A Brief Introduction to Evolutionary Multiobjective Optimization

Dimo Brockhoff

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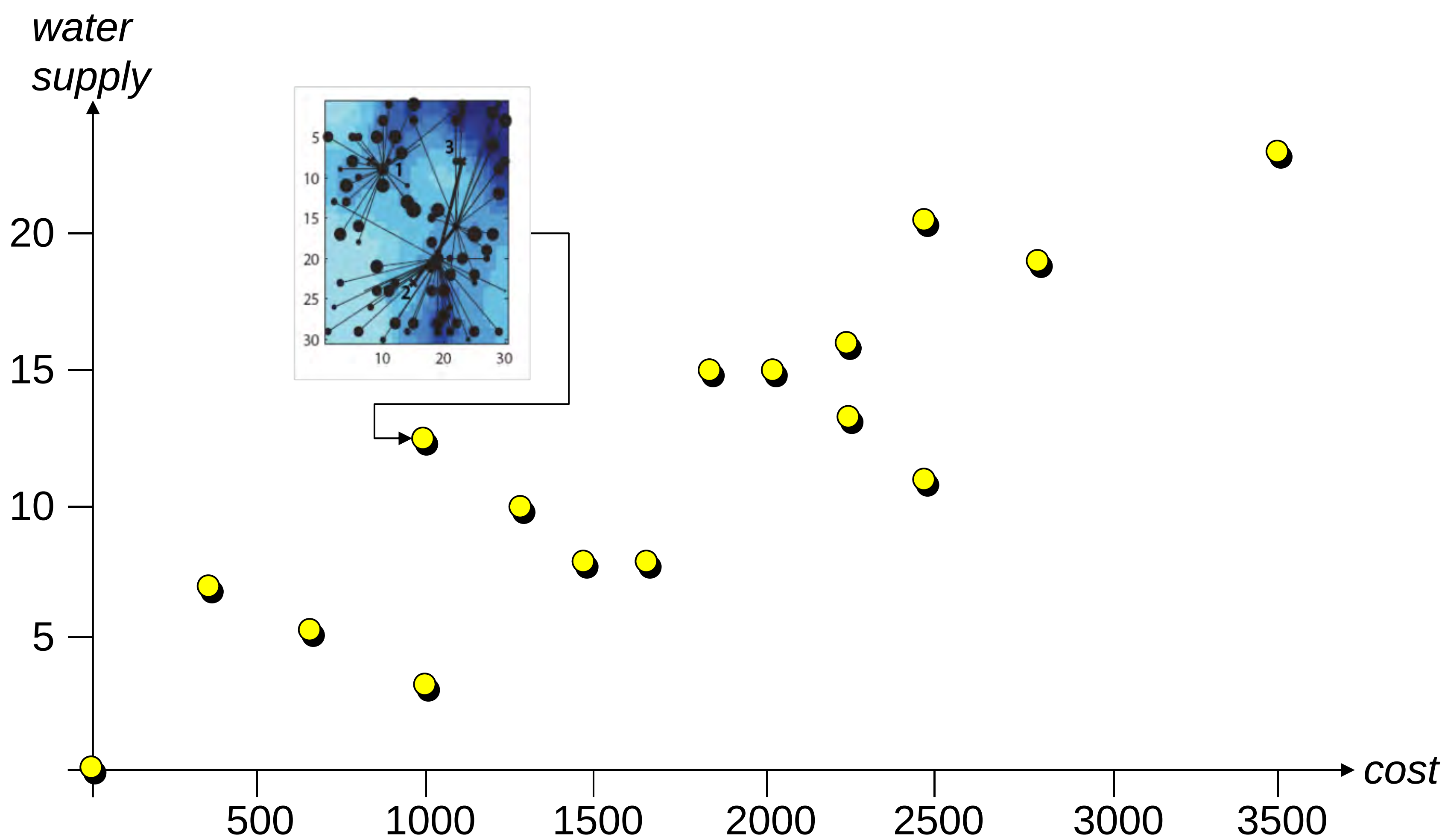
A hypothetical problem: all solutions plotted



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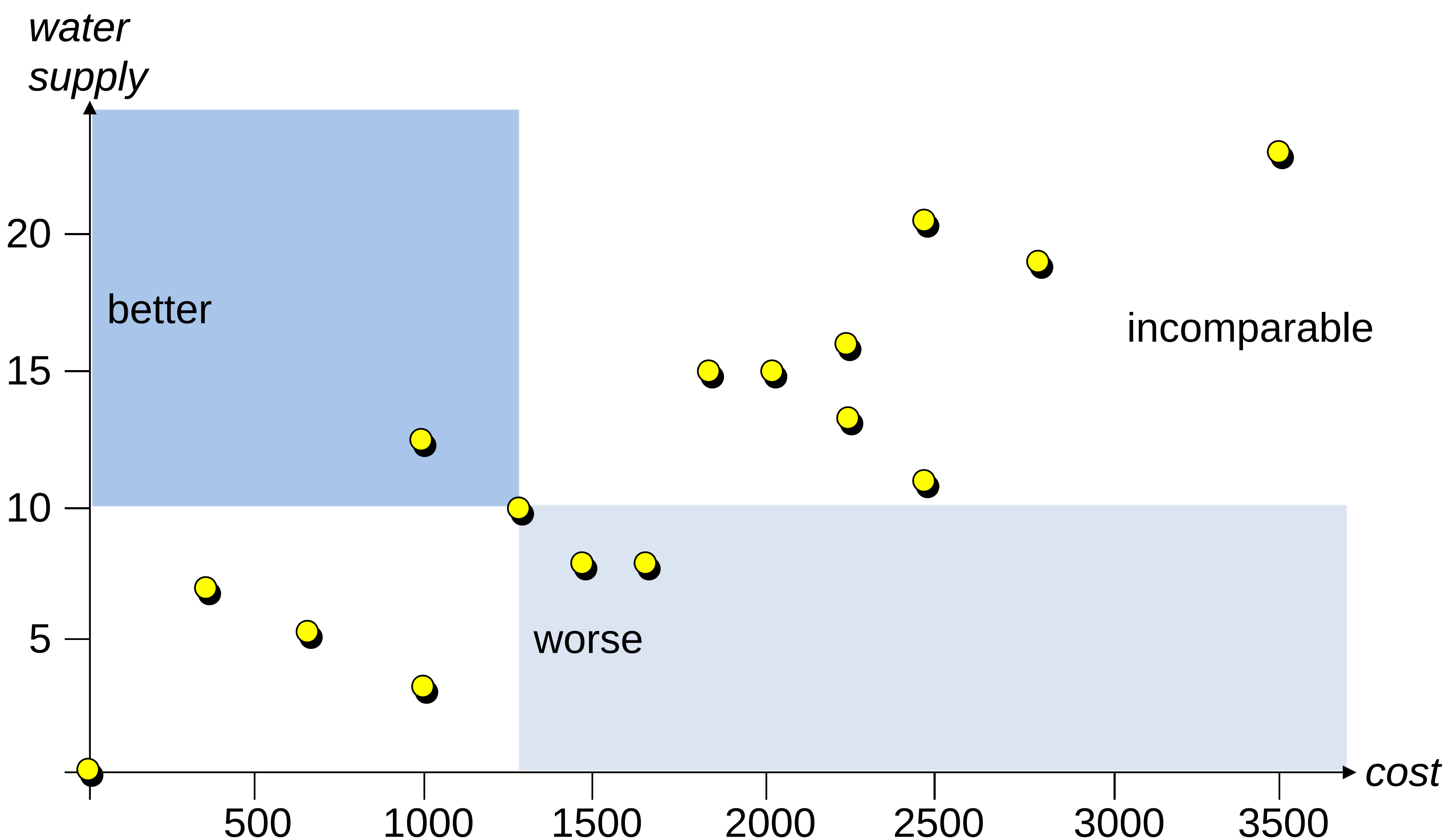
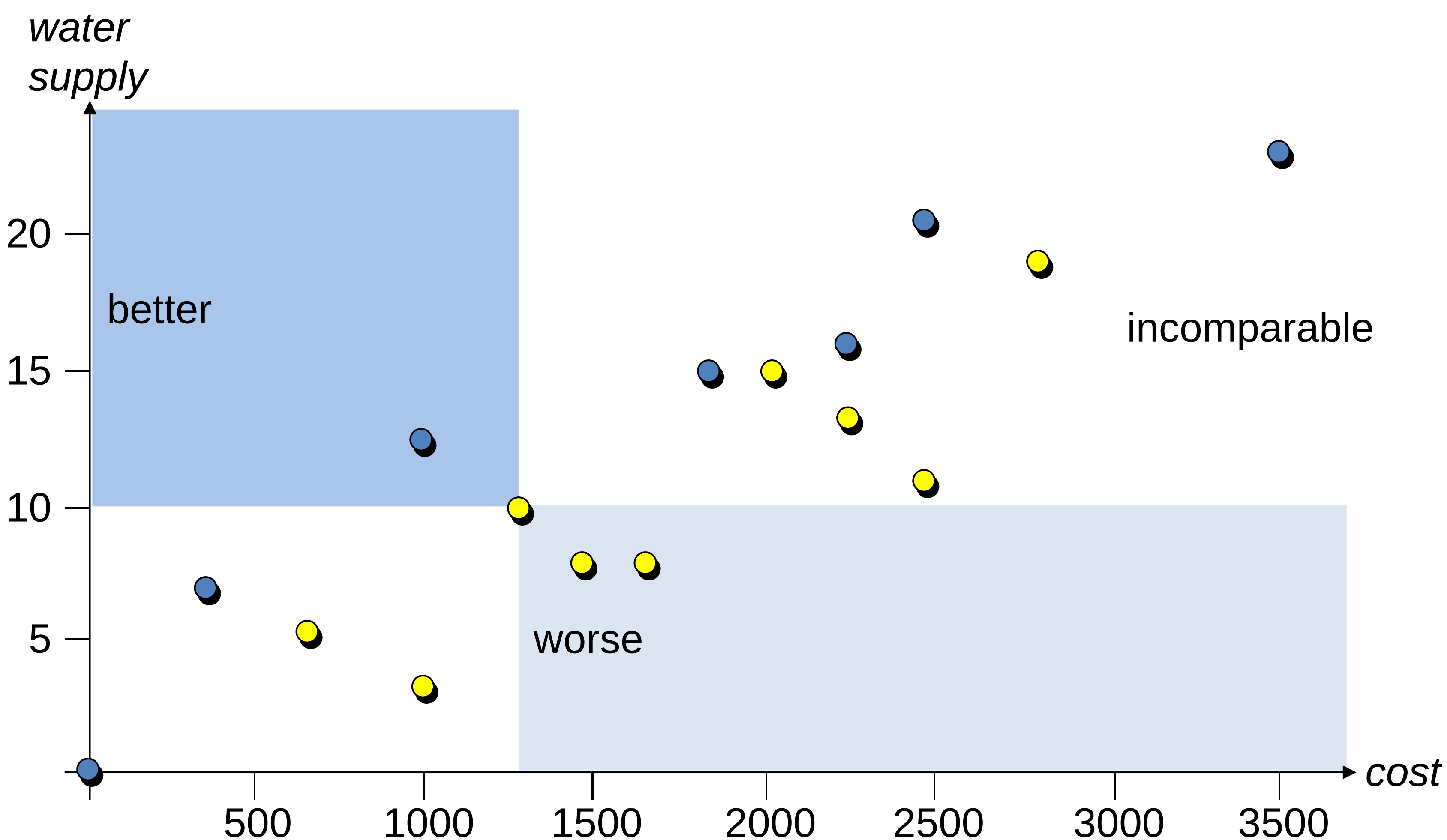
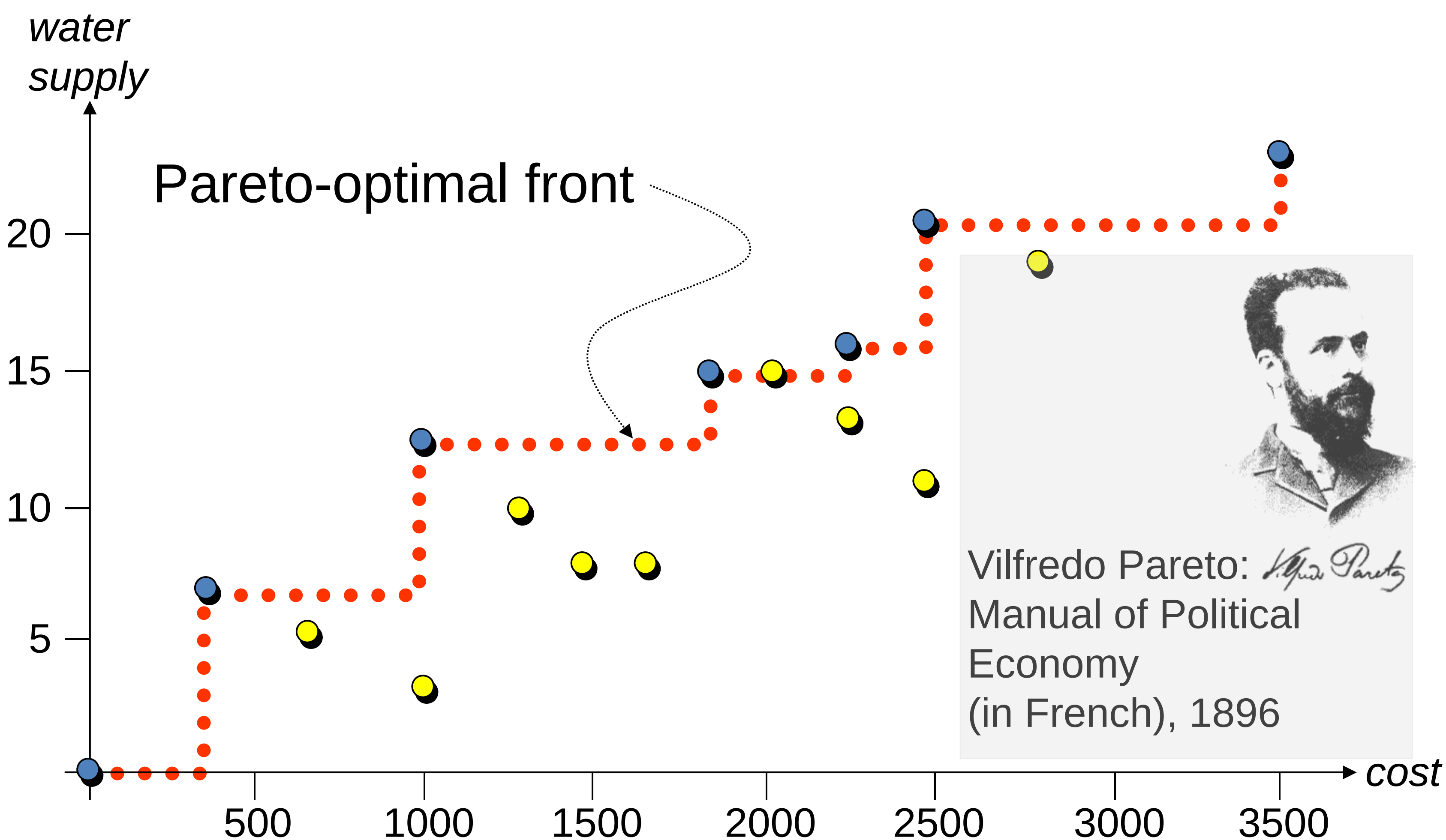


Observations: ❶ there is no single optimal solution, but
❷ some solutions ( ) are better than others ( )



Principles of Multiple Criteria Decision Analysis

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



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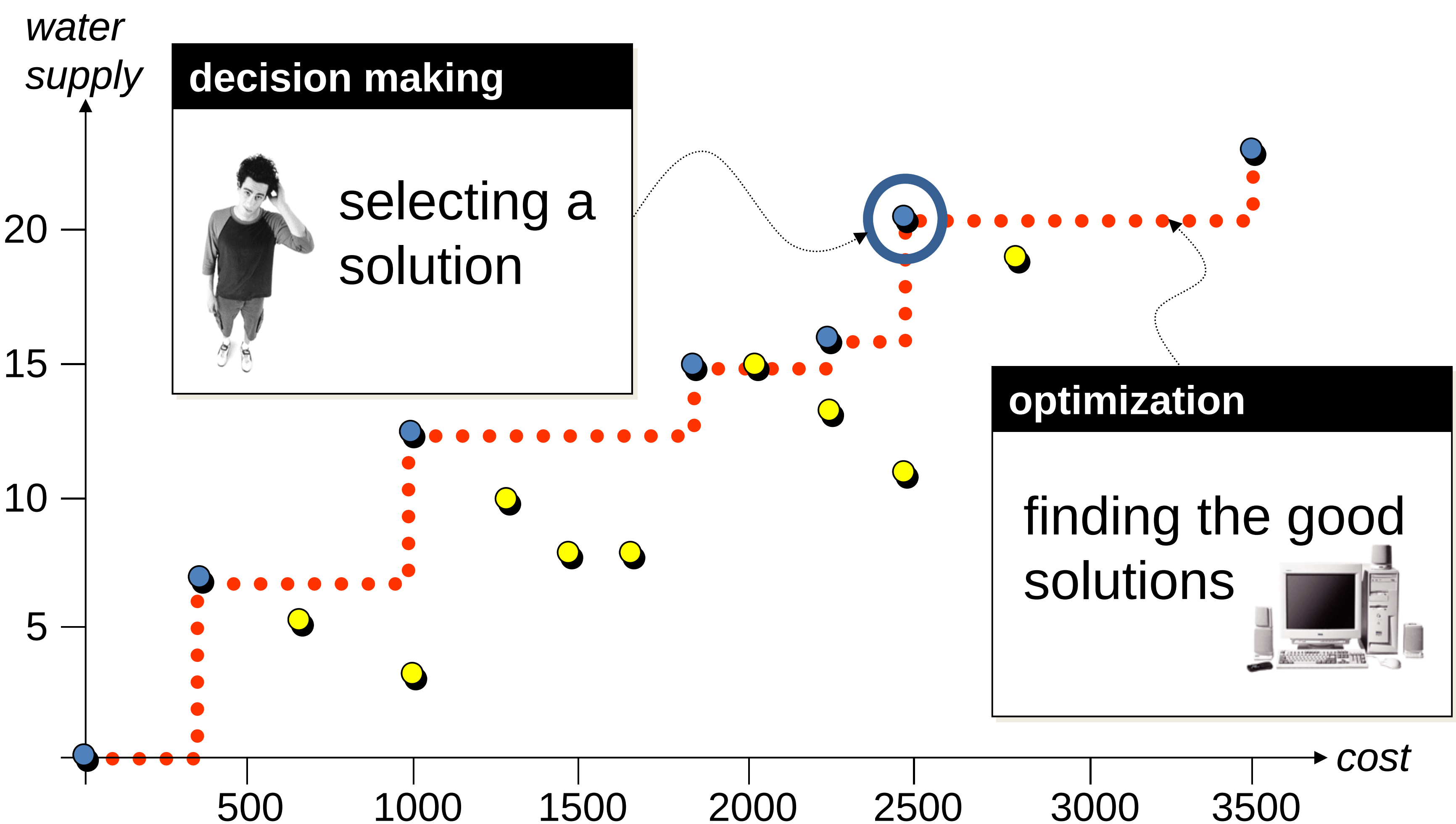
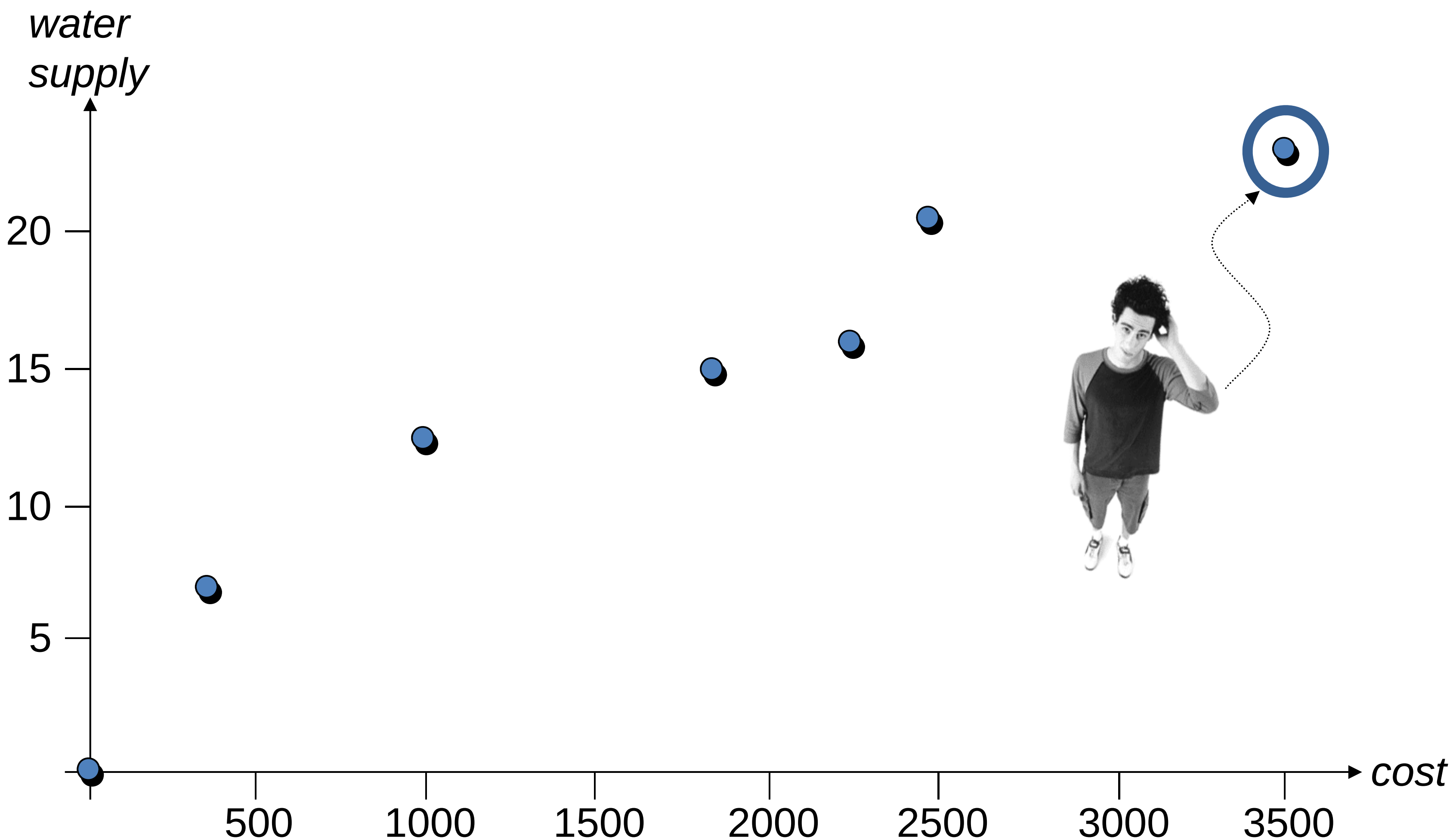


