GECCO 2019 Tutorial on Evolutionary Multiobjective Optimization

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updated slides will be available at http://www.cmap.polytechnique.fr/~dimo.brockhoff/









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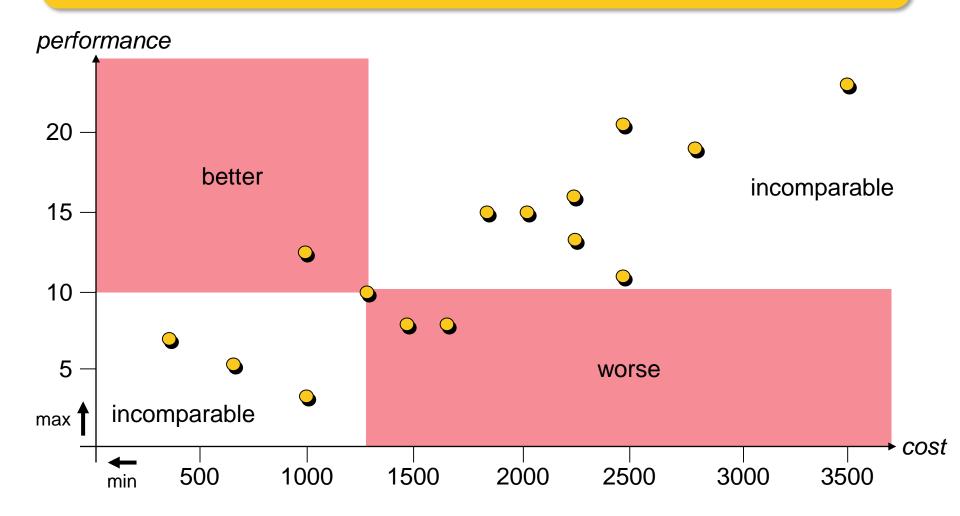
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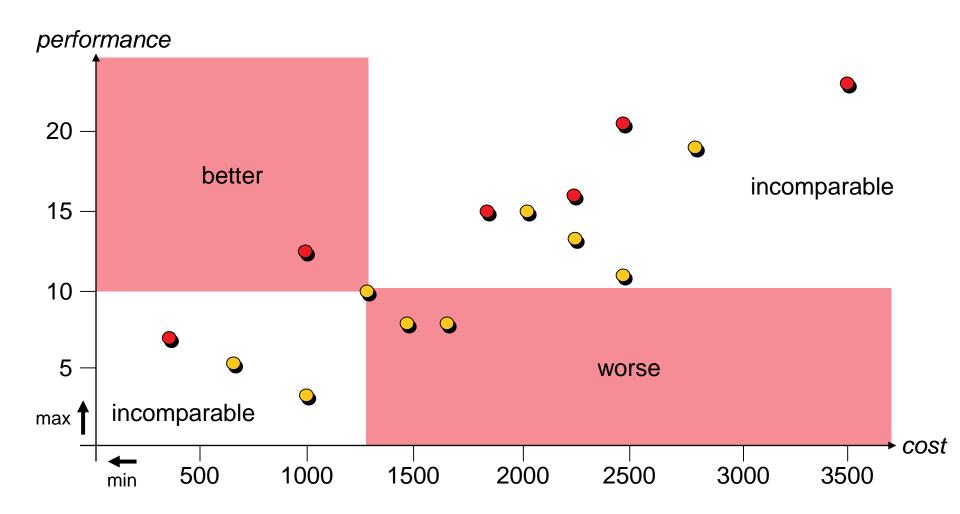
https://doi.org/10.1145/3319619.3323396

Multiobjective Optimization

Multiple objectives that have to be optimized simultaneously

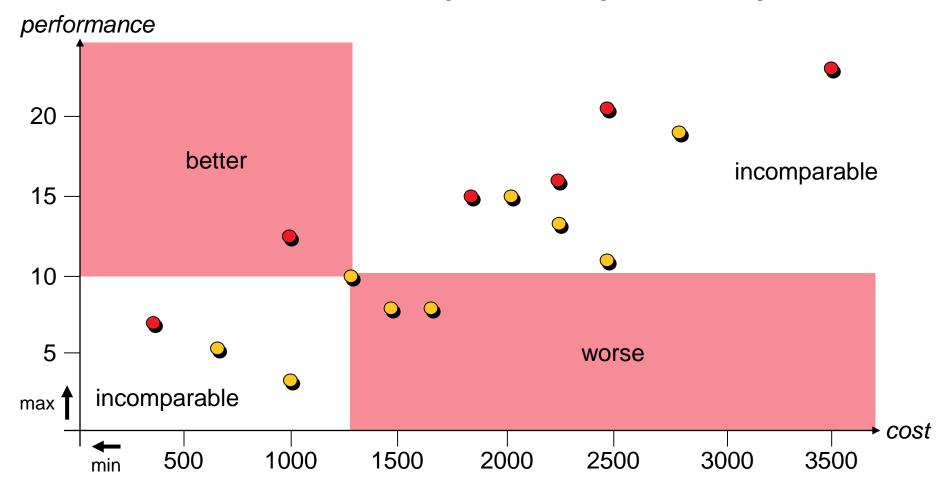


- Observations: there is no single optimal solution, but
 - 2 some solutions (•) are better than others (•)



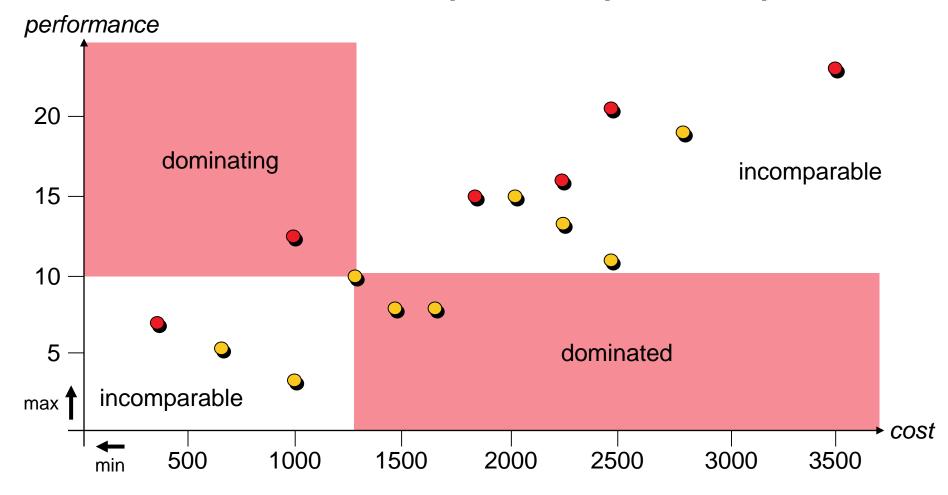
u weakly Pareto dominates v ($u \leq_{par} v$): $\forall 1 \leq i \leq k : f_i(u) \leq f_i(v)$

