(Evolutionary) Multiobjective Optimization

July 5, 2017

CEA/EDF/Inria summer school "Numerical Analysis"

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Overview of the Remaining Lectures & Exercises

Introduction to (Evolutionary) Multiobjective Optimization (now)

- difference to single-objective optimization, the basics
- algorithms and their design principles; MO-CMA-ES

Benchmarking Optimization Algorithms (this morning)

- performance assessment
- automated benchmarking with the COCO platform

Exercise around COCO (this afternoon)

- interpreting available COCO data
- if time allows: looking critically at published results

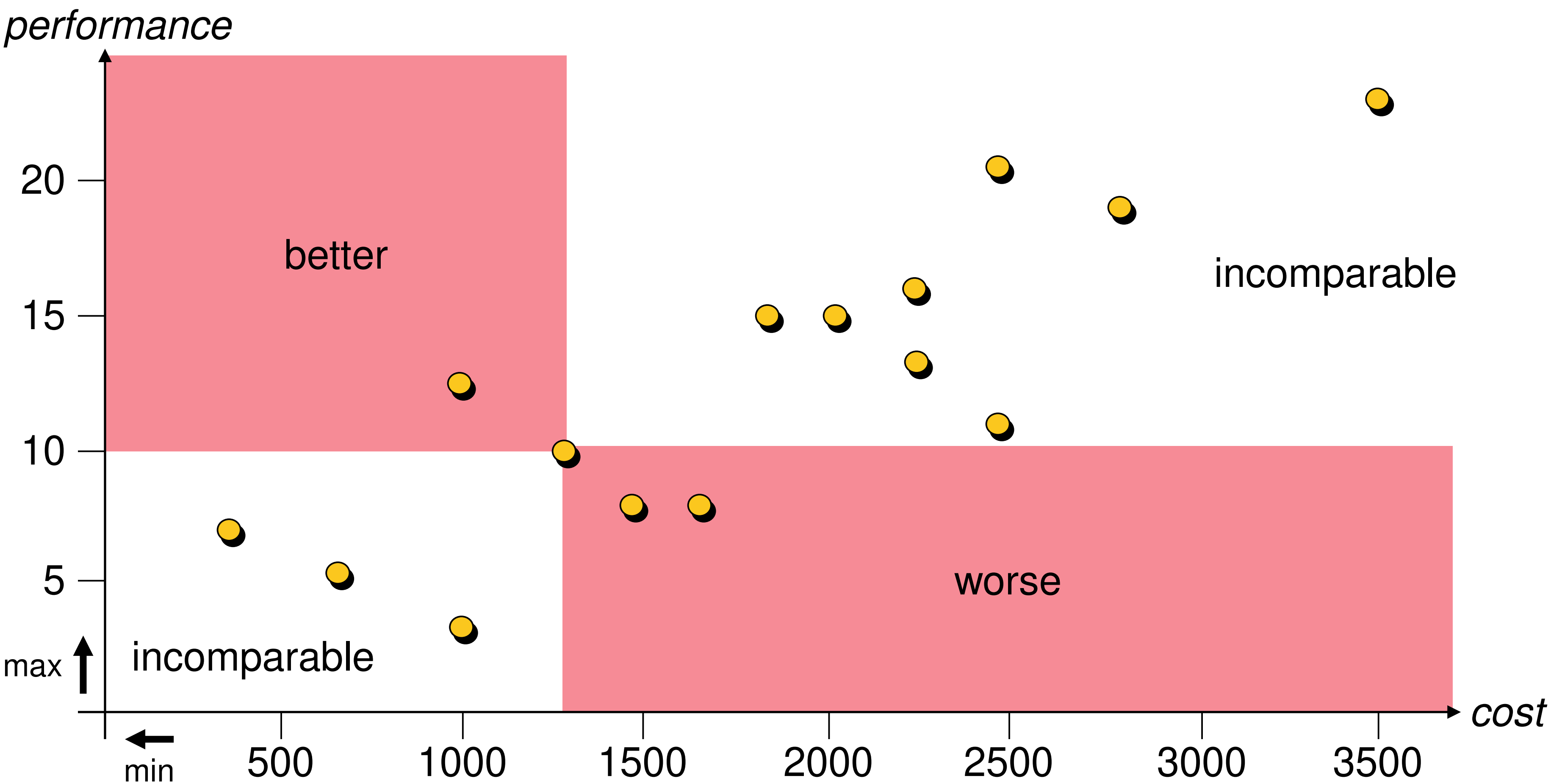
Exercise on Anne's part (tomorrow afternoon)

- The (1+1)-ES, running CMA-ES and interpreting its output, ...

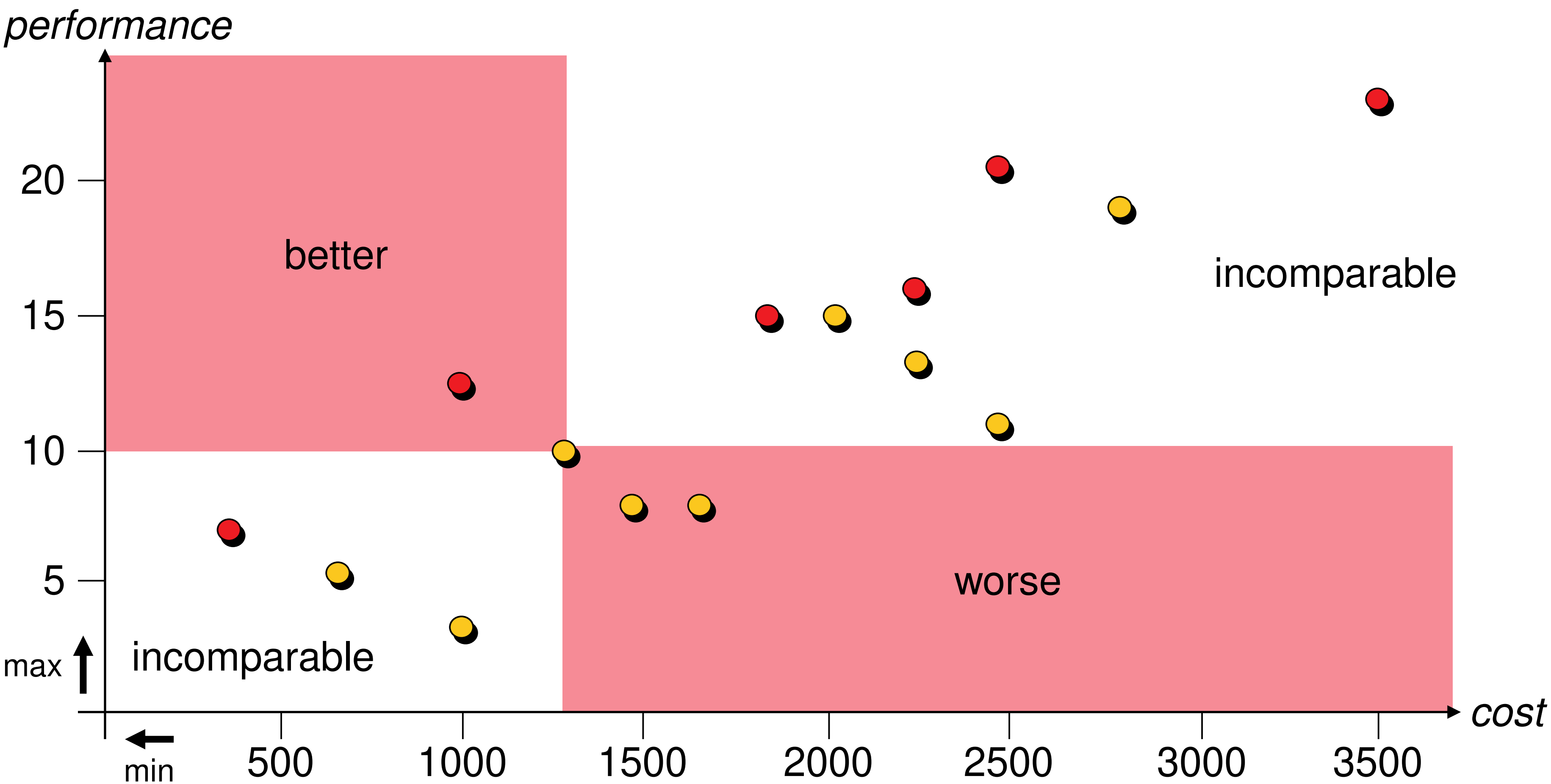
(Evolutionary)
Multiobjective Optimization

Multiobjective Optimization

Multiple objectives that have to be optimized simultaneously

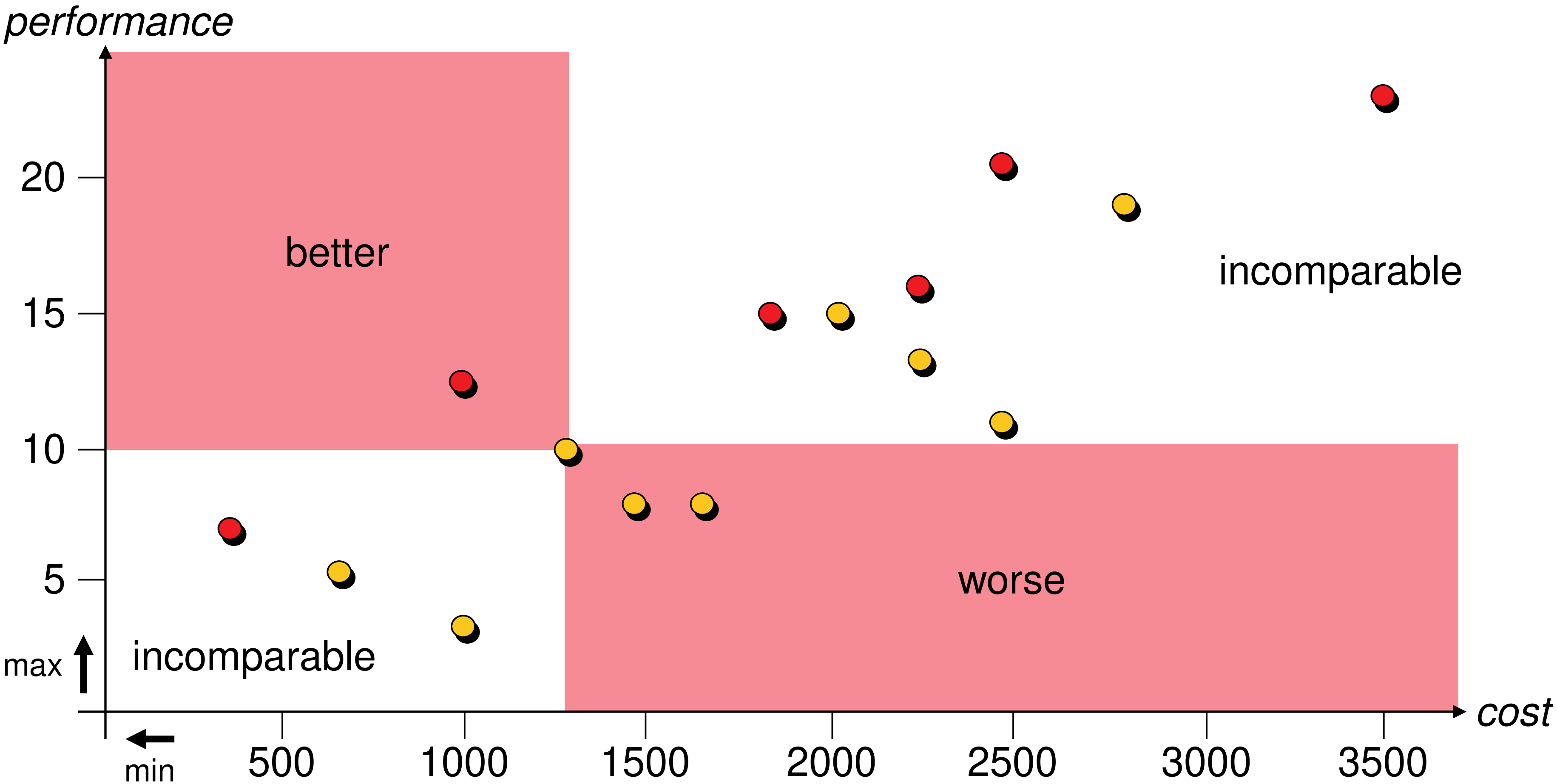


Observations: ❶ there is no single optimal solution, but
❷ some solutions (red) are better than others (yellow)



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

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



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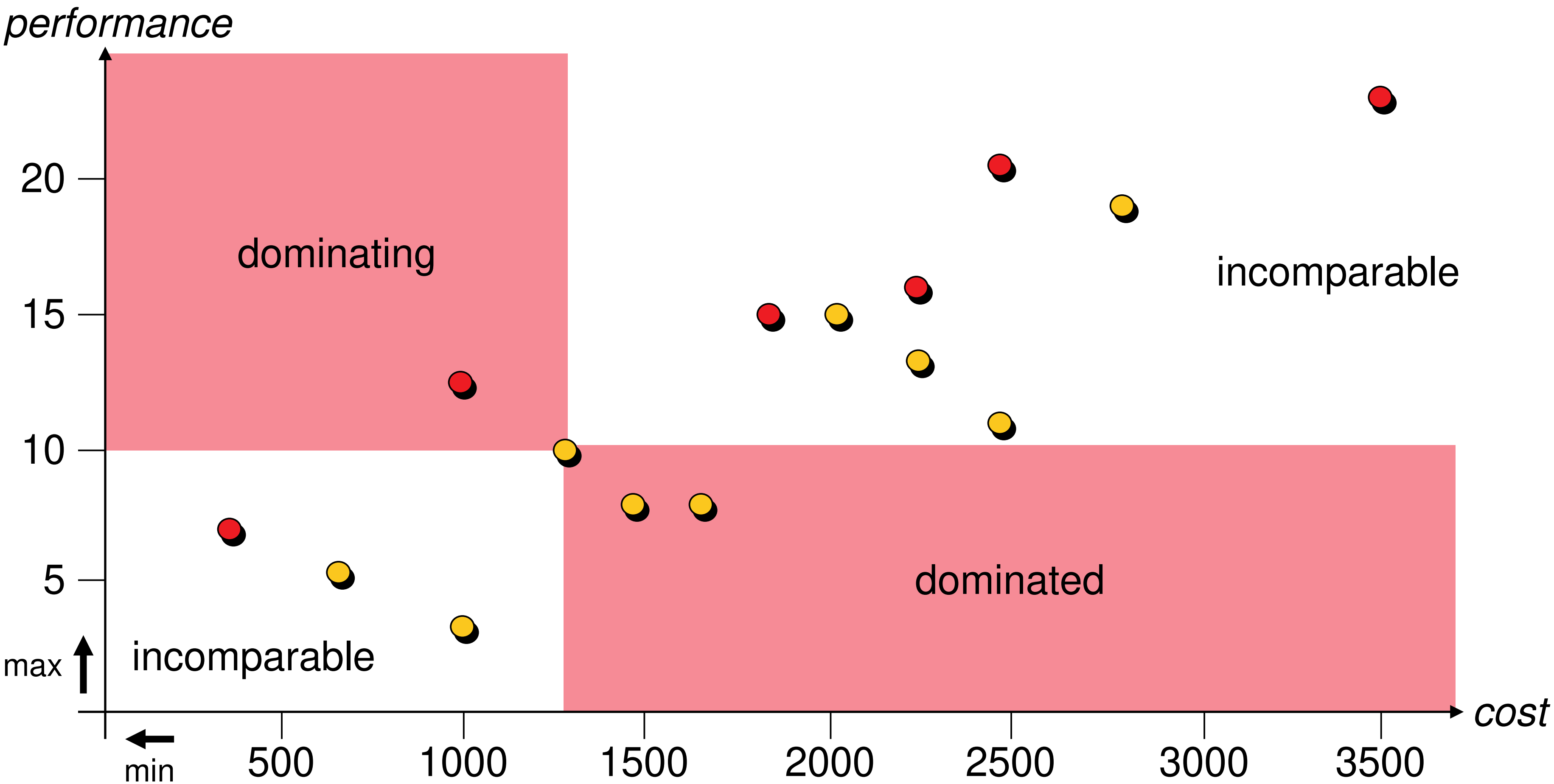


Exercise 1

Show the equivalence between

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

and

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

Exercise 2: Understanding Pareto Dominance

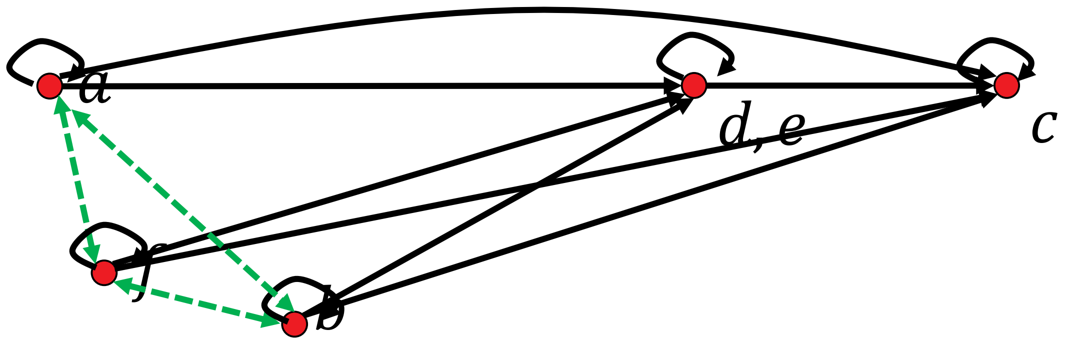
Given the following solutions, tell which ones dominate each other and which don't for the double sphere problem

