Tchebycheff





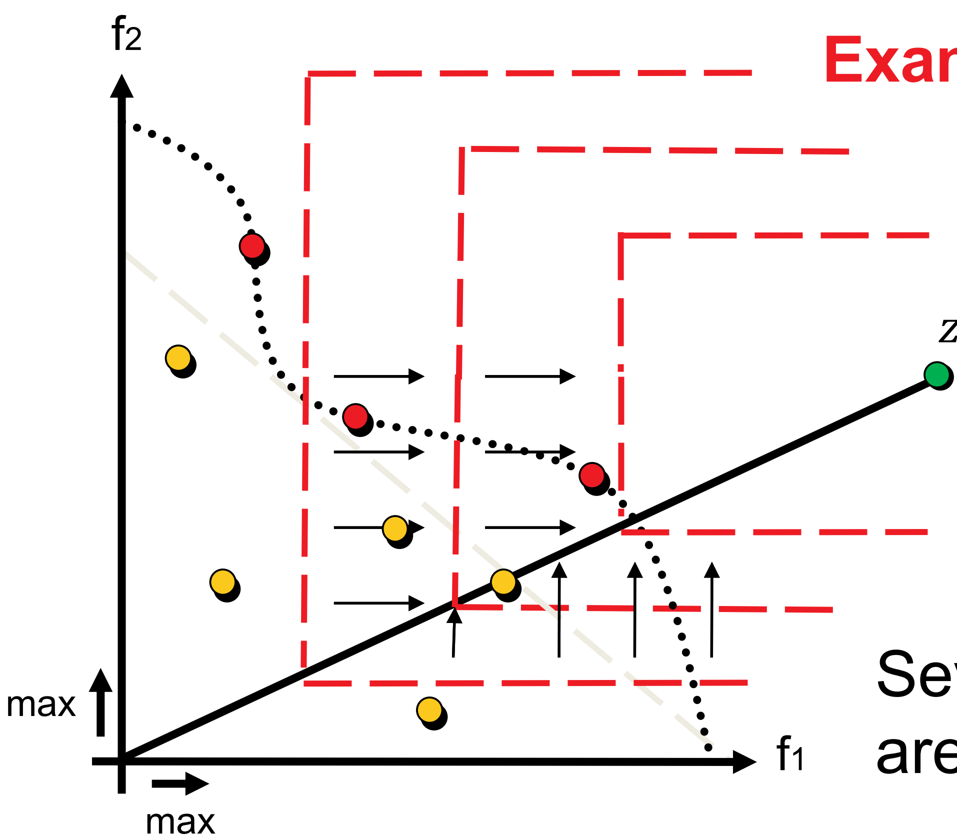
Several other scalarizing functions are known, see e.g. [Miettinen 1999]

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 Tchebycheff



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

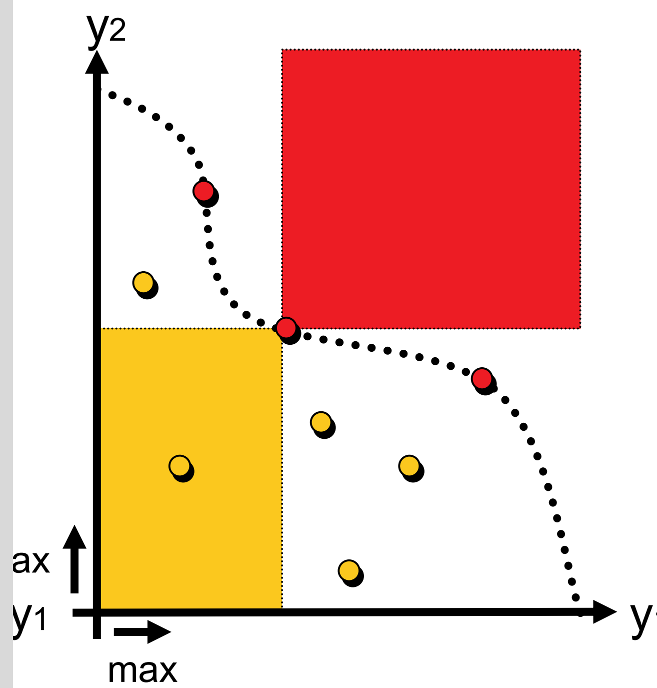
$$y = \max_i \,|\, \lambda_i (u_i - z_i) |$$