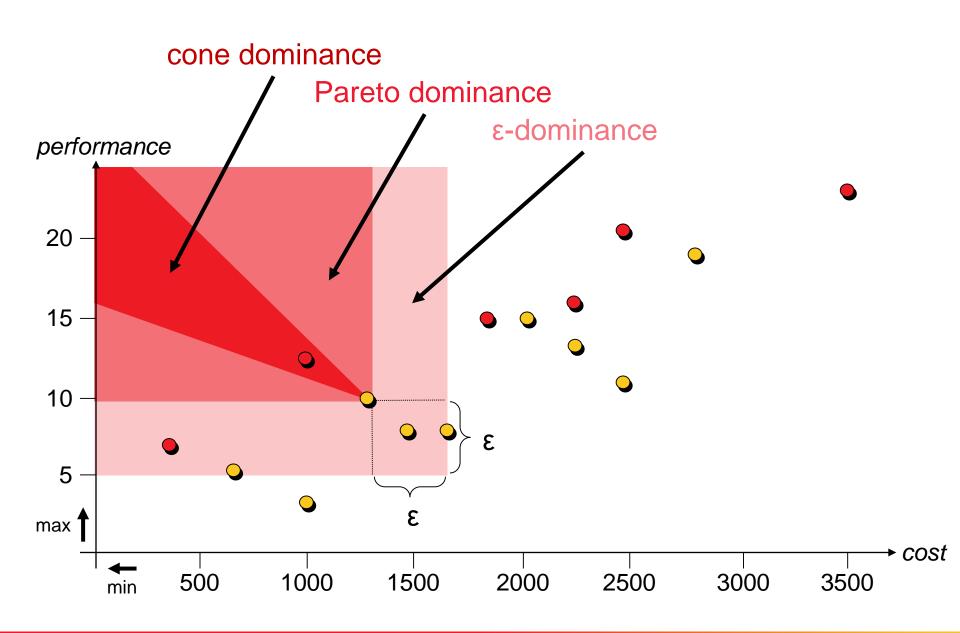
 $u \ Pareto \ dominates \ v \ (u <_{par} v): \ u \leqslant_{par} v \land v \not\leqslant_{par} u$



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

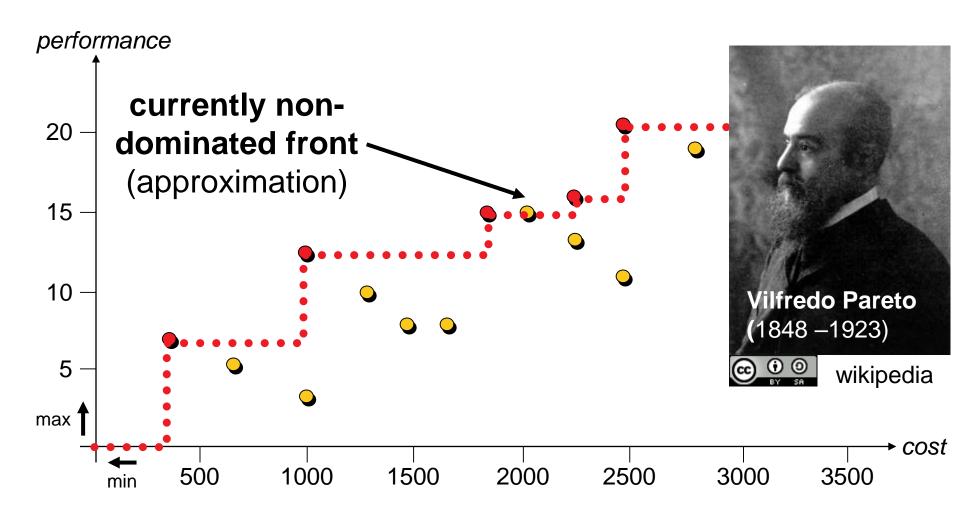
 $u \ Pareto \ dominates \ v \ (u <_{par} v): \ u \leqslant_{par} v \land v \not\leqslant_{par} u$





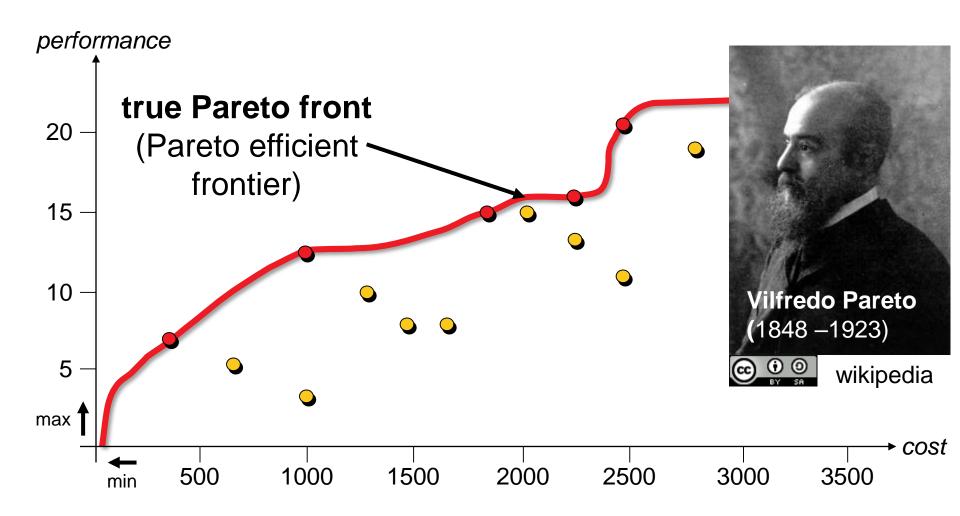
Pareto set: set of all non-dominated solutions (decision space)

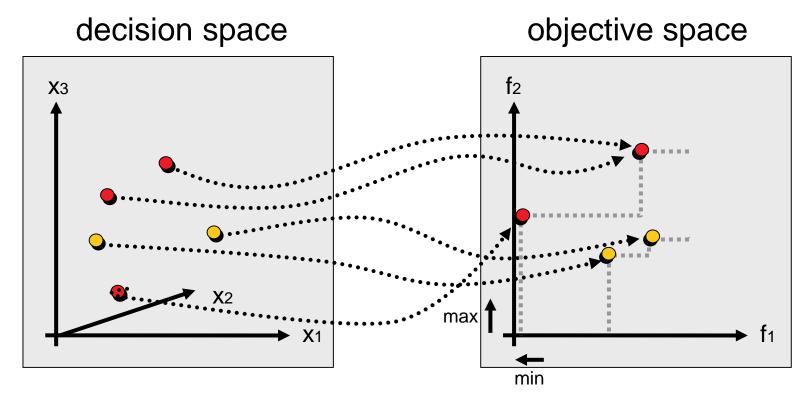
Pareto front: its image in the objective space