Decision Making: Selecting a Solution

Possible Approach:

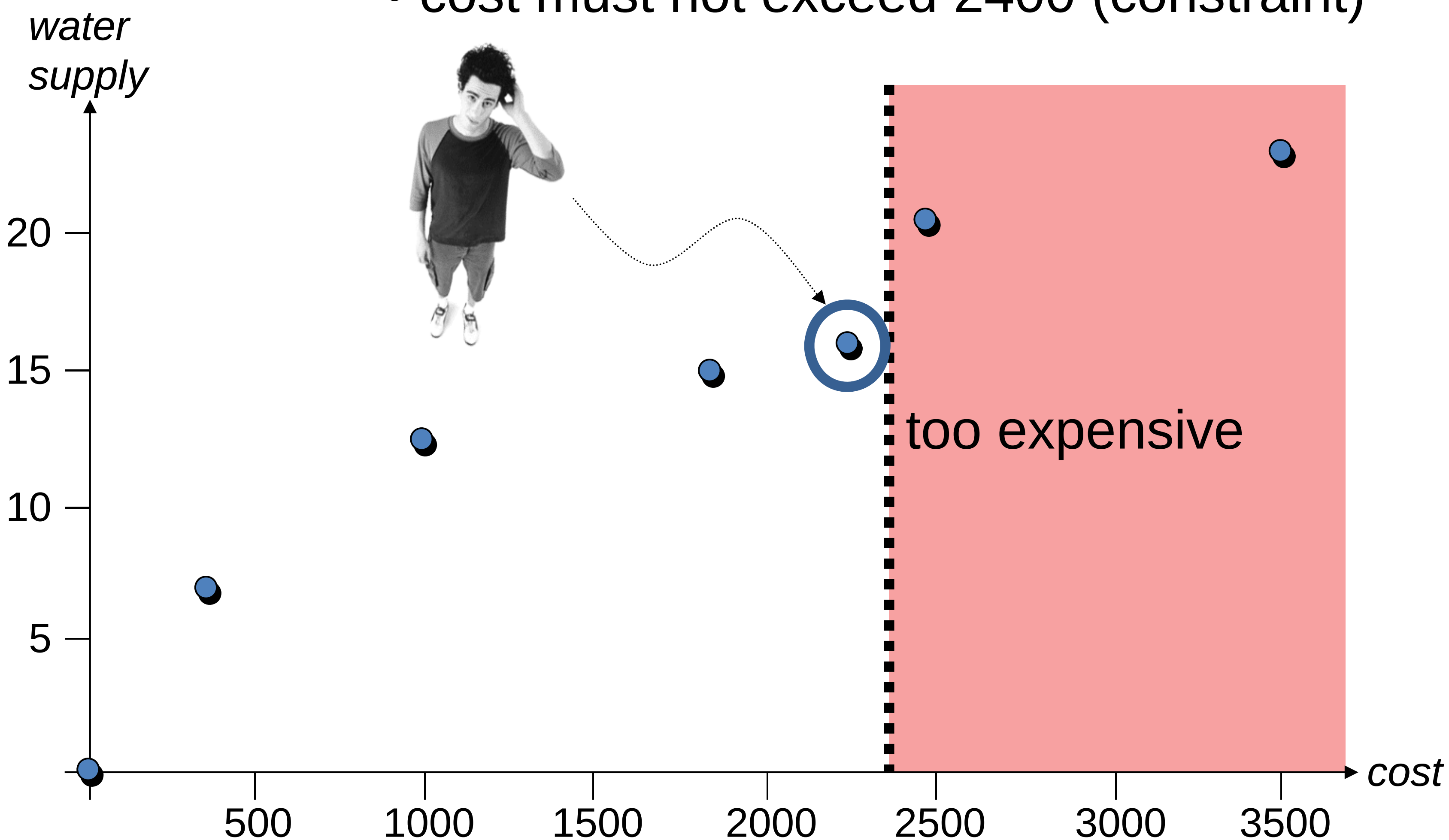
- supply more important than cost (ranking)



Decision Making: Selecting a Solution

Possible Approach:

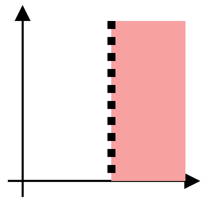
- supply more important than cost (ranking)
- cost must not exceed 2400 (constraint)



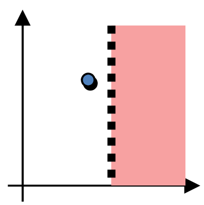
When to Make the Decision

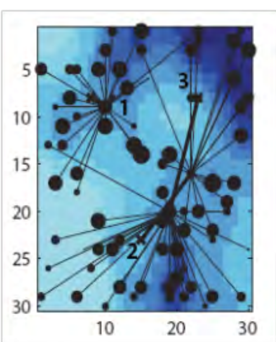
Before Optimization:

rank objectives,
define constraints,…



search for one
(blue) solution





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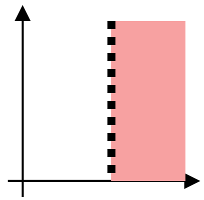

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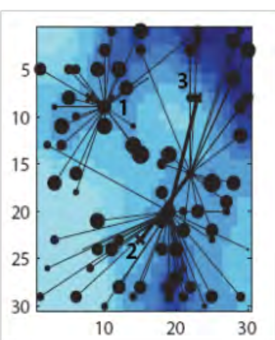

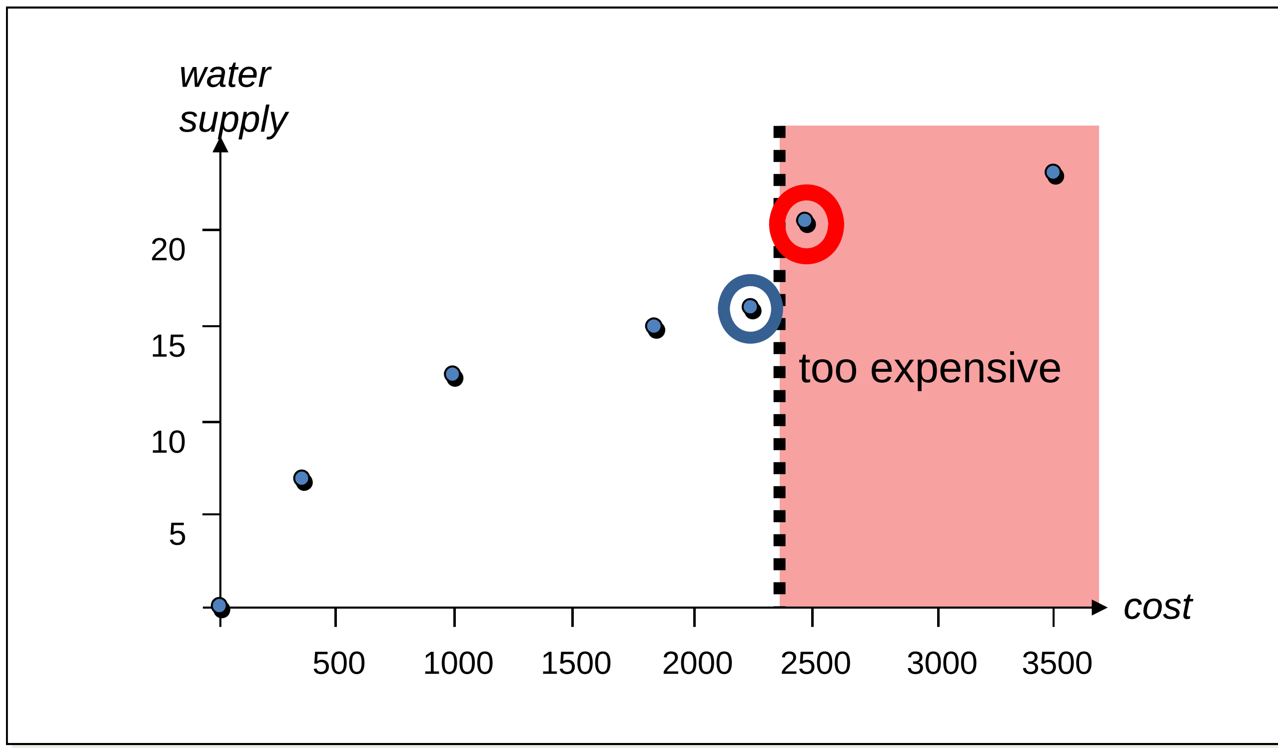

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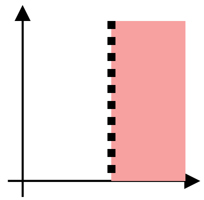

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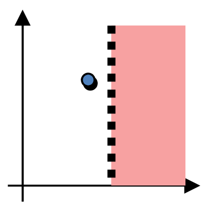
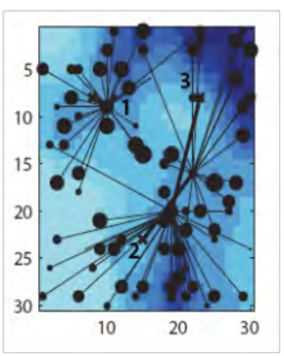
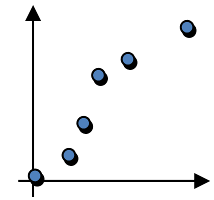


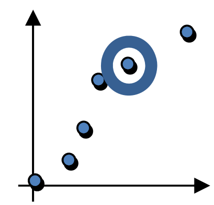


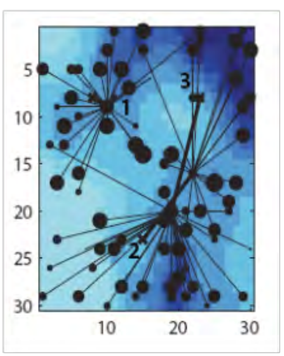
After Optimization:



search for a set of
(blue) solutions

select one solution
considering
constraints, etc.





When to Make the Decision

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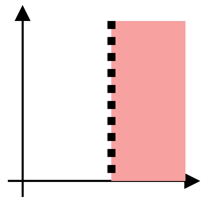

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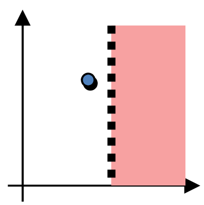

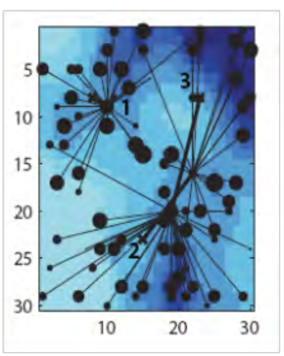

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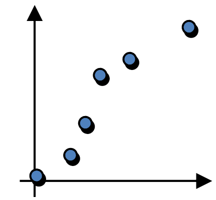

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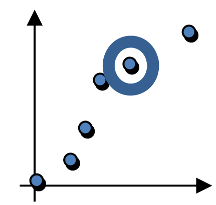


Focus: learning about a problem

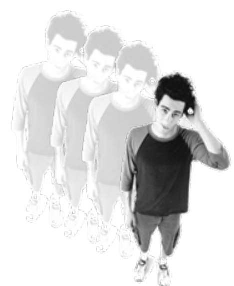
- trade-off surface
- interactions among criteria
- structural information

Multiple Criteria Decision Making (MCDM)

Definition: MCDM

MCDM can be defined as the study of methods and procedures by which concerns about multiple conflicting criteria can be formally incorporated into the management planning process

International Society on Multiple Criteria Decision Making



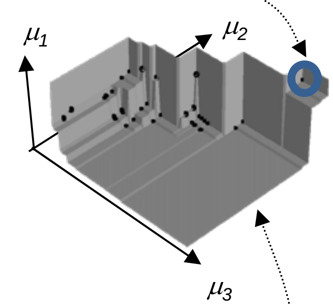
model

$$\min_x \left[\mu_1(x), \mu_2(x), \ldots, \mu_n(x)\right]^T$$
$$s.t.$$
$$g(x) \leq 0$$
$$h(x) = 0$$
$$x_l \leq x \leq x_u$$

decision making

(exact) optimization

trade-off surface



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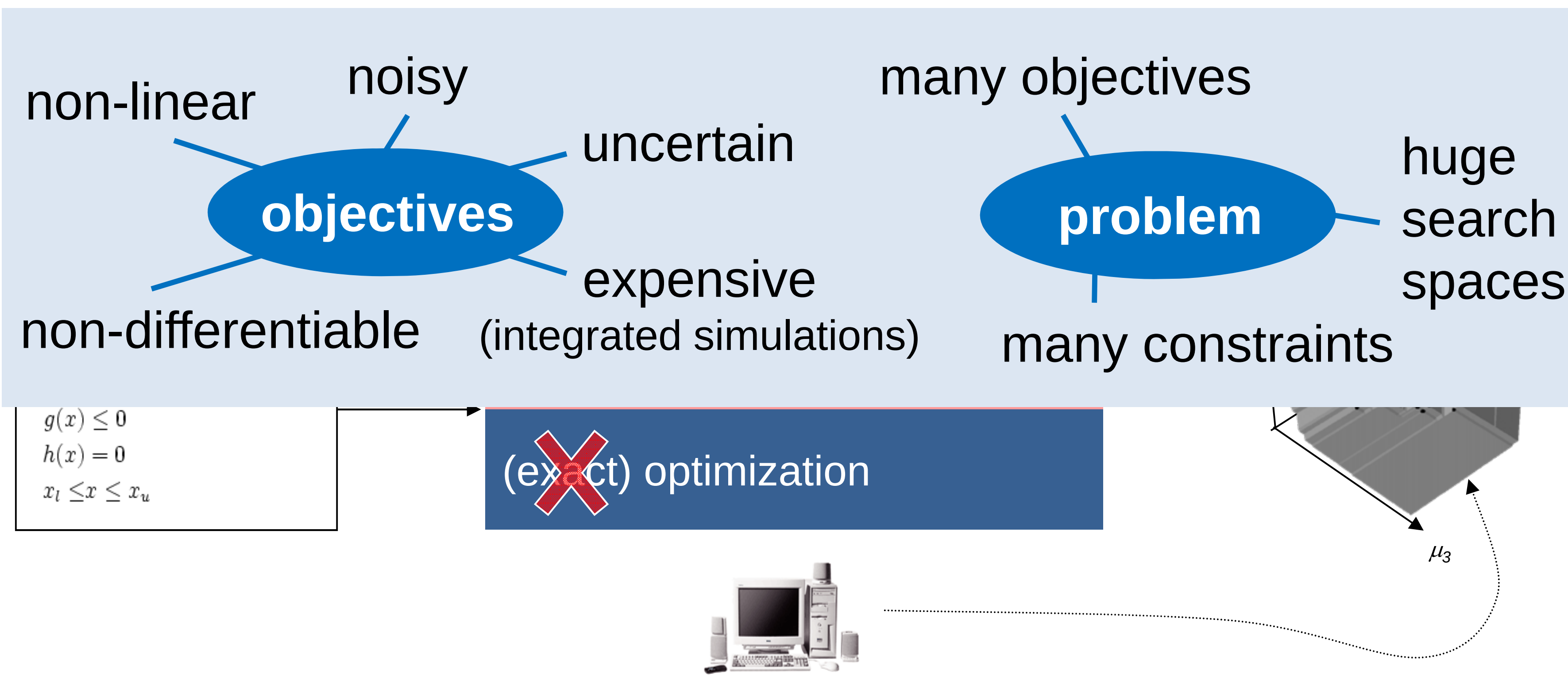

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MCDM can be defined as the study of methods and procedures by which concerns about multiple conflicting criteria can be formally incorporated into the management planning process

International Society on Multiple Criteria Decision Making

non-linear

noisy

many objectives

objectives

uncerta

expens

(integrated si

non-differentiable

$g(x) \leq 0$
$h(x) = 0$
$x_l \leq x \leq x_u$

(~~exact~~) optim

Black box optimization

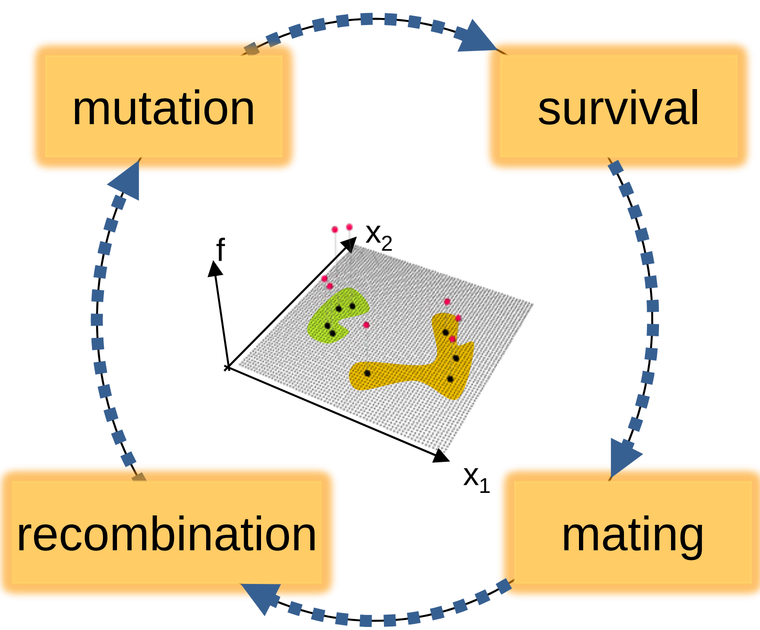
$$x \in X \longrightarrow \boxed{f} \longrightarrow (f_1(x), \ldots, f_k(x))$$

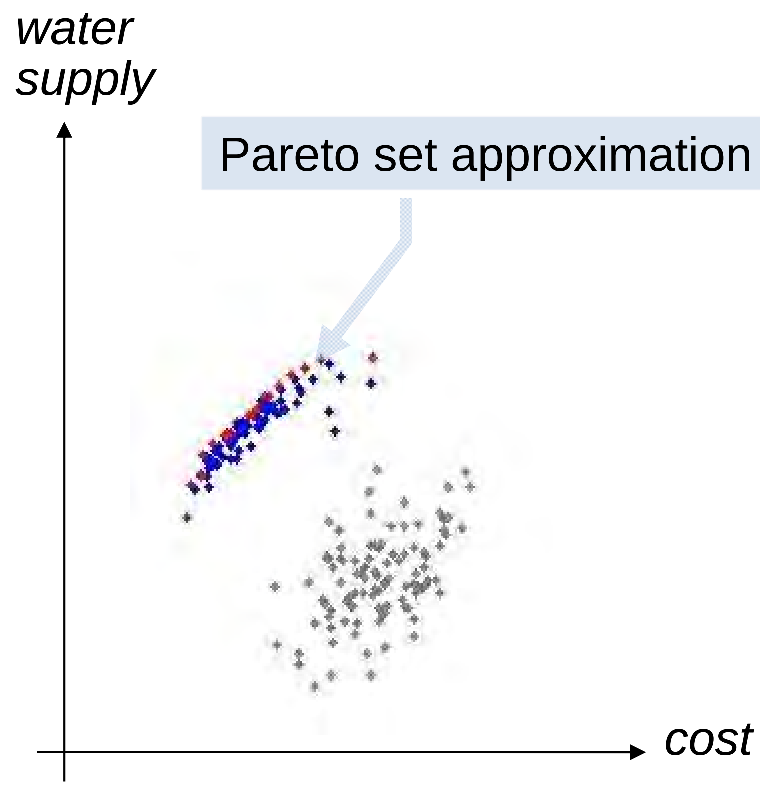
only mild assumptions

Evolutionary Multiobjective Optimization (EMO)

Definition: EMO

EMO = **evolutionary algorithms** / randomized search algorithms
- applied to multiple criteria decision making (in general)
- used to approximate the Pareto-optimal set (mainly)