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

Approaches to Multiobjective Optimization

dominance-based

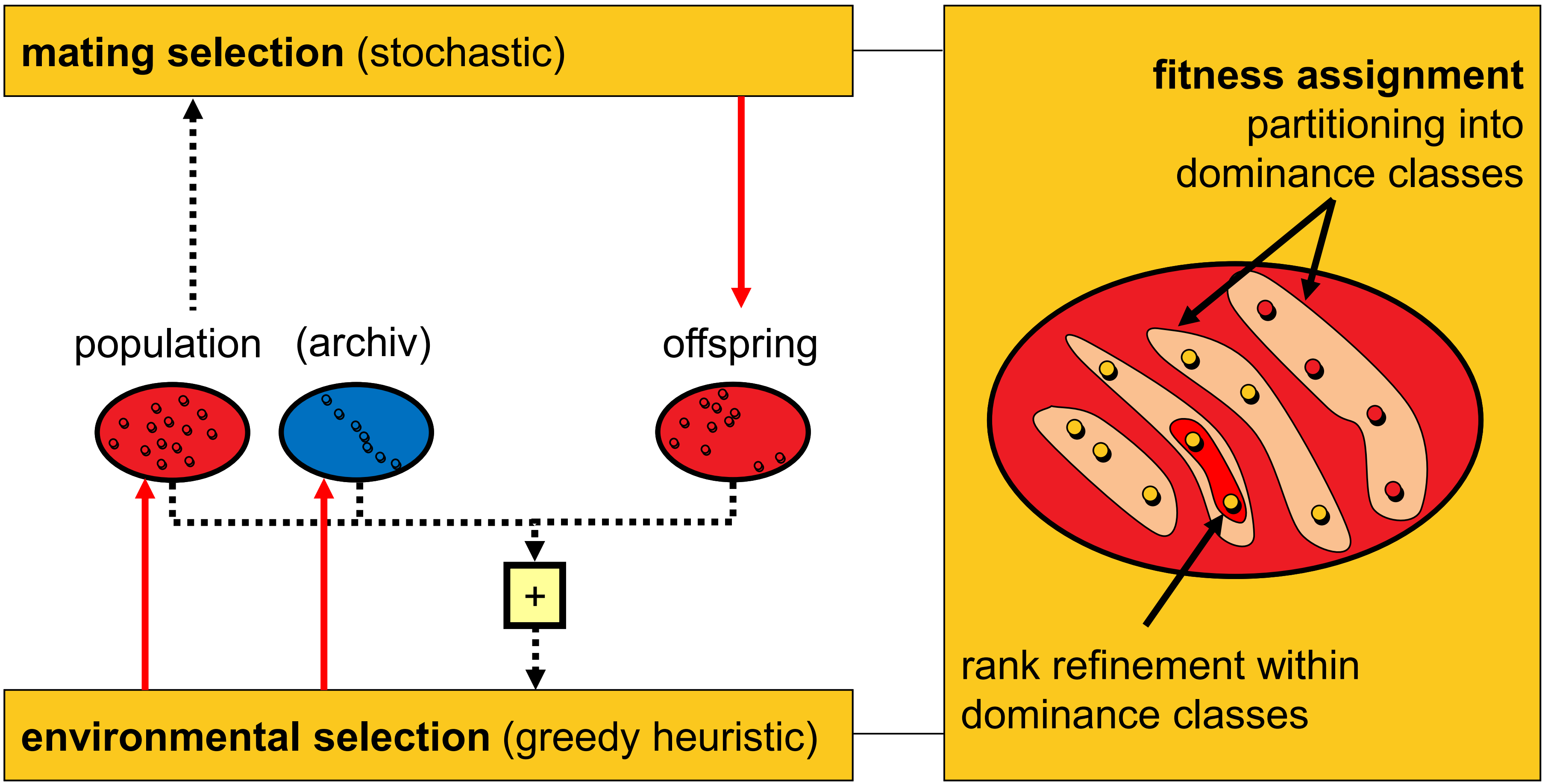
SPEA2, NSGA-II
"modern" EMOA



set-oriented

scaling-independent

General Scheme of Most Set-Oriented EMO

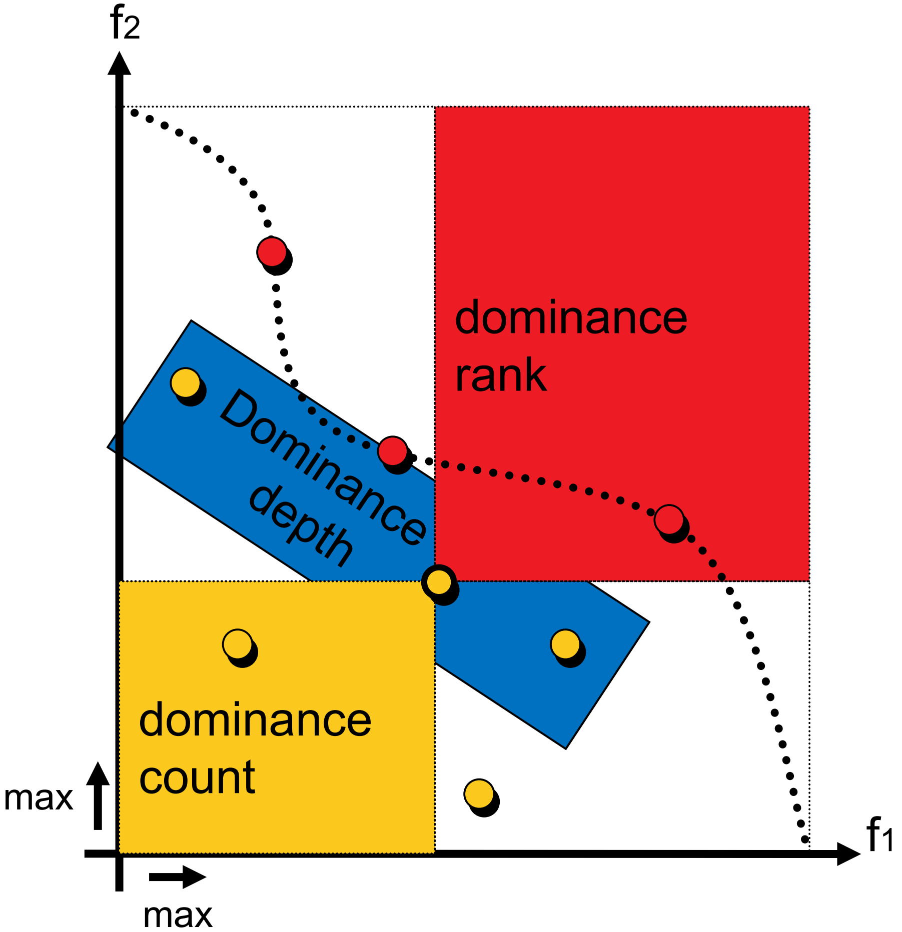


Ranking of the Population Using Dominance

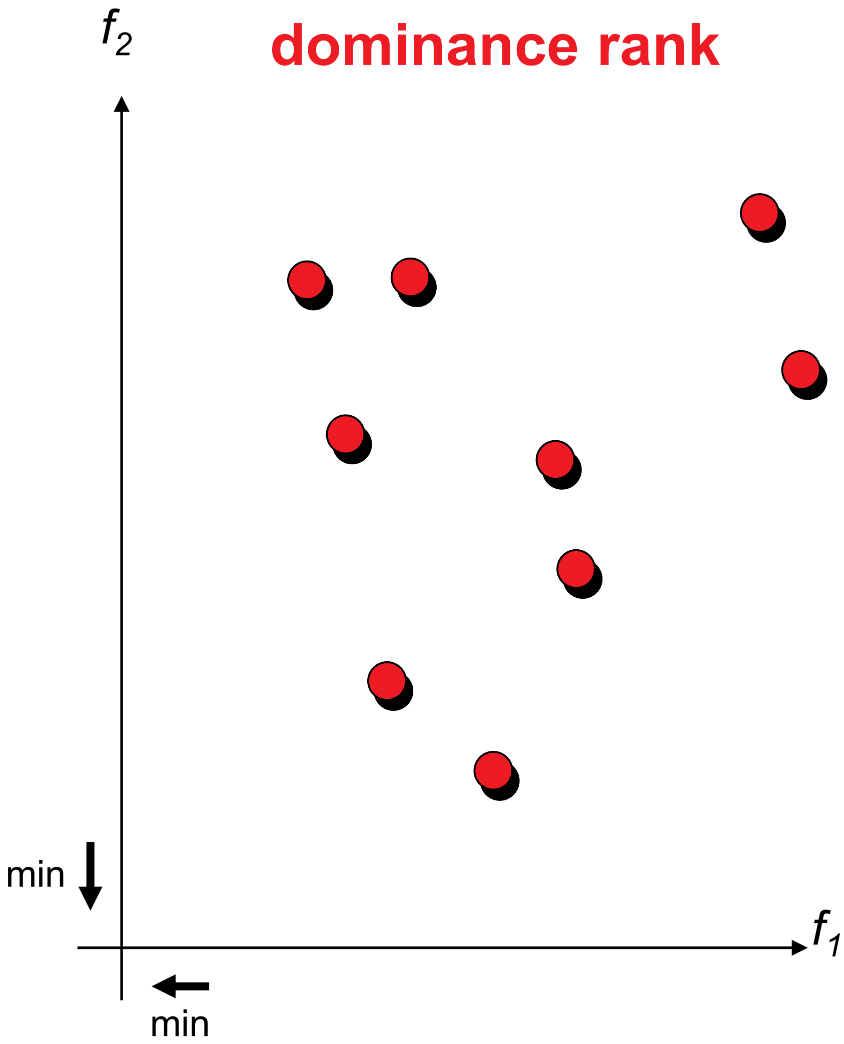
... goes back to a proposal by David Goldberg in 1989.

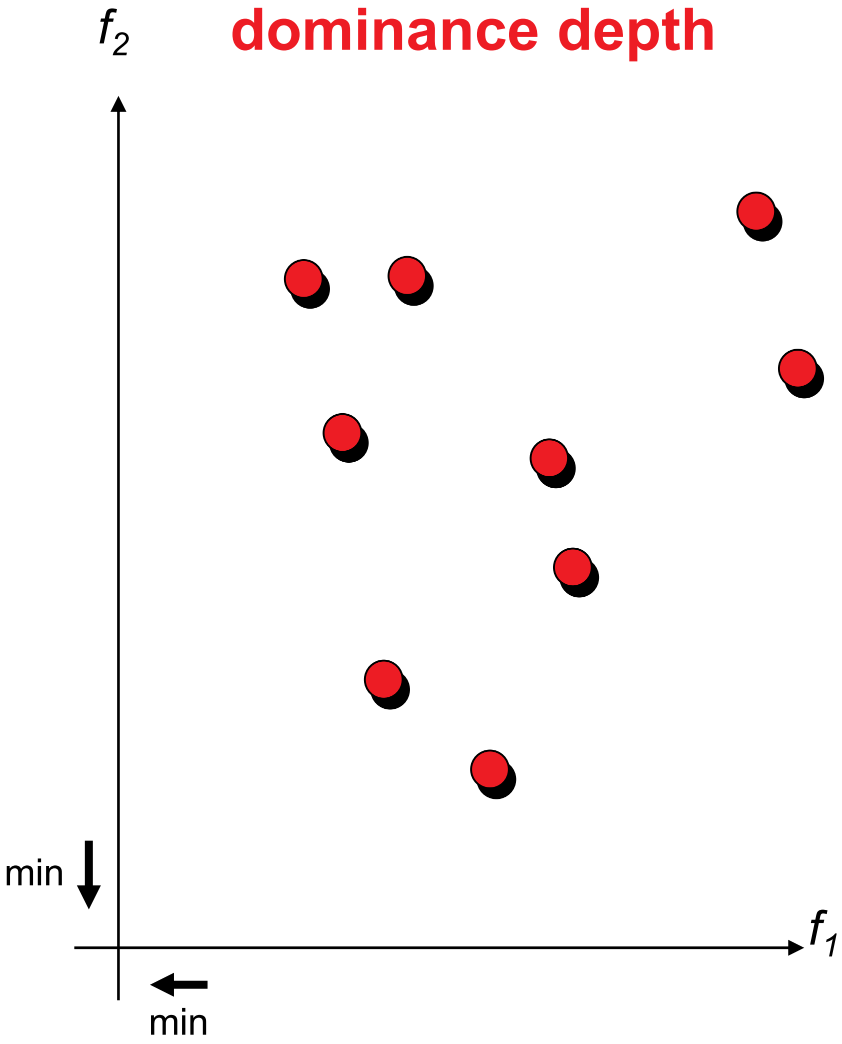
... is based on pairwise comparisons of the individuals only.