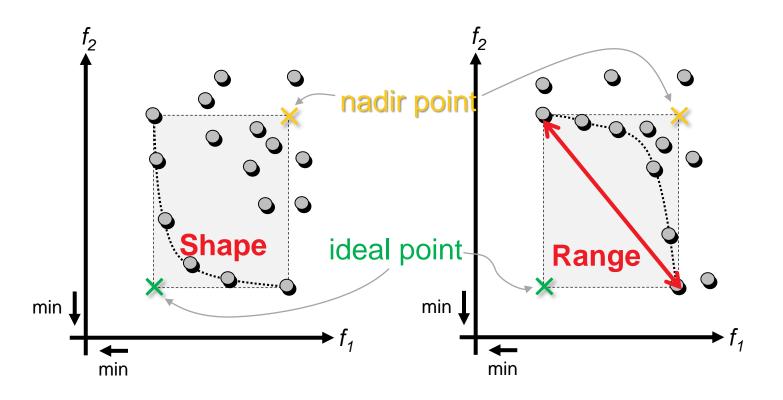
Pareto set: set of all non-dominated solutions (decision space)

Pareto front: its image in the objective space





- solution of Pareto-optimal set non-optimal decision vector
- vector of Pareto-optimal front
- non-optimal objective vector



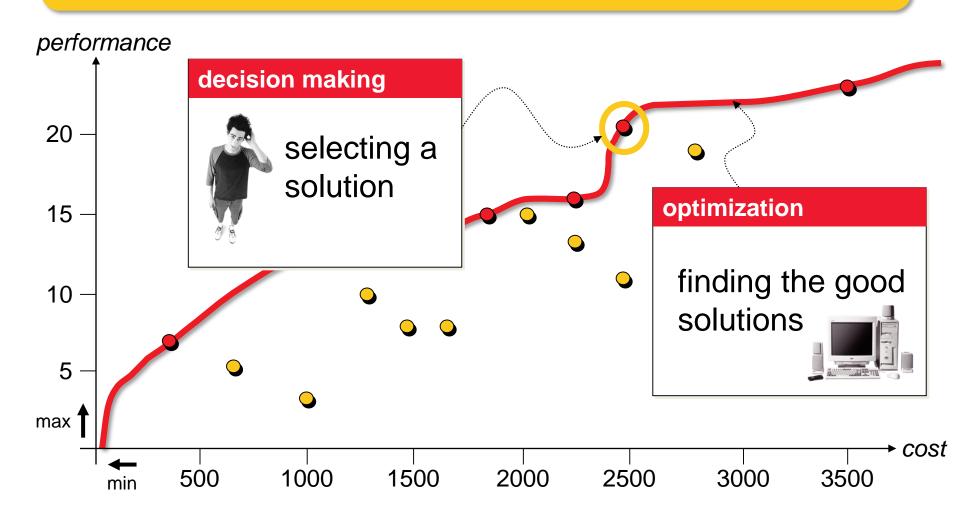
ideal point: best values nadir point: worst values

obtained for Pareto-optimal points

Optimization vs. Decision Making

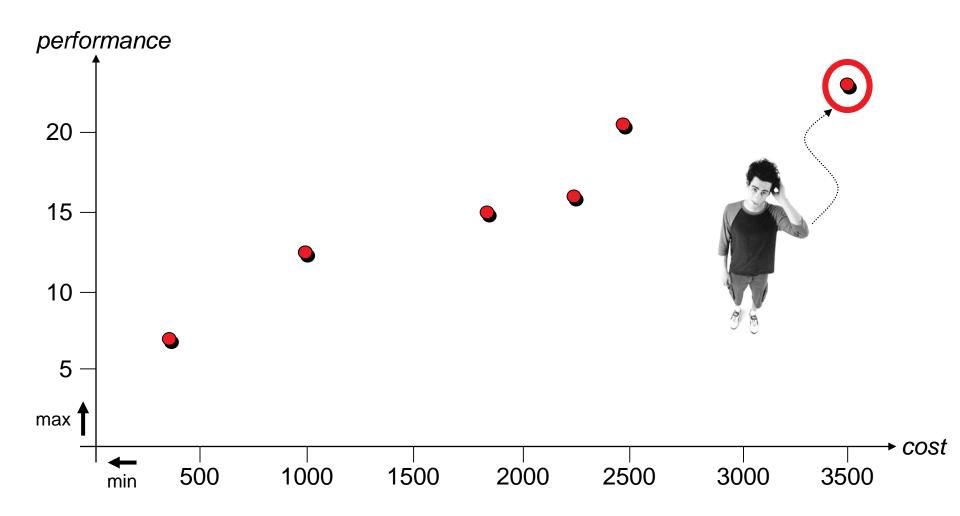
Multiobjective Optimization

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



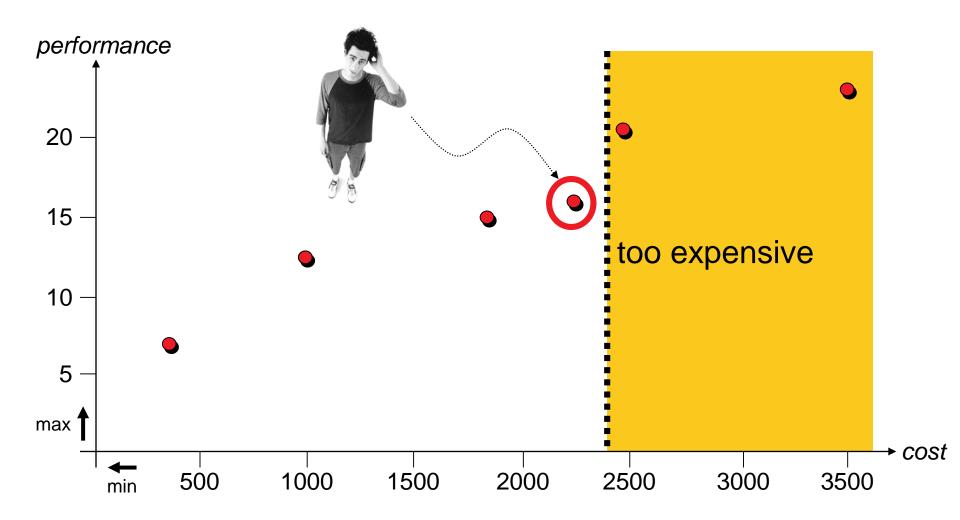
Selecting a Solution: Examples

Possible • ranking: performance more important than cost Approaches:

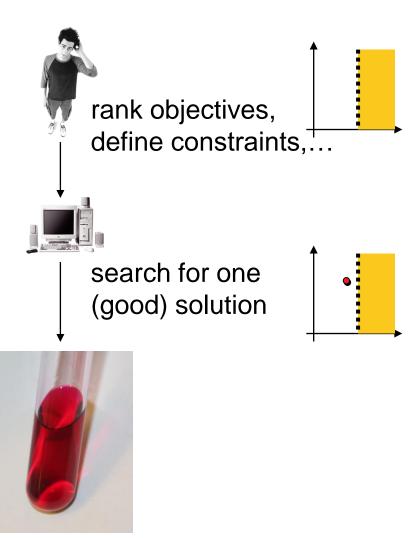


Selecting a Solution: Examples

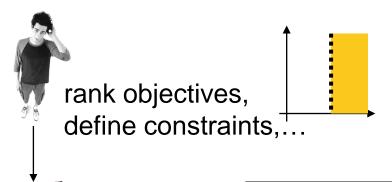
Possible • ranking: performance more important than cost Approaches: 2 constraints: cost must not exceed 2400