The History of EMO At A Glance

1984
first EMO approaches

dominance-based population ranking

1990
dominance-based EMO algorithms with diversity preservation techniques

1995
attainment functions

elitist EMO algorithms preference articulation convergence proofs

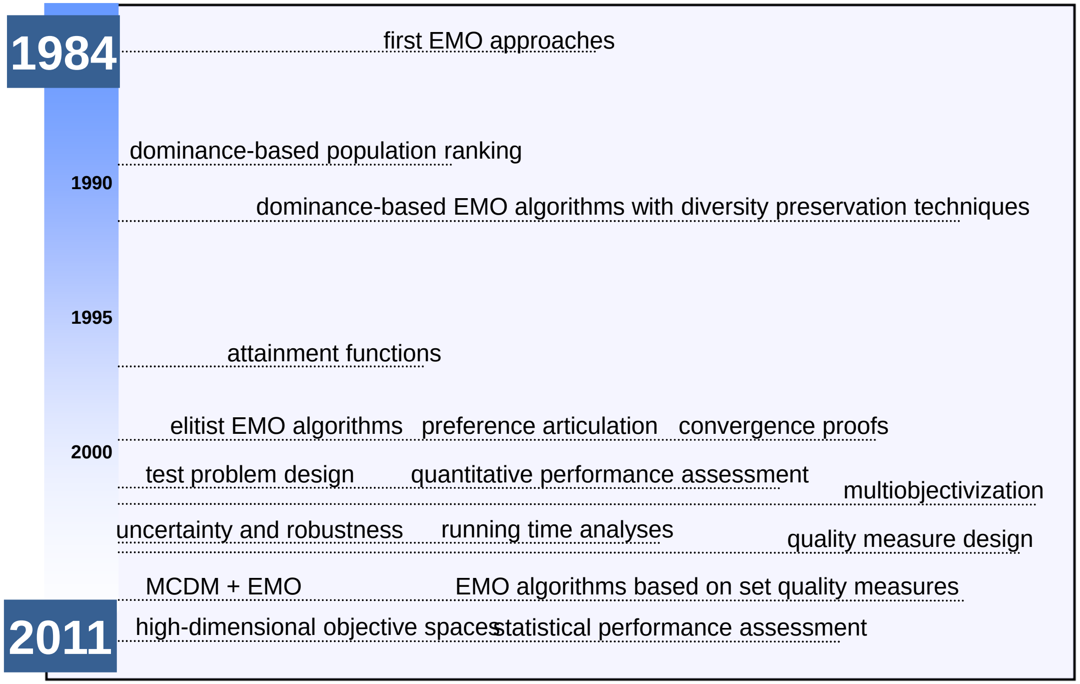
2000
test problem design quantitative performance assessment
multiobjectivization

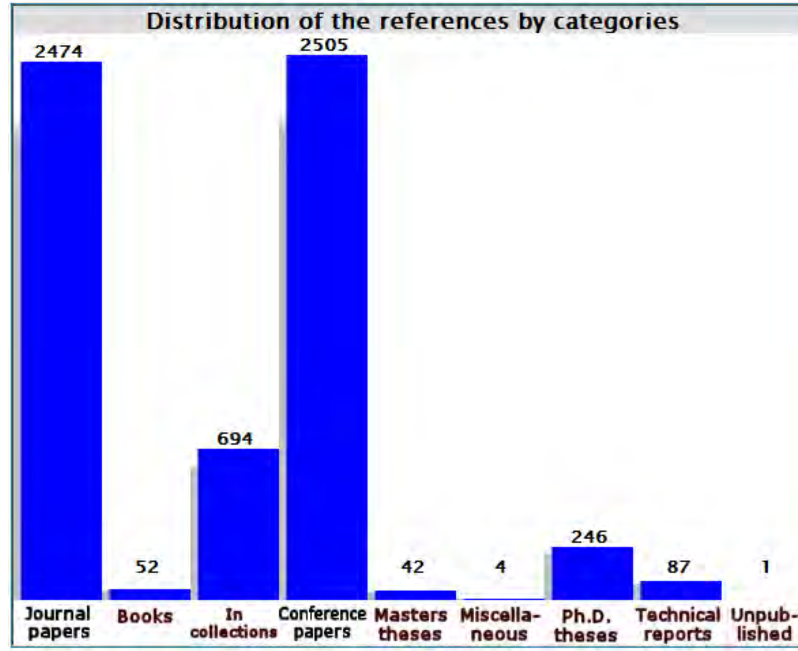
uncertainty and robustness running time analyses quality measure design

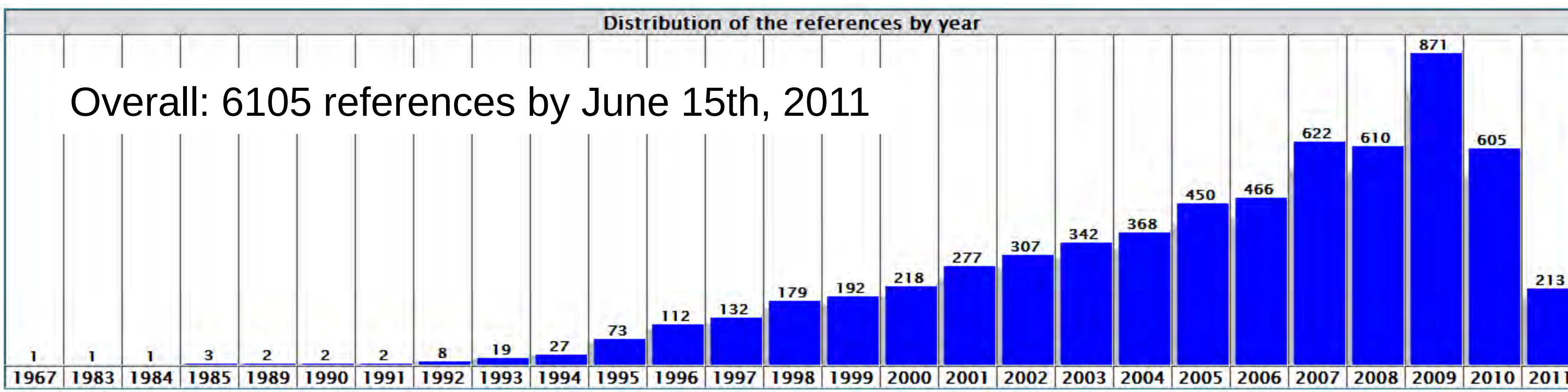
MCDM + EMO quality indicator based EMO algorithms

2010
many-objective optimization statistical performance assessment

The History of EMO At A Glance



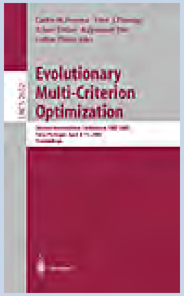
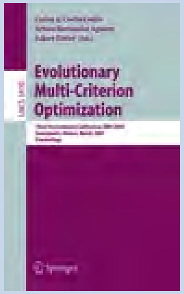
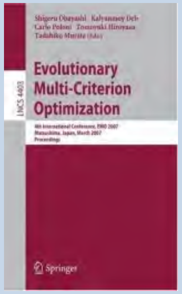
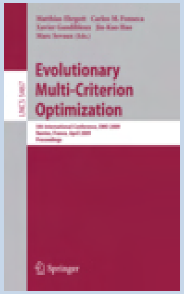
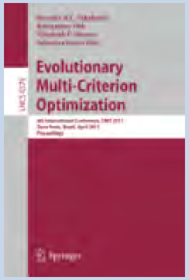




http://delta.cs.cinvestav.mx/~ccoello/EMOO/EMOOstatistics.html

The EMO Community

The EMO conference series:

EMO2001	EMO2003	EMO2005	EMO2007	EMO2009	EMO2011	EMO2013
Zurich	Faro	Guanajuato	Matsushima	Nantes	Ouro Peto	Sheffield
Switzerland	Portugal	Mexico	Japan	France	Brazil	UK
						
45/87	56/100	59/115	65/124	39/72	42/83	?

Many further activities:

special sessions, special journal issues, workshops, tutorials, ...

Overview

A Brief Introduction to EMO

- basics: what is the difference between single- and multiobjective optimization?
- state-of-the-art algorithm design concepts
- performance assessment

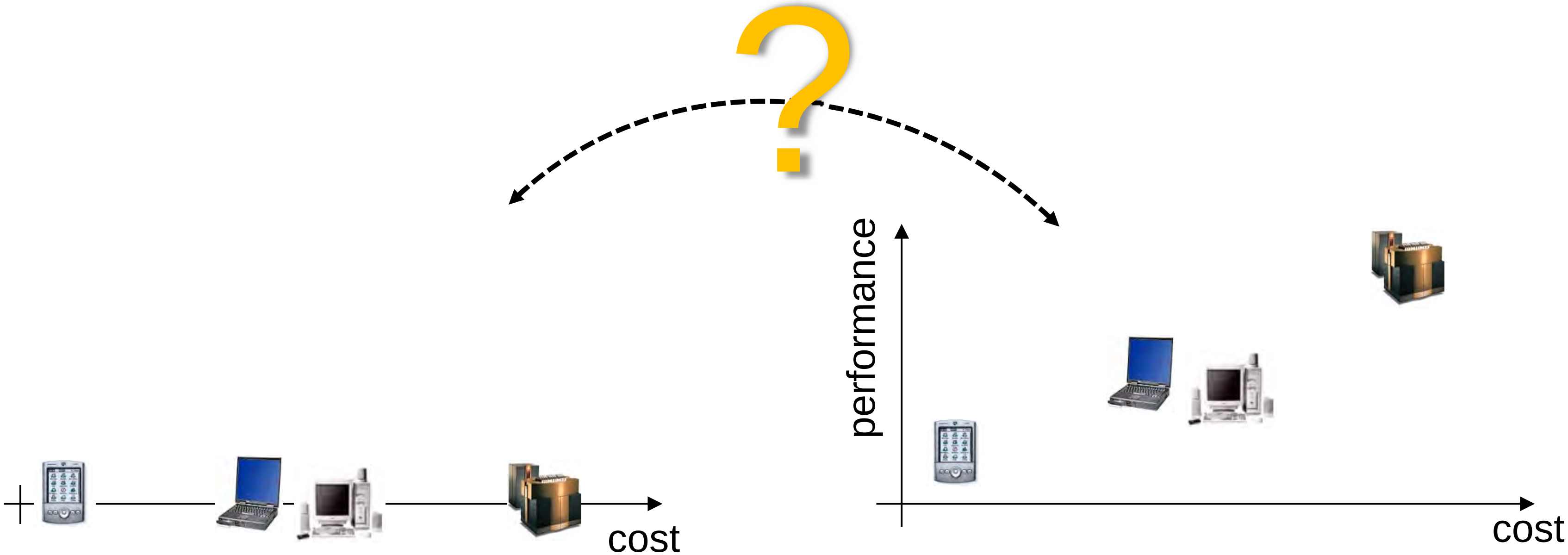
Advanced Concepts Useful in Practice

- objective reduction
- multiobjectivization
- innovization

Examples of Applications

Starting Point

What makes evolutionary multiobjective optimization different from single-objective optimization?



single objective **multiple objectives**

A General (Multiobjective) Optimization Problem

A *multiobjective optimization problem* is defined by a 5-tuple $(X, Z, \mathbf{f}, \mathbf{g}, \leqslant)$ where

- X is the decision space,
- $Z = \mathbb{R}^n$ is the objective space,
- $\mathbf{f} = (f_1, \ldots, f_n)$ is a vector-valued function consisting of n objective functions $f_i : X \mapsto \mathbb{R}$,
- $\mathbf{g} = (g_1, \ldots, g_m)$ is a vector-valued function consisting of m constraint functions $g_i : X \mapsto \mathbb{R}$, and
- $\leqslant \subseteq Z \times Z$ is a binary relation on the objective space.

The goal is to identify a decision vector $\mathbf{a} \in X$ such that (i) for all $1 \leq i \leq m$ holds $g_i(\mathbf{a}) \leq 0$ and (ii) for all $\mathbf{b} \in X$ holds $\mathbf{f}(\mathbf{b}) \leqslant \mathbf{f}(\mathbf{a}) \Rightarrow \mathbf{f}(\mathbf{a}) \leqslant \mathbf{f}(\mathbf{b})$.

Single-Objective Optimization As Special Case

decision space

objective space

objective function

total order $\leq$ on $\mathbb{R}$

$$(X, Z, f: X \rightarrow Z, rel \subseteq Z \times Z)$$

Single-Objective Optimization As Special Case

decision space | objective space | objective function

total order $\leq$ on $\mathbb{R}$

$$(X, Z, f: X \rightarrow Z, rel \subseteq Z \times Z)$$

$$(X, prefrel)$$

total preorder where

$a \; prefrel \; b \Leftrightarrow f(a) \; rel \; f(b)$

Preference Relations in the Multiobjective Case

decision space   objective space   objective functions

partial order

$(X, Z, f\colon X \to Z, rel \subseteq Z \times Z)$

preorder where

$a \; prefrel \; b :\Leftrightarrow f(a) \; rel \; f(b)$

$(X, prefrel)$

most of the time not total!

$$(X, \preccurlyeq_{par})$$

$$\downarrow$$

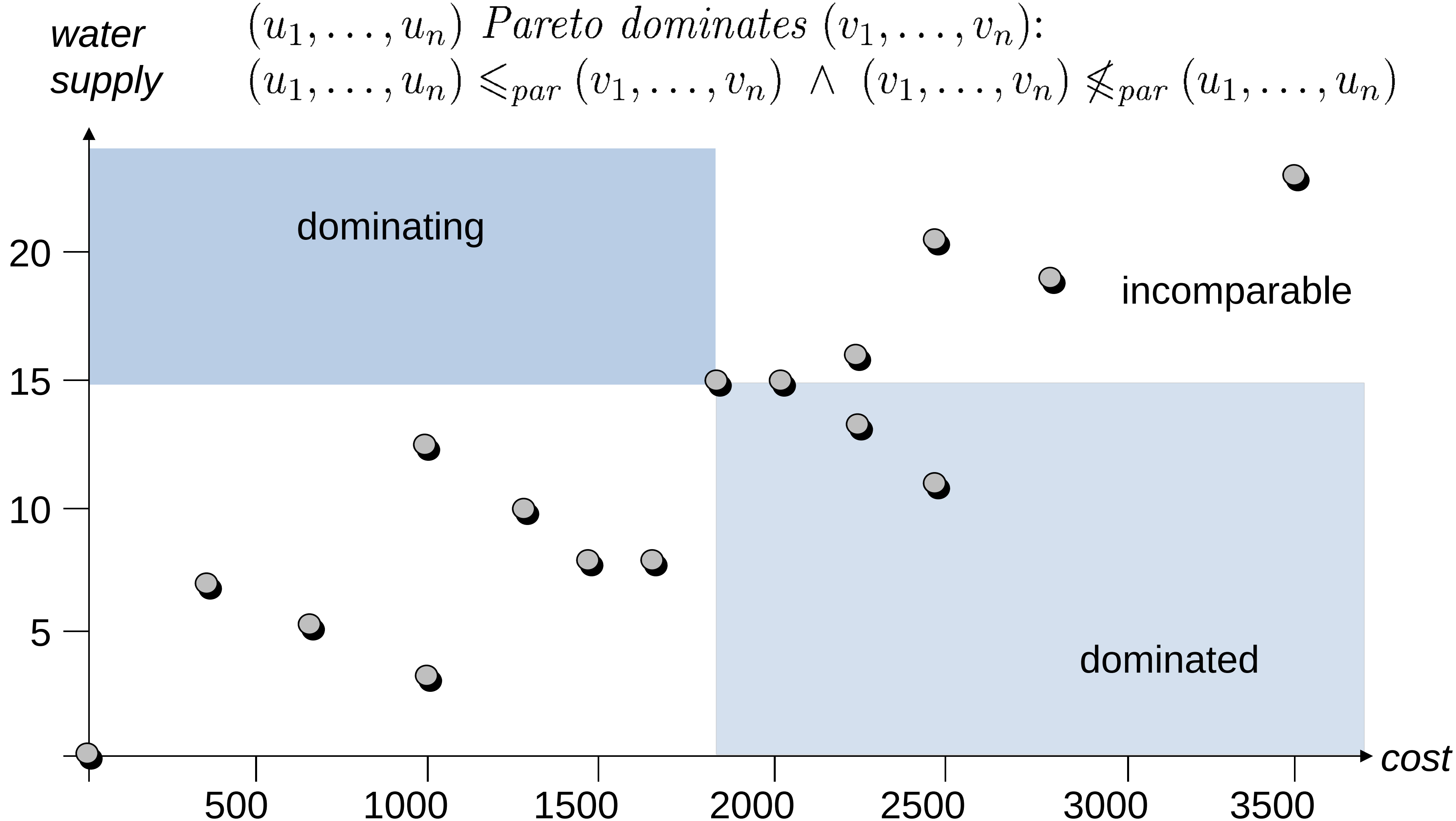
$$a \preccurlyeq_{par} b :\Leftrightarrow f(a) \leqslant_{par} f(b)$$

Example:
weak
Pareto dominance

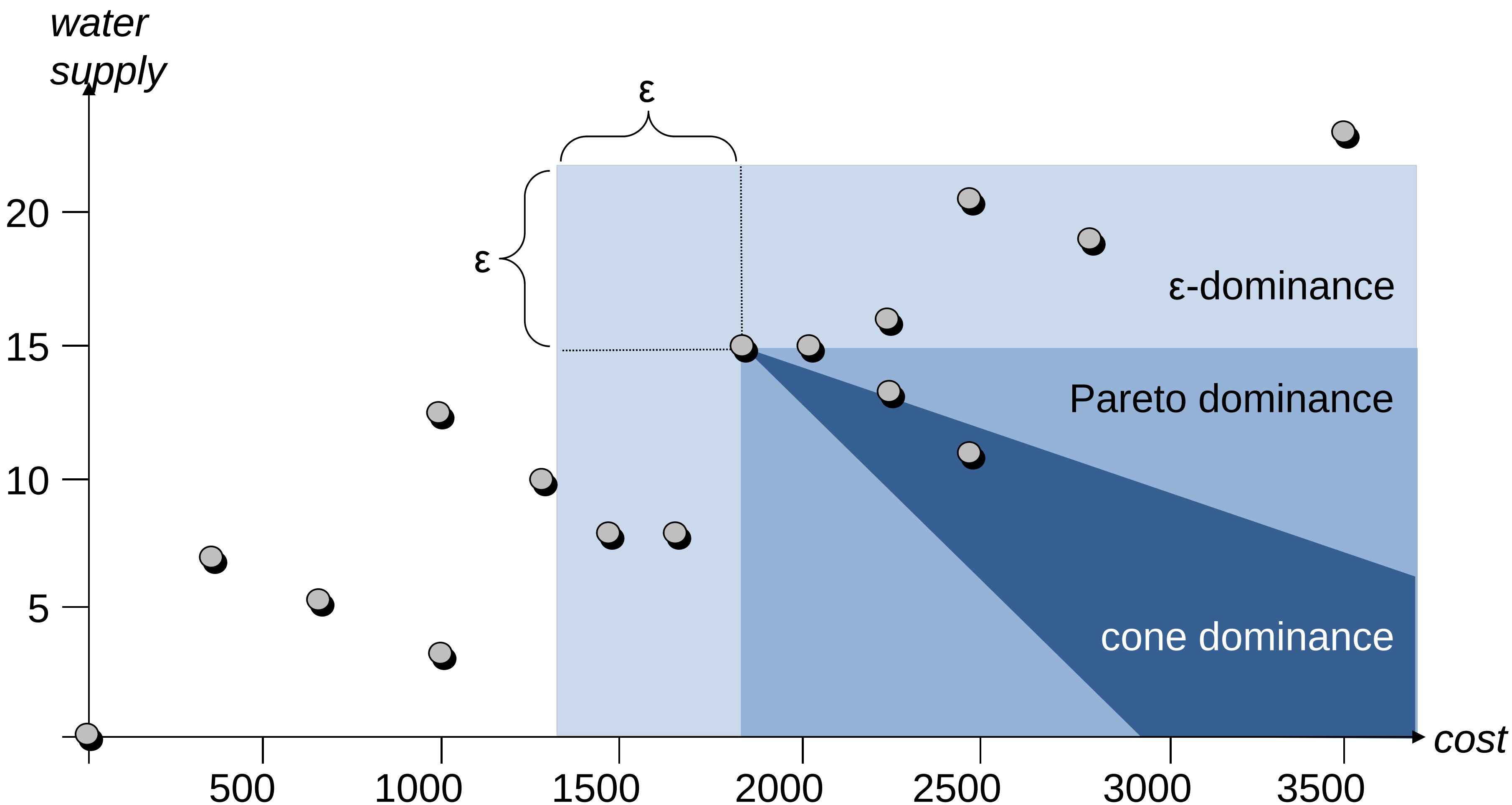
Pareto Dominance

$$(u_1, \ldots, u_n) \textit{ weakly Pareto dominates } (v_1, \ldots, v_n):$$
$$(u_1, \ldots, u_n) \leqslant_{par} (v_1, \ldots, v_n) :\Leftrightarrow \forall 1 \leq i \leq n : u_i \leq v_i$$

$$(u_1, \ldots, u_n) \textit{ Pareto dominates } (v_1, \ldots, v_n):$$
$$(u_1, \ldots, u_n) \leqslant_{par} (v_1, \ldots, v_n) \;\wedge\; (v_1, \ldots, v_n) \not\leqslant_{par} (u_1, \ldots, u_n)$$