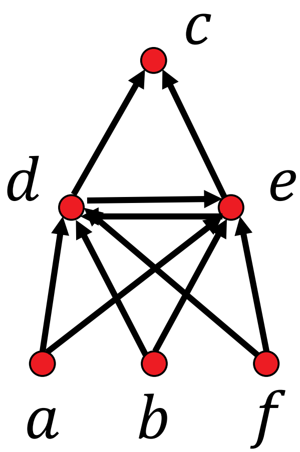
$$f_{\text{doublesphere}}: x \mapsto \left(\sum_{i=1}^{n} x_i^2\,,\ \sum_{i=1}^{n} (x_i - 1)^2\right).$$

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

Visualizing Dominance Relations as Graphs

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



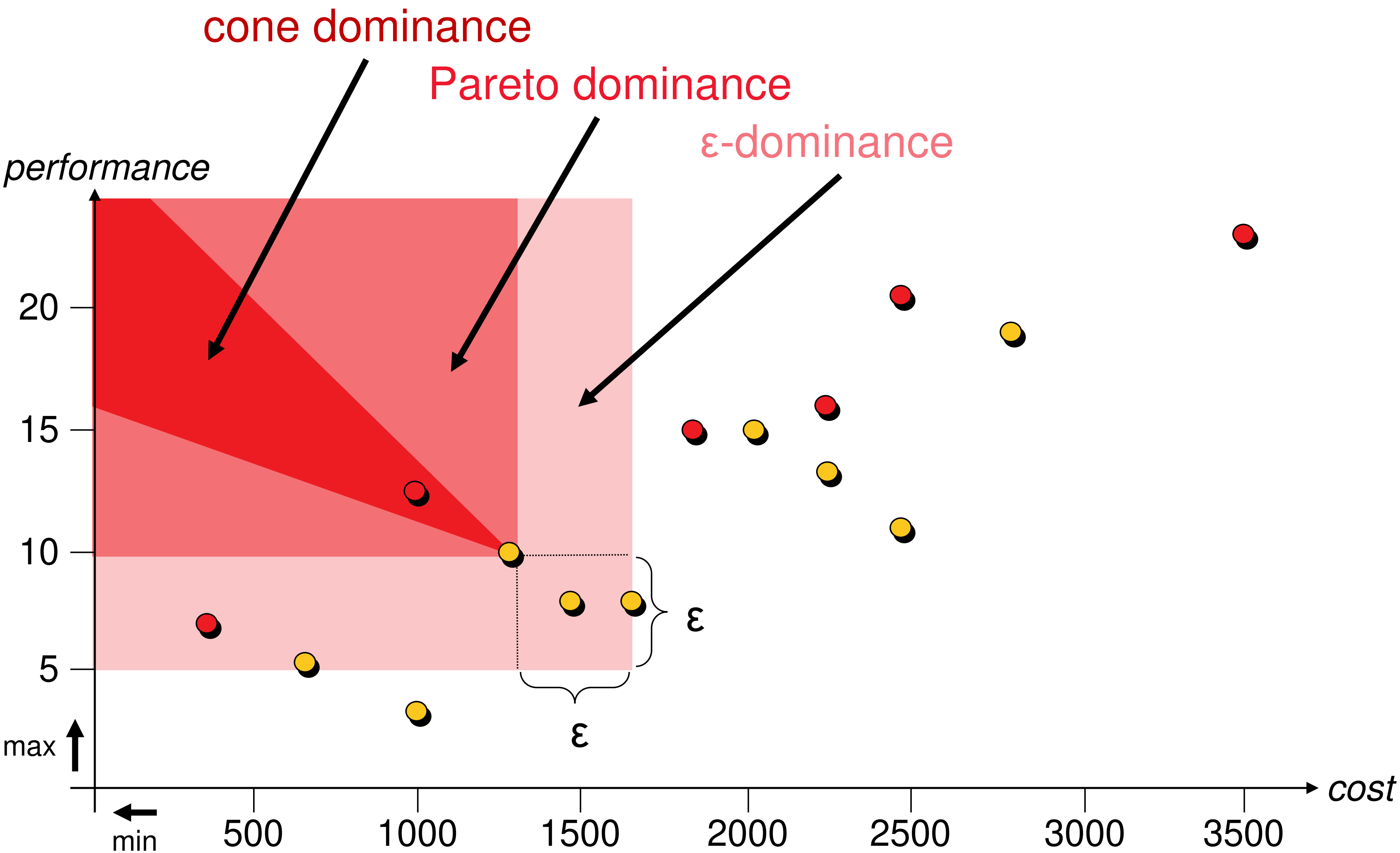


The weak Pareto dominance is a preorder, i.e. a relation that is

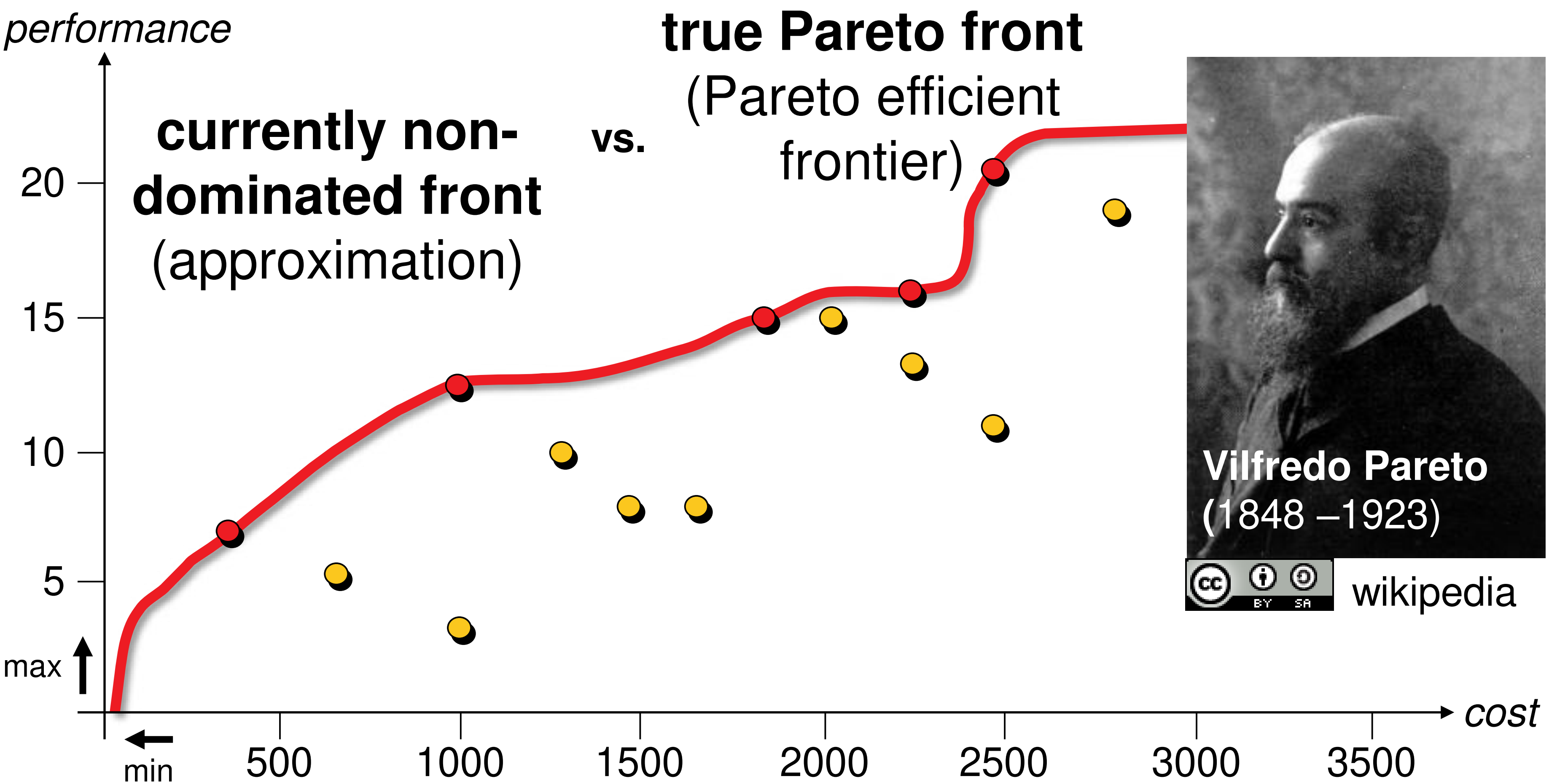
- reflexive and transitive
- minimal elements = Pareto-optimal solutions

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.

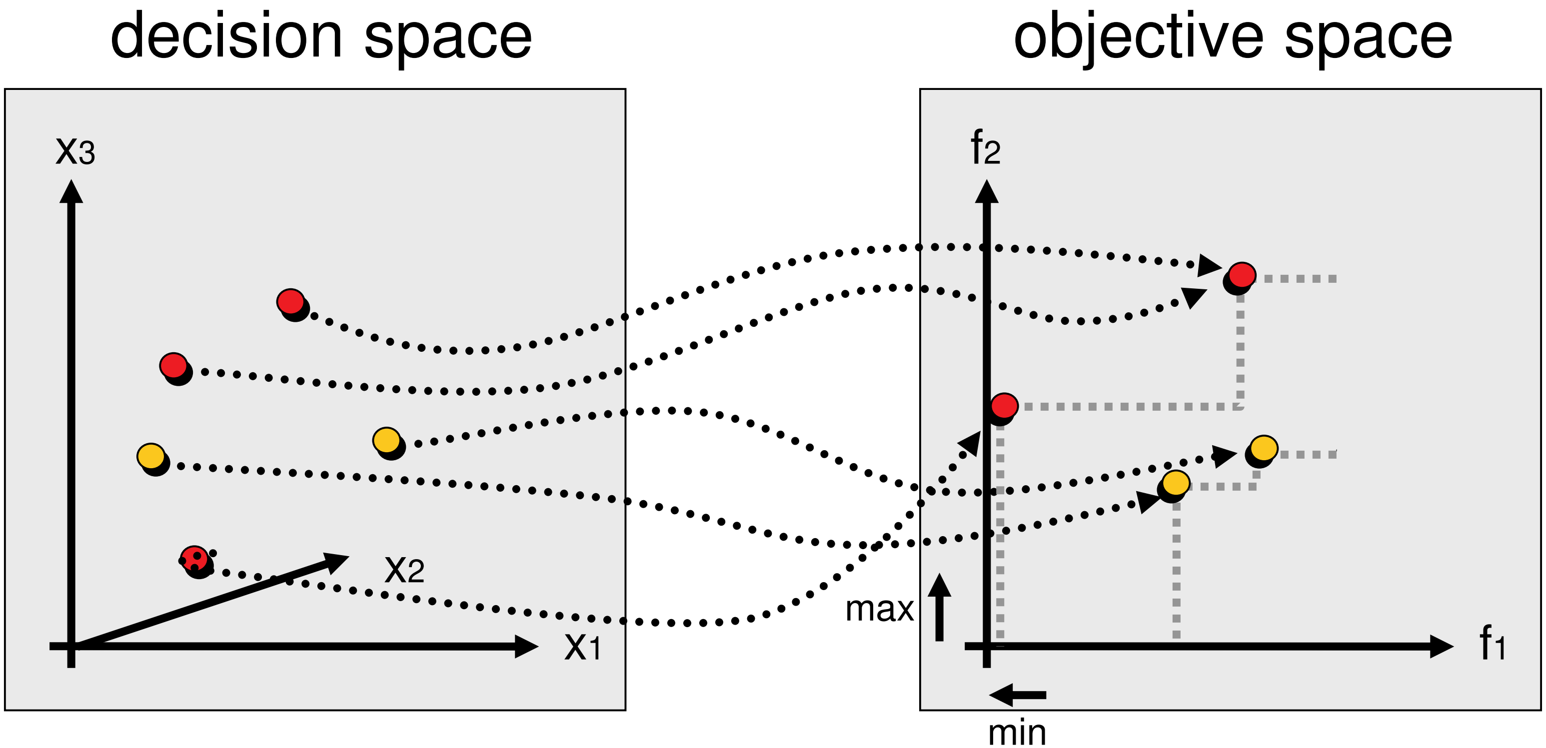
! The Pareto dominance itself is not reflexive and thus, never a poset!


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

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



wikipedia



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

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

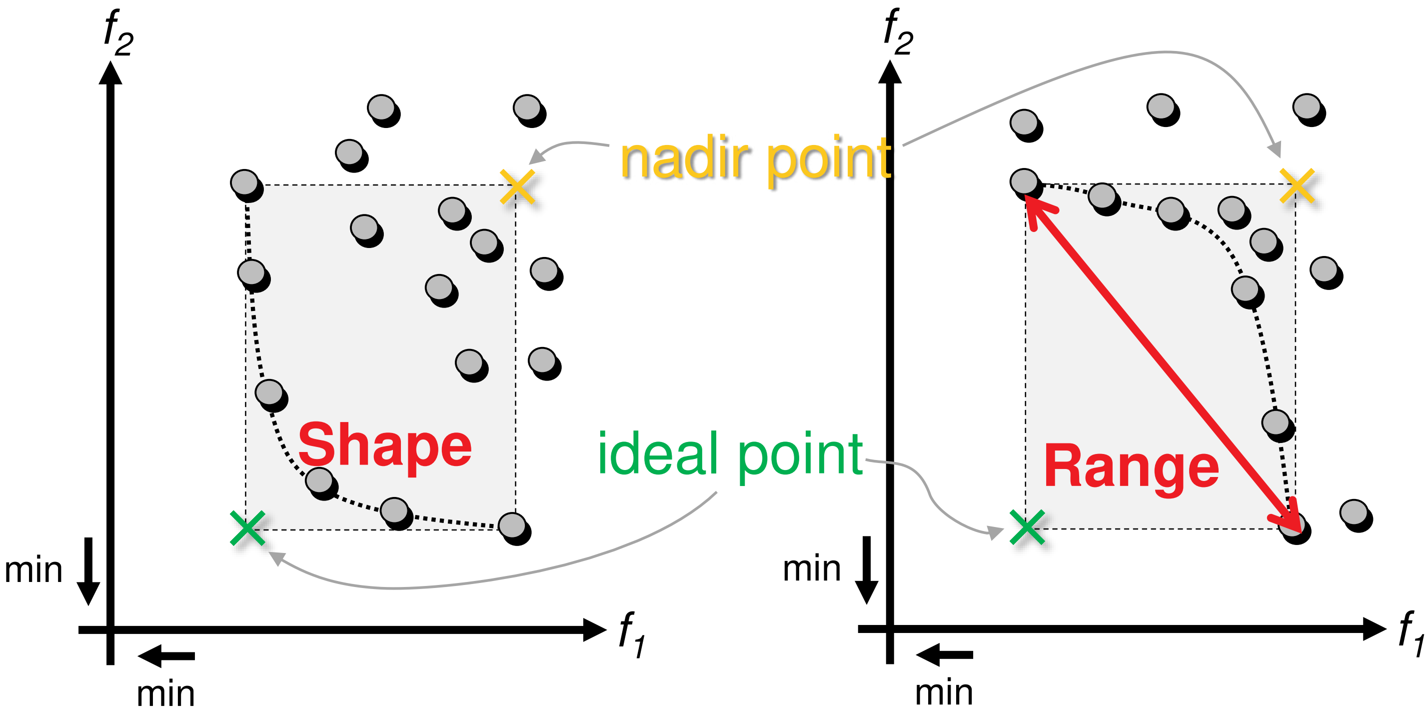
a) what is the Pareto set?