- **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





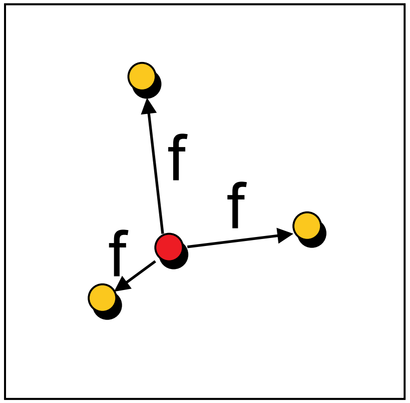
Refinement of Dominance Rankings

Goal: rank incomparable solutions within a dominance class

❶ Diversity information

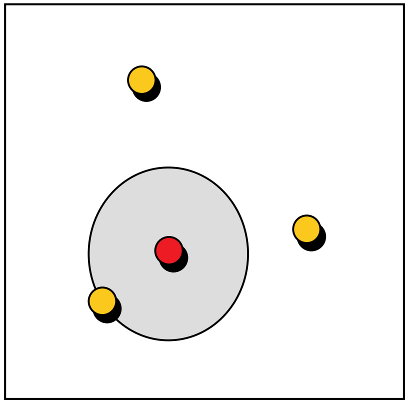
Kernel method

diversity =
function of the
distances



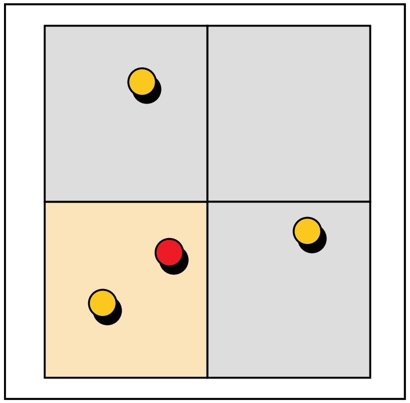
k-th nearest neighbor

diversity =
function of distance
to k-th nearest neighbor



Histogram method

diversity =
number of elements
within box(es)