Different Notions of Dominance



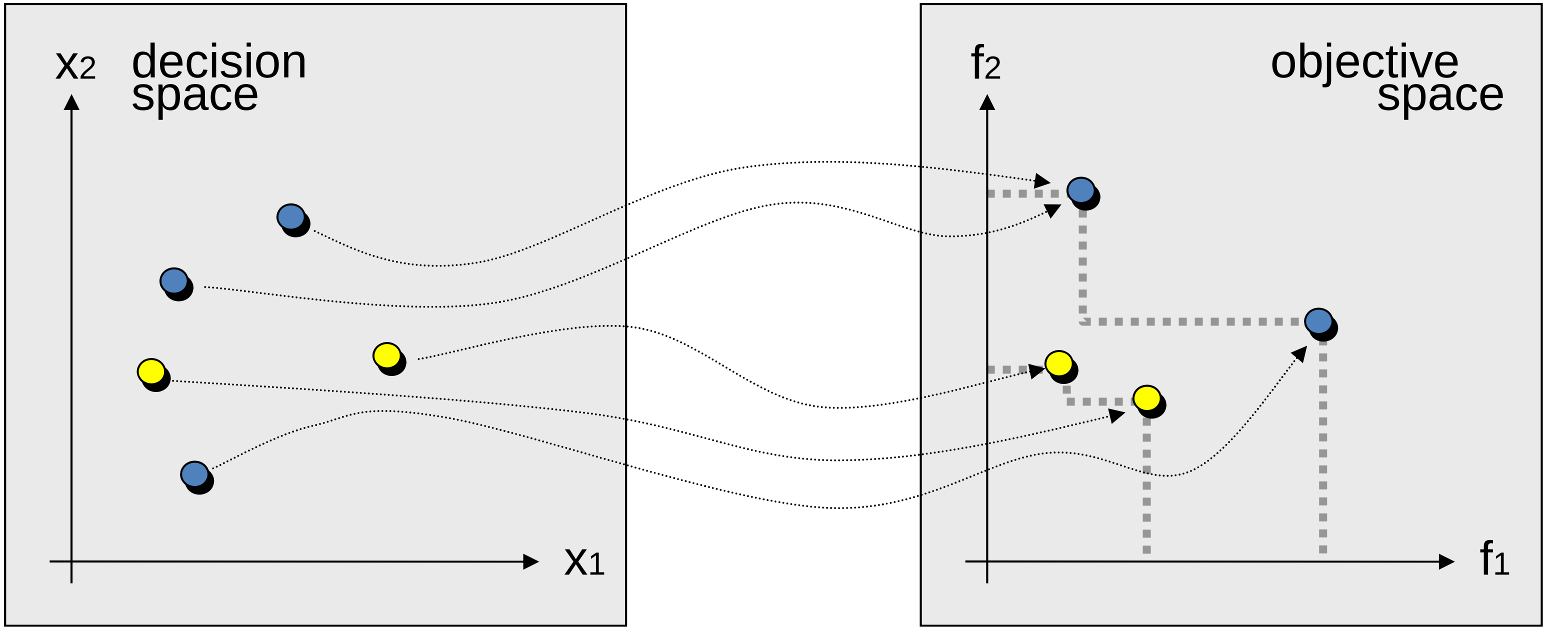
The Pareto-optimal Set

The *minimal set* of a preordered set $(Y, \leqq)$ is defined as

$$Min(Y, \leqq) := \{a \in Y \mid \forall b \in Y : b \leqq a \Rightarrow a \leqq b\}$$

Pareto-optimal set $Min(X, \preccurlyeq_{par})$ — Pareto-optimal front

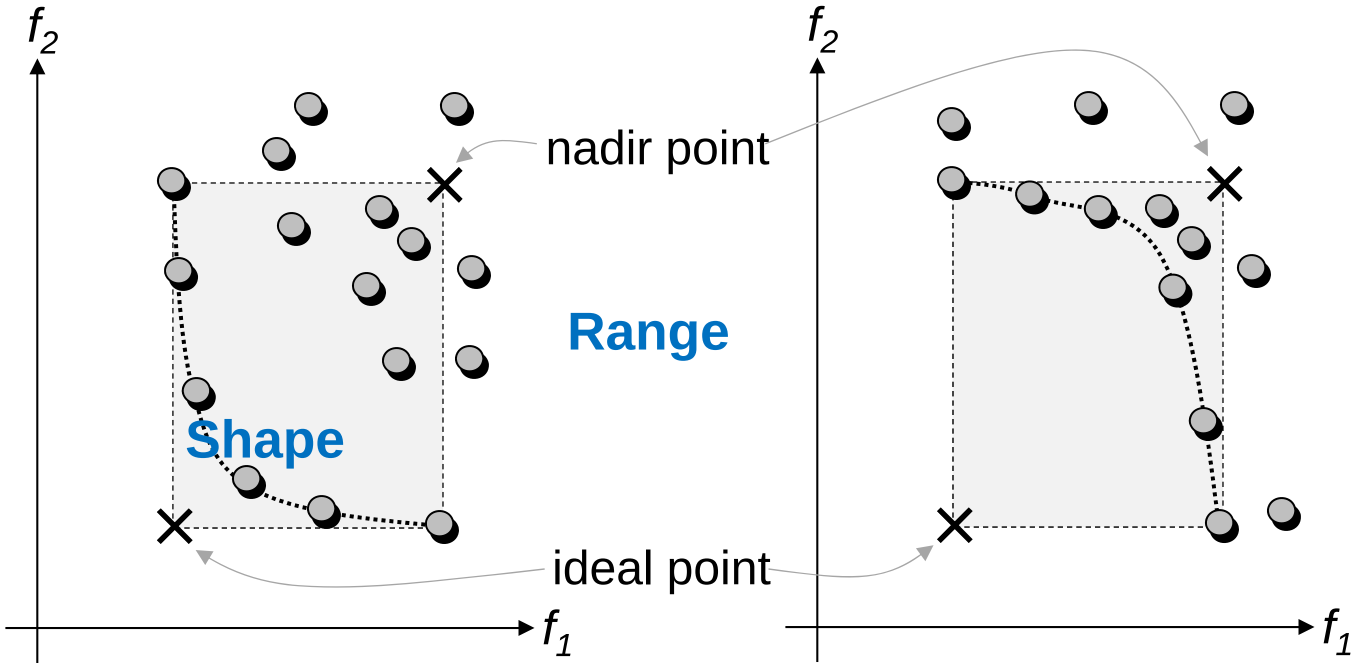
non-optimal decision vector — non-optimal objective vector



Computational complexity:

multiobjective variants can become NP- and #P-complete

Size: Pareto set can be exponential in the input length (e.g. shortest path [Serafini 1986], MST [Camerini et al. 1984])



Approaches To Multiobjective Optimization

A multiobjective problem is as such underspecified

…because not any Pareto-optimum is equally suited!

Additional preferences are needed to tackle the problem:

Solution-Oriented Problem Transformation:
Induce a total order on the decision space, e.g., by aggregation.

Set-Oriented Problem Transformation:

First transform problem into a set problem and then define an objective function on sets.

Preferences are needed in any case, but the latter are weaker!

Problem Transformations and Set Problems

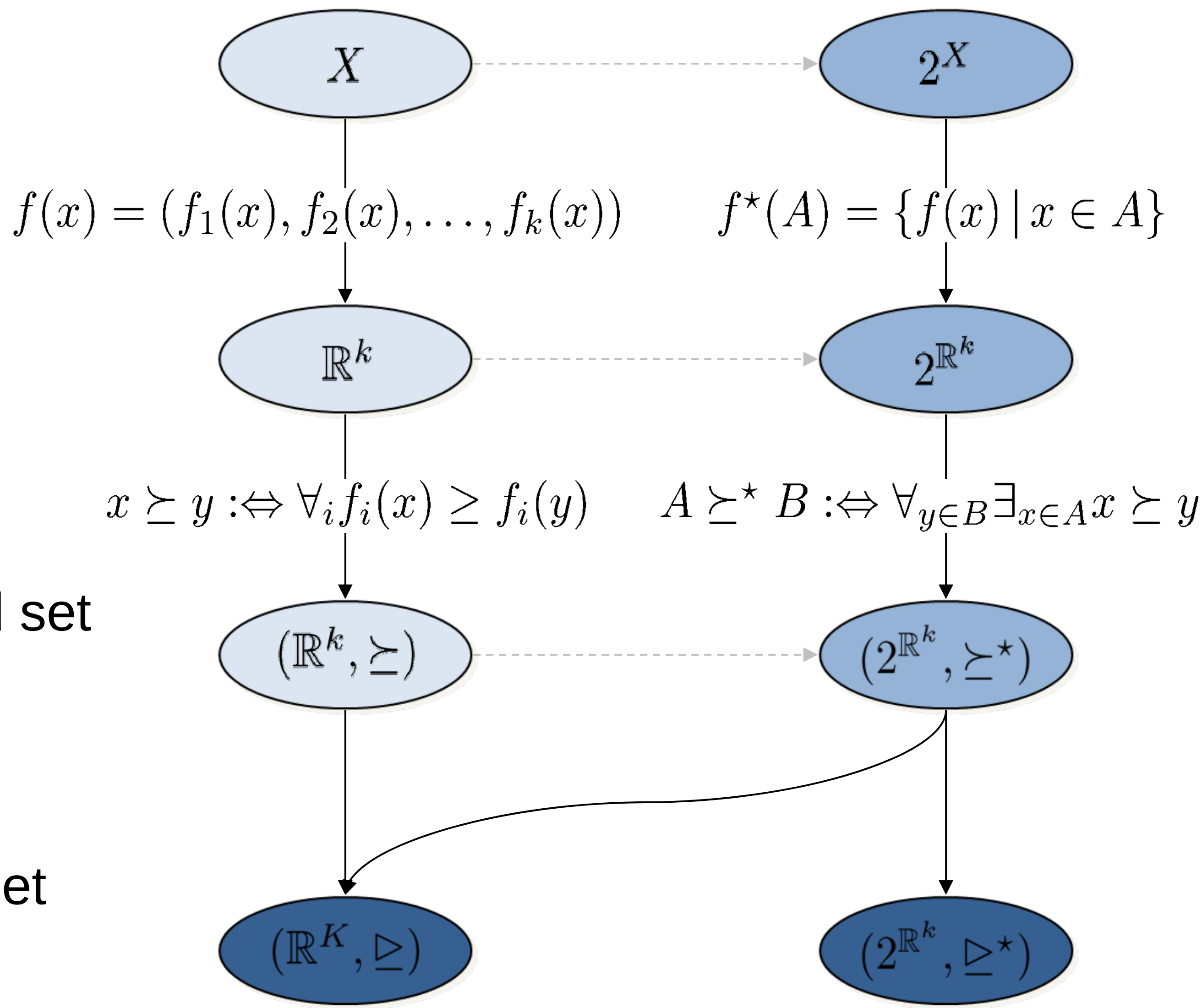
single solution problem | **set problem**

search space

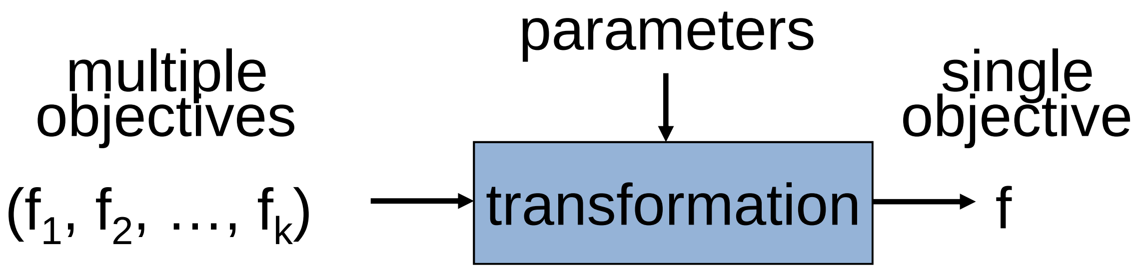
objective space

(partially) ordered set

(totally) ordered set



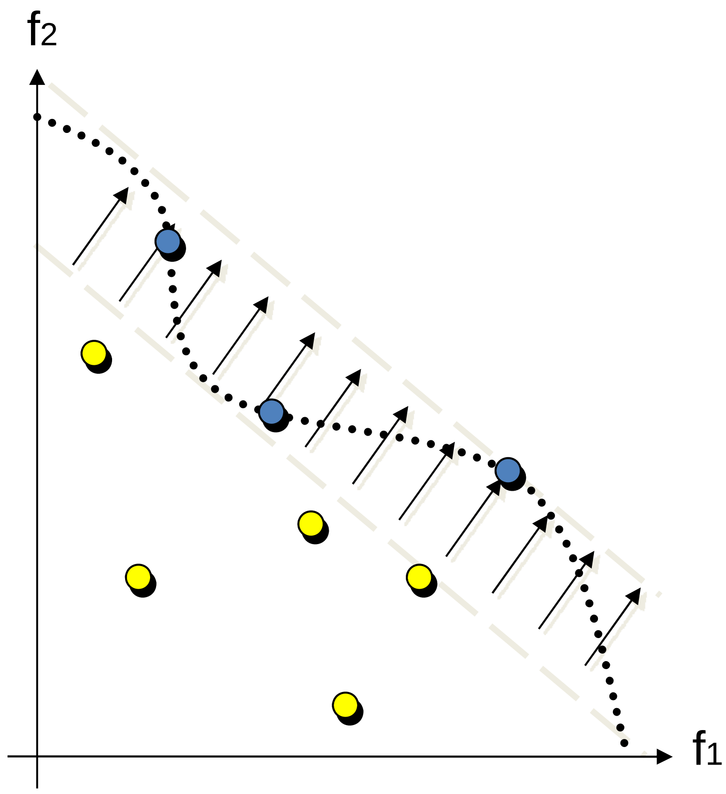
Solution-Oriented Problem Transformations



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

Aggregation-Based Approaches

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



Example: weighting approach

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

→ $y = w_1 y_1 + \ldots + w_k y_k$ →

Other example: Tchebycheff

$$y = \max w_i(u_i - z_i)$$

Set-Oriented Problem Transformations

For a multiobjective optimization problem $(X, Z, \mathbf{f}, \mathbf{g}, \leqslant)$, the associated *set problem* is given by $(\Psi, \Omega, F, \mathbf{G}, \preccurlyeq)$ where

- $\Psi = 2^X$ is the space of decision vector sets, i.e., the powerset of X,
- $\Omega = 2^Z$ is the space of objective vector sets, i.e., the powerset of Z,
- F is the extension of $\mathbf{f}$ to sets, i.e., $F(A) := \{\mathbf{f}(\mathbf{a}) \,:\, \mathbf{a} \in A\}$ for $A \in \Psi$,
- $\mathbf{G} = (G_1, \ldots, G_m)$ is the extension of $\mathbf{g}$ to sets, i.e., $G_i(A) := \max\{g_i(\mathbf{a}) \,:\, \mathbf{a} \in A\}$ for $1 \leq i \leq m$ and $A \in \Psi$,
- $\preccurlyeq$ extends $\leqslant$ to sets where $A \preccurlyeq B :\Leftrightarrow \forall \mathbf{b} \in B \; \exists \mathbf{a} \in A : \mathbf{a} \leqslant \mathbf{b}$.

Another approach:
define relation via quality indicators

Quality of Pareto Set Approximations

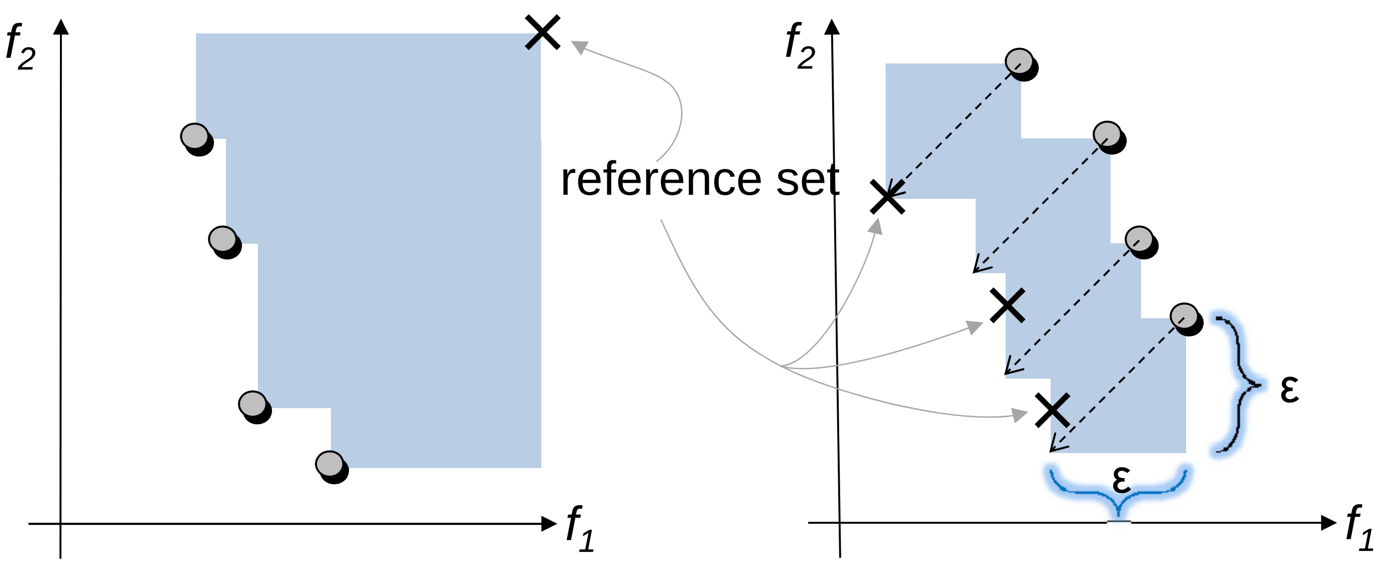
A (unary) *quality indicator* I is a function $I : \Psi \mapsto \mathbb{R}$ that assigns a Pareto set approximation a real value.

$$A \overset{\text{ref}}{\preccurlyeq} B :\Leftrightarrow I(A) \geq I(B)$$

$$A \overset{\text{ref}}{\preccurlyeq} B :\Leftrightarrow I(A,R) \leq I(B,R)$$

I(A) = volume of weakly dominated area in objective space

I(A,R) = how much needs A to be moved to weakly dominate R



hypervolume indicator

epsilon indicator

Refinements

Not all preference relations are useful...

$\overset{\text{ref}}{\preccurlyeq}$ **refines** the weak dominance relation $\preccurlyeq$ iff

$$A \preccurlyeq B \wedge B \not\preccurlyeq A \Rightarrow A \overset{\text{ref}}{\preccurlyeq} B \wedge B \overset{\text{ref}}{\not\preccurlyeq} A \qquad \textit{(better} \Rightarrow \textit{better)}$$

…sought are total refinements

such as the hypervolume indicator

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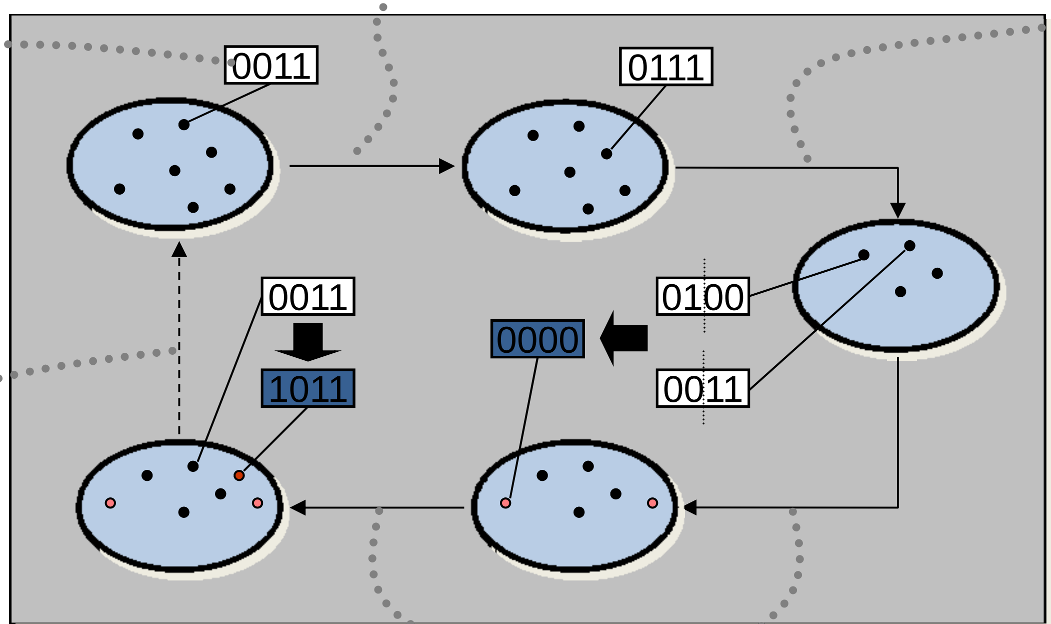
- innovization

Examples of Applications

Algorithm Design: Particular Aspects

representation 1 fitness assignment mating selection

parameters



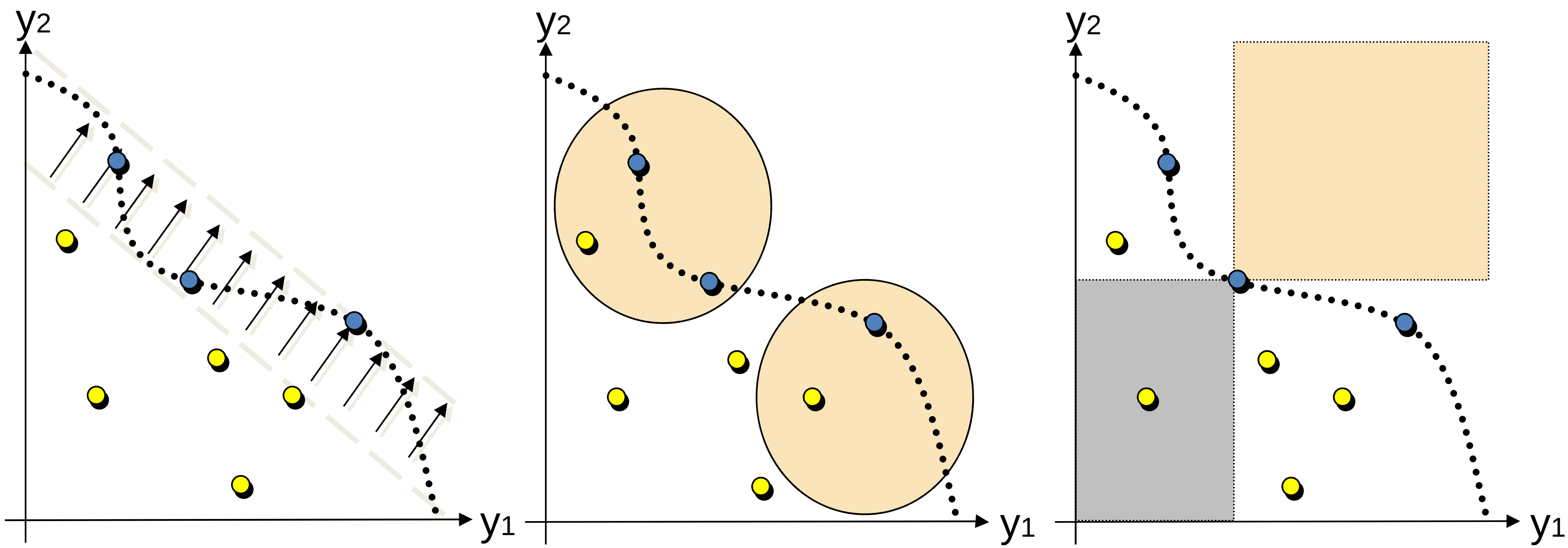
2 environmental selection variation operators