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)

Ideal and Nadir Point



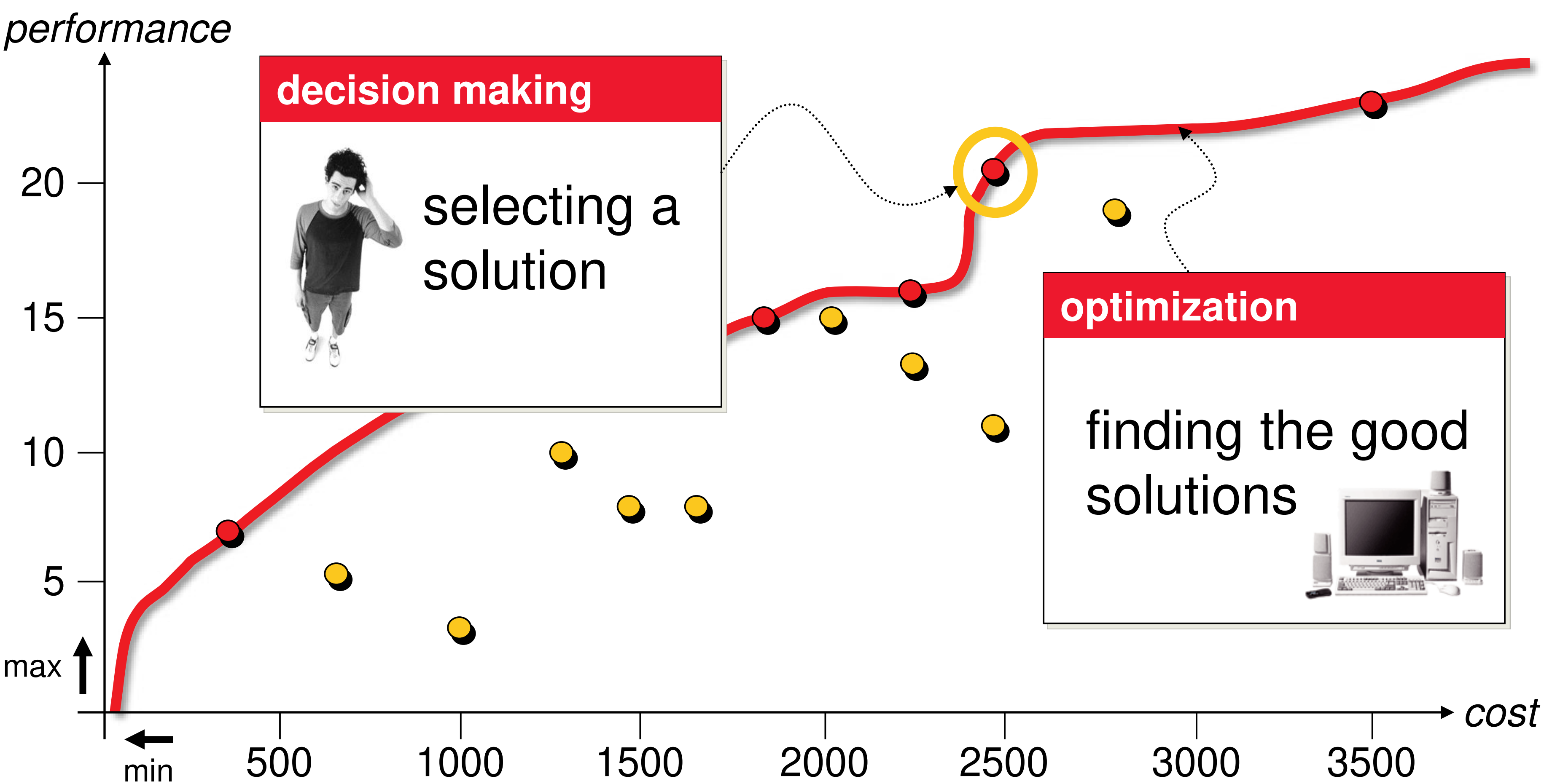
ideal point: best values
nadir point: worst values

} obtained for *Pareto-optimal* points

Optimization vs. Decision Making

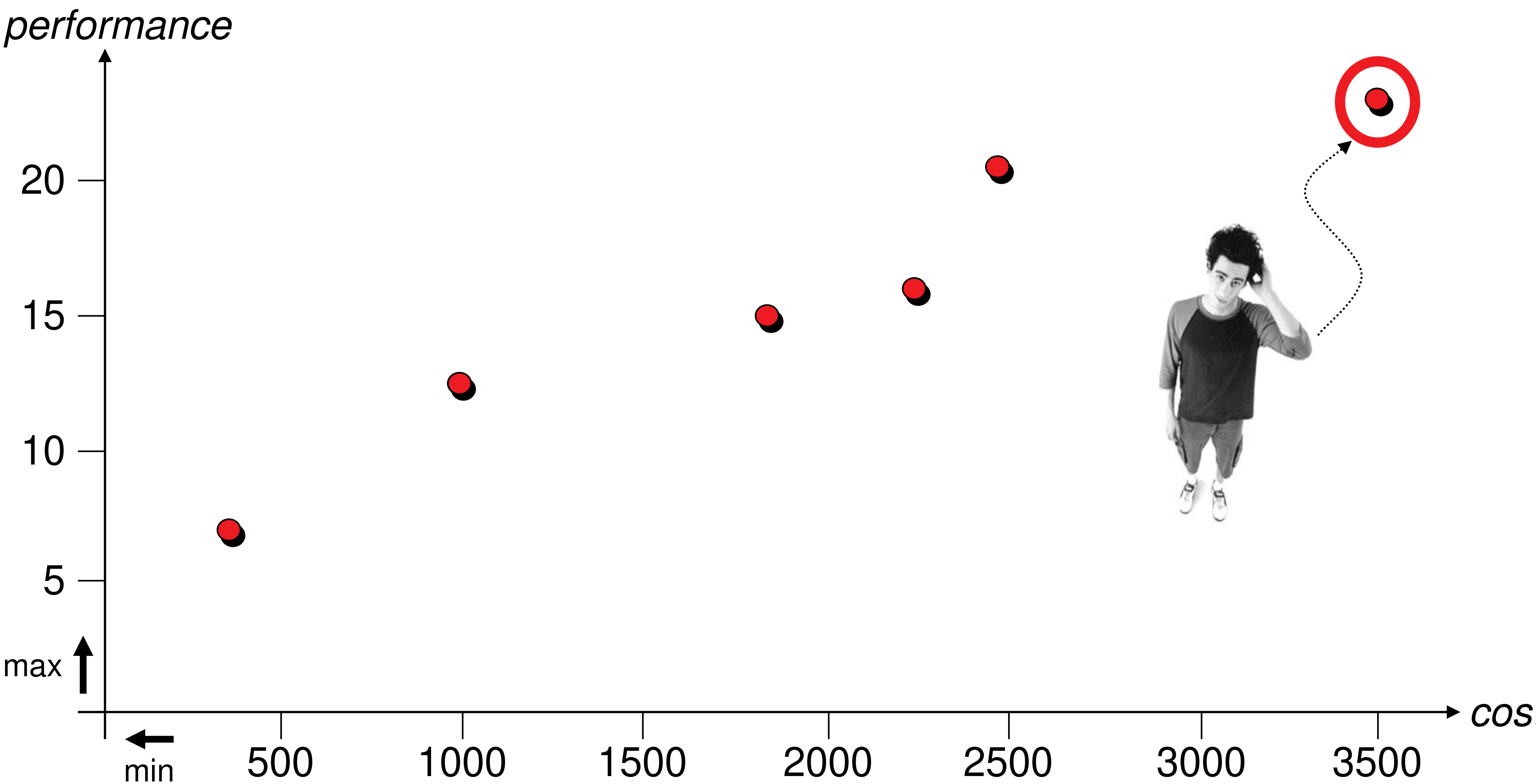
Multiobjective Optimization

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



Possible Approaches:

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

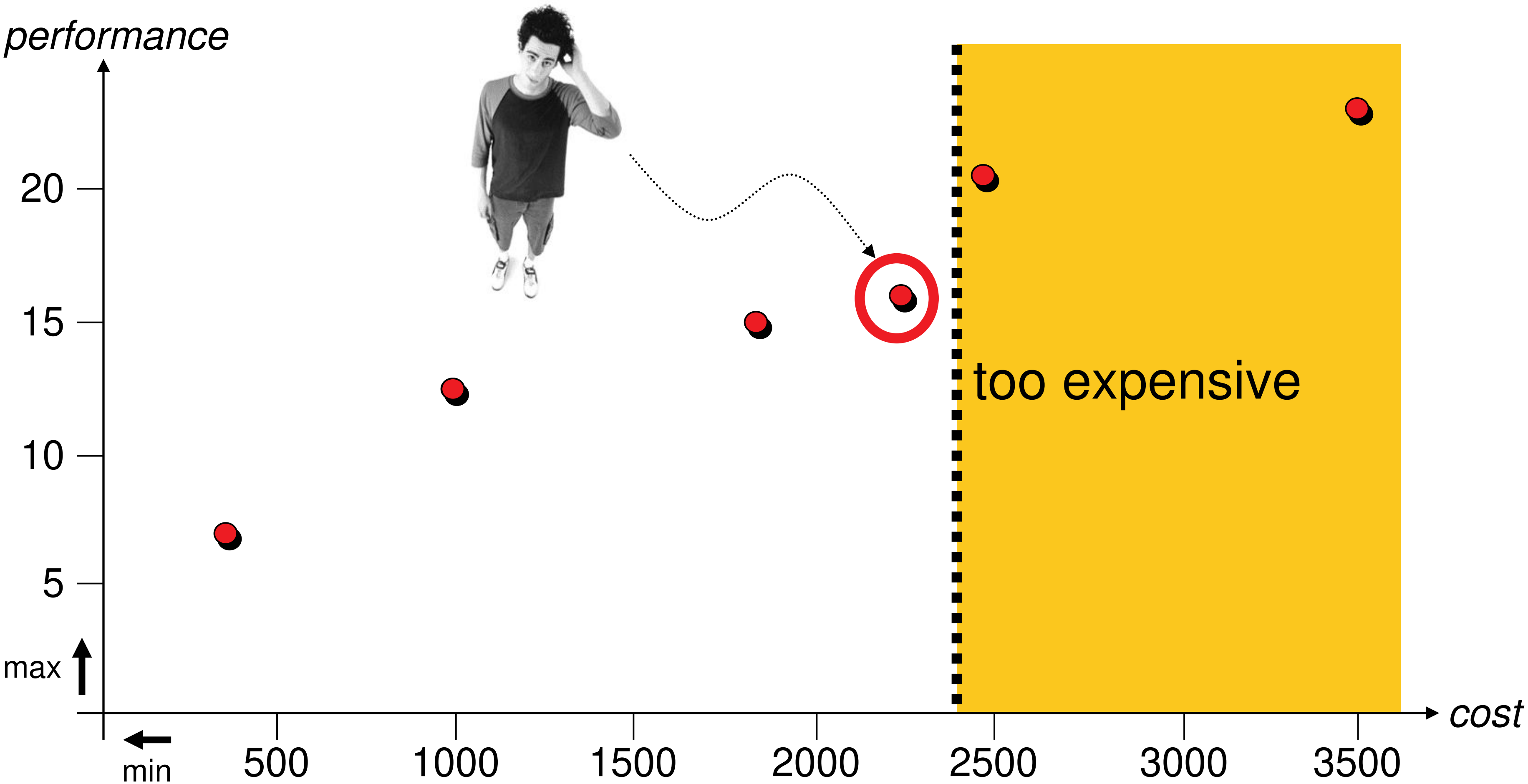


Selecting a Solution: Examples

Possible Approaches:

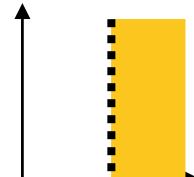
❶ ranking: performance more important than cost

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

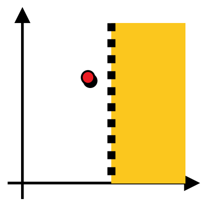


Before Optimization:

rank objectives,
define constraints,…



search for one
(good) solution



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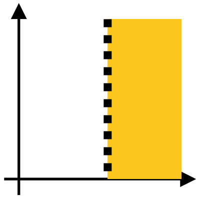

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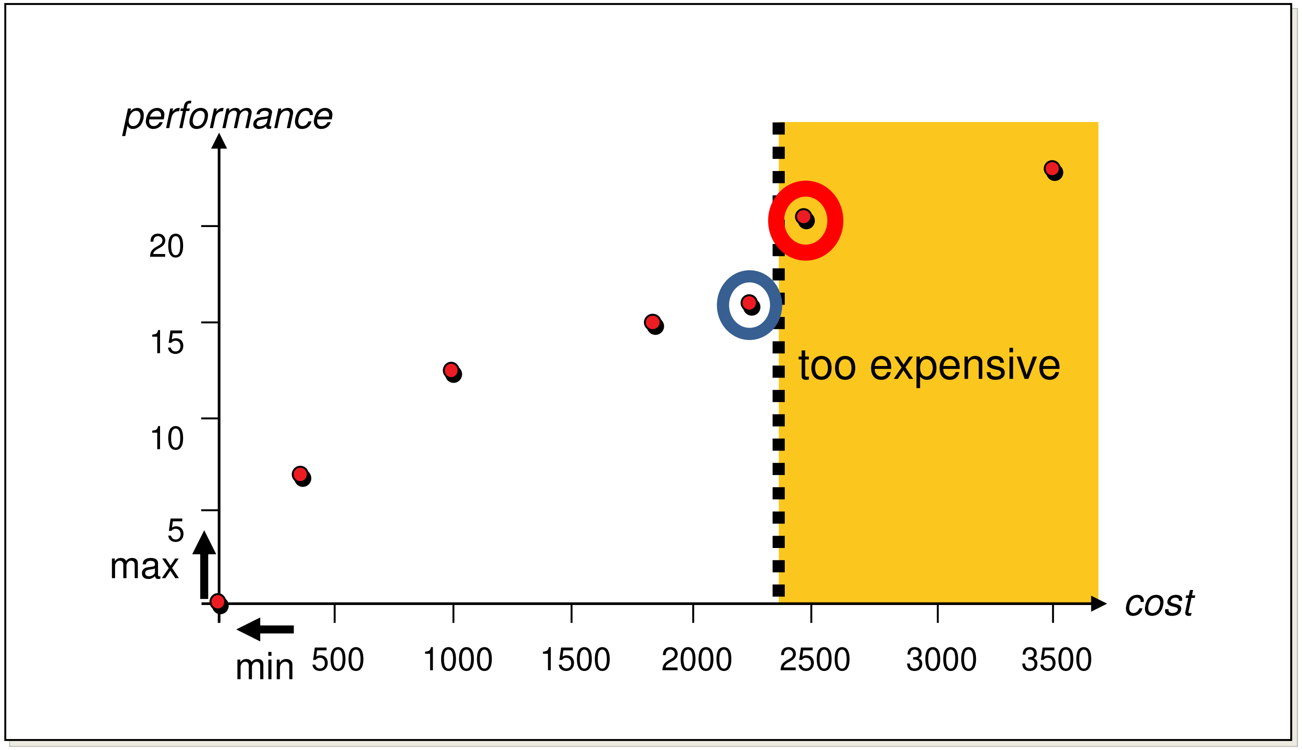
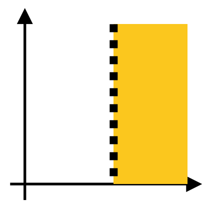


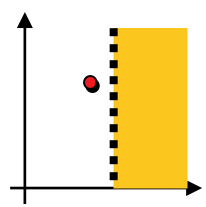
When to Make the Decision

Before Optimization:

rank objectives,
define constraints,…

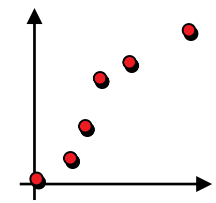


search for one
(good) solution

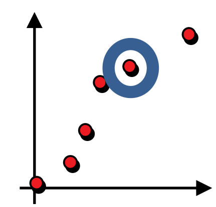


After Optimization:

search for a set of
(good) solutions



select one solution
considering
constraints, etc.



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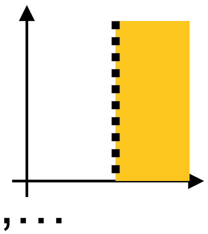

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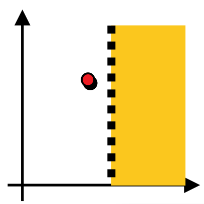

After Optimization:

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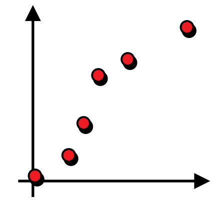

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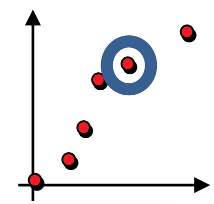


Focus: learning about a problem

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

Two Communities...