Before Optimization:

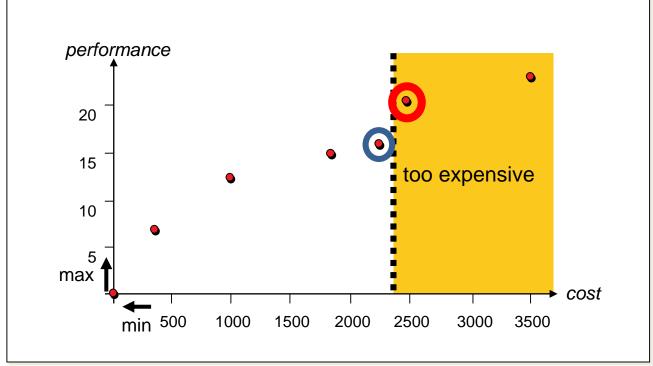


Before Optimization:

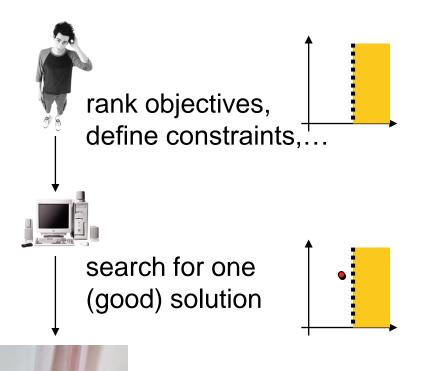


search for one (good) solution

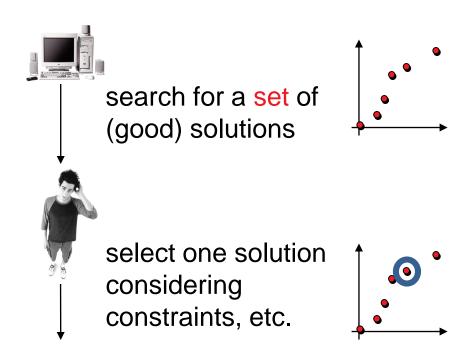




Before Optimization:

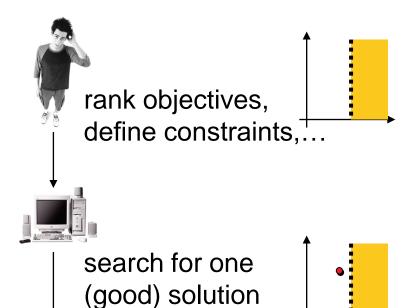


After Optimization:

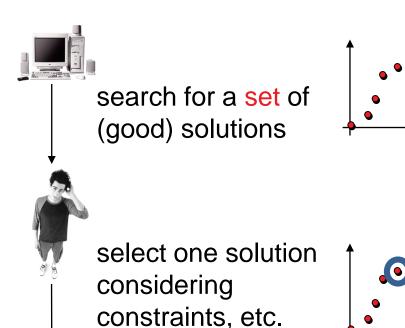




Before Optimization:



After Optimization:

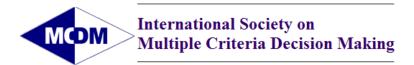




Focus: learning about a problem

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

Two Communities...





- established field (beginning in 1950s/1960s)
- bi-annual conferences since1975
- background in economics, math, management and social sciences
- focus on optimization and decision making

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

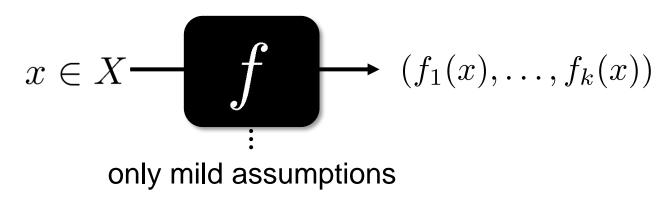
...Slowly Merge Into One



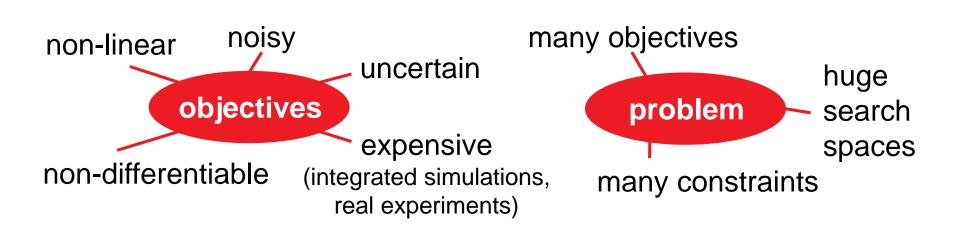
- MCDM track at EMO conference since 2009
- special sessions on EMO at the MCDM conference since 2008
- joint Dagstuhl seminars since 2004

One of the Main Differences

Blackbox optimization



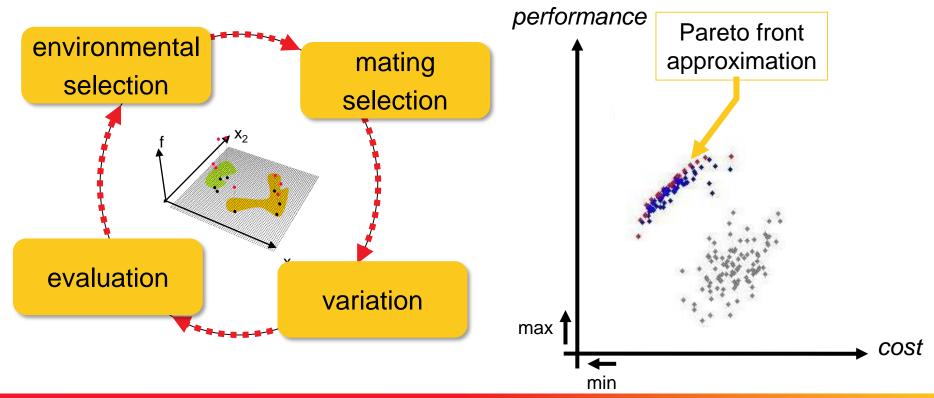
→ EMO therefore well-suited for real-world engineering problems



The Other Main Difference

Evolutionary Multiobjective Optimization

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

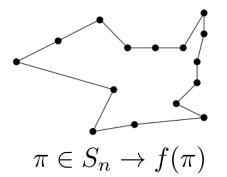


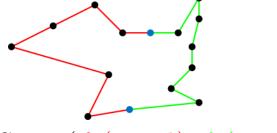
Multiobjectivization

Some problems are easier to solve in a multiobjective scenario

example: TSP

[Knowles et al. 2001]





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

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], ...