Fitness Assignment: Principal Approaches

aggregation-based *weighted sum*

criterion-based *VEGA*

dominance-based *SPEA2*

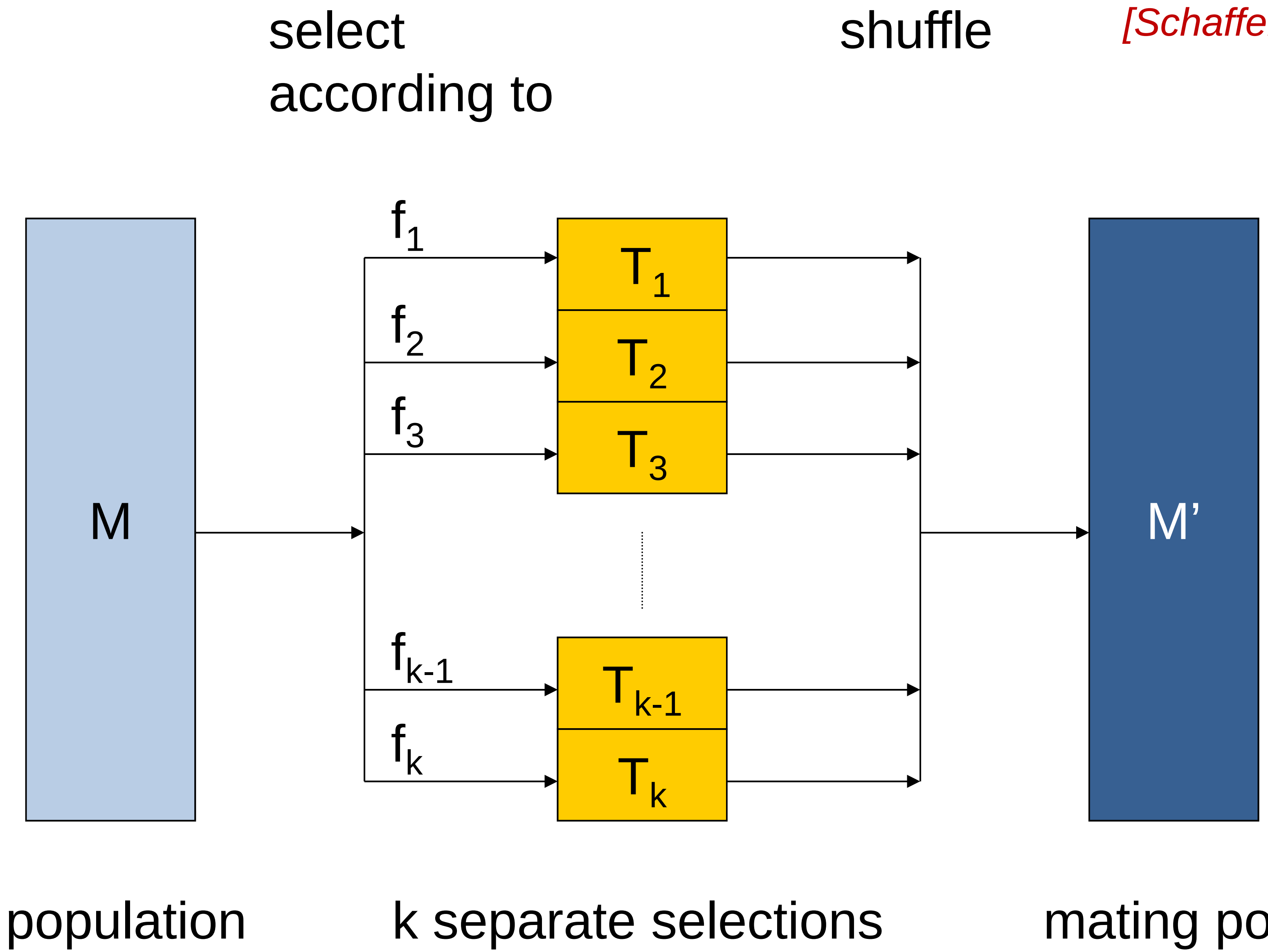


parameter-oriented
scaling-dependent

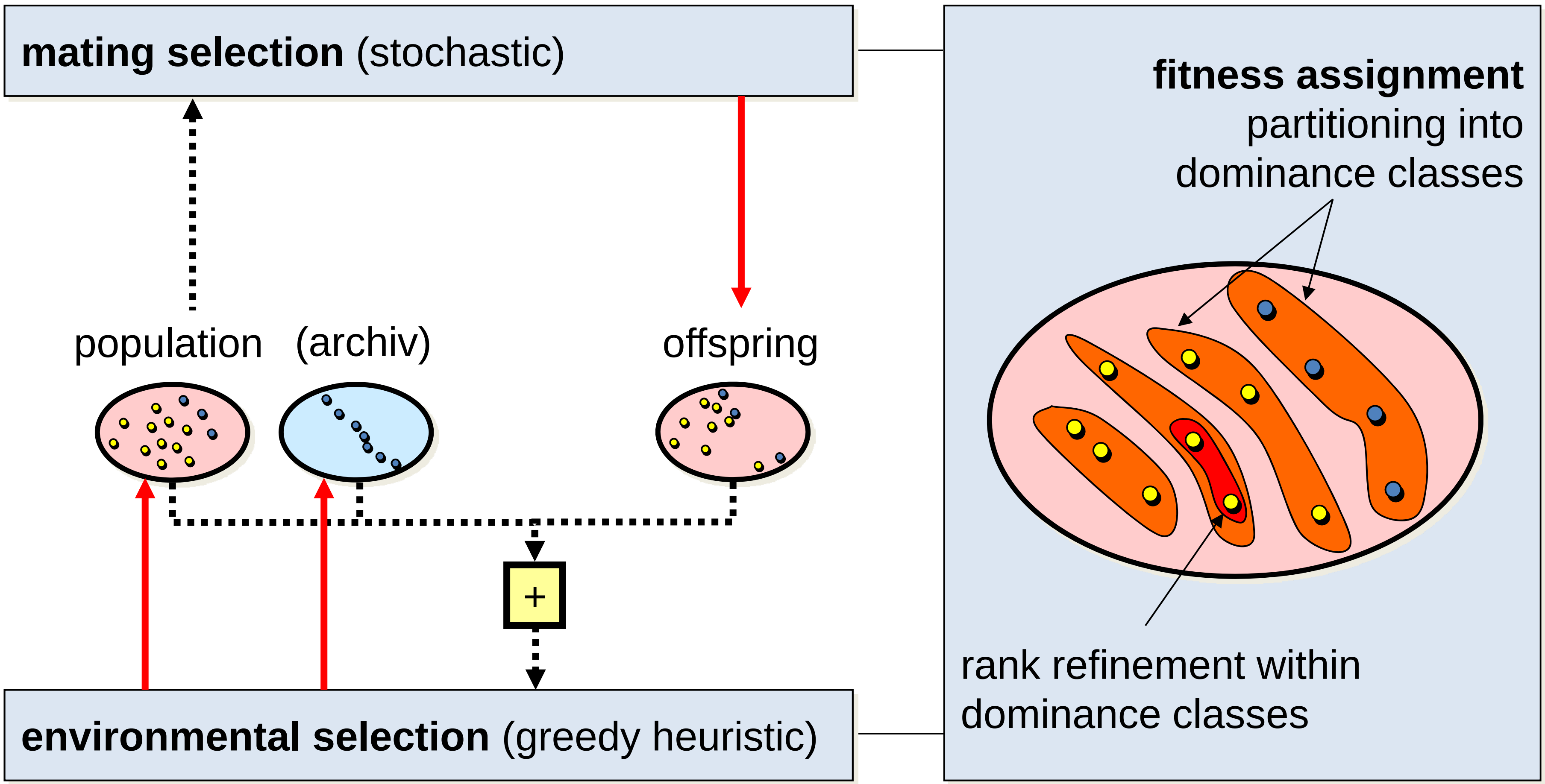
set-oriented
scaling-independent

Criterion-Based Selection: VEGA

[Schaffer 1985]



General Scheme of Dominance-Based 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

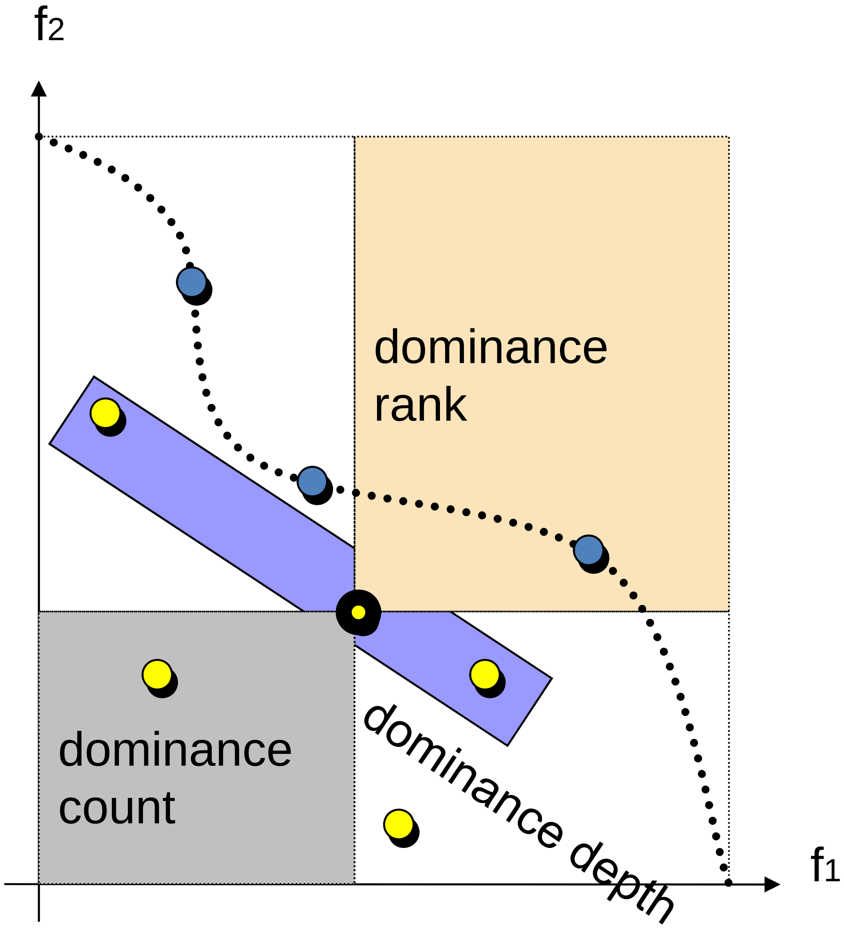
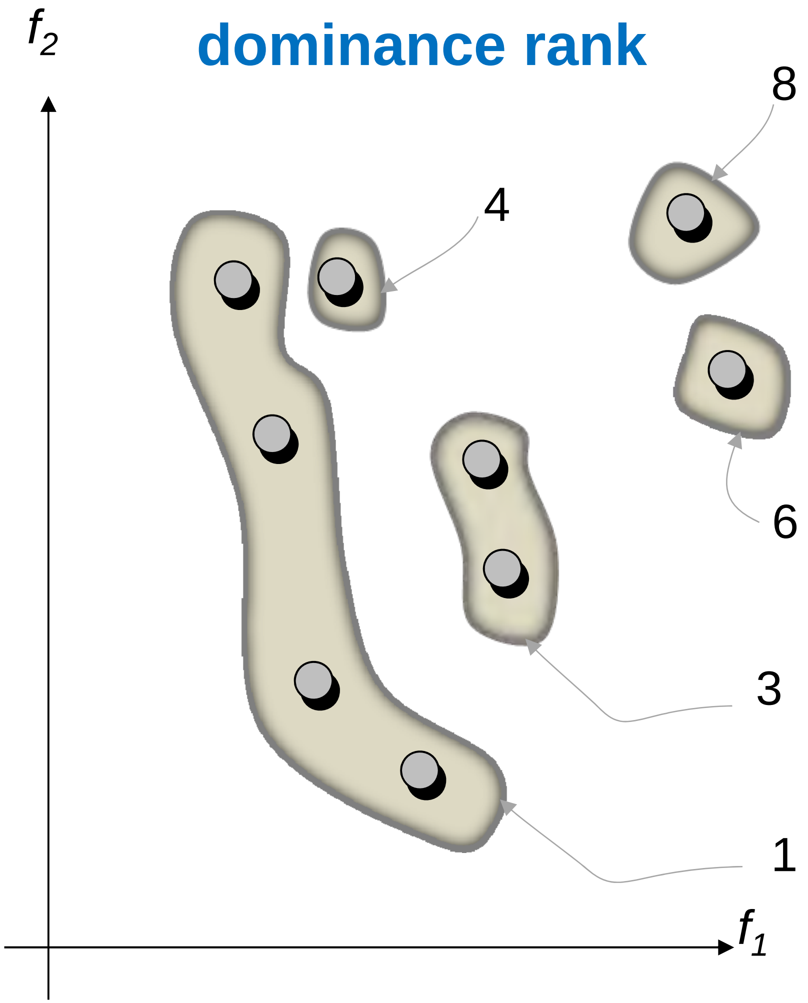
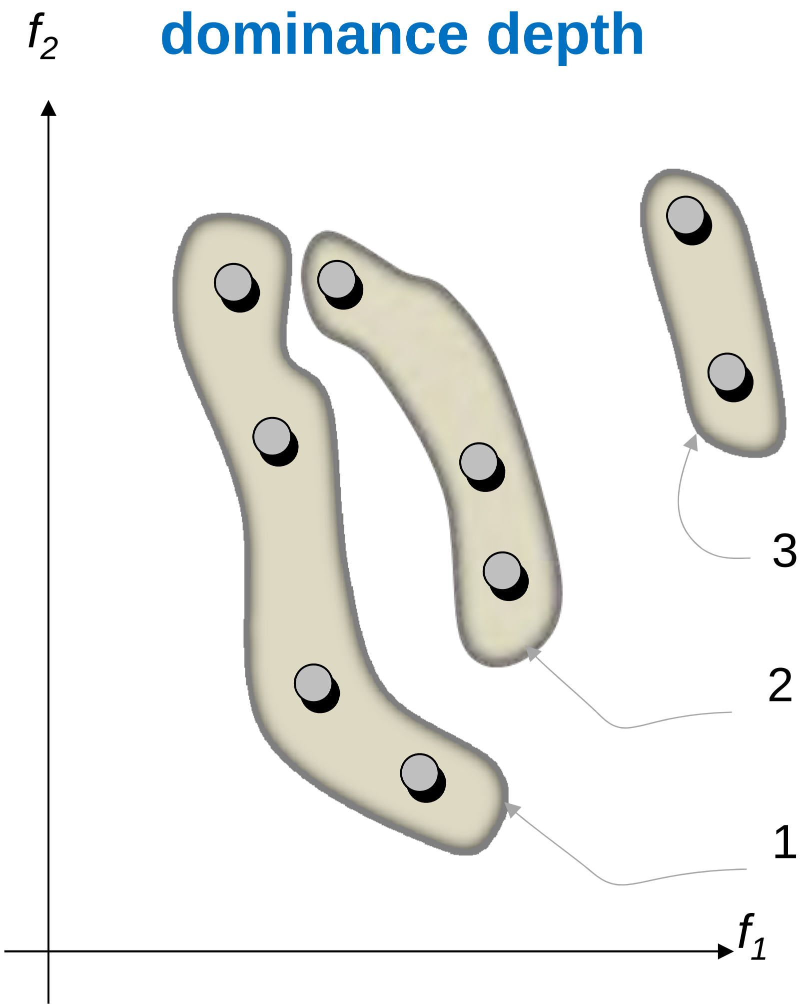


Illustration of Dominance-based Partitioning





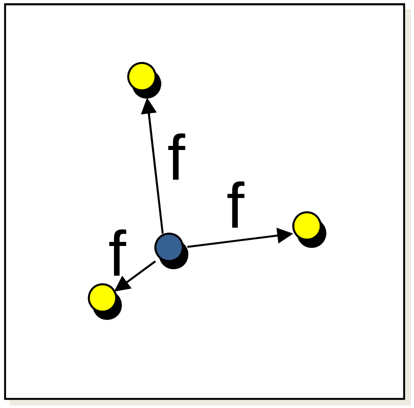
Refinement of Dominance Rankings

Goal: rank incomparable solutions within a dominance class

❶ Density information (good for search, but usually no refinements)

Kernel method

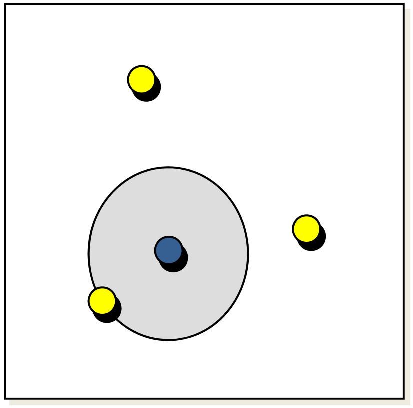
density =
function of the
distances



e.g. NSGA-II

k-th nearest neighbor

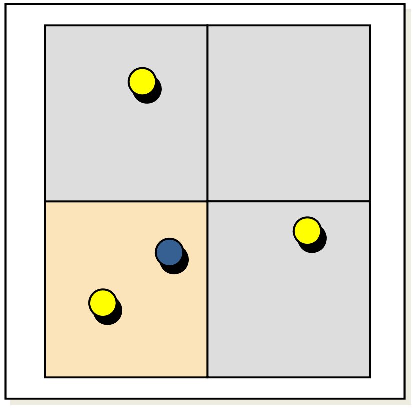
density =
function of distance
to k-th neighbor



e.g. SPEA2

Histogram method

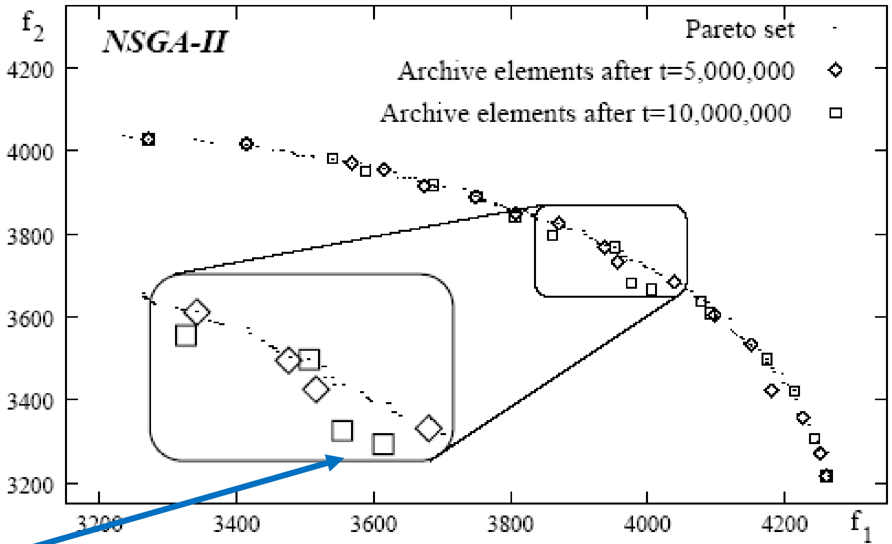
density =
number of elements
within box



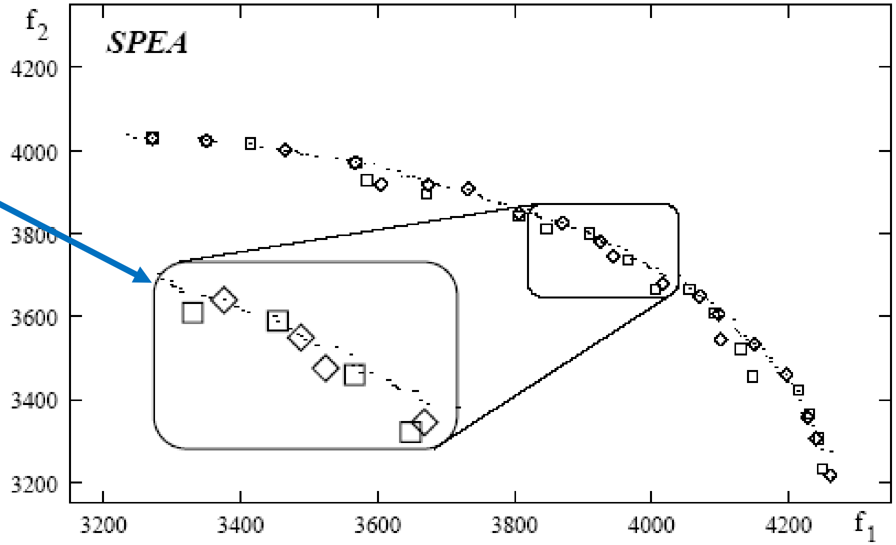
❷ Quality indicator (good for set quality): soon...