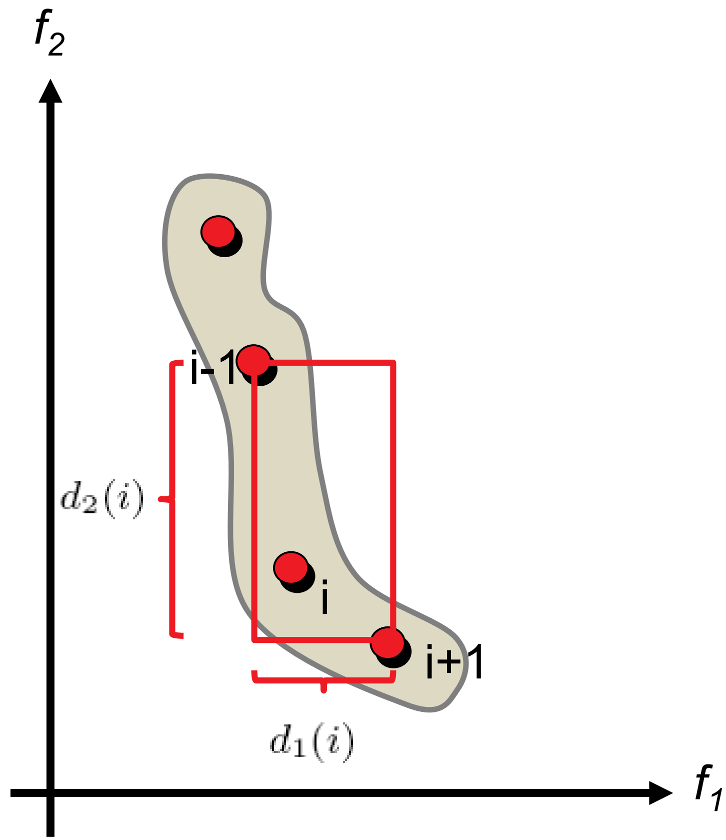


❷ (Contribution to a) quality indicator

Example: NSGA-II Diversity Preservation

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

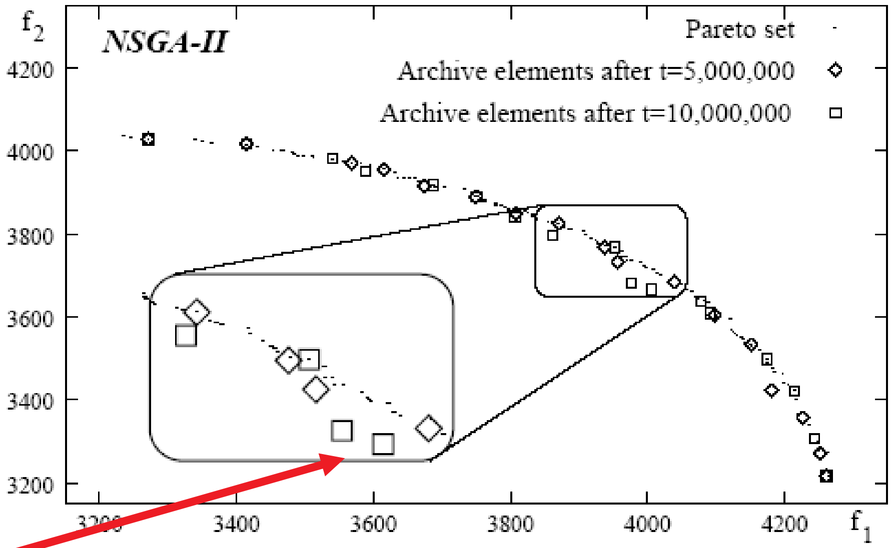


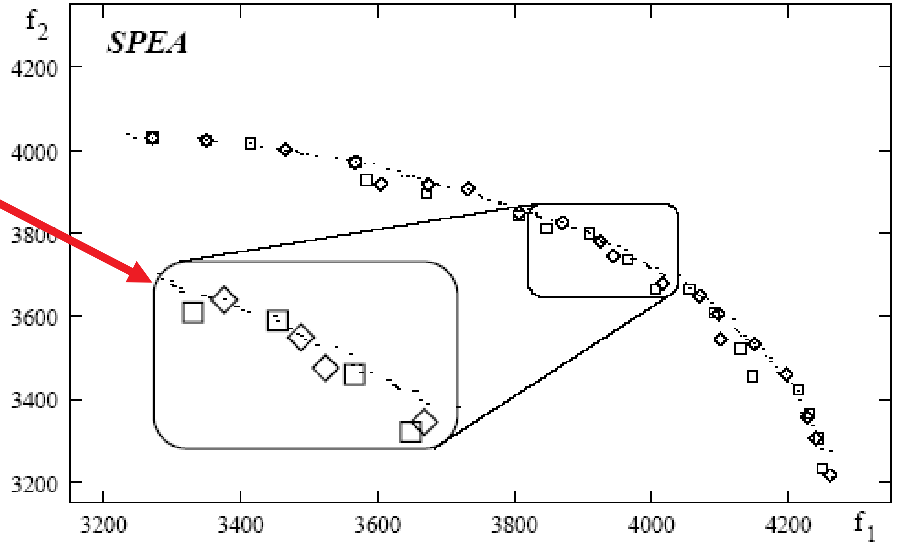
$$\mathrm{CD}(i) = \frac{d_1(i)}{f_{1,\max} - f_{1,\min}} + \cdots + \frac{d_m(i)}{f_{m,\max} - f_{m,\min}}$$

SPEA2 and NSGA-II: Deteriorative Cycles

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

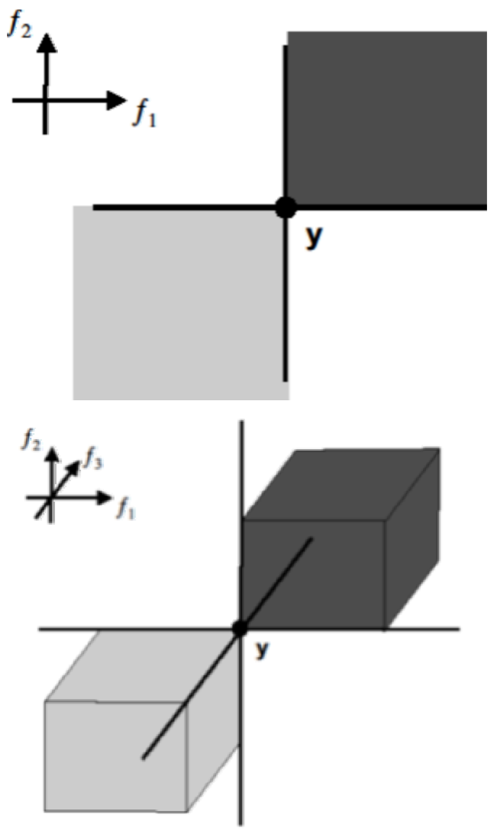
non-dominated solutions already found can be lost