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

- 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

One of the Main Differences

Blackbox optimization

$$x \in X \longrightarrow \boxed{f} \longrightarrow (f_1(x), \dots, f_k(x))$$

only mild assumptions

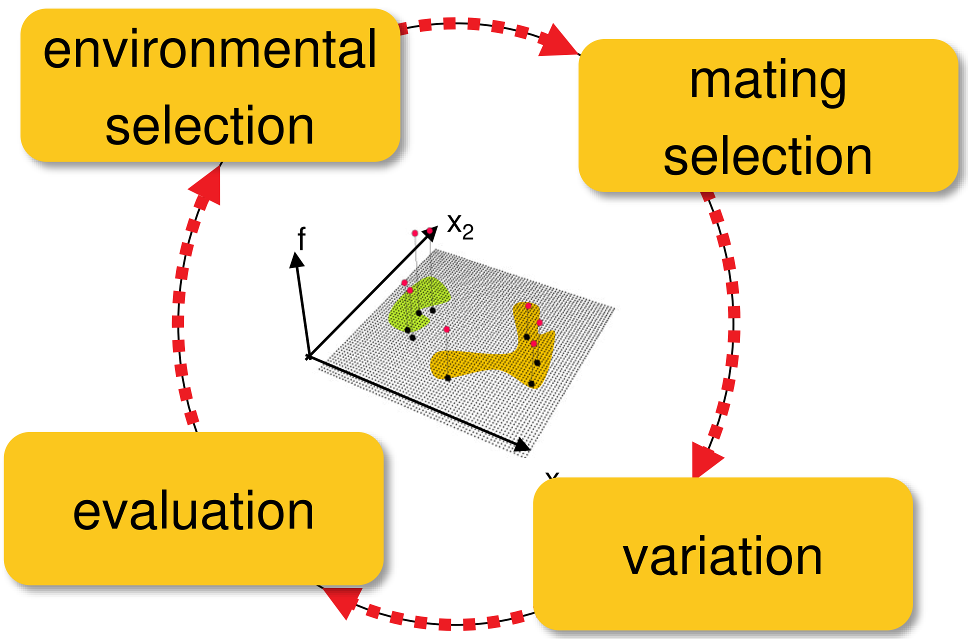
→ EMO therefore well-suited for real-world engineering problems

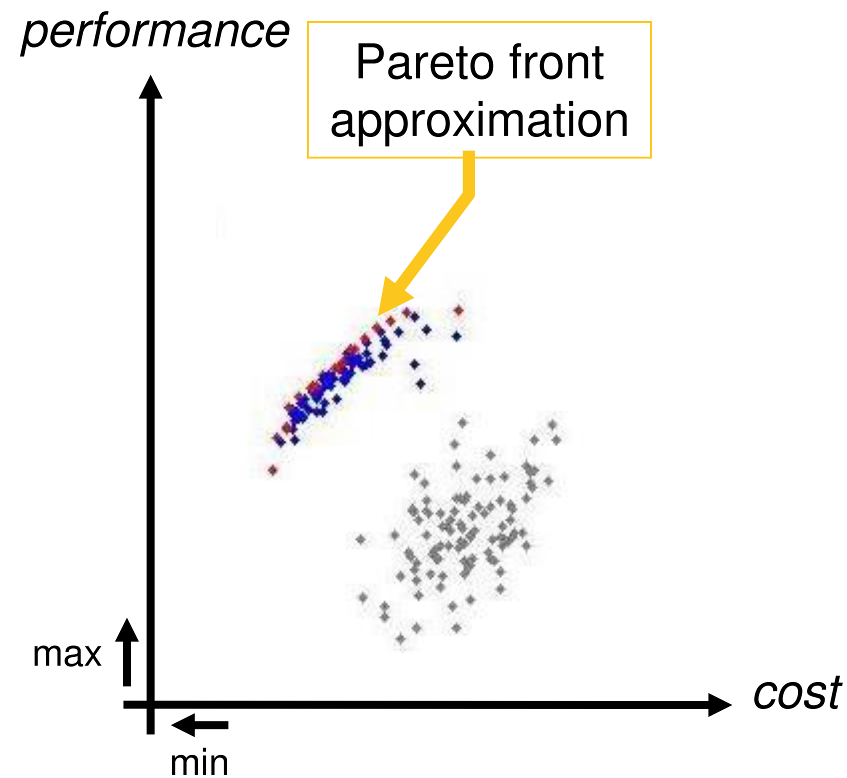
objectives
- non-linear
- noisy
- uncertain
- non-differentiable
- expensive (integrated simulations, real experiments)

problem
- many objectives
- huge search spaces
- many constraints

Evolutionary Multiobjective Optimization

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

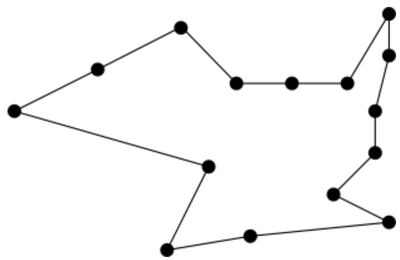




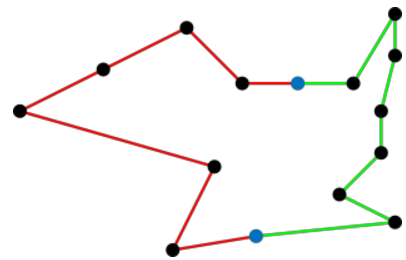
Multiobjectivization

Some problems are easier to solve in a multiobjective scenario

example: TSP
[Knowles et al. 2001]



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



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

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], ...

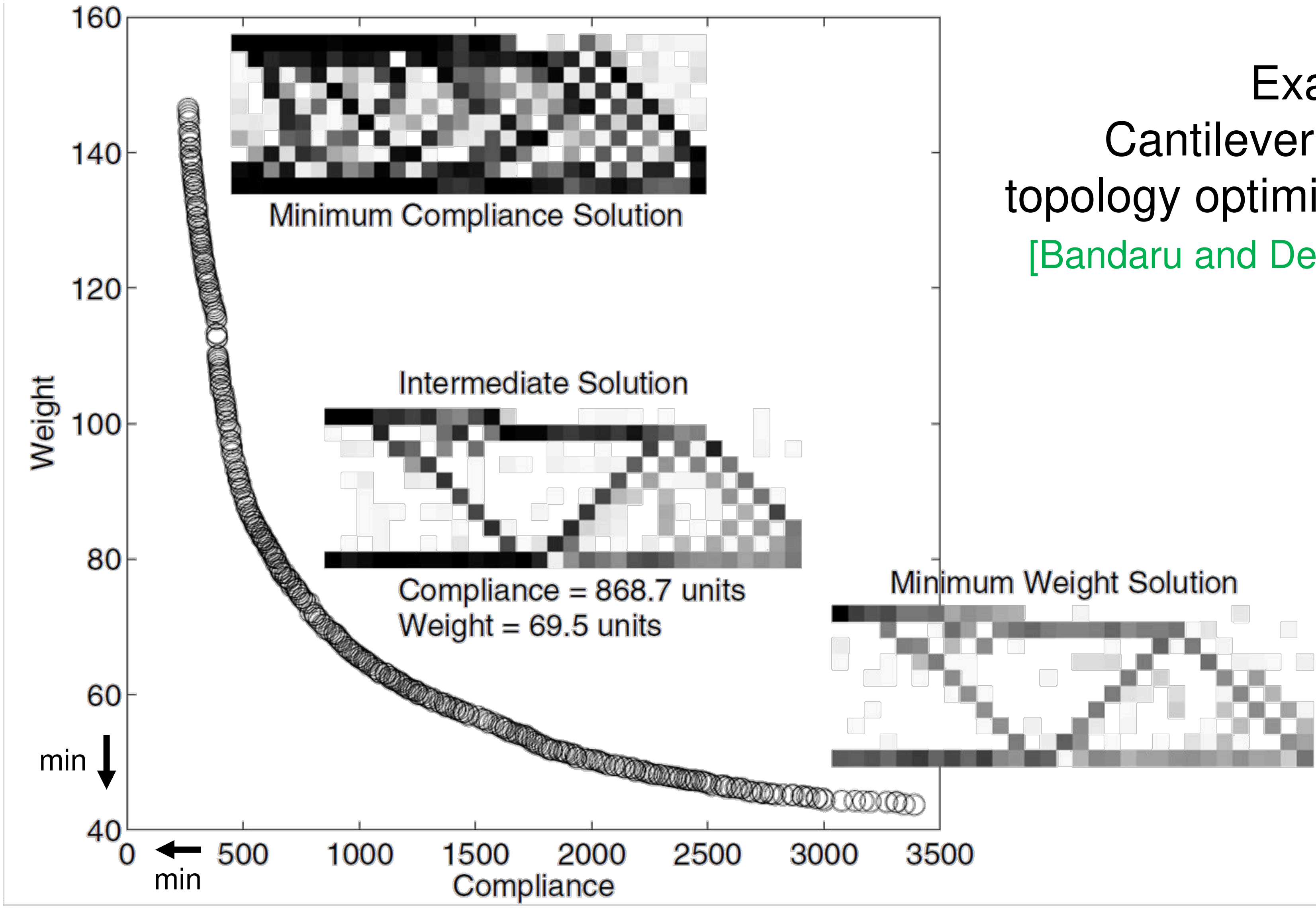
also backed up by theory e.g. [Brockhoff et al. 2009, Handl et al. 2008b]

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

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

Innovization

Often innovative design principles among solutions are found



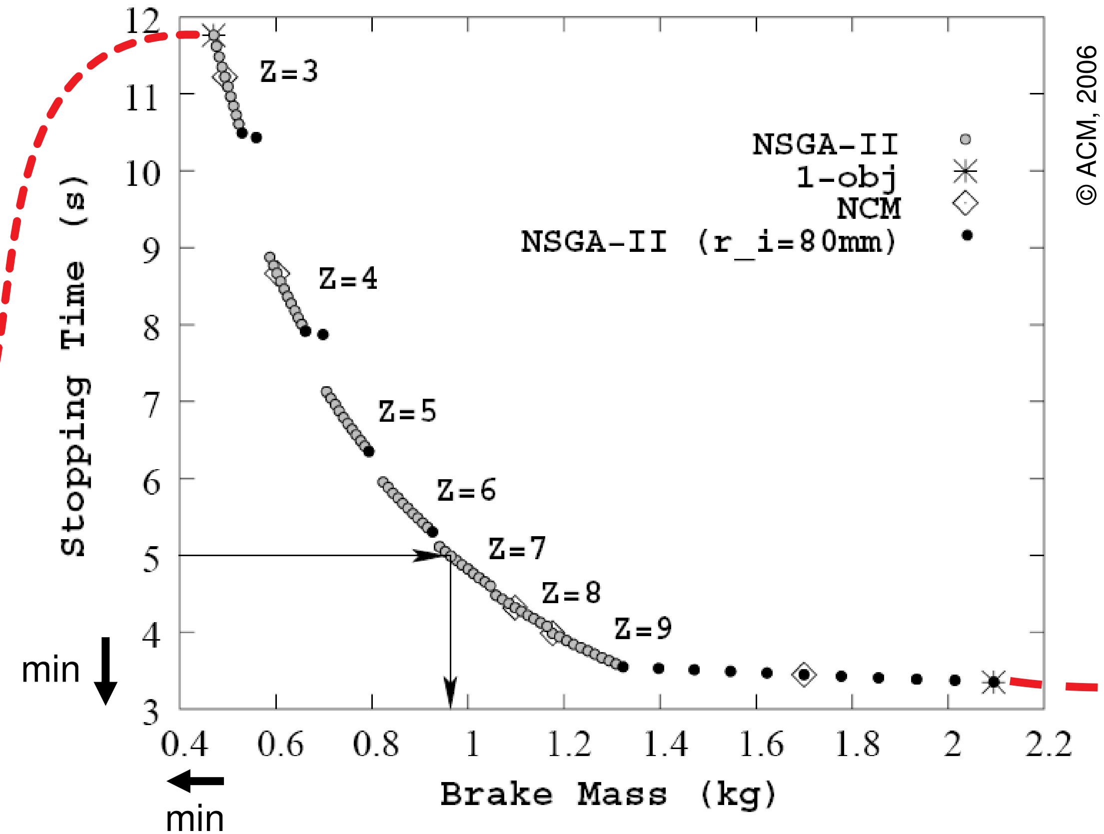
Example:
Cantilever beam
topology optimization
[Bandaru and Deb 2015]

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]

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Approaches to Multiobjective Optimization

aggregation-based

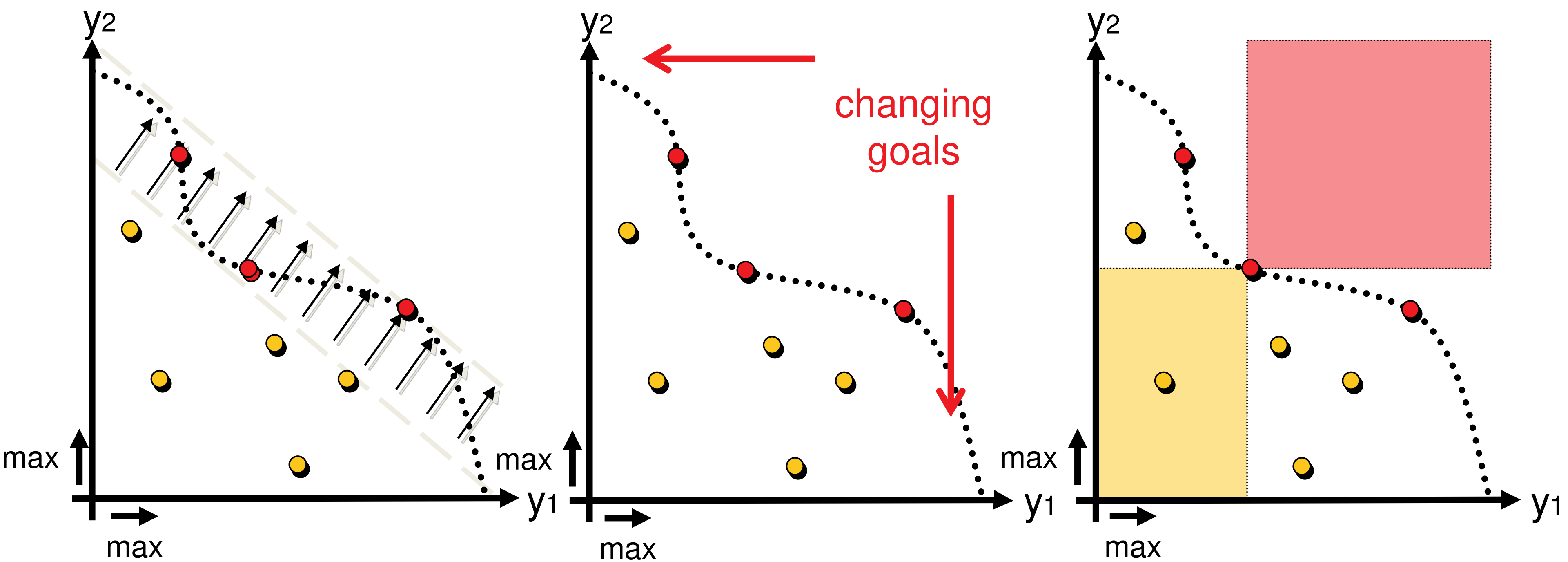
problem decomposition (multiple single-objective optimization problems)

criterion-based

VEGA

dominance-based

SPEA2, NSGA-II "modern" EMOA



solution-oriented
scaling-dependent

set-oriented
less scaling-independent

Solution-Oriented Problem Transformations

parameters

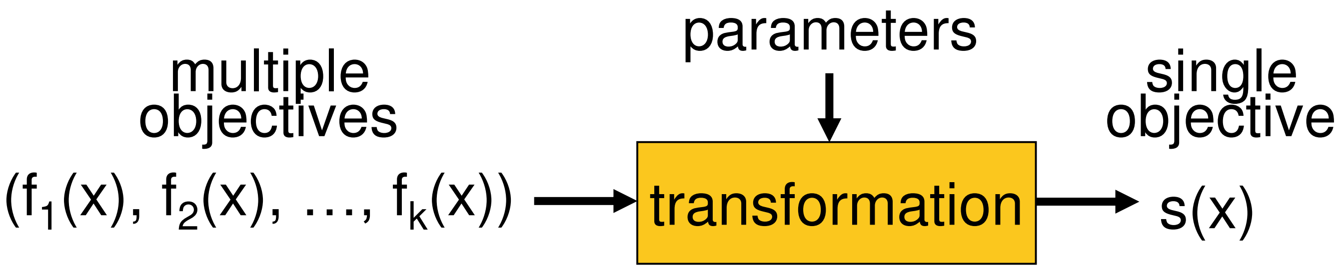
multiple objectives

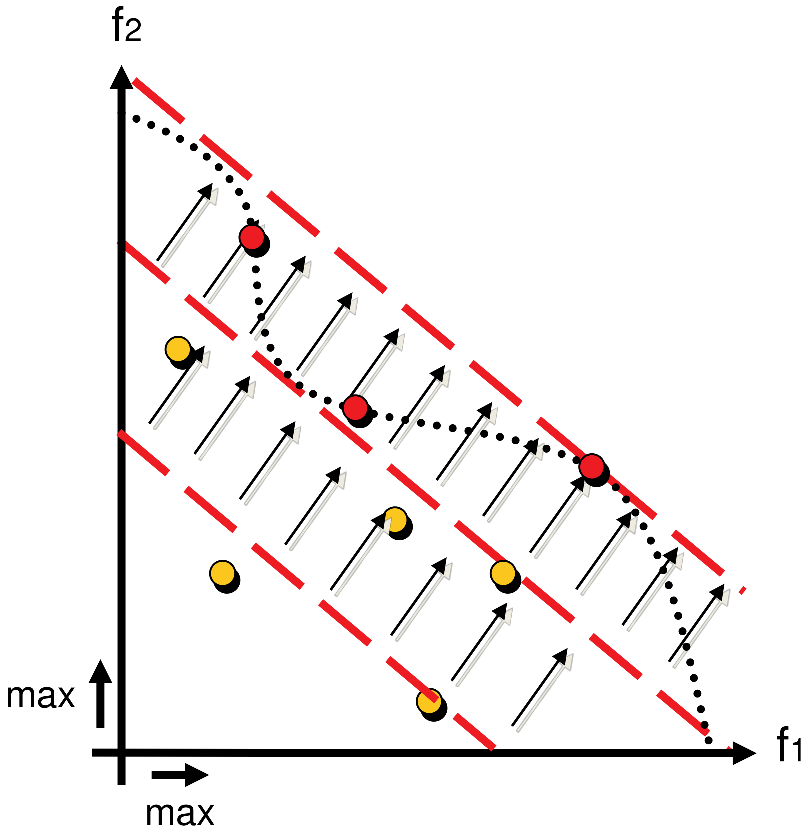
$(f_1(x), f_2(x), \ldots, f_k(x)) \longrightarrow \boxed{\text{transformation}} \longrightarrow s(x)$

single objective

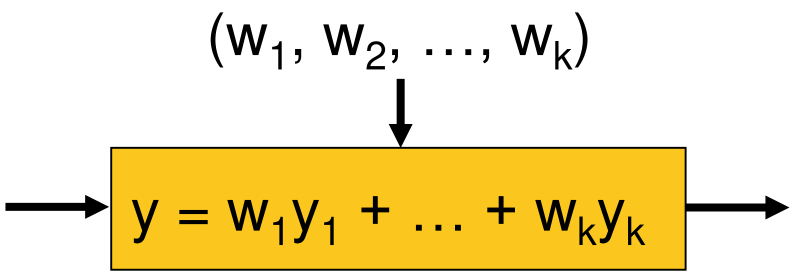
A scalarizing function s is a function $s : Z \rightarrow \mathbb{R}$ that maps each objective vector $u = (u_1, \ldots, u_n) \in Z$ to a real value $s(u) \in \mathbb{R}$