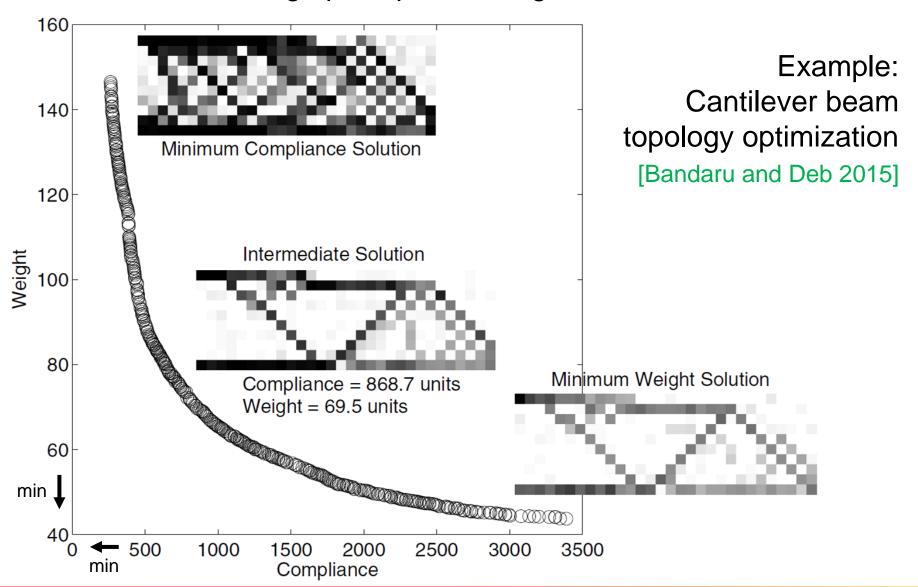
also backed up by theory e.g. [Brockhoff et al. 2009, Handl et al. 2008b]

related to constrained and multimodal single-objective optimization

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

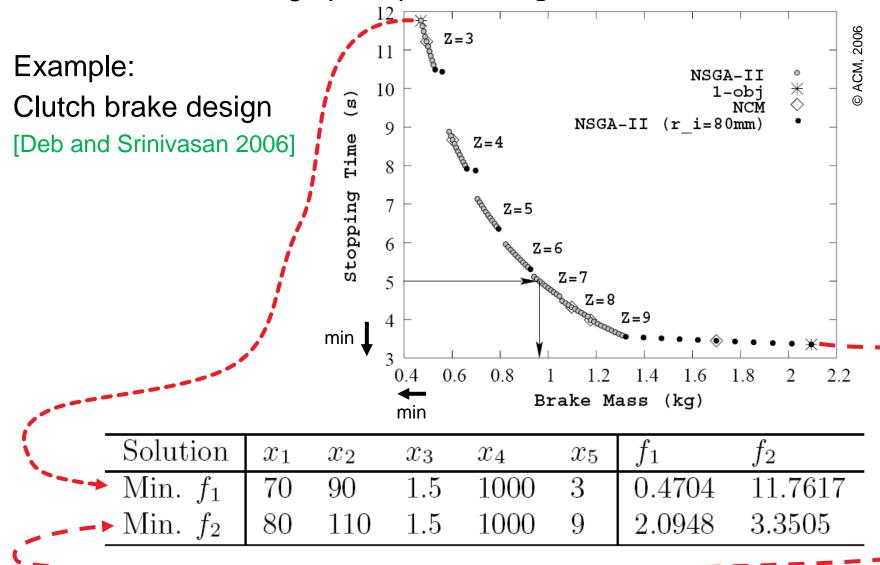
Innovization

Often innovative design principles among solutions are found



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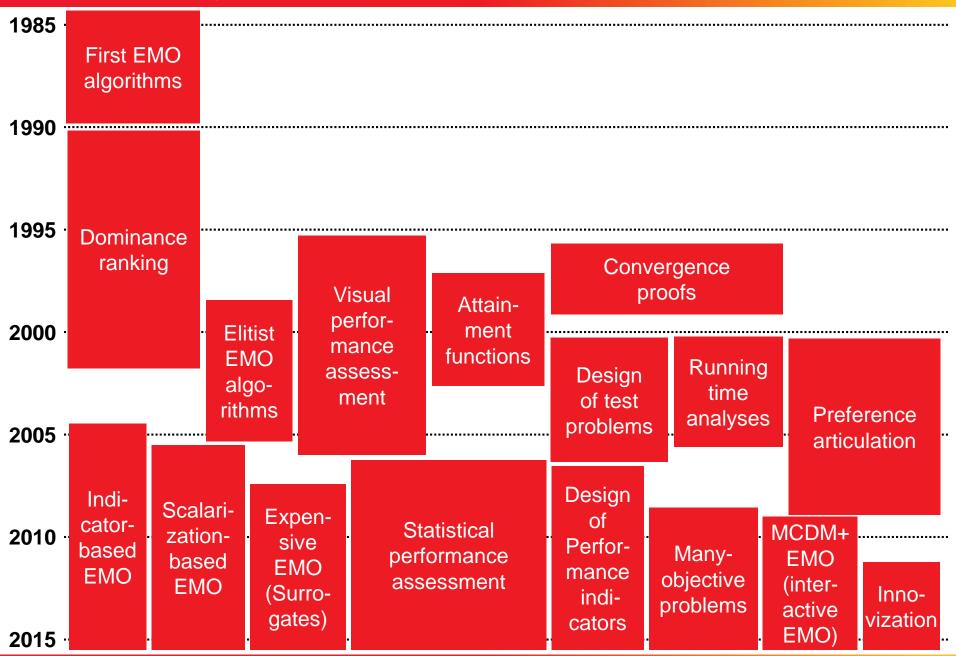
Innovization [Deb and Srinivasan 2006]

- = using machine learning techniques to find new and innovative design principles among solution sets
- = learning from/about a multi-objective optimization problem

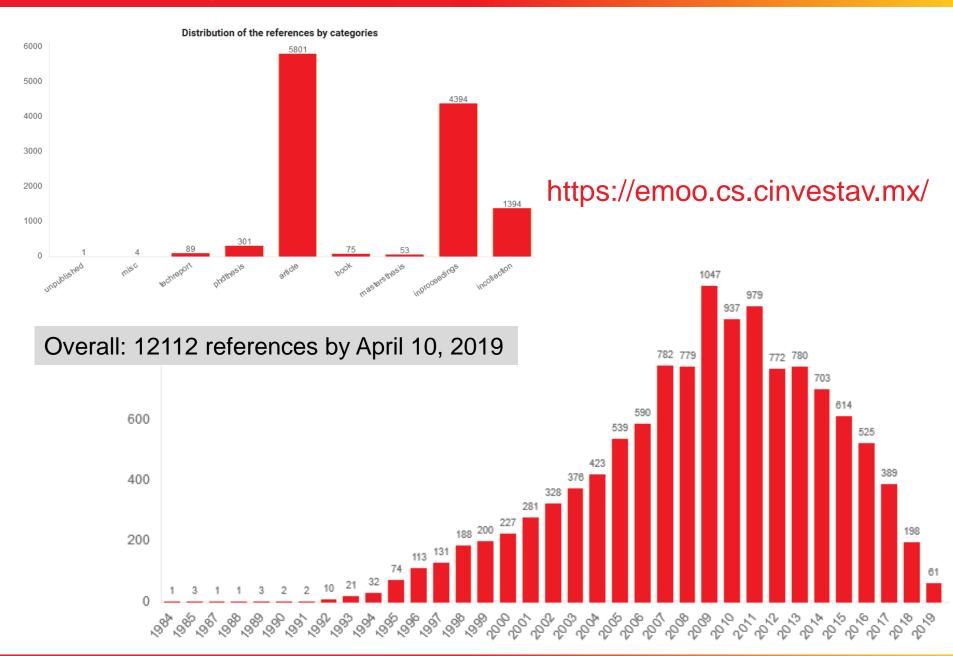
Other examples:

- SOM 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]

The History of EMO At A Glance



The History of EMO At A Glance



The EMO Community



Overview

The Big Picture

Basic Algorithm Design Principles and Concepts

Performance Assessment and Benchmarking

Preference Articulation

Fitness Assignment: Principal Approaches

aggregation-based

problem decomposition (multiple single-objective optimization problems)

scaling-dependent

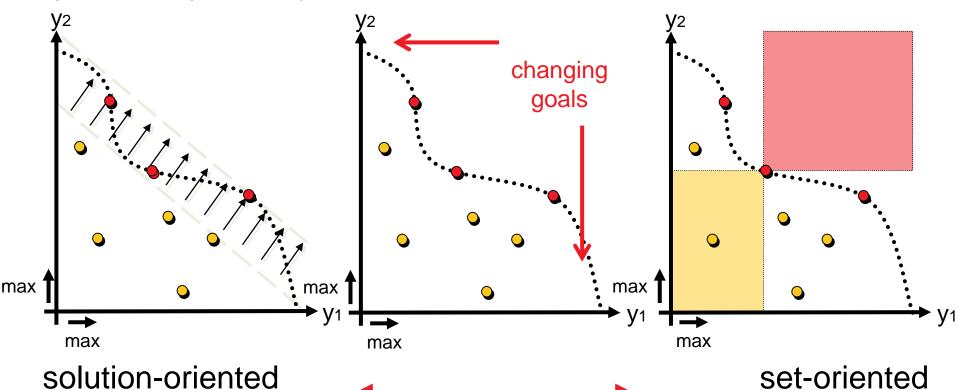
criterion-based

VEGA

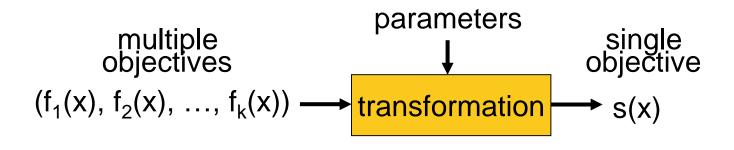
dominance-based

SPEA2, NSGA-II "modern" EMOA

scaling-independent

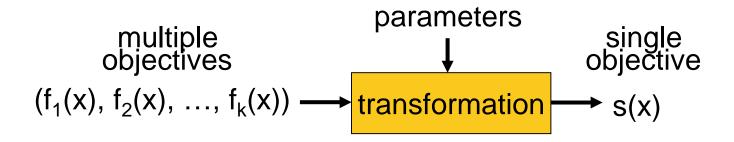


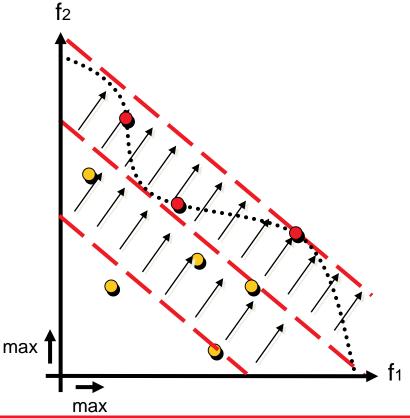
Solution-Oriented Problem Transformations



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

Solution-Oriented Problem Transformations





Example 1: weighted sum approach

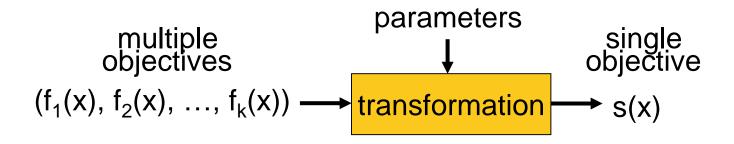
$$(w_1, w_2, ..., w_k)$$

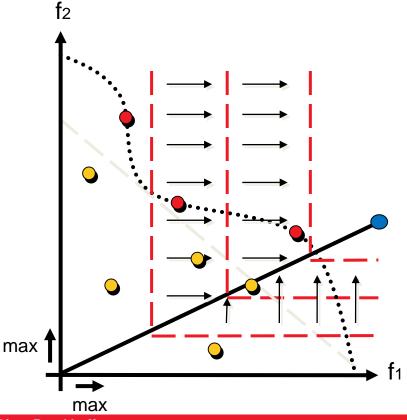
$$\downarrow$$

$$y = w_1y_1 + ... + w_ky_k$$

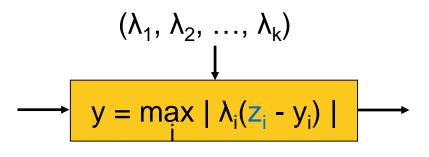
Disadvantage: not all Paretooptimal solutions can be found if the front is not convex