Selection in SPEA2 and NSGA-II can result in

deteriorative cycles



non-dominated solutions already found can be lost



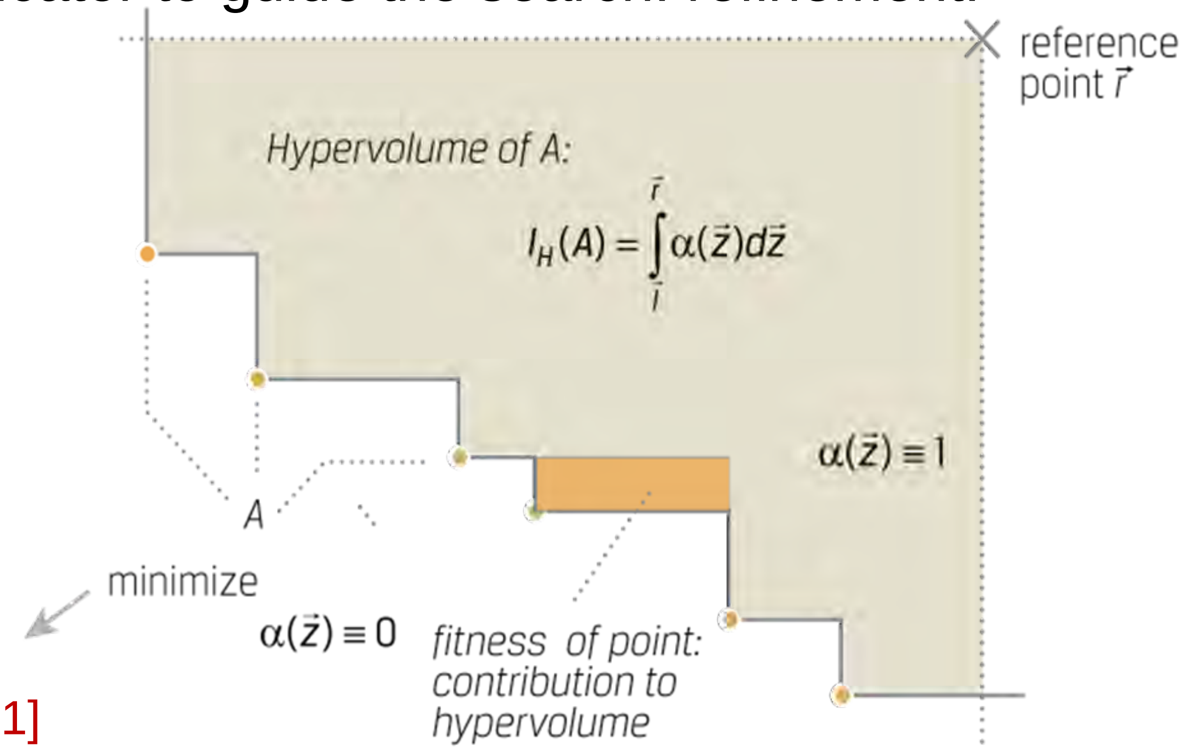
Hypervolume-Based Selection

Latest Approach (e.g. SMS-EMOA [Beume et al. 2007], MO-CMA-ES [Igel et al. 2007])

use hypervolume indicator to guide the search: refinement!

Main idea

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



But: can also result in cycles [Judt et al. 2011] and is expensive [Bringmann and Friedrich 2009]

Therefore: HypE [Bader and Zitzler 2011]

Sampling + Contribution if more than 1 solution deleted

A Brief Introduction to EMO

- basics: what is the difference between single- and multiobjective optimization?
- state-of-the-art algorithm design concepts
- **performance assessment**

Advanced Concepts Useful in Practice

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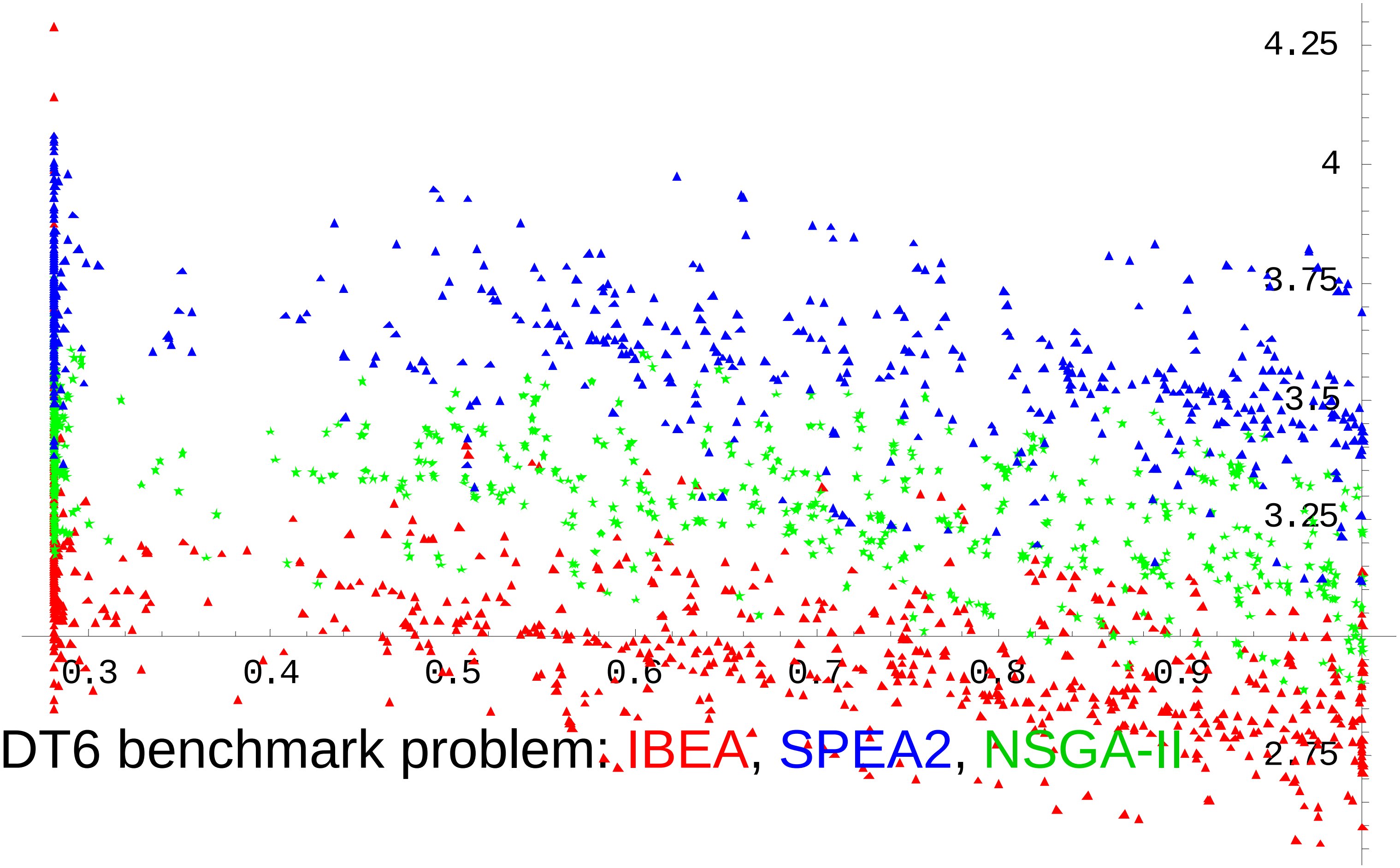
- innovization

Examples of Applications

Once Upon a Time...

... multiobjective EAs were mainly compared visually:



ZDT6 benchmark problem: IBEA, SPEA2, NSGA-II

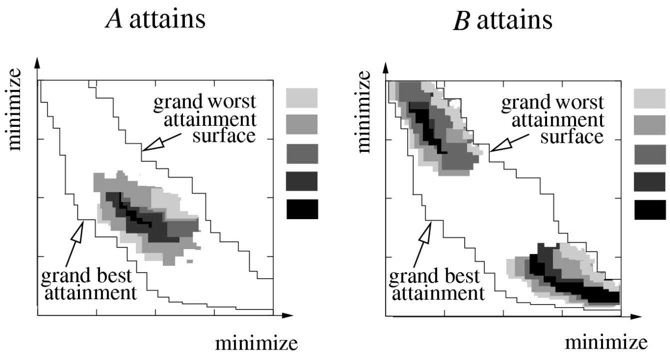
Two Approaches for Empirical Studies

Attainment function approach:

- Applies statistical tests directly to the samples of approximation sets
- Gives detailed information about how and where performance differences occur

Quality indicator approach:

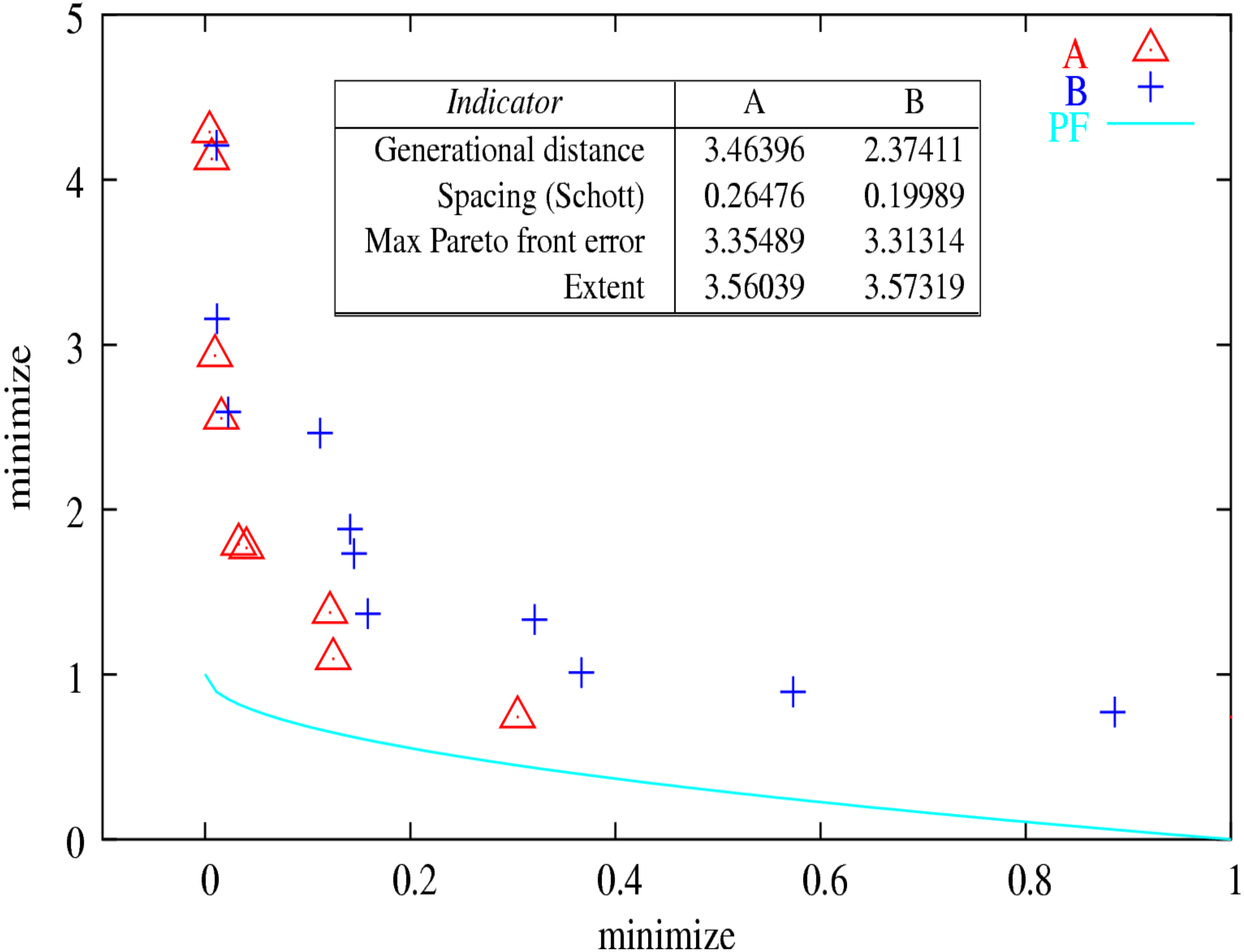
- First, reduces each approximation set to a single value of quality
- Applies statistical tests to the samples of quality values



Indicator	A	B
Hypervolume indicator	6.3431	7.1924
ϵ-indicator	1.2090	0.12722
R_2 indicator	0.2434	0.1643
R_3 indicator	0.6454	0.3475

see e.g. [Zitzler et al. 2003]

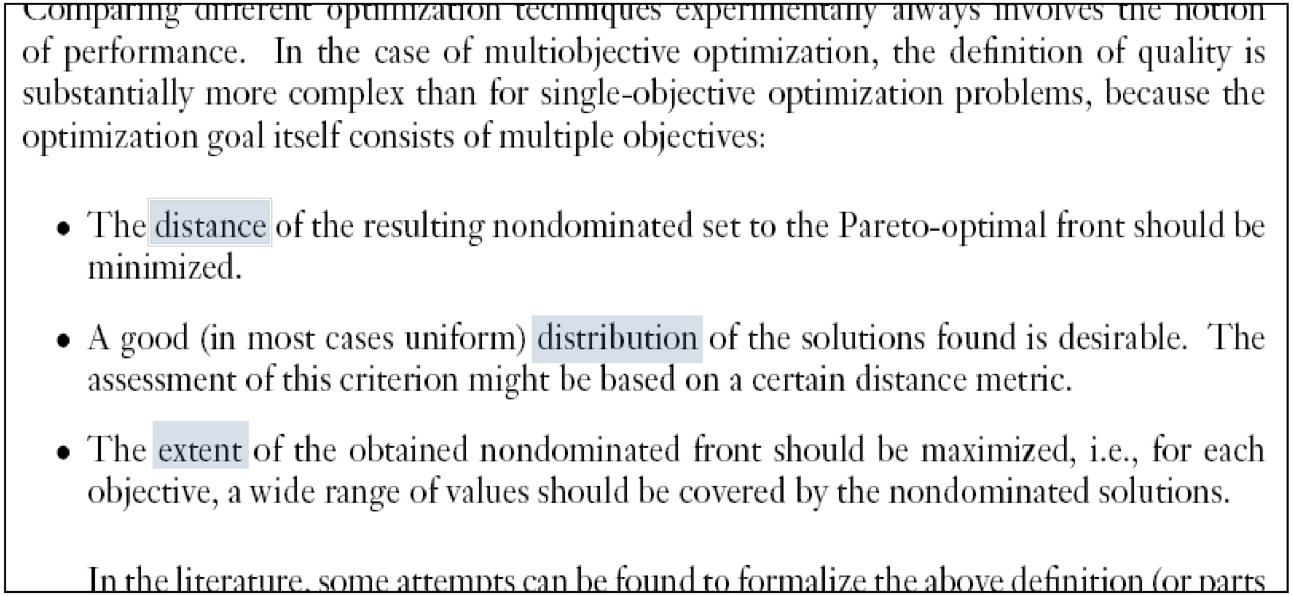
Problems With Non-Compliant Indicators



Indicator	A	B
Generational distance	3.46396	2.37411
Spacing (Schott)	0.26476	0.19989
Max Pareto front error	3.35489	3.31314
Extent	3.56039	3.57319

What Are Good Set Quality Measures?

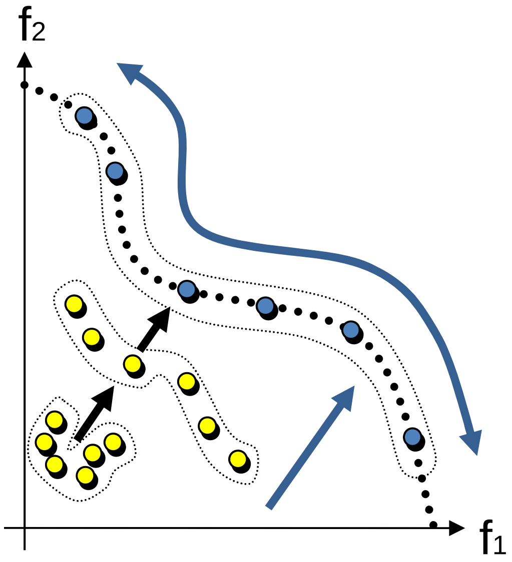
There are **three aspects** [Zitzler et al. 2000]



Comparing different optimization techniques experimentally always involves the notion of performance. In the case of multiobjective optimization, the definition of quality is substantially more complex than for single-objective optimization problems, because the optimization goal itself consists of multiple objectives:

- The distance of the resulting nondominated set to the Pareto-optimal front should be minimized.
- A good (in most cases uniform) distribution of the solutions found is desirable. The assessment of this criterion might be based on a certain distance metric.
- The extent of the obtained nondominated front should be maximized, i.e., for each objective, a wide range of values should be covered by the nondominated solutions.

In the literature, some attempts can be found to formalize the above definition (or parts



Wrong! [Zitzler et al. 2003]

An infinite number of unary set measures is needed to detect in general whether A is better than B

But: total (weak) refinement nice → hypervolume (or R2) indicator

Overview

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Examples of Applications

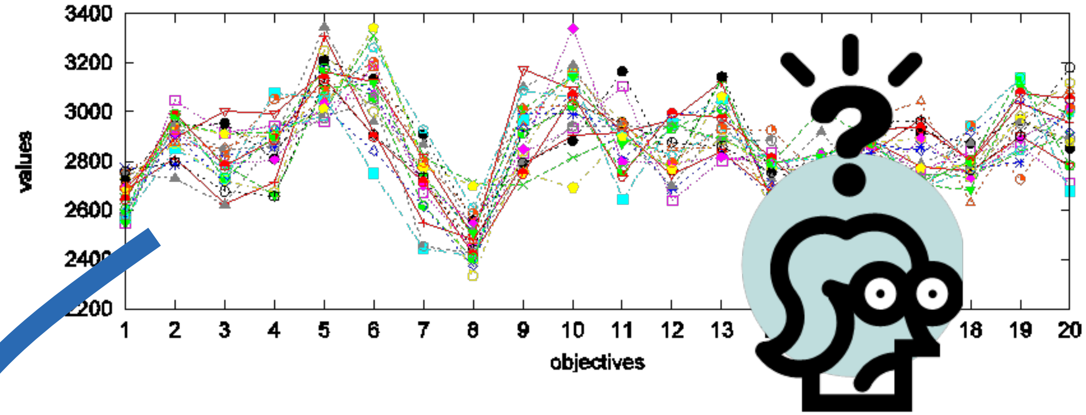
Motivation

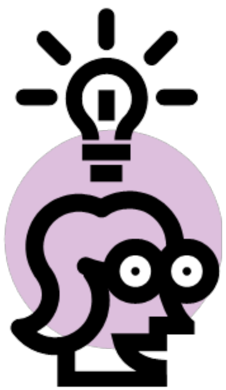
multiobjective problem

$$\begin{array}{l} \text{min. } \{f_1(\mathbf{x}), \ldots, f_k(\mathbf{x})\} \\ \text{subject to } \mathbf{x} \in S \\ \text{and } f_i : \mathbb{R}^n \to \mathbb{R} \end{array}$$

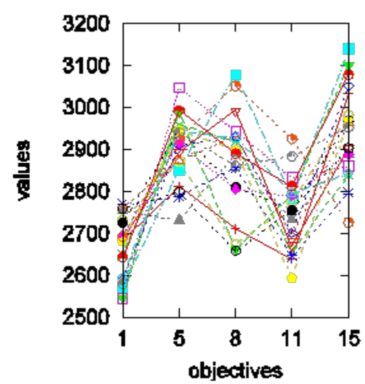
optimizer

(approximation of) Pareto front



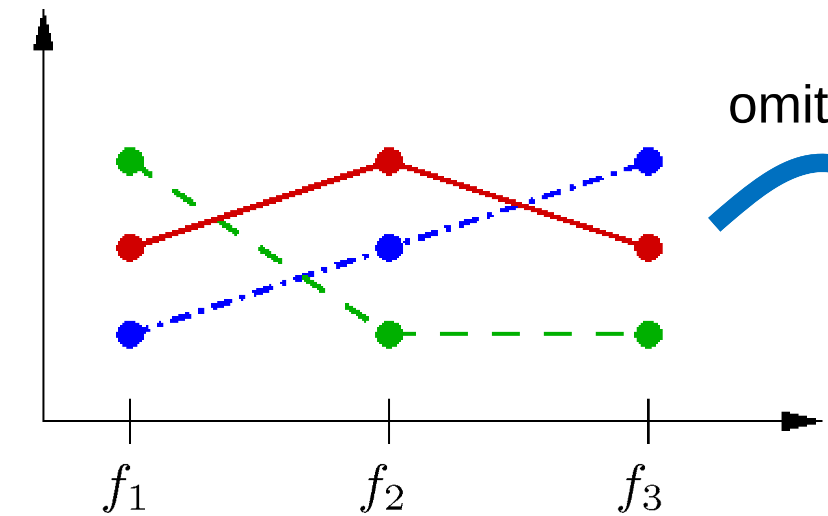


reduce number of objectives / detect redundant objectives

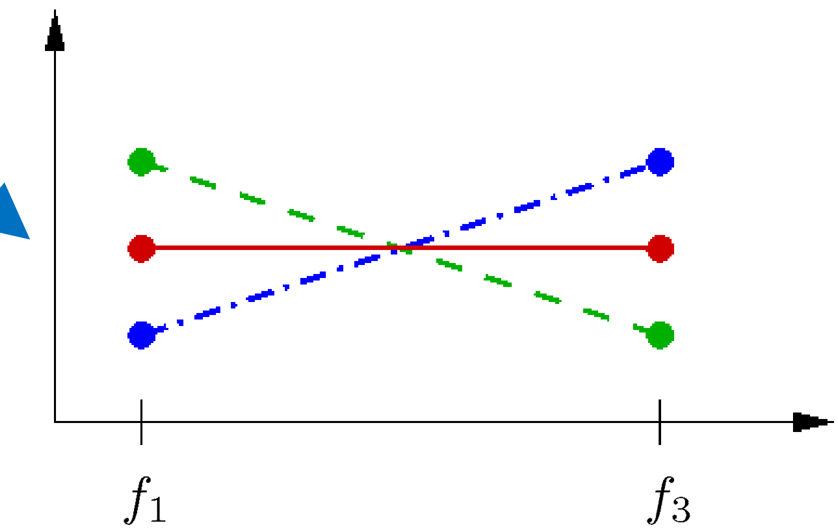


$\Rightarrow$ assist the decision maker

$\Rightarrow$ learn about the problem



omit f_2



$a||b$ $\quad$ $b||c$ $\quad$ $a||c$ $\quad\longrightarrow\quad$ $a||b$ $\quad$ $b||c$ $\quad$ $a||c$

still the same relations

Key questions

- Objective reduction possible without changing the problem?
- How to compute a minimum objective set?
- Applicable to real problems?