Solution-Oriented Problem Transformations

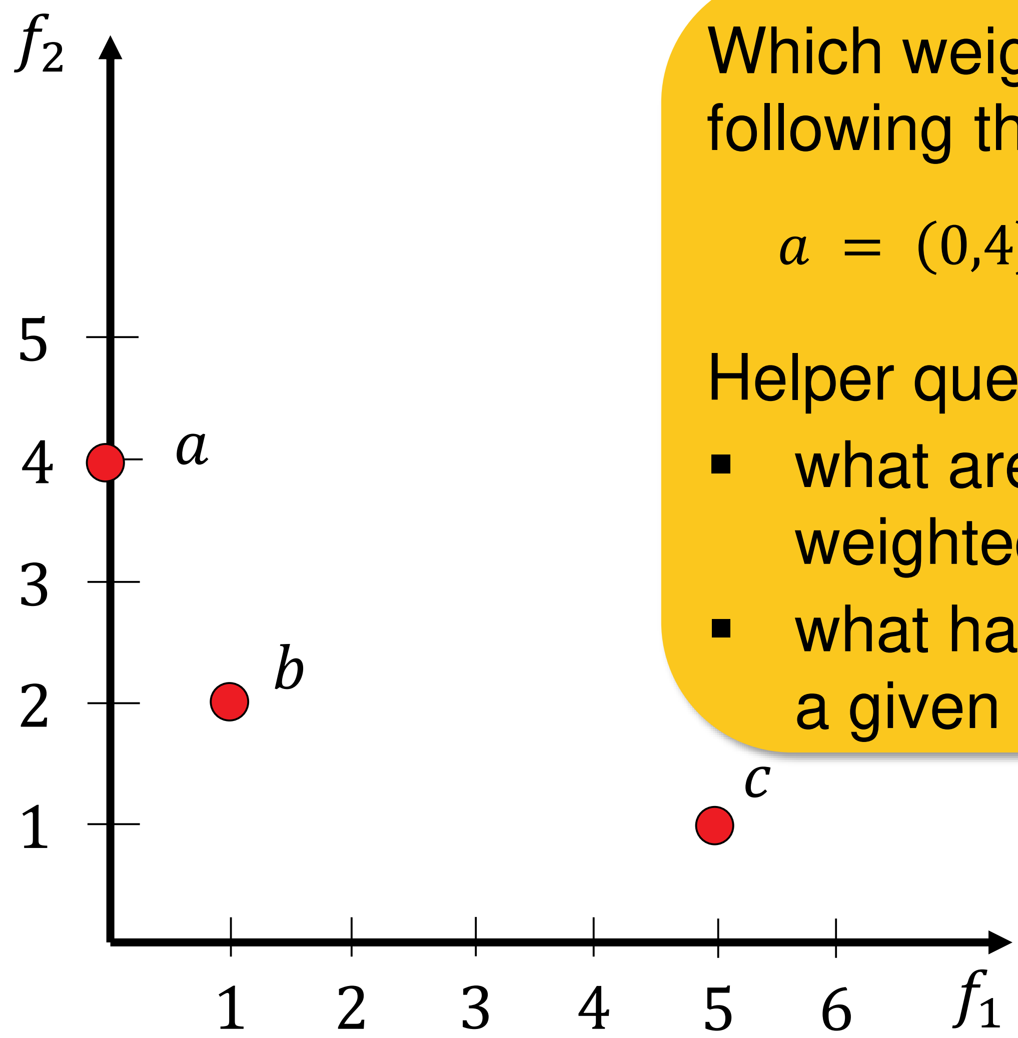




Example 1: weighted sum approach



Exercise 4: Weighted Sum



Which weights are optimal for the following three points?

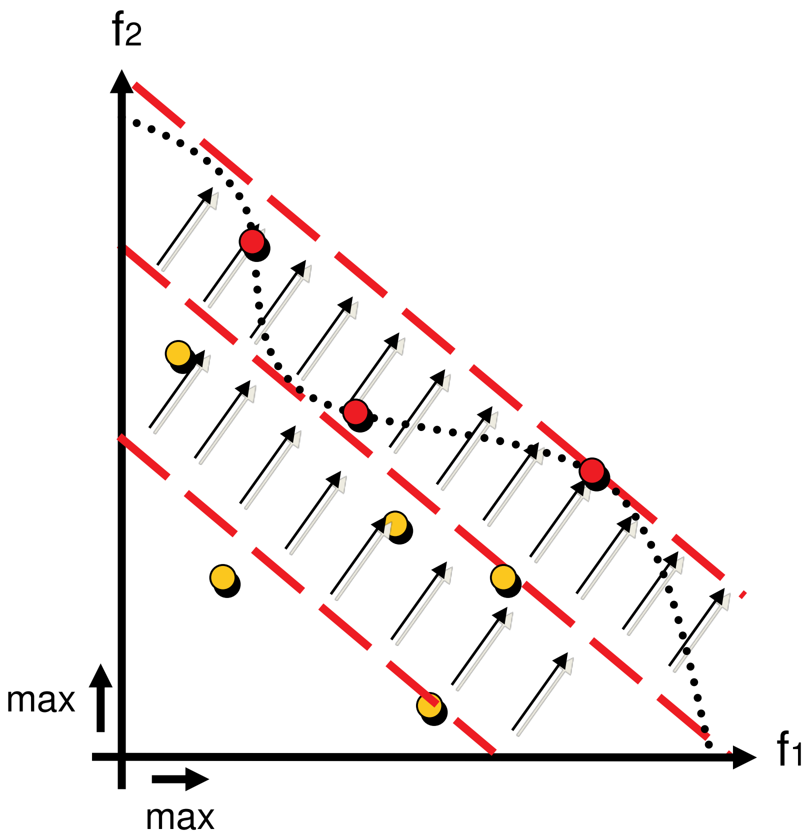
$$a = (0,4) \quad b = (1,2) \quad c = (5,1)$$

Helper questions:

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

multiple objectives

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



Example 1: weighted sum approach

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

→ $y = w_1y_1 + \ldots + w_ky_k$ →

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

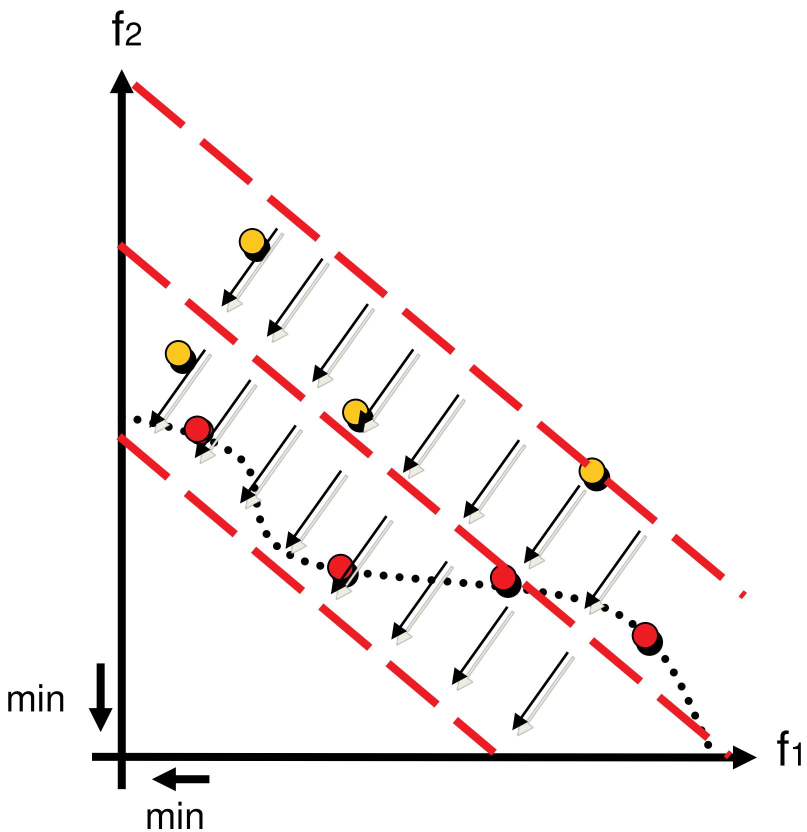
Solution-Oriented Problem Transformations

multiple objectives

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

parameters

single objective



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Solution-Oriented Problem Transformations

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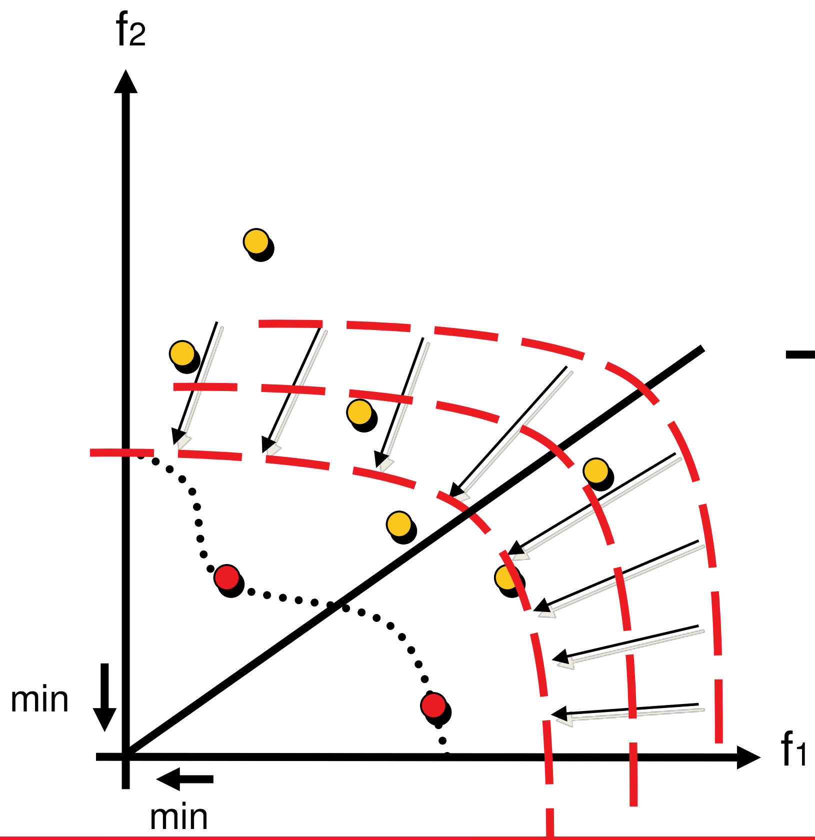


Example 2: weighted p-norm

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

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

$p = 1$: weighted sum

$p = \infty$: weighted Tchebycheff

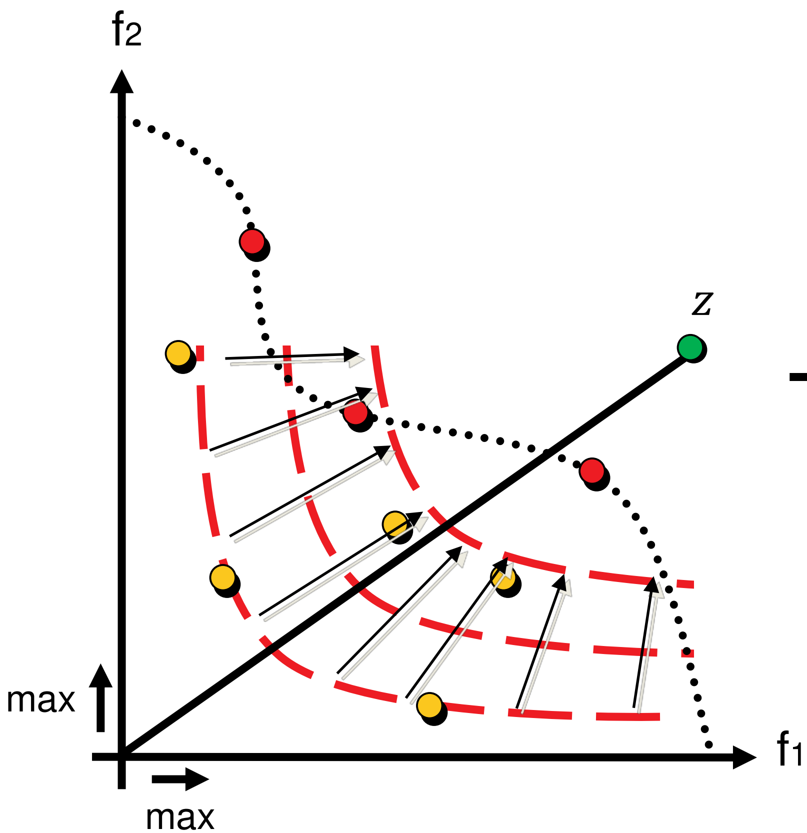
Solution-Oriented Problem Transformations

parameters

multiple objectives

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

single objective



Example 2: weighted p-norm

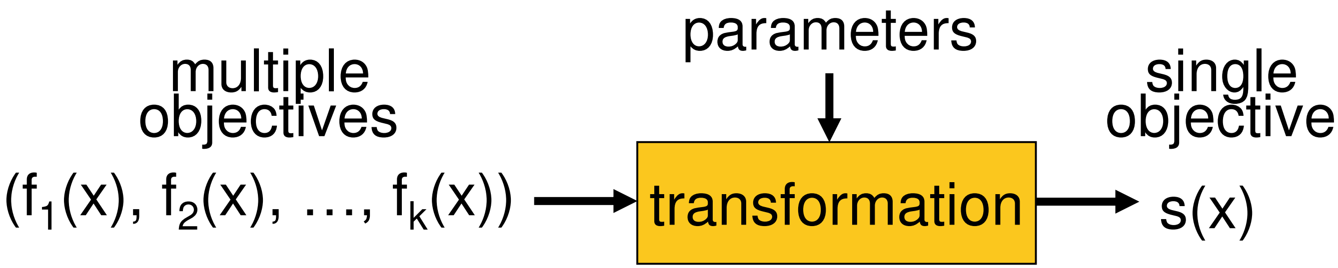
$(w_1, w_2, \ldots, w_k)$

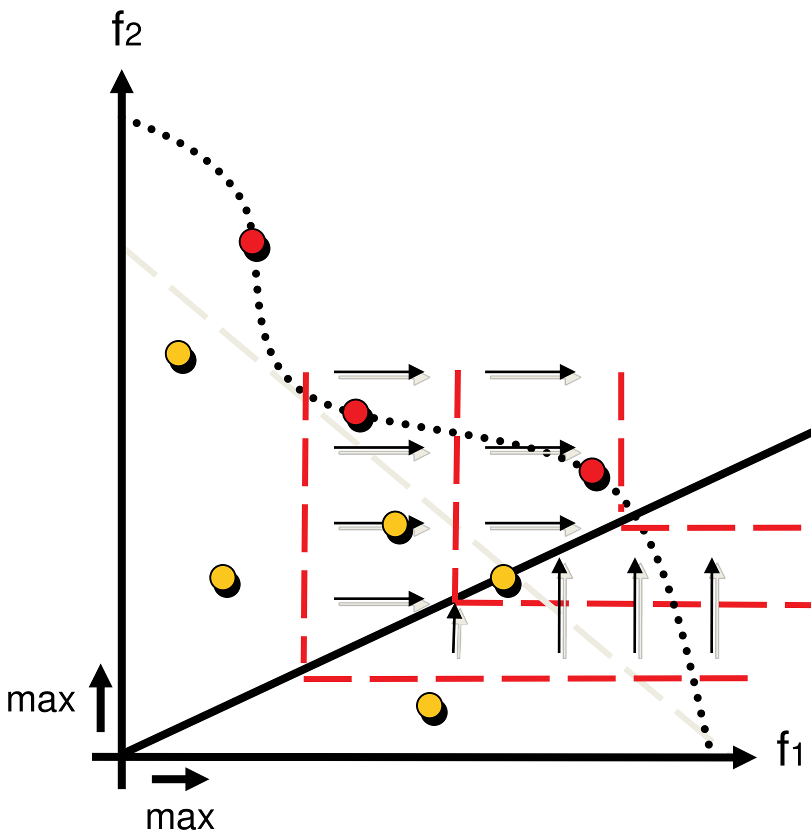
$$y = \sqrt[p]{\sum_{i=1}^{k} (|w_1(y_1 - z_i)|)^p}$$