Solution-Oriented Problem Transformations



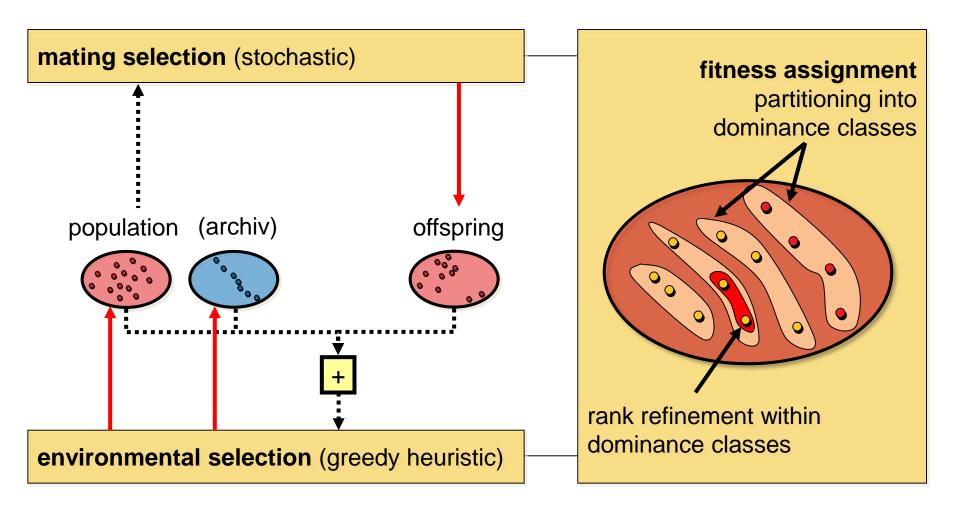


Example 2: weighted Tchebycheff



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

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

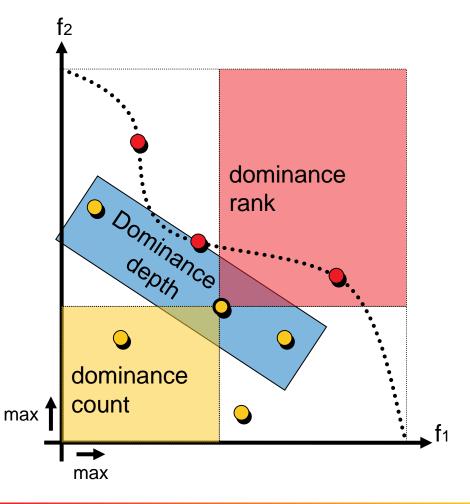
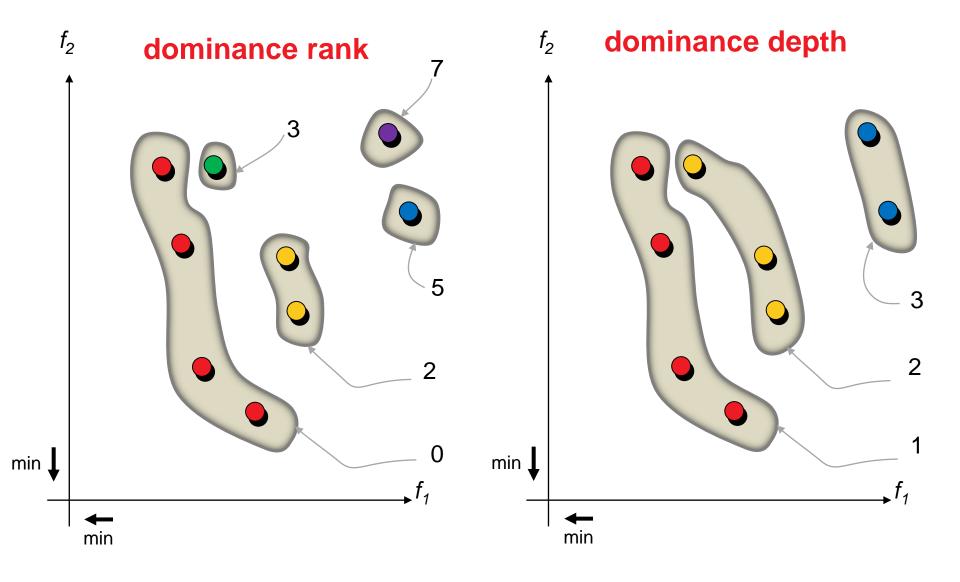


Illustration of Dominance-Based Partitioning



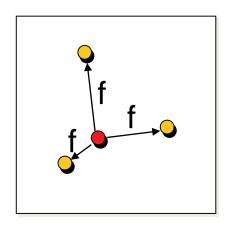
Refinement of Dominance Rankings

Goal: rank incomparable solutions within a dominance class

Diversity information

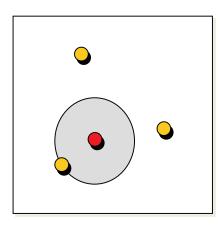
Kernel method

diversity = function of the distances



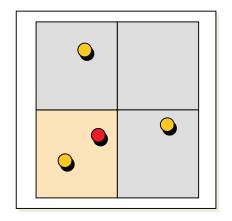
k-th nearest neighbor

diversity =
function of distance
to k-th nearest neighbor



Histogram method

diversity =
number of elements
 within box(es)

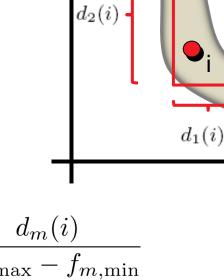


2 (Contribution to a) quality indicator

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



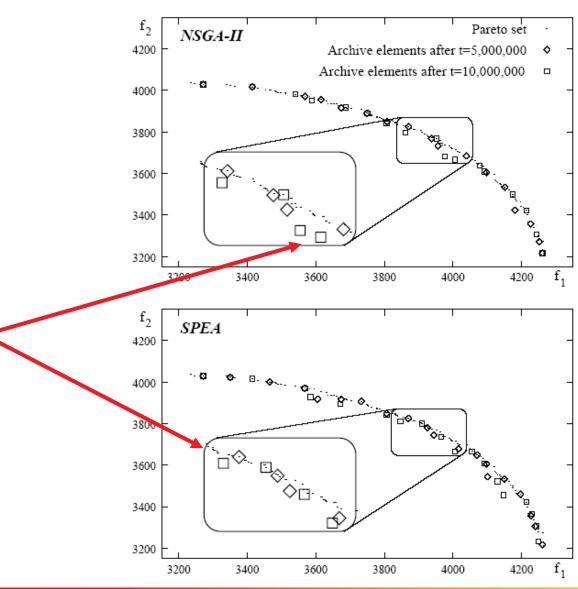
distance to the neighbors in each objective
$$\mathrm{CD}(i) = \frac{d_1(i)}{f_{1,\max} - f_{1,\min}} + \dots + \frac{d_m(i)}{f_{m,\max} - f_{m,\min}}$$

SPEA2 and NSGA-II: Deteriorative Cycles

Selection in SPEA2 and NSGA-II can result in

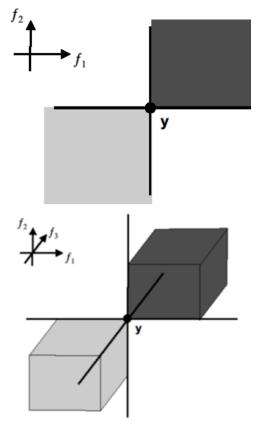
deteriorative cycles

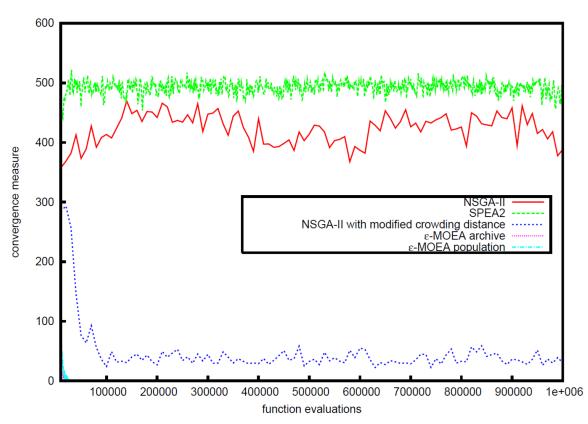
non-dominated solutions already found can be lost