Objective Reduction Approaches

Omitting redundant objectives [Agrell 1997], [Gal and Leberling 1977]

- Not suitable for black-box optimization

PCA based objective reduction [Deb and Saxena 2005-2008]

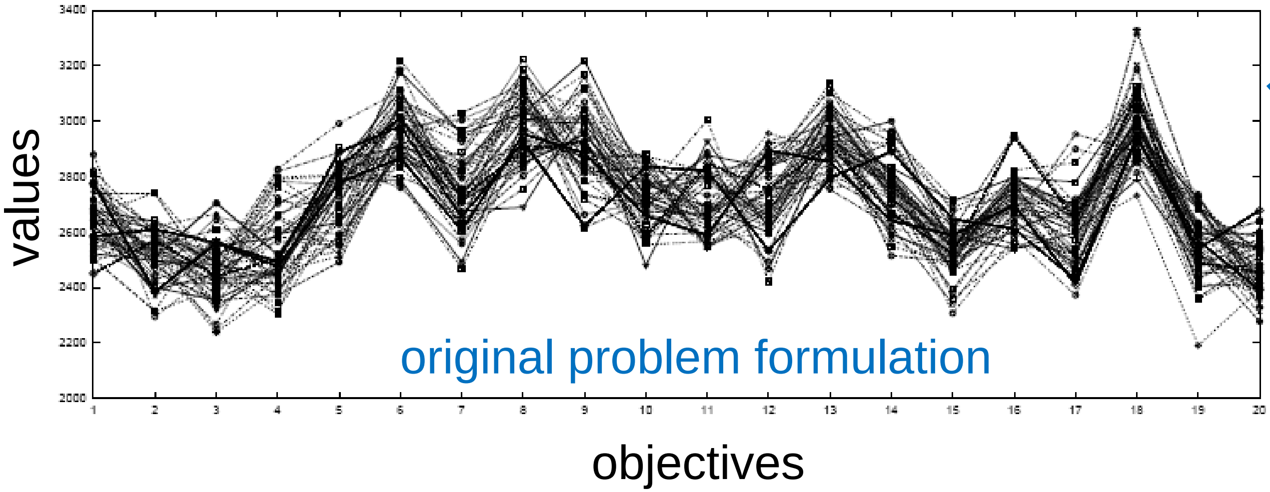
- Cannot guarantee preservation of dominance structure
- Works well in practice

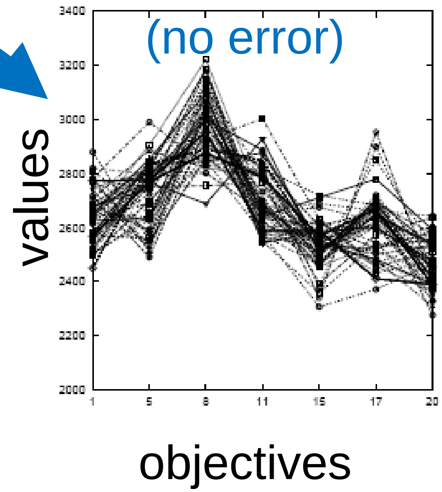
Dominance Relation Preservation [Brockhoff and Zitzler 2006-2009] [López Jaimes et al. 2008, 2009]

- Goal: find minimal set of objectives that preserve dominance relation
- Efficient greedy algorithms available
  [http://www.tik.ee.ethz.ch/sop/download/supplementary/objectiveReduction/]

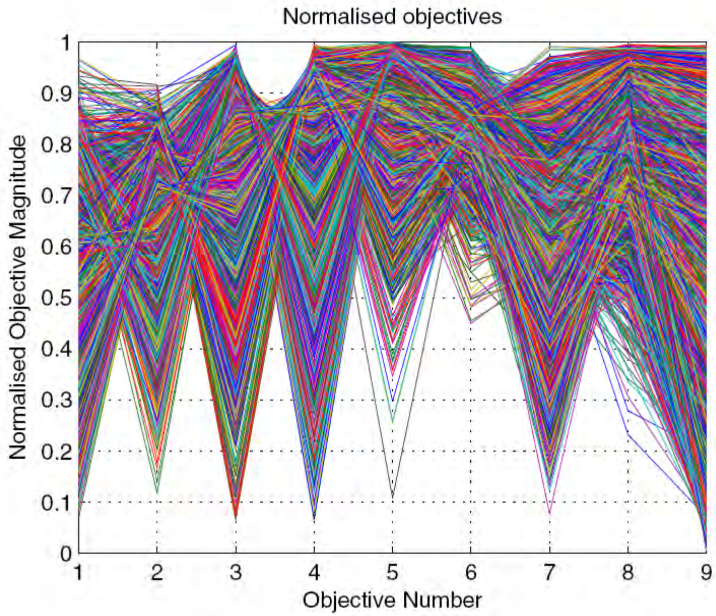
Objective Reduction: Examples

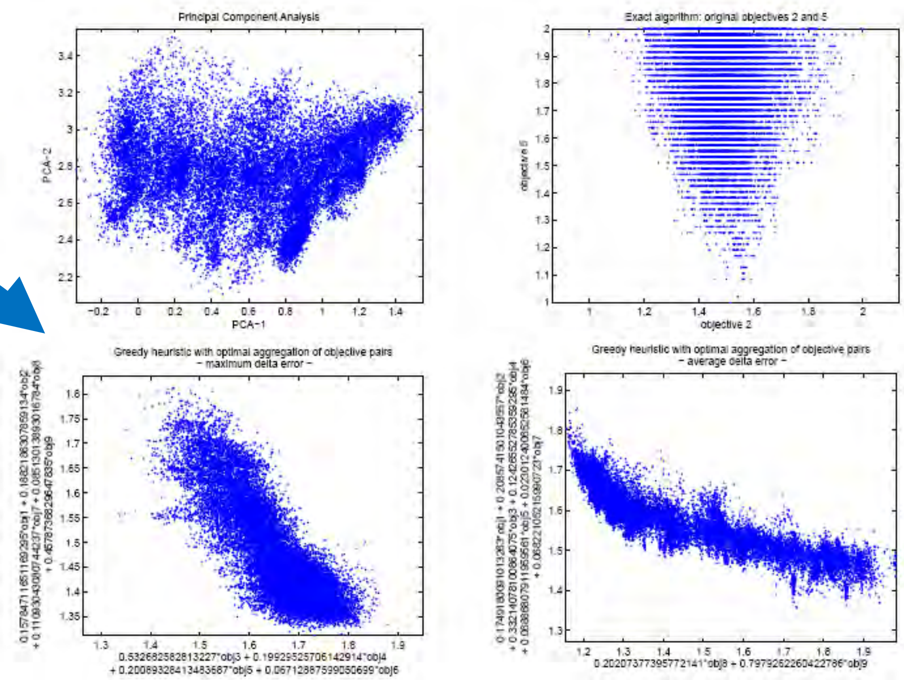
Knapsack Problem





Radar Waveform Problem



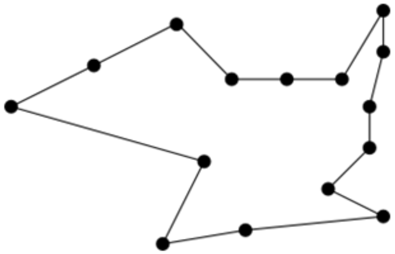


The Opposite: Multiobjectivization

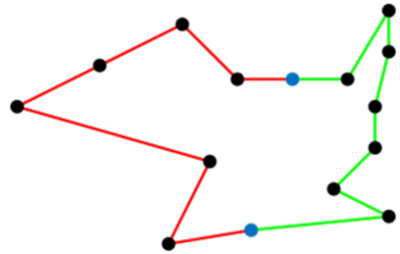
Some problems are easier to solve in a multiobjective scenario

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], theoretical (runtime) analyses [Brockhoff et al. 2009]
- 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], theoretical (runtime) analyses [Handl et al. 2008b]

Innovization

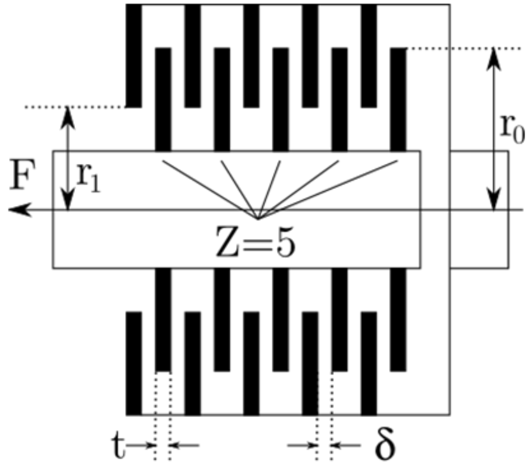
Often innovative design principles among solutions are found

example:

clutch brake design

[Deb and Srinivasan 2006]

min. mass +
stopping time



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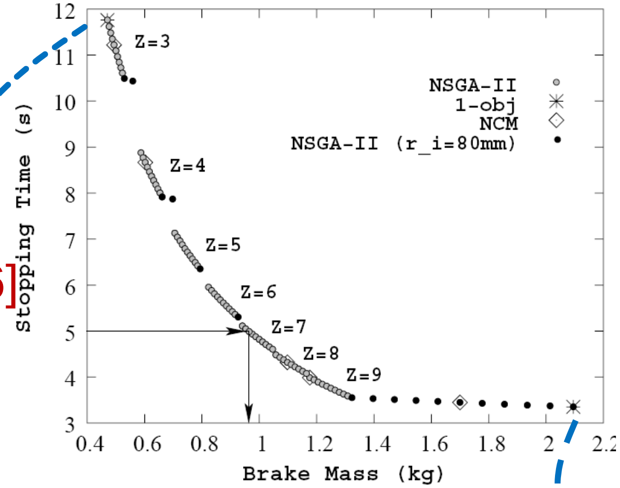
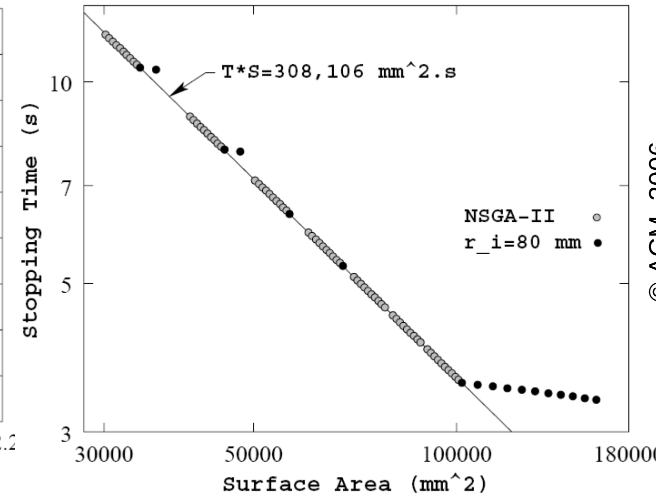




Solution	x_1	x_2	x_3	x_4	x_5	f_1	f_2
Min. f_1	70	90	1.5	1000	3	0.4704	11.7617
Min. f_2	80	110	1.5	1000	9	2.0948	3.3505

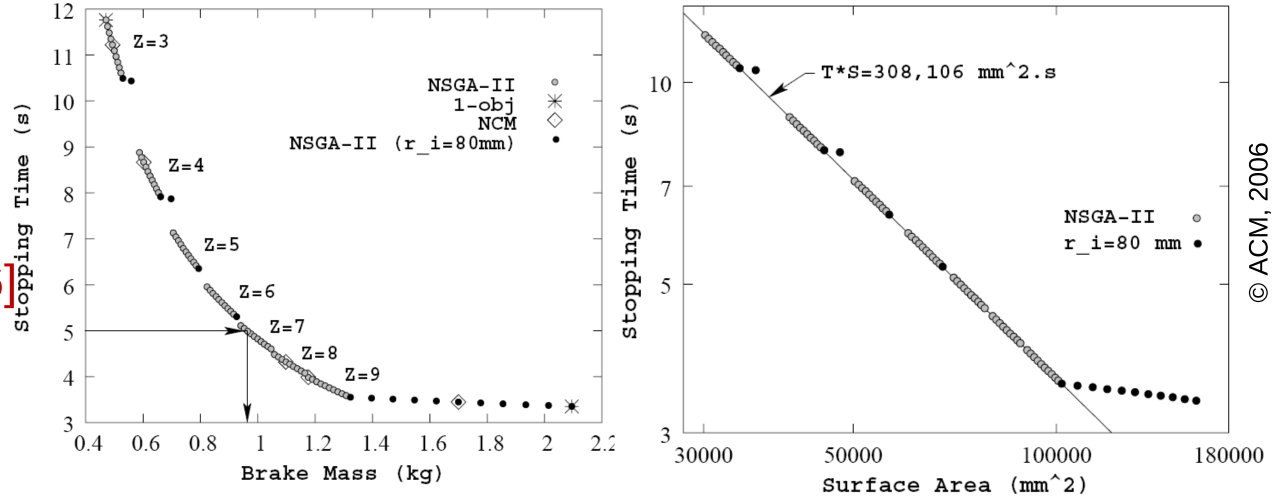
Innovization

Often innovative design principles among solutions are found

example:

clutch brake design

[Deb and Srinivasan 2006]



Innovization [Deb and Srinivasan 2006]

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

= learning about a multiobjective optimization problem

Other examples:

- SOM for supersonic wing design [Obayashi and Sasaki 2003]
- biclustering for processor design and KP [Ulrich et al. 2007]

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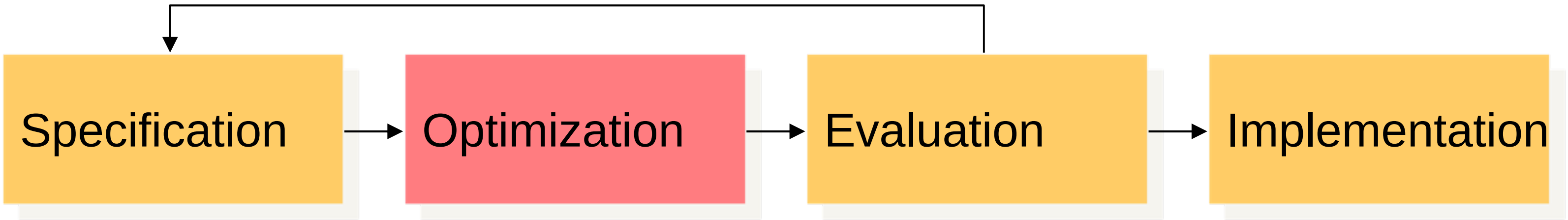
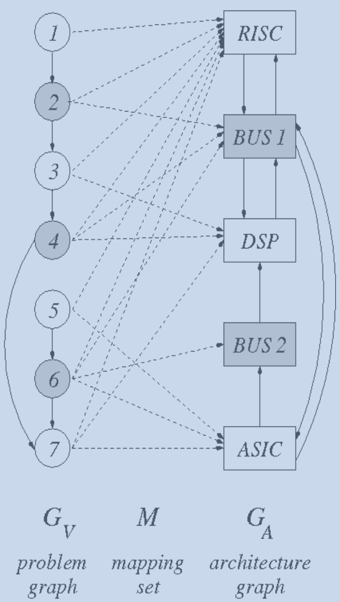
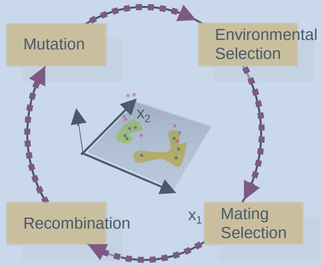
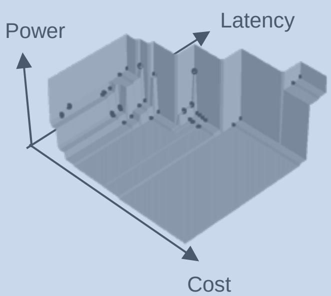
Examples of Applications