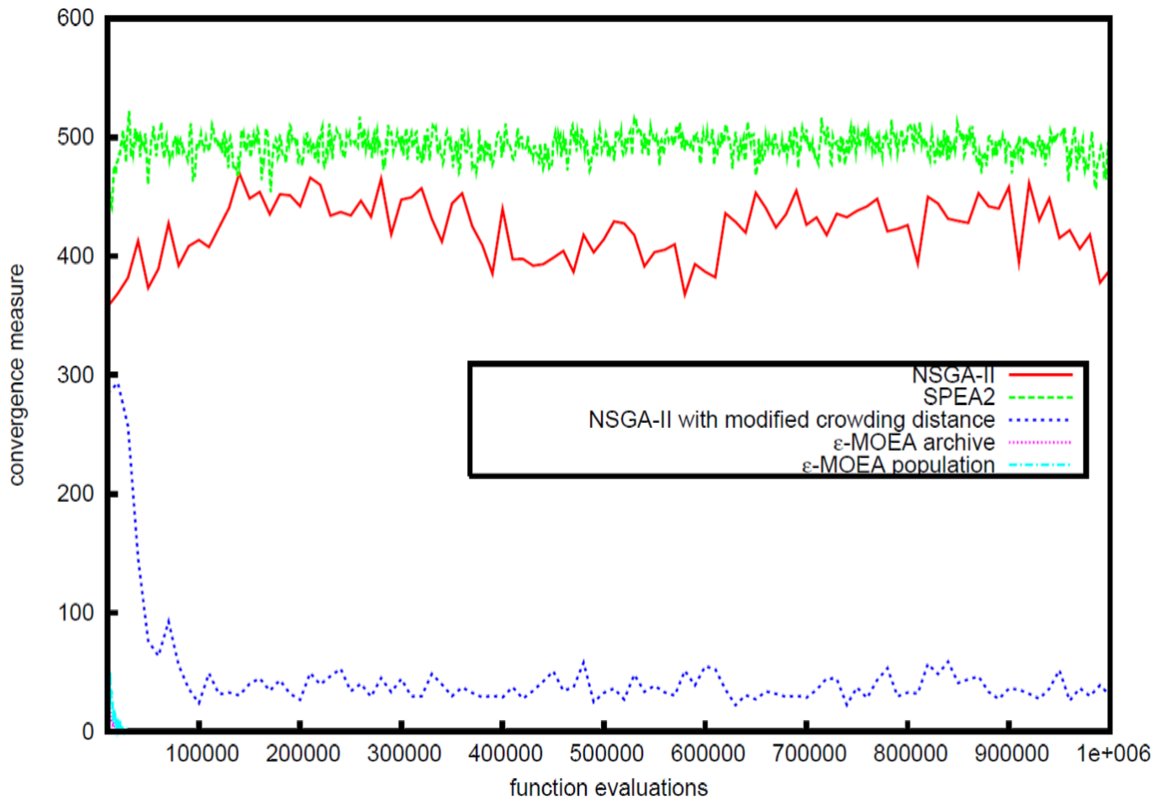




Remark: Many-Objective Optimization

- 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





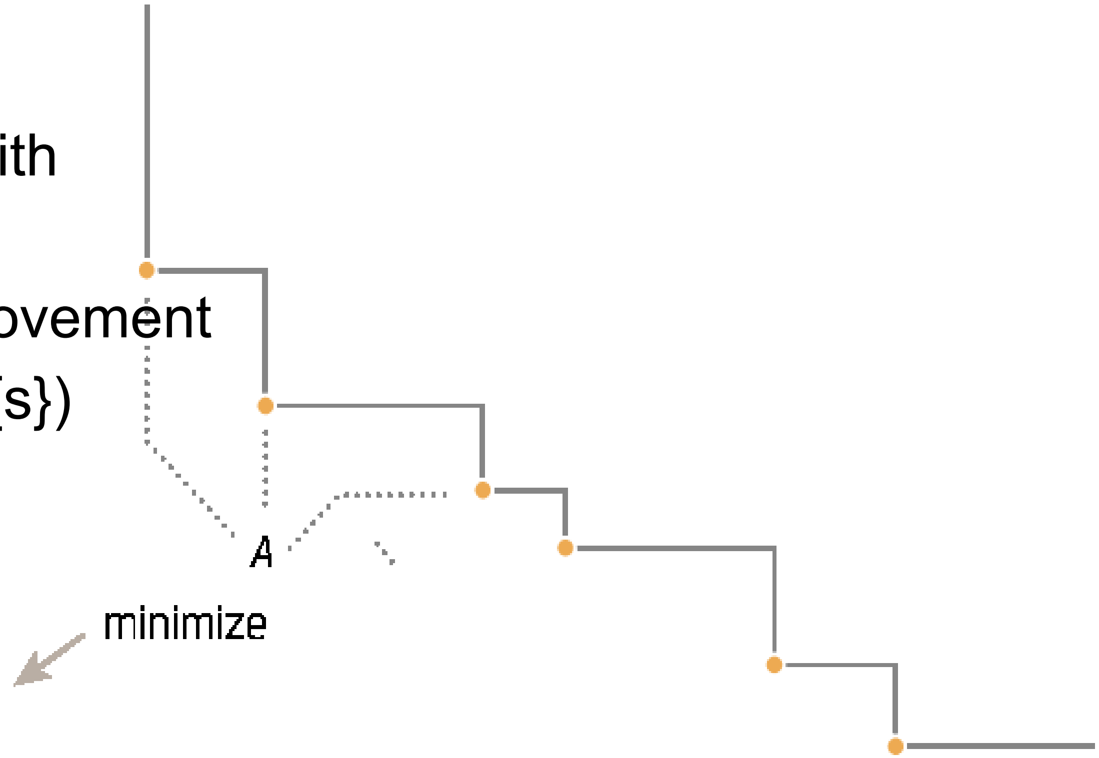
Hypervolume-Based Selection