$p = 1$: weighted sum

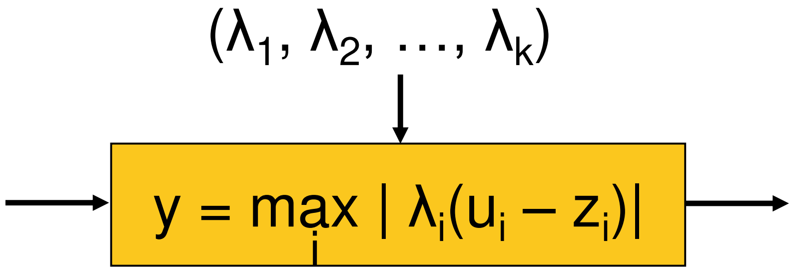
$p = \infty$: weighted Tchebycheff

Solution-Oriented Problem Transformations



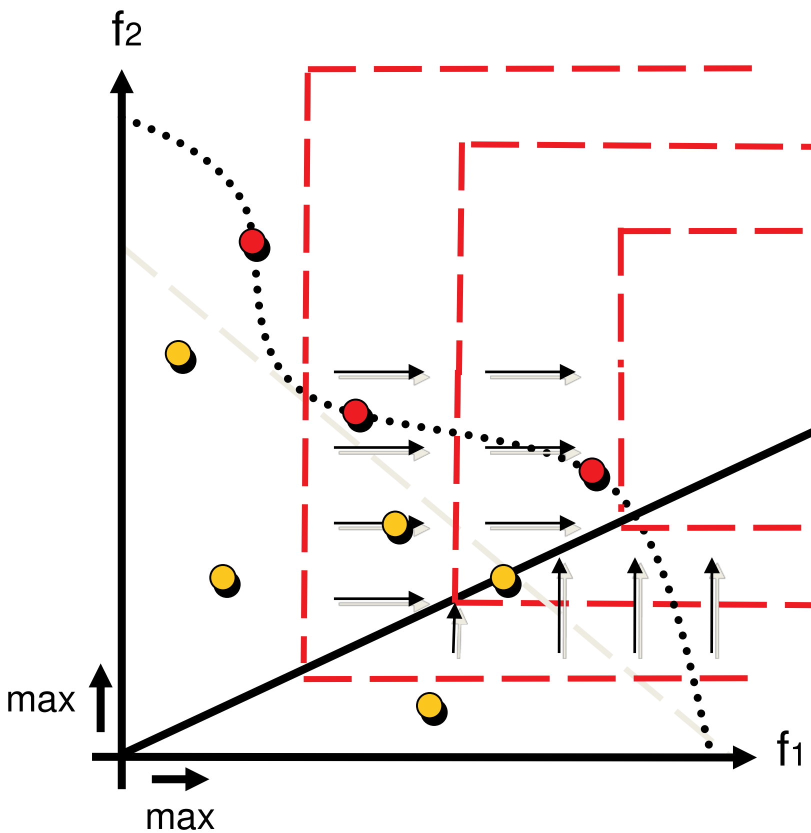


Example 2: weighted Tchebycheff



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

Code Walk: a Weighted Sum with CMA-ES

+ the Ask&Tell Interface to Optimization

Code Walk

Simple Implementation of a Weighted Sum Approach:

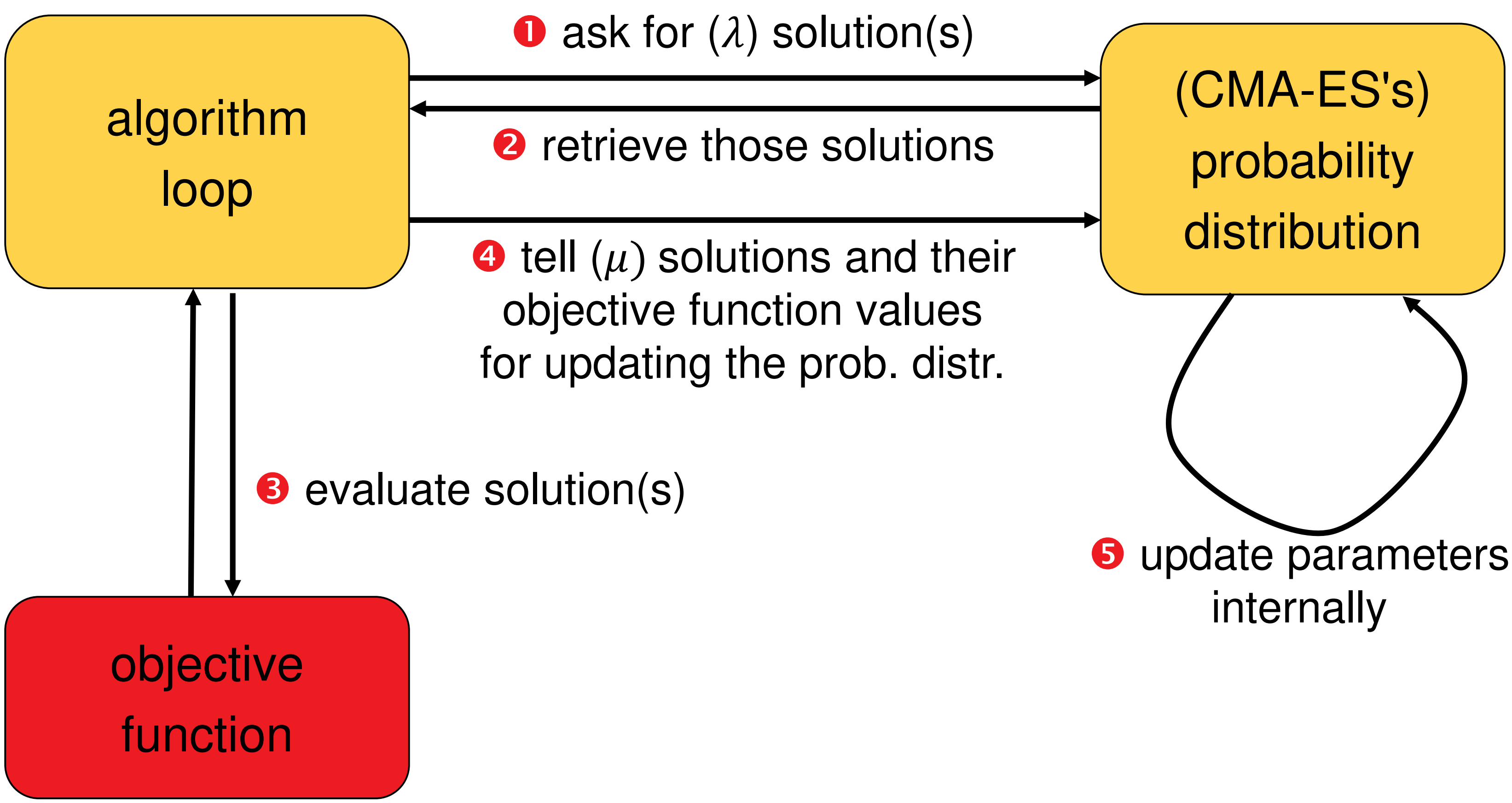
- N scalarizing functions, optimized by CMA-ES with restarts
- Python: use CMA-ES after `pip install cma` (more details here: `https://pypi.python.org/pypi/cma`)
- Assume COCO interface to objective function (later today)
- use ask and tell interface (next slide)
- CMA-ES parameters as default (with $\sigma_{init} \approx 30\%$ of initial search range)
- would need to be improved in practice:
  - how to normalize the objectives and estimate z?
  - in which order do we optimize the N scalarizing functions?
  - how to smartly distribute the budget?
  - intertwine restarts
  - ...

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.fcts.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)



Code Walk: Weighted Sum

```
from __future__ import division
import cma

def weighted_sum_search(fun, budget):
    """Simplest weighted sum of N weights, optimized
       with CMA-ES.
    """
    N = 50 # number of different weights
    maxrunlength = (budget//N + 1) * fun.dimension

    curr_weight = 1
    while curr_weight >= 0:
        runCMAESWithWeightedSum(fun, curr_weight,
                                maxrunlength)
        curr_weight -= 1/(N-1)
        if curr_weight < 0 and curr_weight > -1e-15:
            curr_weight = 0
```

Code Walk: Optimizing Weighted Sum w/ CMA-ES

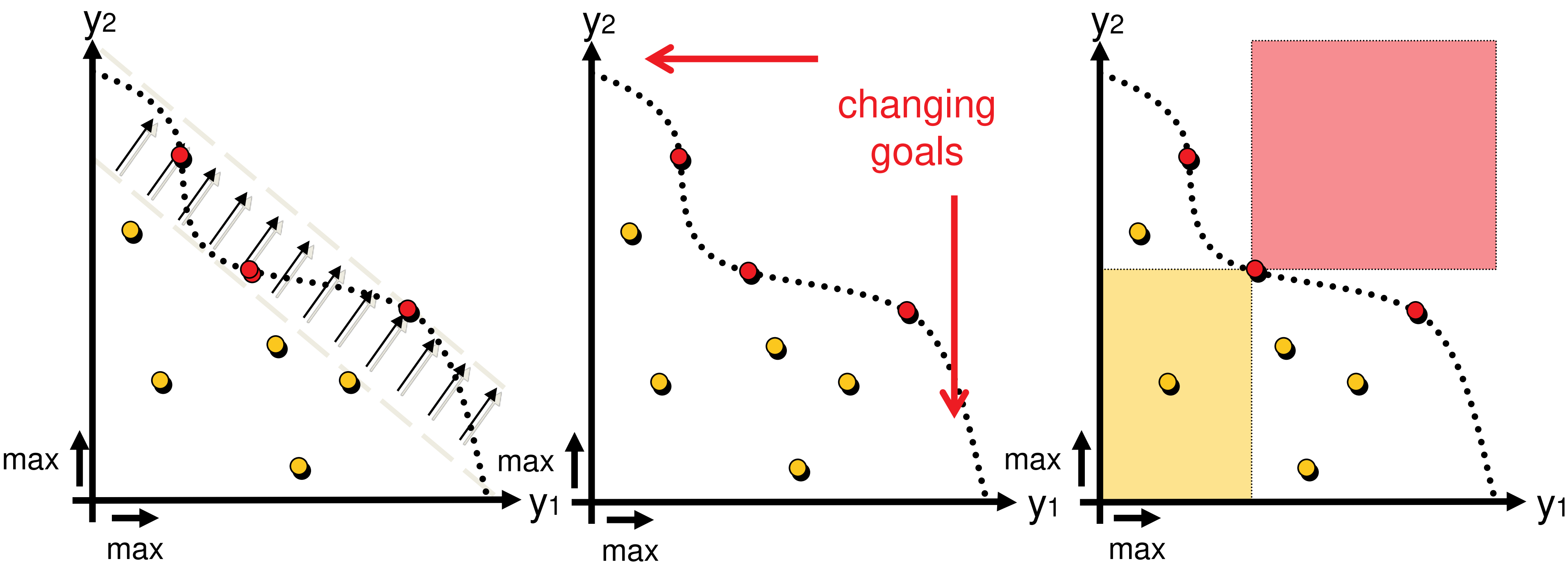
```
def runCMAESWithWeightedSum(fun, weight, budget):
    """ Restarted CMA-ES on weighted sum of fun"""

    while budget > 0:
        es = cma.CMAEvolutionStrategy(fun.dimension
        * [5] - 10*np.random.rand(fun.dimension), 3)
        while not es.stop() and budget > 0:
            solutions = es.ask()
            budget -= len(solutions)
            # evaluation:
            obj_vectors = np.array(
                            [fun(s) for s in solutions])
            # computation of weigted sum:
            F = (weight * obj_vectors[:,0] +
                       (1-weight) * obj_vectors[:,1])
            # update of strategy parameters
            es.tell(solutions, F)
```