Application: Design Space Exploration

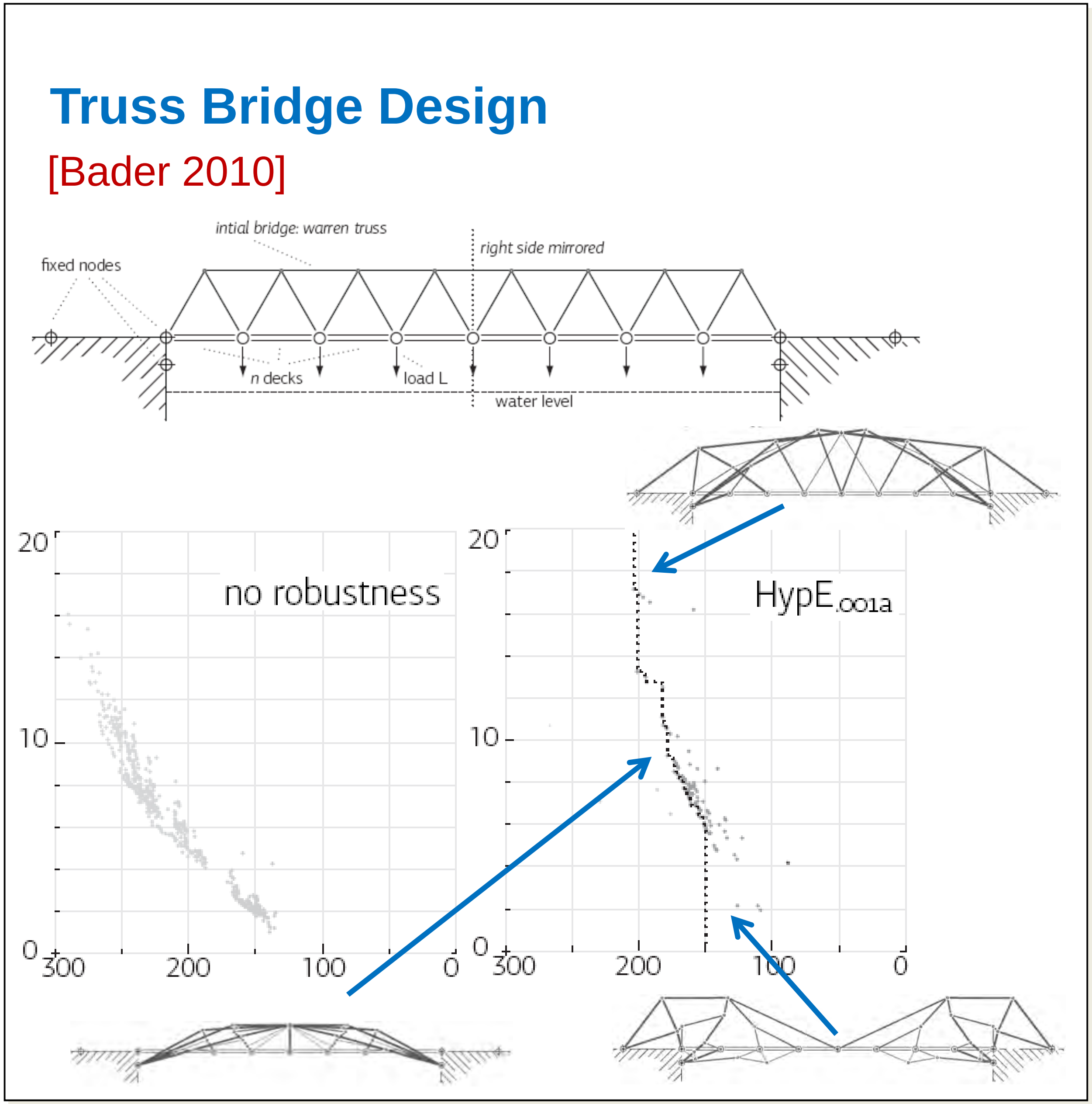


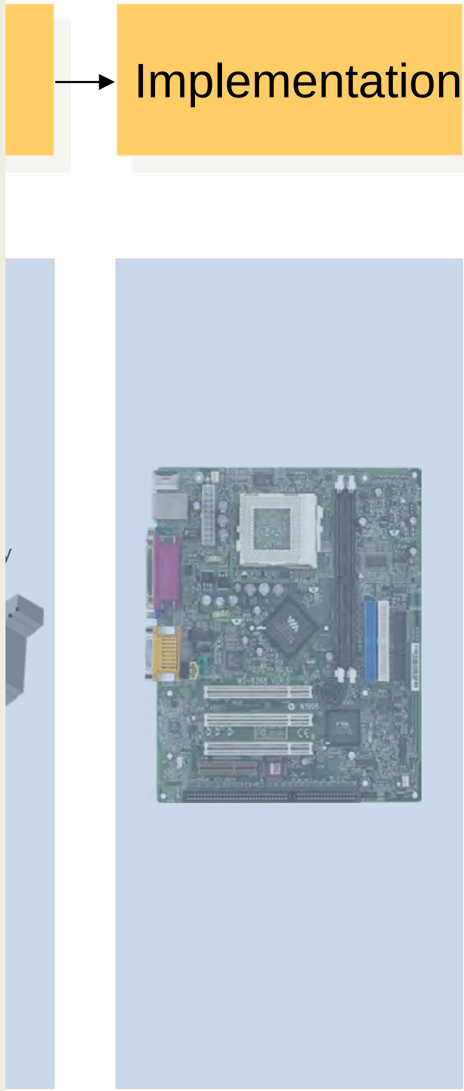






Application: Design Space Exploration

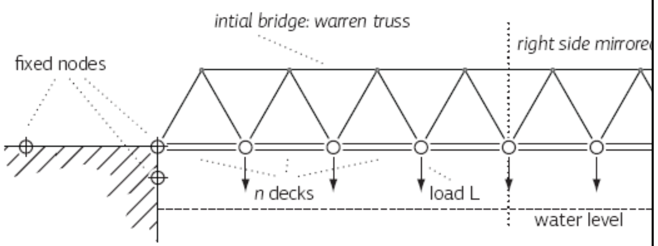


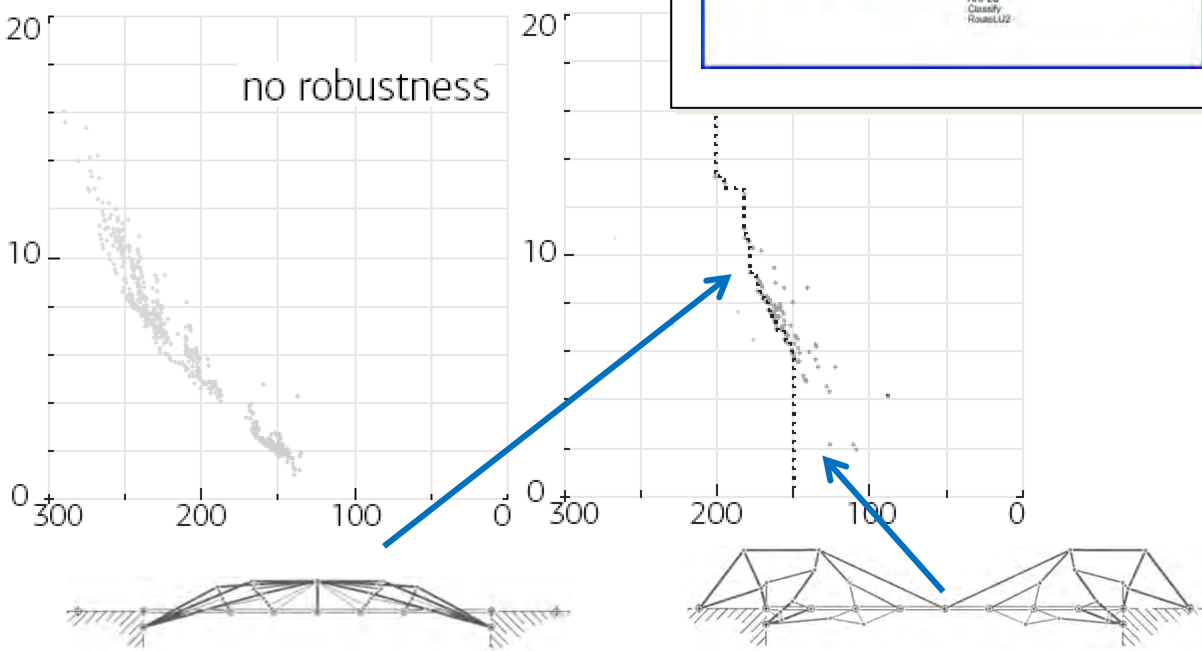


Application: Design Space Exploration

Truss Bridge Design

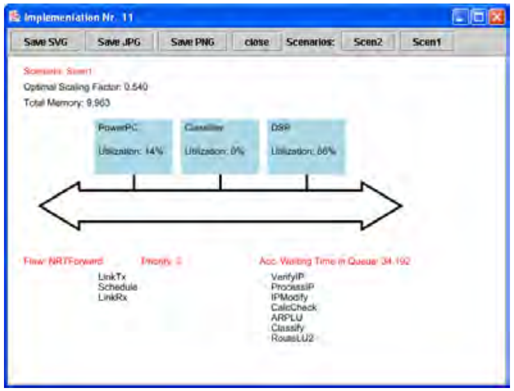
[Bader 2010]

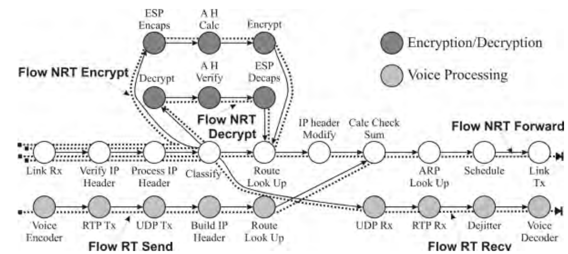


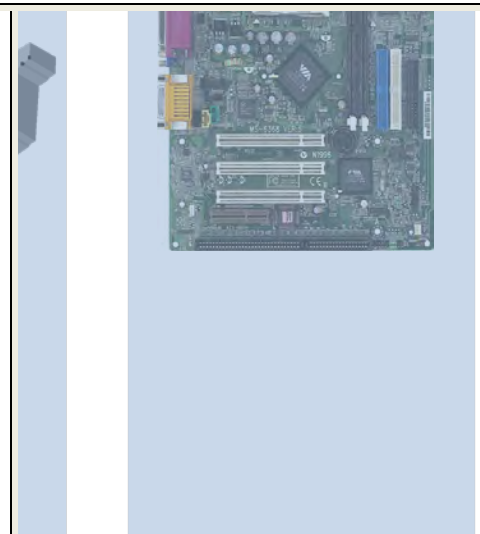


Network Processor Design

[Thiele et al. 2002]







Application: Design Space Exploration

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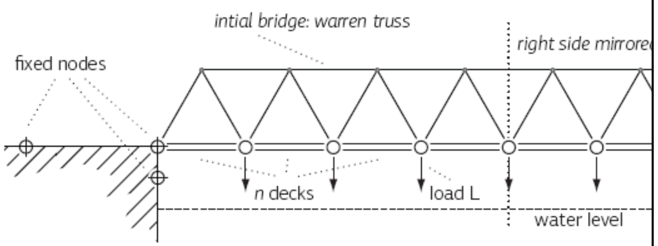
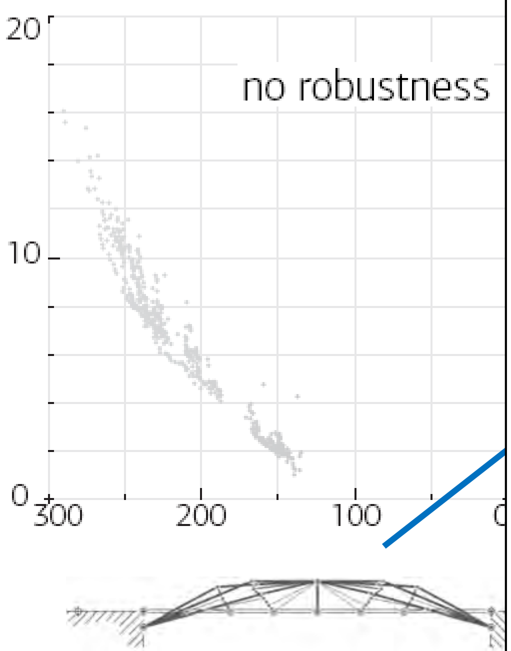
[Bader 2010]





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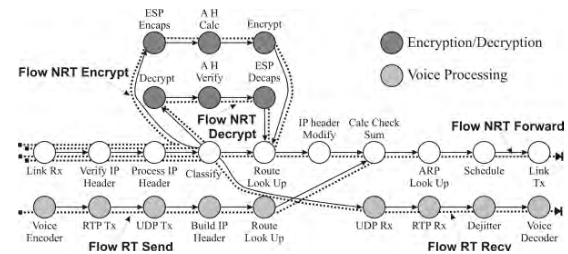
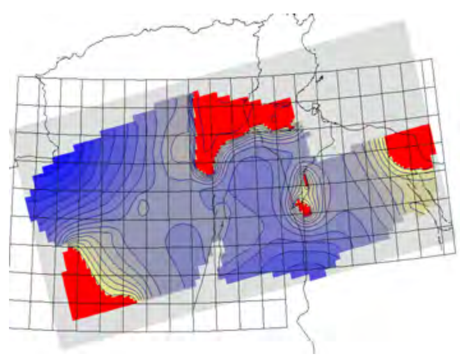
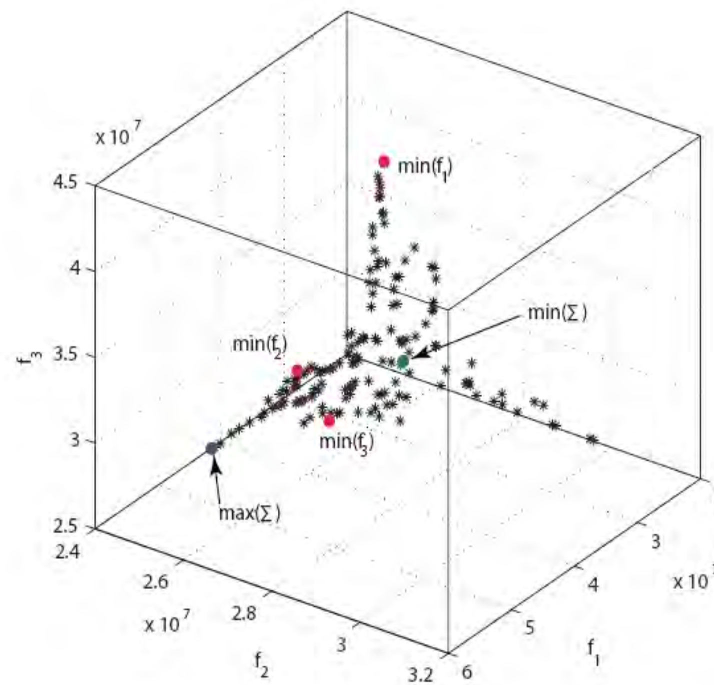
[Thiele et al. 2002]



Water resource management

[Siegfried et al. 2009]

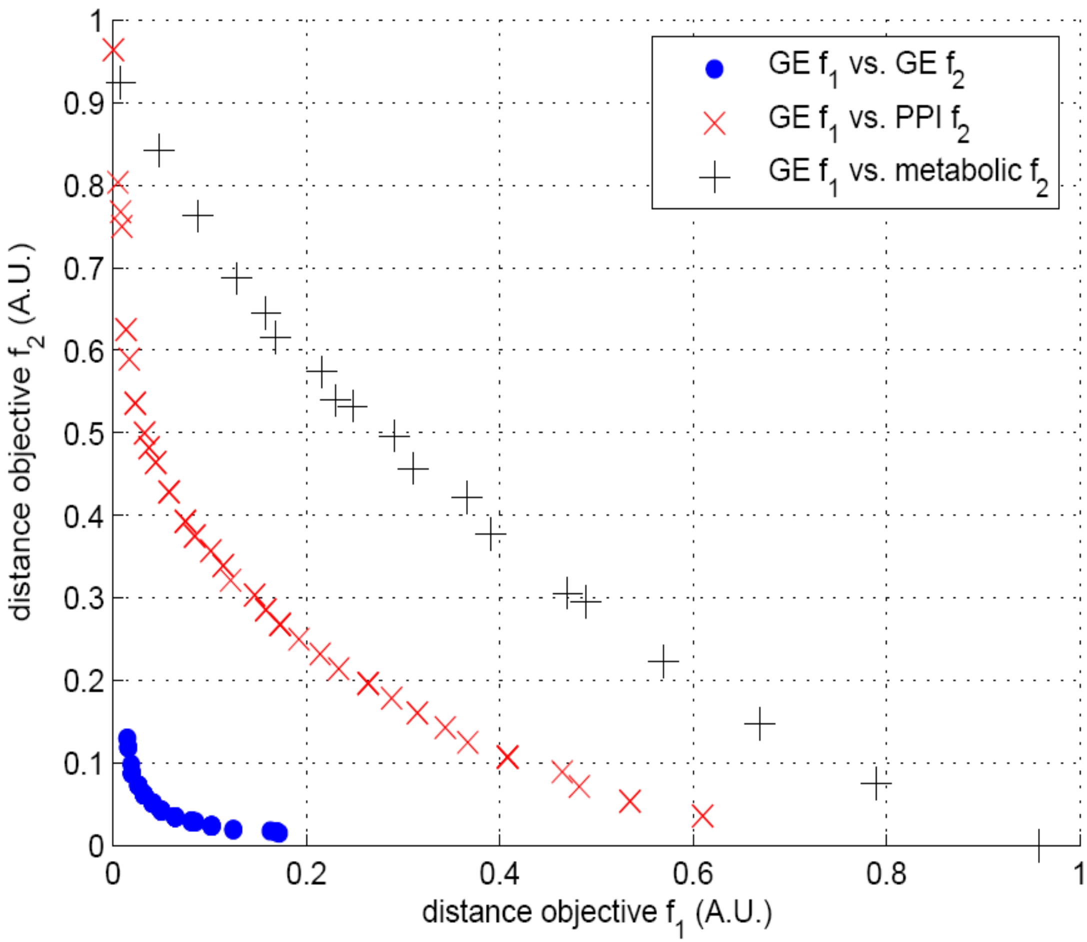




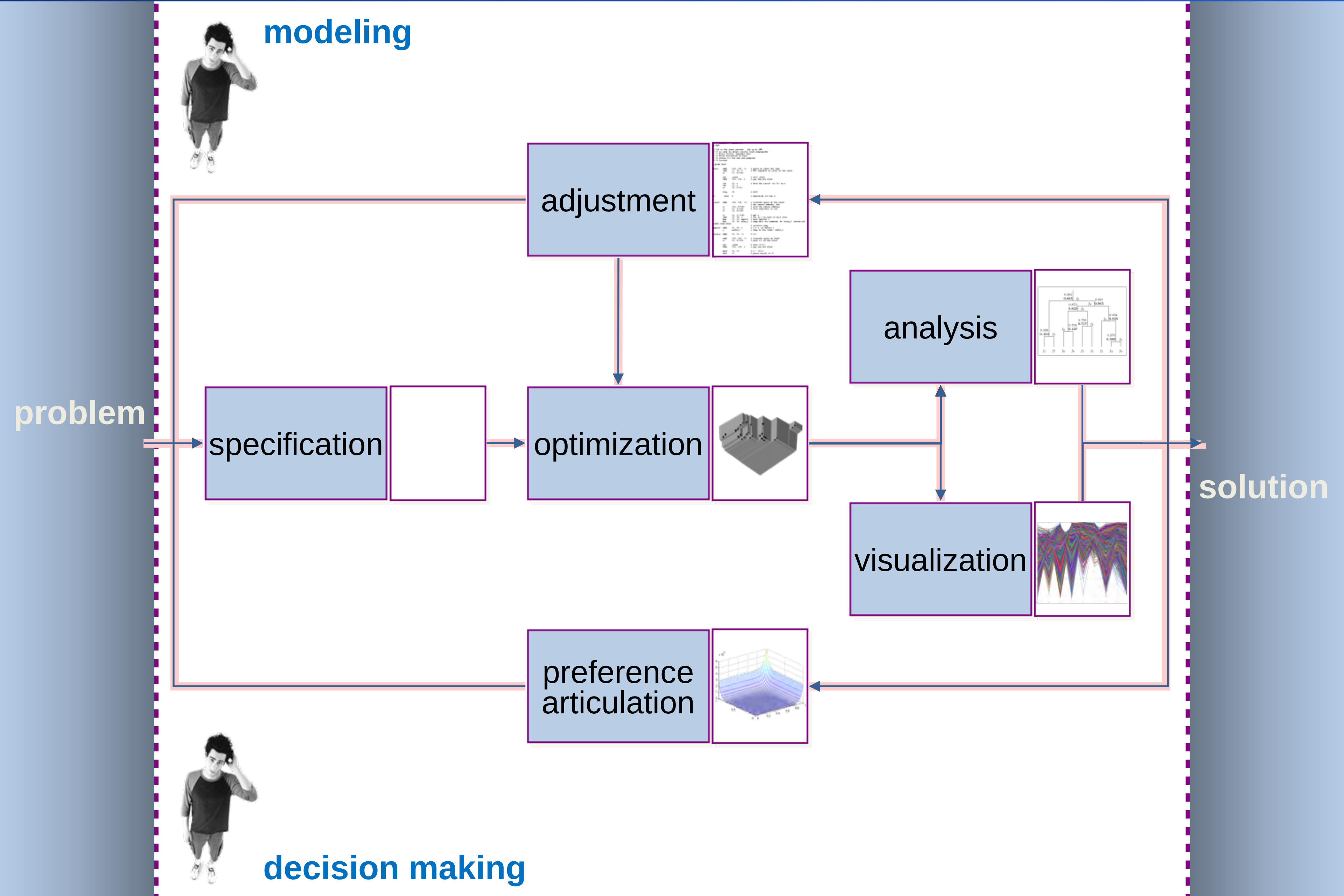
Module identification from biological data [Calonder et al. 2006]

Find group of genes wrt different data types:

- similarity of gene expression profiles
- overlap of protein interaction partners
- metabolic pathway map distances



Conclusions: EMO as Interactive Decision Support



The EMO Community

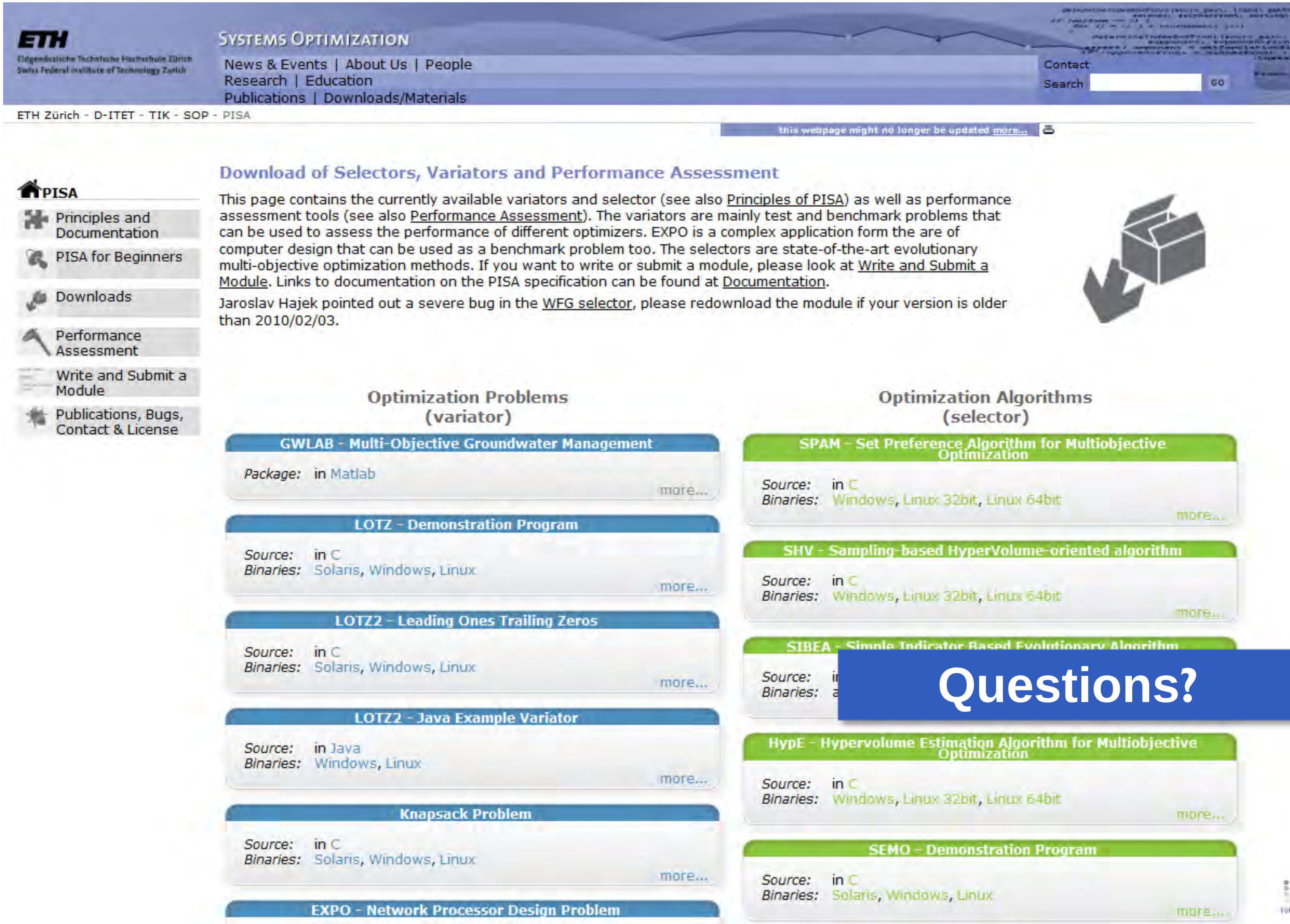
Links:

- EMO mailing list: *http://w3.ualg.pt/lists/emo-list/*
- EMO bibliography: *http://www.lania.mx/~ccoello/EMOO/*
- EMO conference series: *http://www.mat.ufmg.br/emo2011/*

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, 2^{nd} Ed. 2007
- **Multiobjective Optimization—Interactive and Evolutionary Approaches**, J. Branke, K. Deb, K. Miettinen, and R. Slowinski, editors, volume 5252 of *LNCS*. Springer, 2008
- and more…

PISA: http://www.tik.ee.ethz.ch/pisa/



Questions?

References

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