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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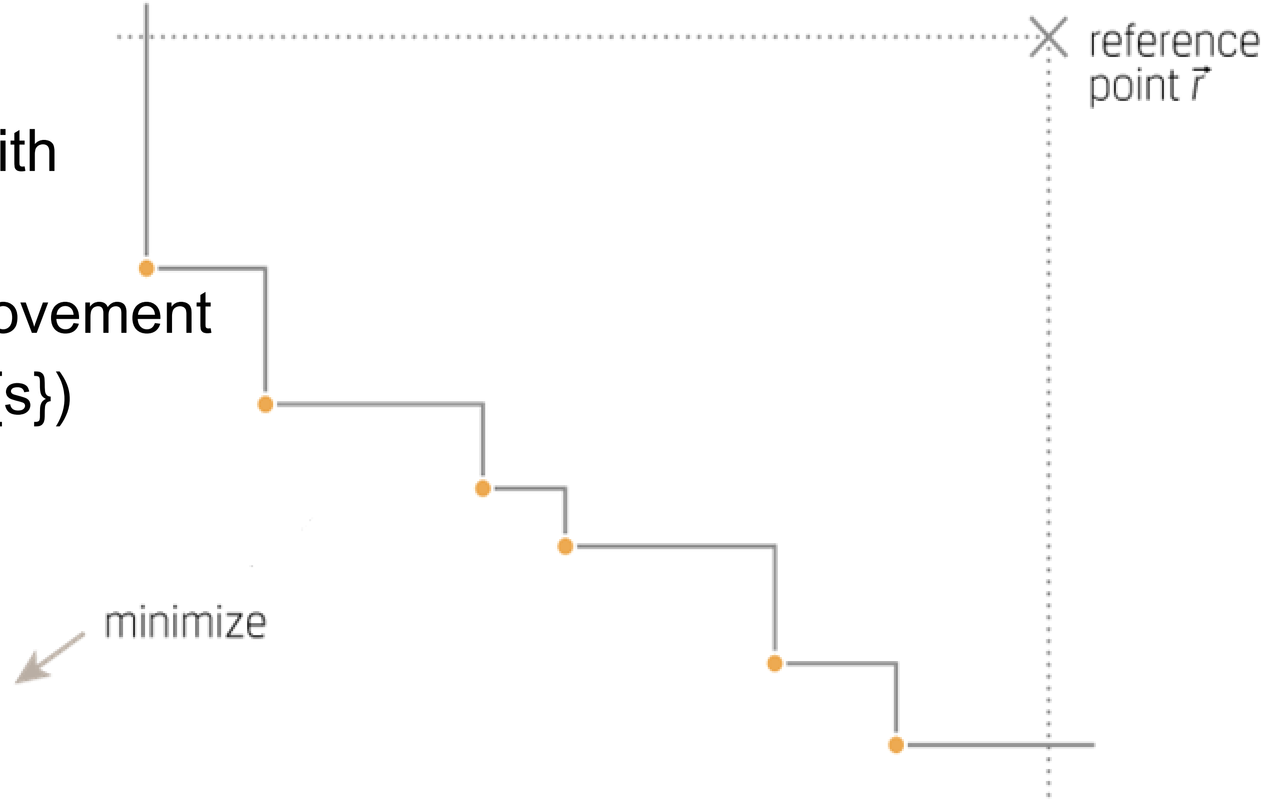

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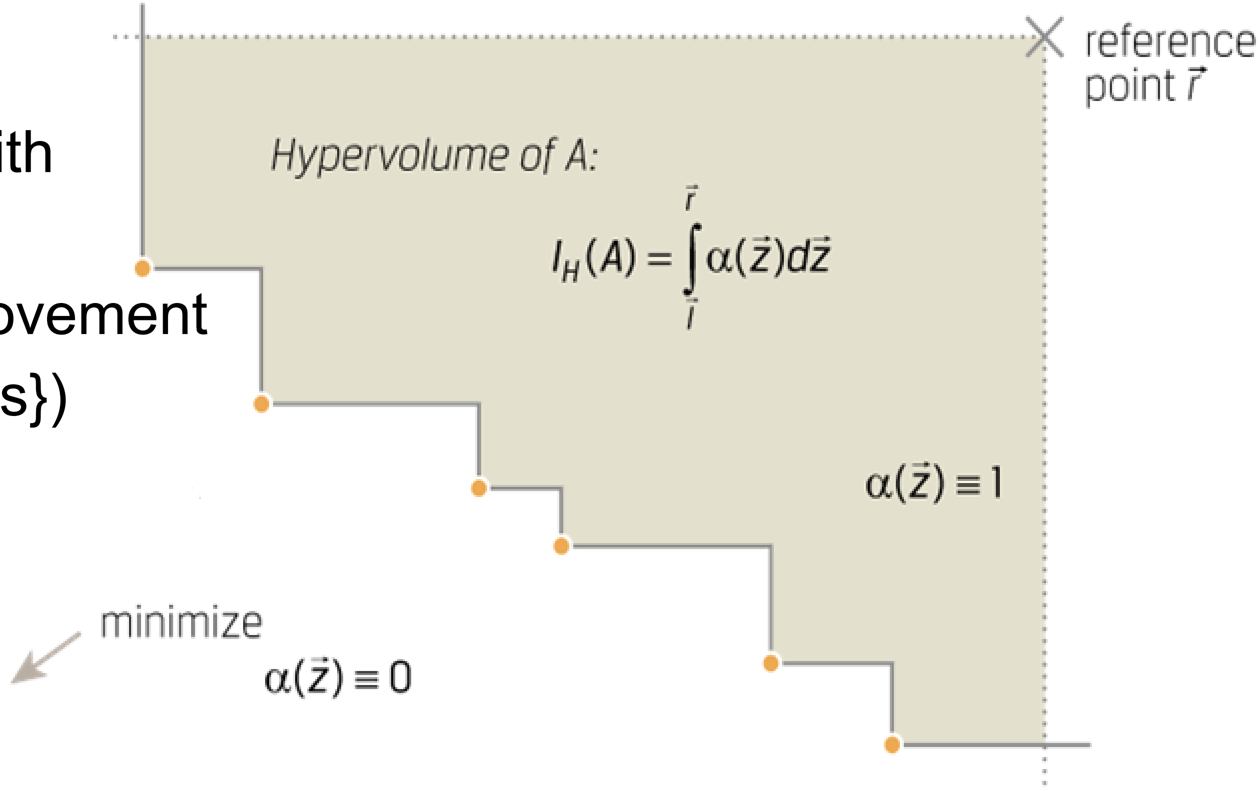