Approaches to Multiobjective Optimization

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

criterion-based
VEGA

dominance-based
SPEA2, NSGA-II
"modern" EMOA

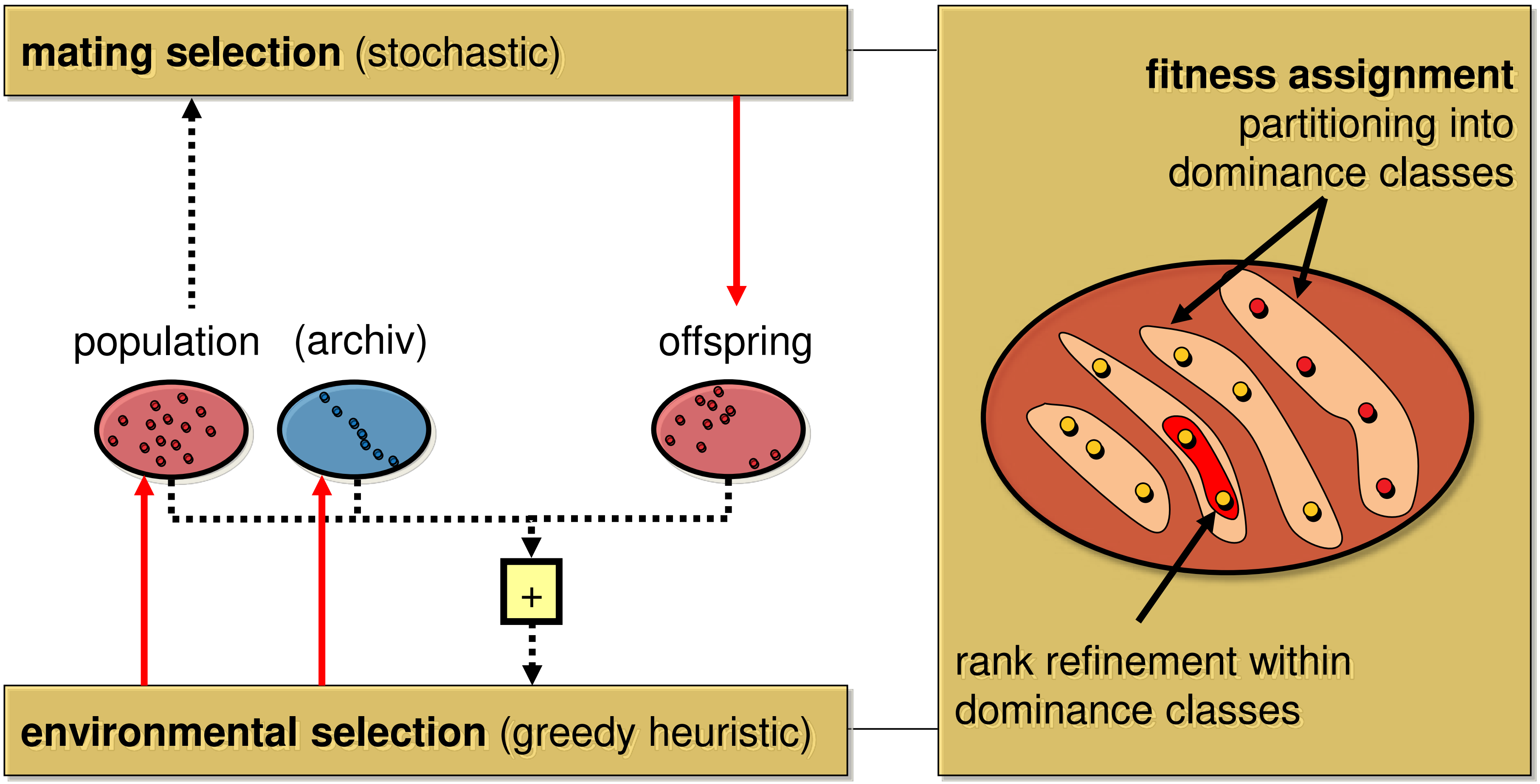


solution-oriented
scaling-dependent

set-oriented
less scaling-independent

Set-Oriented Approaches

General Scheme of Most Set-Oriented EMO

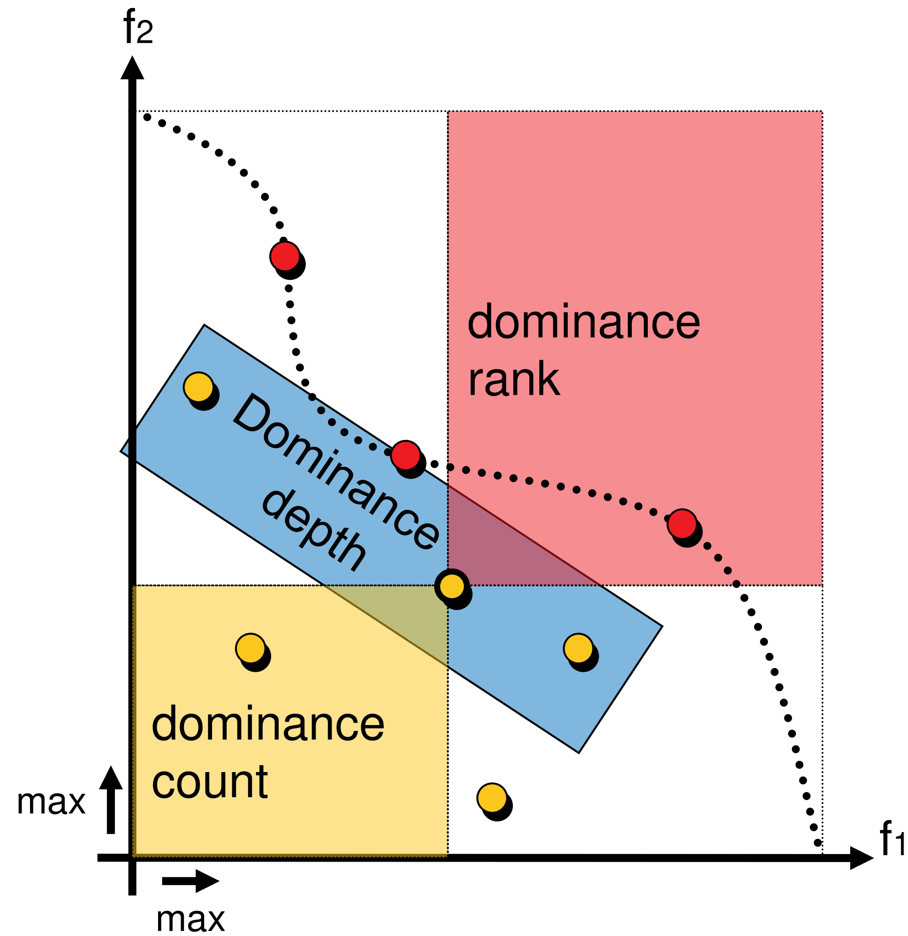


Ranking of the Population Using Dominance

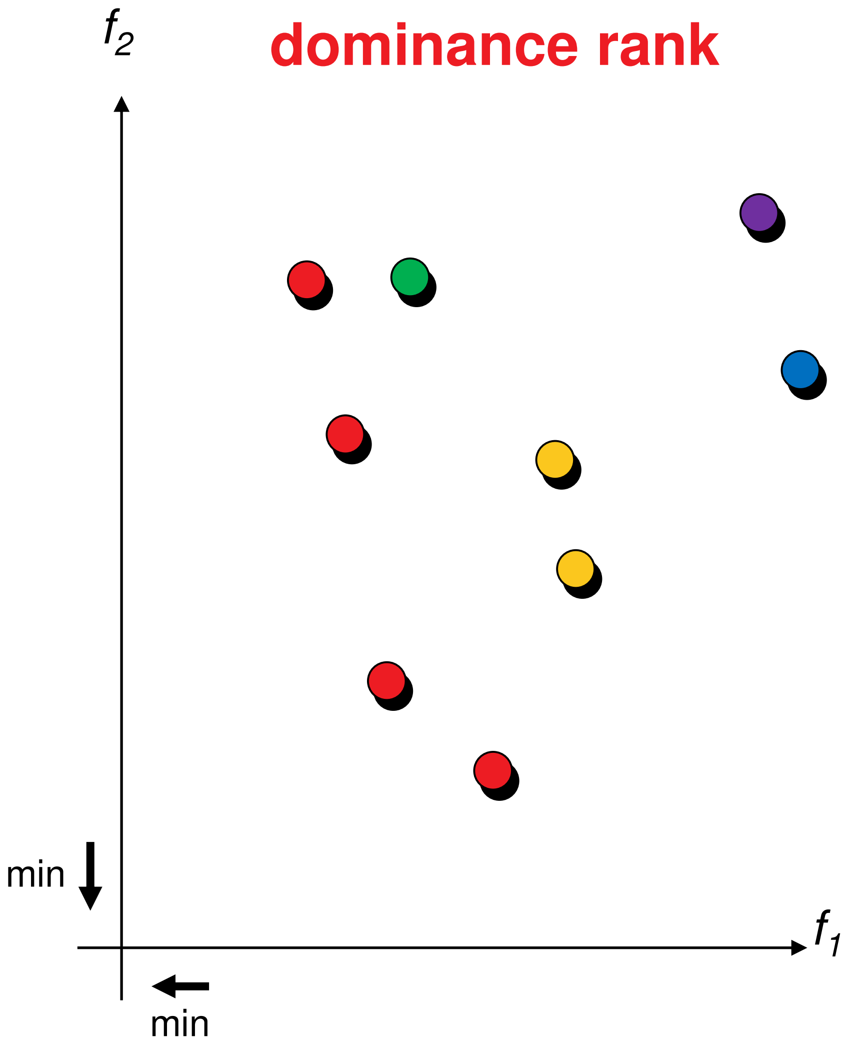
... goes back to a proposal by David Goldberg in 1989.

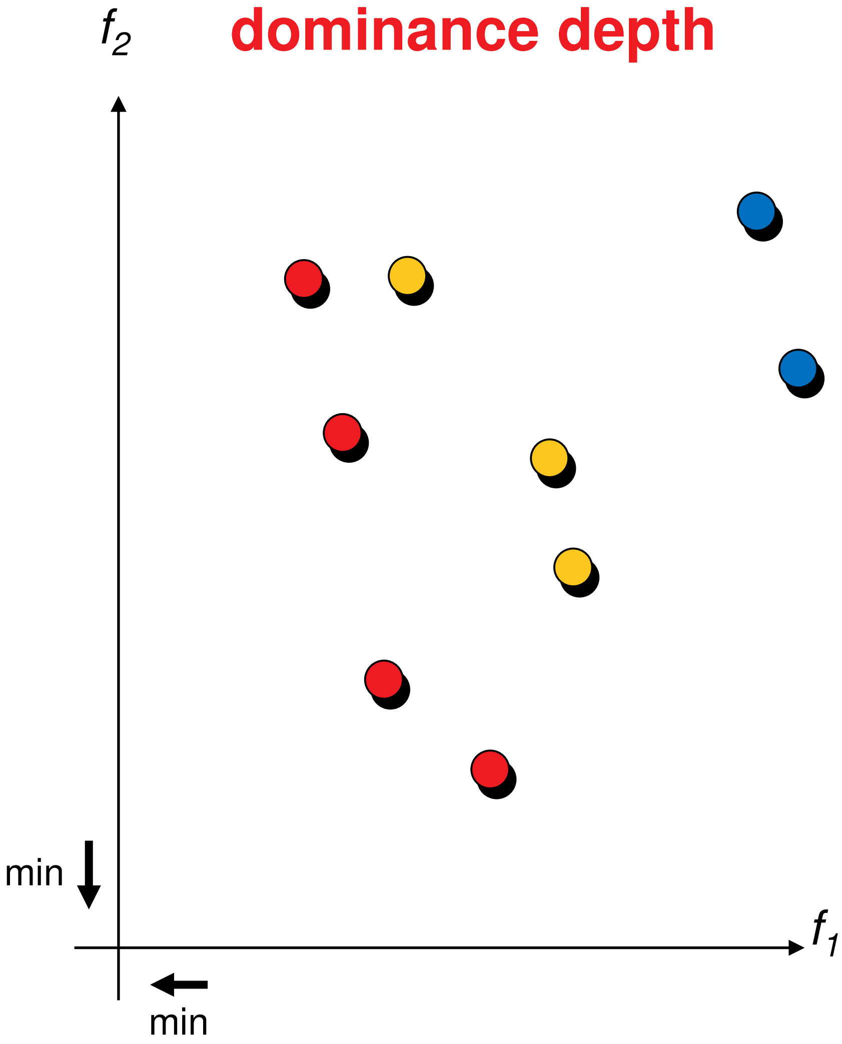
... is based on pairwise comparisons of the individuals only.

- **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





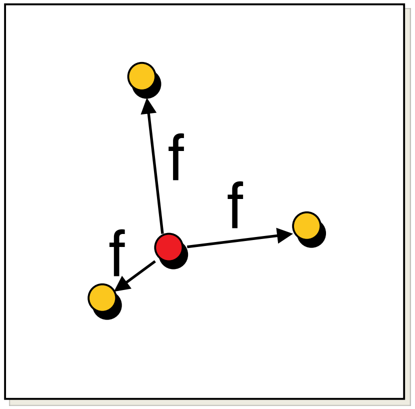
Refinement of Dominance Rankings

Goal: rank incomparable solutions within a dominance class

❶ Diversity information

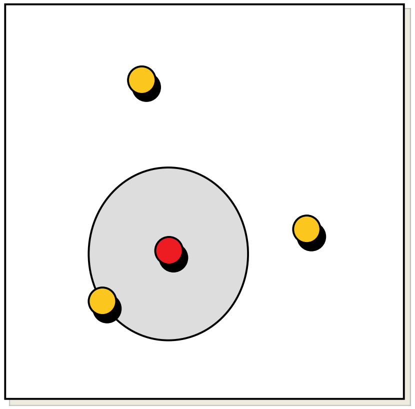
Kernel method

diversity =
function of the
distances



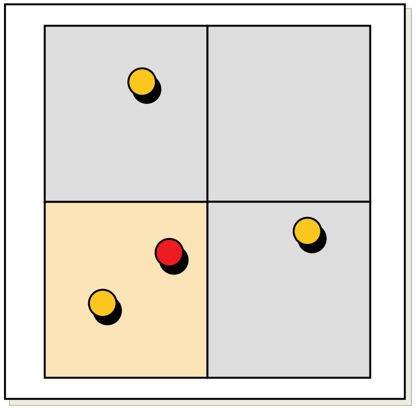
k-th nearest neighbor

diversity =
function of distance
to k-th nearest neighbor



Histogram method

diversity =
number of elements
within box(es)

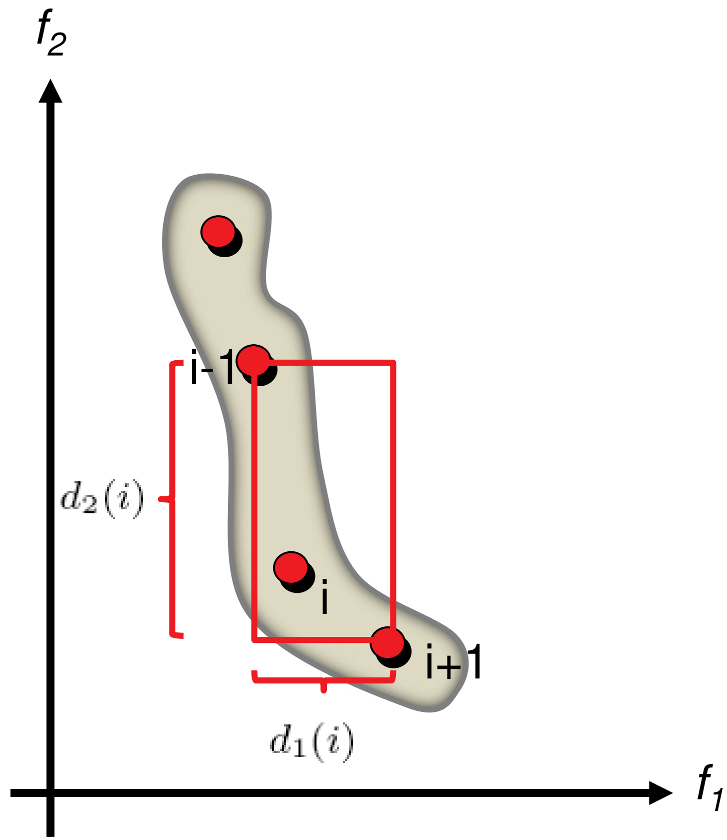


❷ (Contribution to a) quality indicator

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



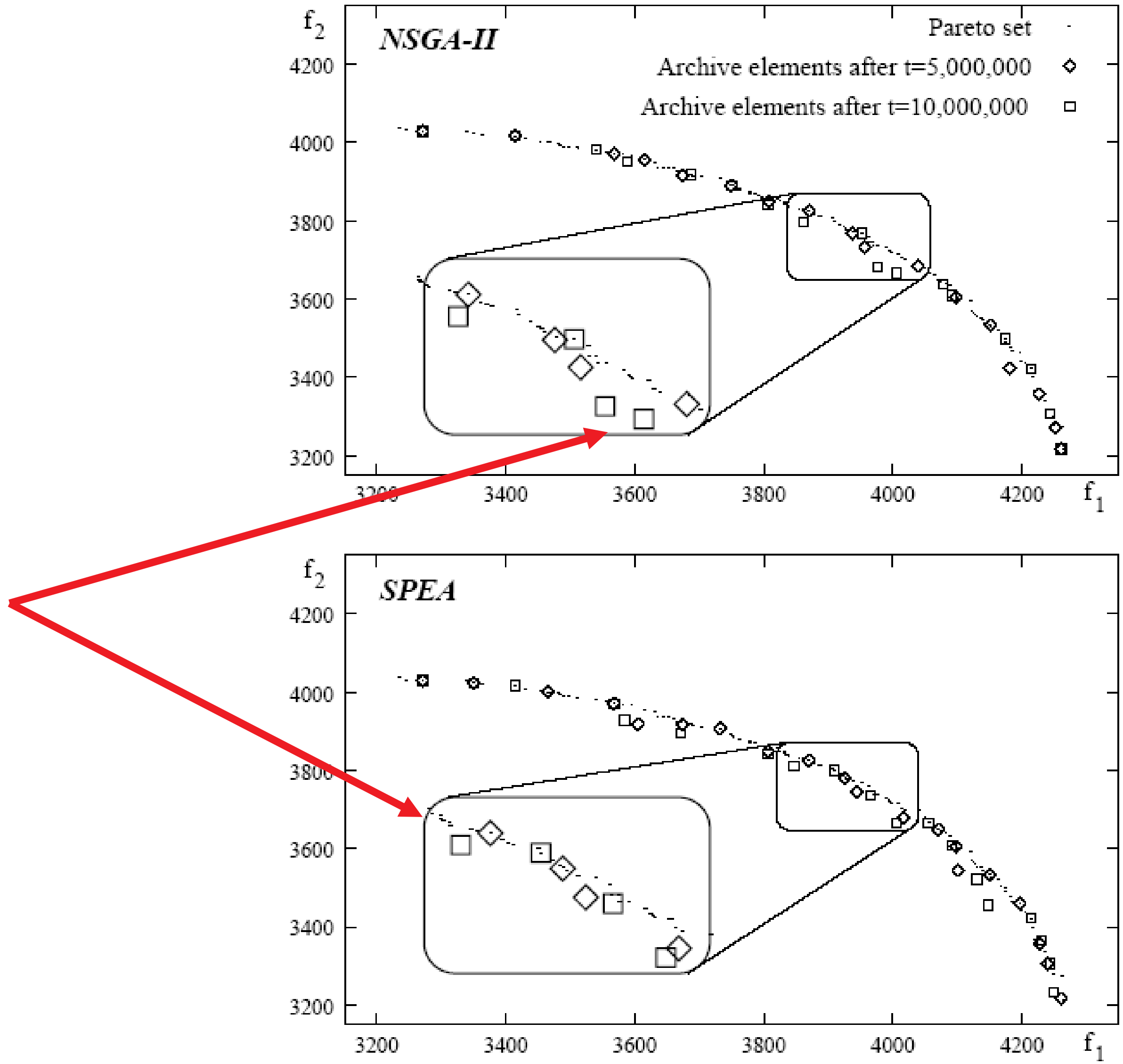
$$\mathrm{CD}(i) = \frac{d_1(i)}{f_{1,\max} - f_{1,\min}} + \cdots + \frac{d_m(i)}{f_{m,\max} - f_{m,\min}}$$

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



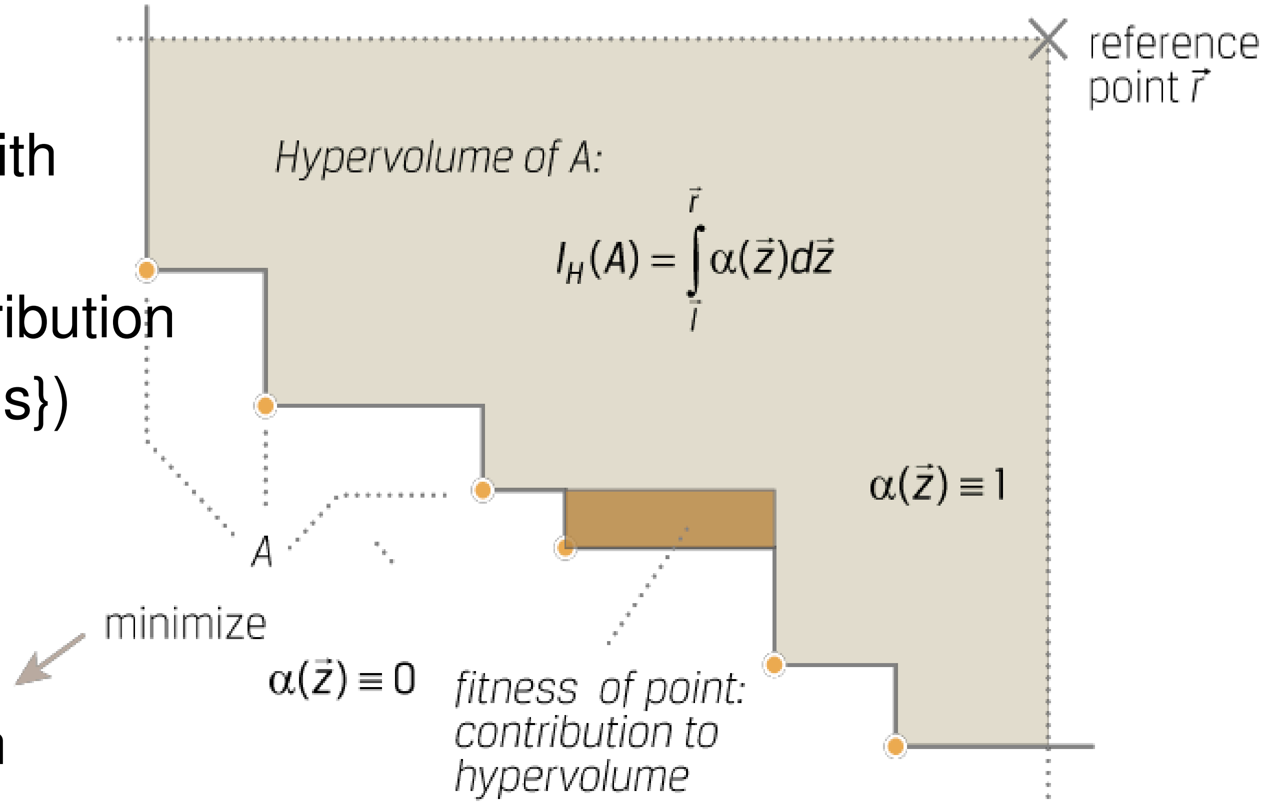
Hypervolume-Based Selection

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 contribution $d(s) = I_H(P) - I_H(P / \{s\})$ iteratively



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]

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

Three Other Mentionable Algorithms

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

MO-CMA-ES: Multiobj. variant of the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) [Igel et al. 2007] [Voß et al. 2010]

RM-MEDA: Regularity Model-Based Multiobjective Estimation of Distribution Algorithm [Zhang et al. 2008]

For the first two: several variants and enhancements exist

MOEA/D

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

- optimizes N scalarizing functions in parallel
- uses best solutions of neighbor subproblems for mating
- keeps best for each scalarizing function and updates neighbors

MO-CMA-ES

MO-CMA-ES: Multiobj. variant of the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) [Igel et al. 2007] [Voß et al. 2010]

- each population member is a single-objective CMA-ES instance
- each CMA-ES instance generates points according to its multivariate Gaussian distribution
- multiobjective selection based on hypervolume loss
- probability distribution is adapted based on ranking within the selection
- most recent: recombination of covariance matrix [Krause et al. 2016]

RM-MEDA

RM-MEDA: Regularity Model-Based Multiobjective Estimation of Distribution Algorithm [Zhang et al. 2008]

- builds a piecewise linear model of the Pareto **set** and samples from it:
  - clustering the points in K clusters
  - for each cluster, fit a linear (hyper-)plane of dimension n-1
- for sampling new points:
  - sample first uniformly at random a (hyper-)plane
  - uniformly at random a point within the (hyper-)plane
  - add a small random uniform vector as noise to it

Many More Algorithms Exist...

...and many more are proposed every day

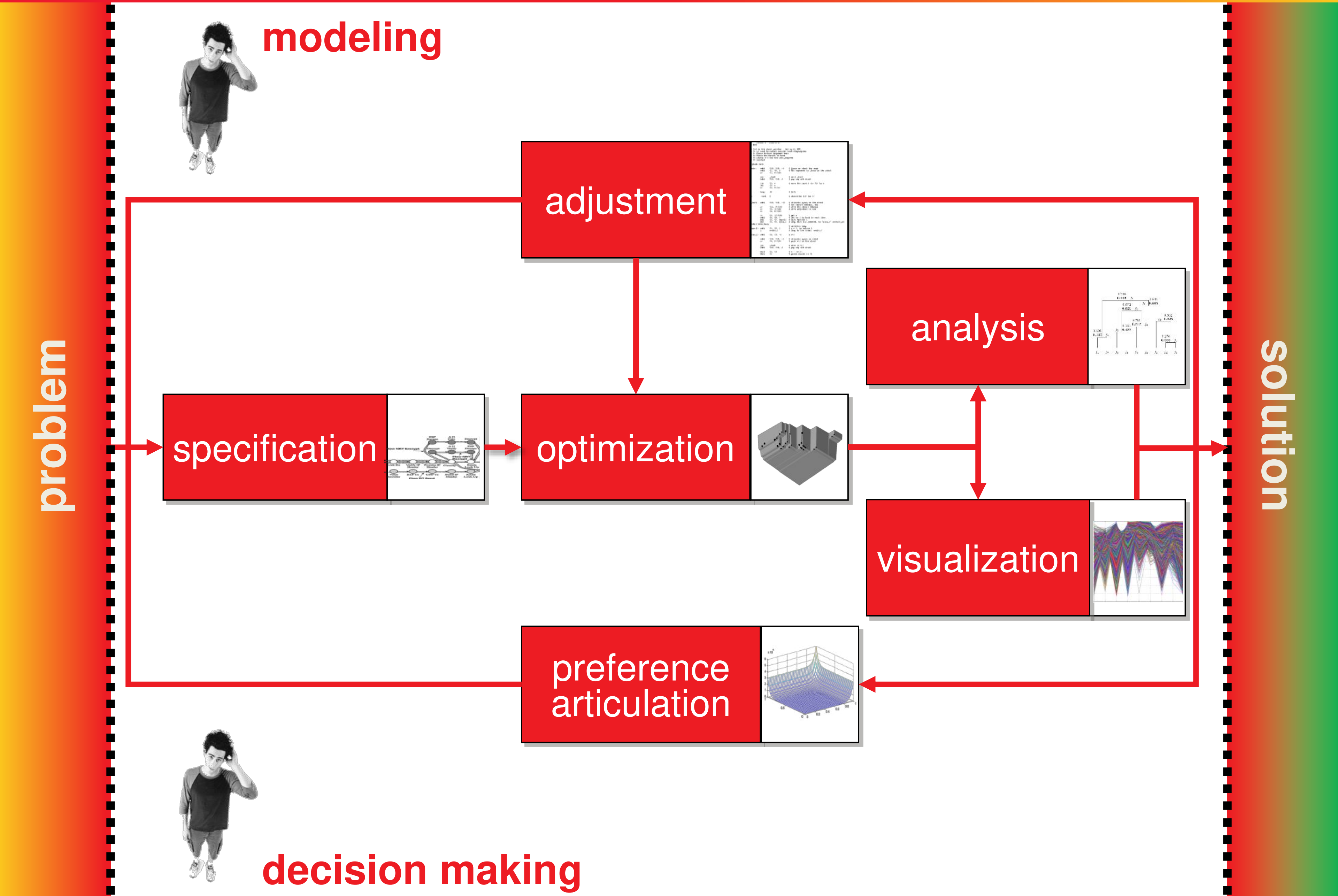
The Main Practical Question Right Now:

which algorithm to use on my problem?

→ needs benchmarking to recommend algorithms

the second step: how to improve the current best algos?

Conclusions: EMO as Interactive Decision Support



The EMO Community

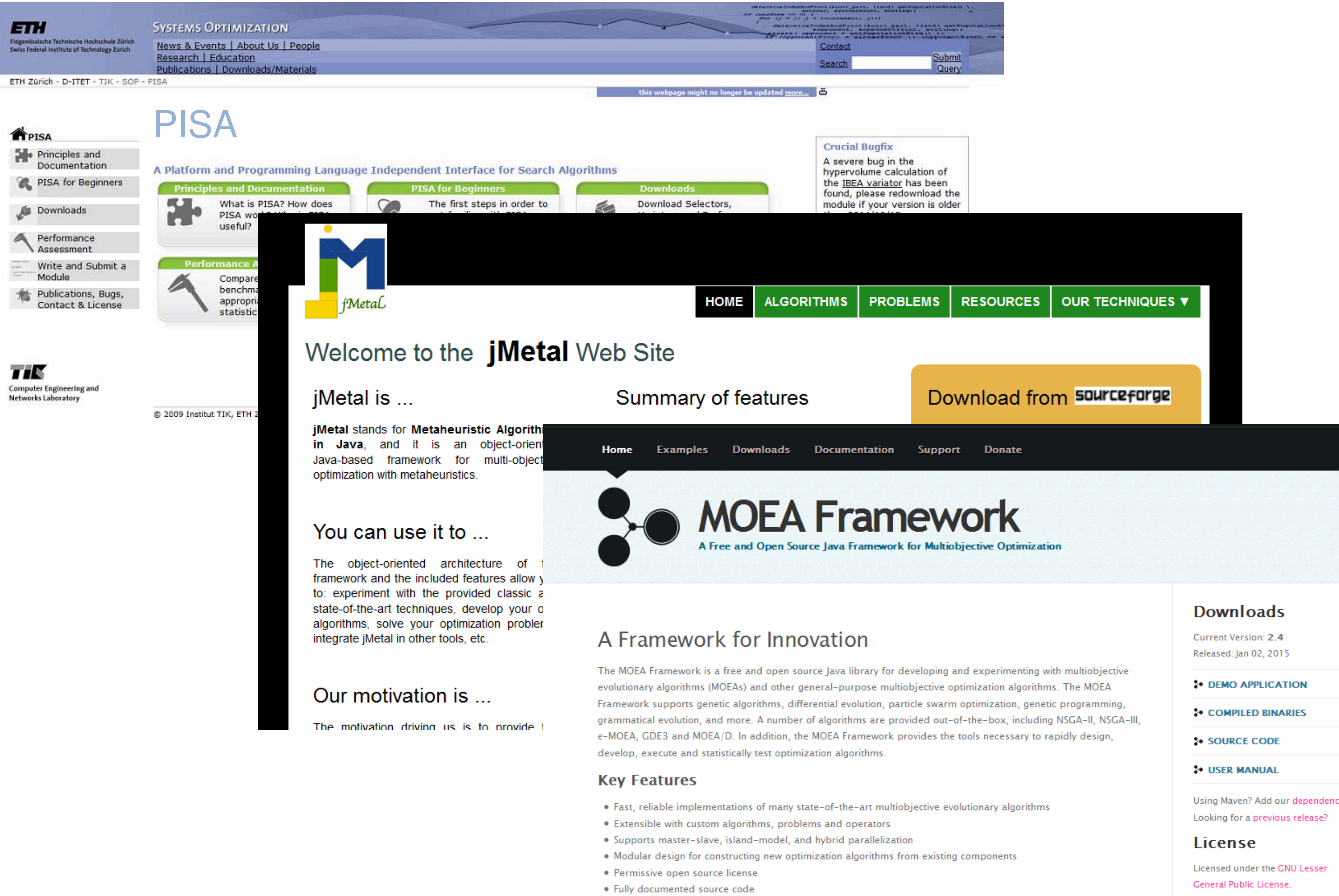
Links:

- EMO mailing list: *https://lists.dei.uc.pt/mailman/listinfo/emo-list*
- MCDM mailing list: *http://lists.jyu.fi/mailman/listinfo/mcdm-discussion*
- EMO bibliography: *http://www.lania.mx/~ccoello/EMOO/*
- EMO conference series: *http://www.emo2017.org/*

Books:

- ***Multi-Objective Optimization using Evolutionary Algorithms***
  Kalyanmoy Deb, Wiley, 2001
- ***Evolutionary Algorithms for Solving Multi Evolutionary Algorithms for Solving Multi-Objective Problems Objective Problems***, Carlos A. Coello Coello, David A. Van Veldhuizen & Gary B. Lamont, Kluwer, 2nd Ed. 2007
- **Multiobjective Optimization—Interactive and Evolutionary Approaches**, J. Branke, K. Deb, K. Miettinen, and R. Slowinski, editors, volume 5252 of *LNCS*. Springer, 2008 [(still) many open questions!]
- and more…

Software



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A Framework for Innovation
The MOEA Framework is a free and open source Java library for developing and experimenting with multiobjective evolutionary algorithms (MOEAs) and other general-purpose multiobjective optimization algorithms. The MOEA Framework supports genetic algorithms, differential evolution, particle swarm optimization, genetic programming, grammatical evolution, and more. A number of algorithms are provided out-of-the-box, including NSGA-II, NSGA-III, ε-MOEA, GDE3 and MOEA/D. In addition, the MOEA Framework provides the tools necessary to rapidly design, develop, execute and statistically test optimization algorithms.
Key Features
Fast, reliable implementations of many state-of-the-art multiobjective evolutionary algorithms
Extensible with custom algorithms, problems and operators
Supports master-slave, island-model, and hybrid parallelization
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Fully documented source code
Downloads
Current Version: 2.4
Released: Jan 02, 2015
DEMO APPLICATION
COMPILED BINARIES
SOURCE CODE
USER MANUAL
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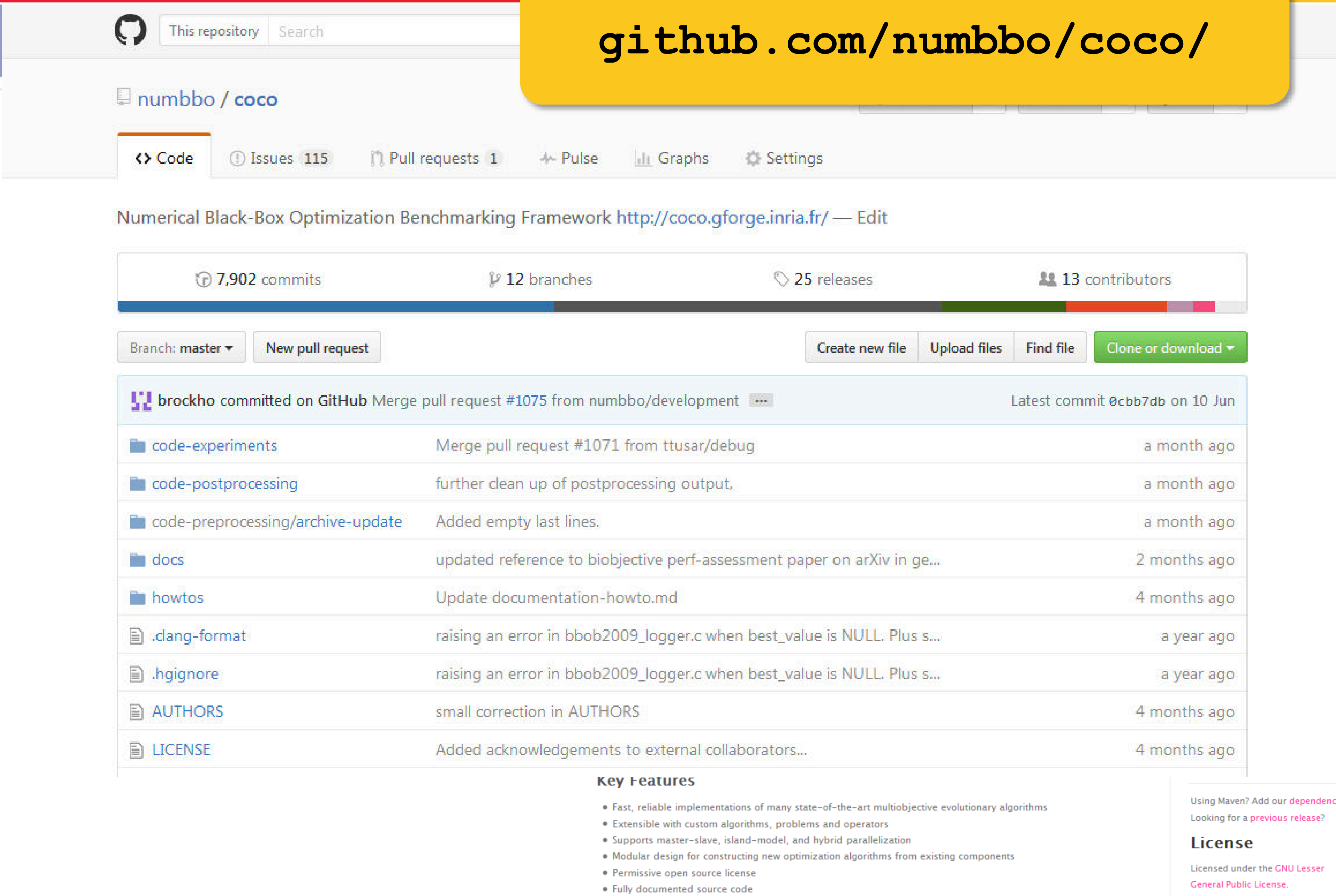
Software

github.com/numbbo/coco/



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