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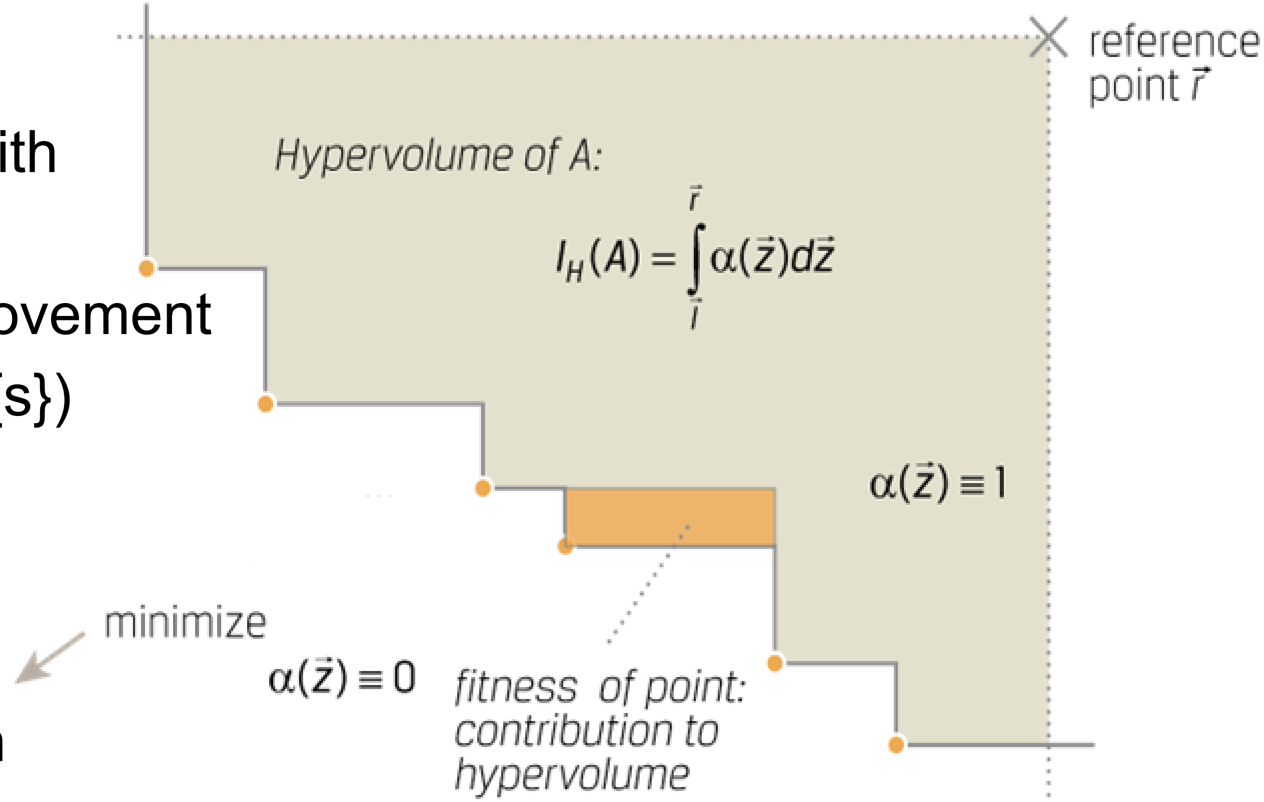
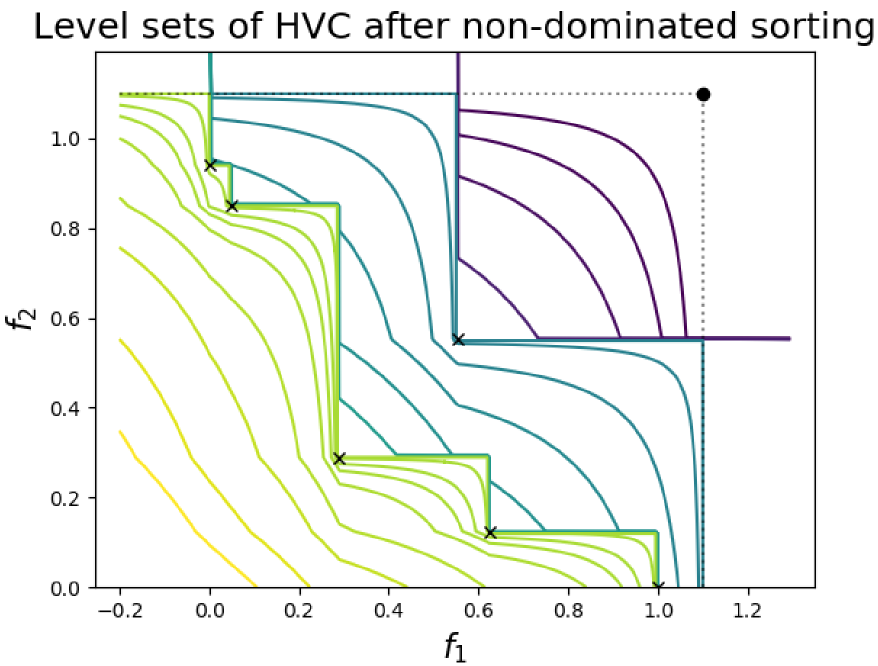
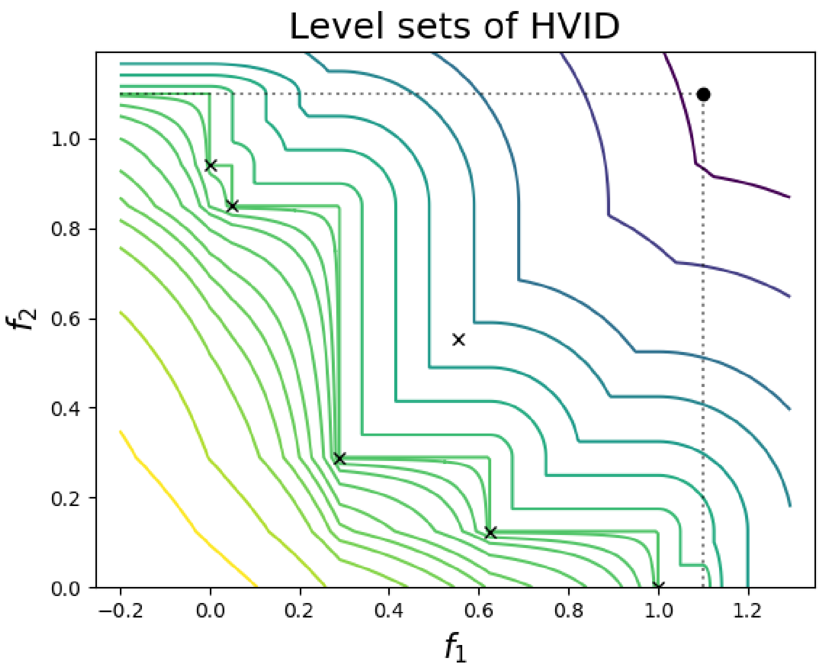


But: can also result in cycles if reference point is not constant [Judt et al. 2011] and is expensive to compute exactly [Bringmann and Friedrich 2009]

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.

Multiobjective Problem $\xrightarrow{\text{Indicator}}$ 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

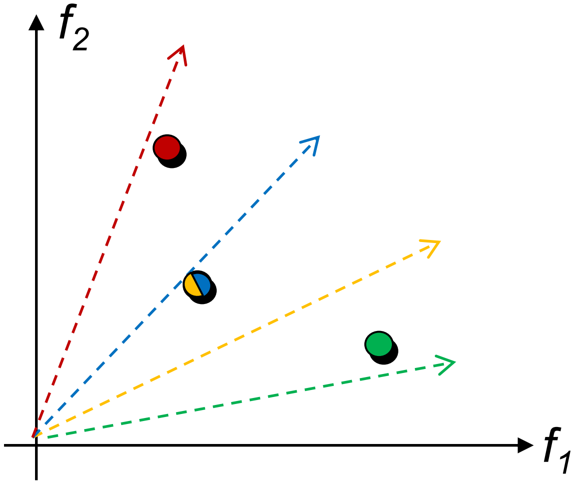
  HypE [Bader and Zitzler 2011]: Hypervolume sampling + contribution if more than 1 (random) solution deleted

Decomposition-Based Selection: MOEA/D

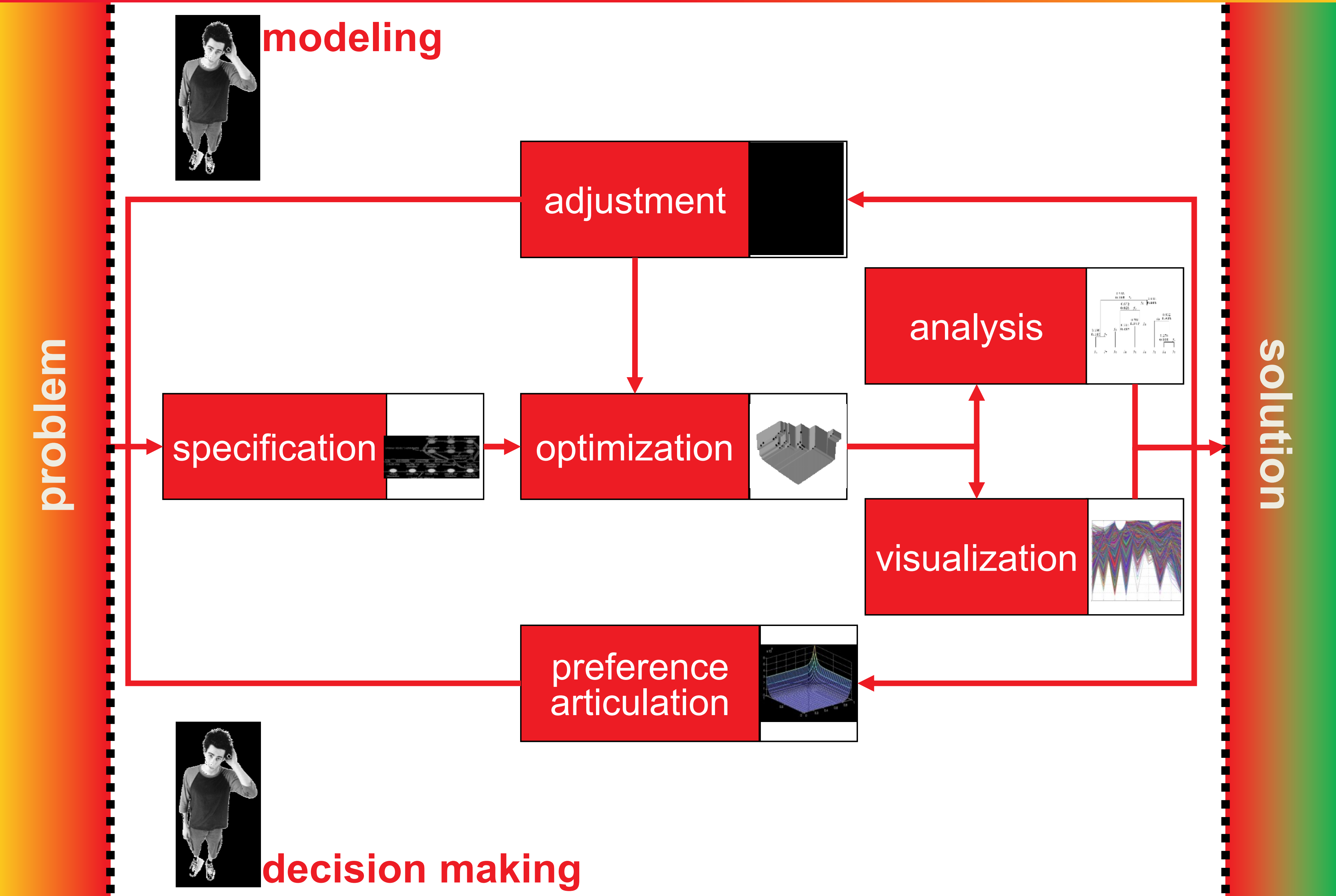
MOEA/D: Multiobjective Evolutionary Algorithm Based on Decomposition [Zhang and Li 2007]

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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