Remark: Many-Objective Optimization

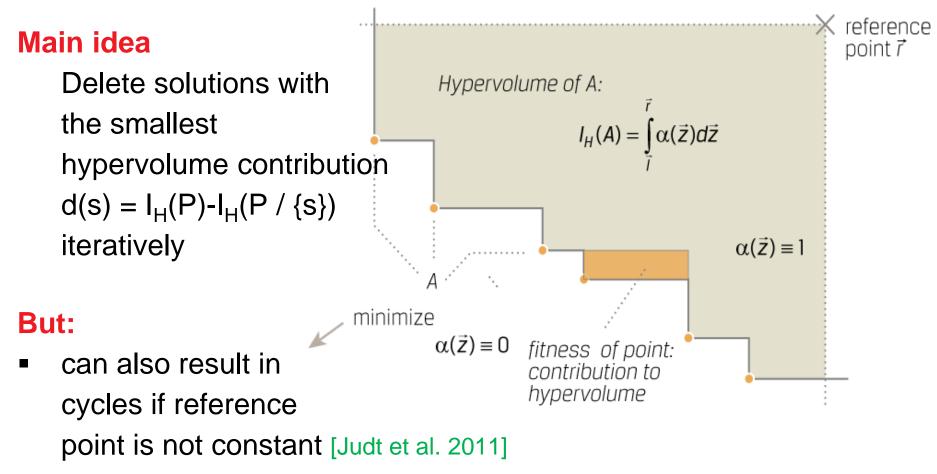
- high number of objectives
 - → percentage of non-dominated solutions within a random sample quickly approaches 100 %
 - > optimization is mainly guided by diversity criterion
 - → apply secondary criterion compliant with dominance relation





Hypervolume-Based Selection

Latest Approach (SMS-EMOA, MO-CMA-ES, HypE, ...) use hypervolume indicator to guide the search: refines dominance



- expensive to compute exactly [Bringmann and Friedrich 2009]
- but less and less practical restrictions [Guerreiro and Fonseca 2017]

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 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

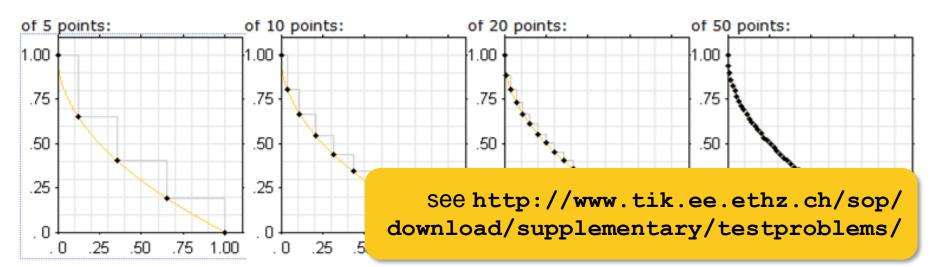
The Optimization Goal in Indicator-Based EMO

When the goal is to maximize a unary indicator...

- we have a single-objective problem on sets
- but what is the optimum?
- important: population size μ plays a role!

Optimal µ-Distribution:

A set of μ solutions that maximizes a certain unary indicator I among all sets of μ solutions is called optimal μ -distribution for I. [Auger et al. 2009a]



Optimal µ-Distributions for the Hypervolume

Hypervolume indicator refines dominance relation

 \Rightarrow most results on optimal μ -distributions for hypervolume

Optimal µ-Distributions (example results)

[Auger et al. 2009a]:

- contain equally spaced points iff front is linear
- density of points $\propto \sqrt{-f'(x)}$ with f' the slope of the front
- optimal μ-distributions known on convex-quadratic functions with same Hessian [Touré et al. 2019a]

[Friedrich et al. 2011]:

optimal μ-distributions for the hypervolume correspond to ε-approximations of the front

OPT
$$1 + \frac{\log(\min\{A/a, B/b\})}{n}$$
HYP
$$1 + \frac{\sqrt{A/a} + \sqrt{B/b}}{n - 4}$$

$$\log HYP \quad 1 + \frac{\sqrt{\log(A/a)\log(B/b)}}{n - 2}$$

(probably) does not hold for > 2 objectives

Indicator-Based EMO

Open Questions:

- how do the optimal μ-distributions look like for >2 objectives?
- how to compute certain indicators quickly in practice?
 - several recent improvements for the hypervolume indicator [Yildiz and Suri 2012], [Bringmann 2012], [Bringmann 2013]
 [Guerreiro and Fonseca 2018]
- how to do indicator-based subset selection quickly?
 - also here several recent improvements
 [Kuhn et al. 2014], [Bringmann et al. 2014], [Guerreiro et al. 2015]
- what is the best strategy for the subset selection?
- is the hypervolume the right performance measure for >2 objectives?

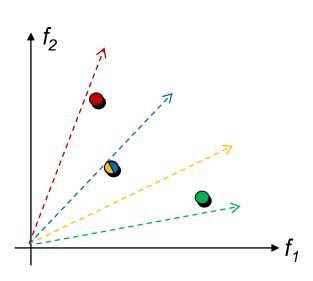
further open questions on indicator-based EMO available at http://simco.gforge.inria.fr/doku.php?id=openproblems

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



https://sites.google.com/view/moead/home

Remark: Variation in EMO

- at first sight not different from single-objective optimization
- most research on selection mechanisms (until now)
- but: convergence to a set ≠ convergence to a point

Open Question:

how to achieve fast convergence to a set?

Related work:

- set-based gradient of the HV [Emmerich et al. 2007]
- multiobjective CMA-ES [Igel et al. 2007, Voß et al. 2010, Krause et al. 2016]
- RM-MEDA [Zhang et al. 2008]
- set-based variation [Bader et al. 2009]
- set-based fitness landscapes [Verel et al. 2011]
- offline and online configuration based on libraries of variation operators [Bezerra et al. 2015, Hadka and Reed 2013]
- COMO-CMA-ES [Touré et al. 2019b, EMO1@Monday]

Overview

The Big Picture

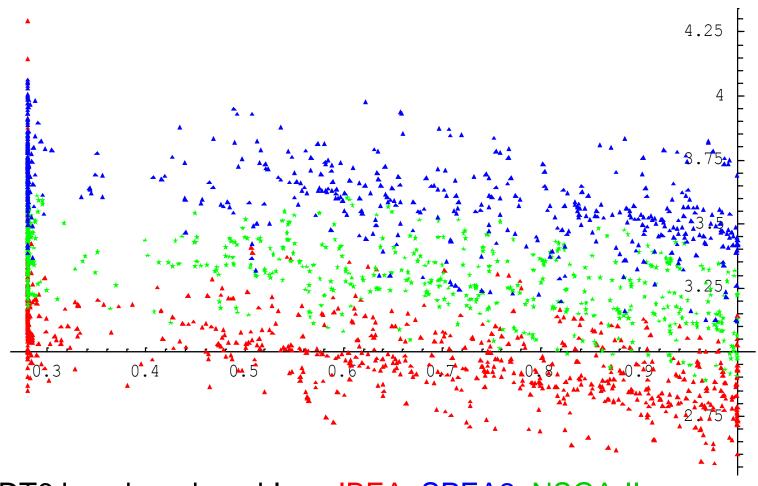
Basic Algorithm Design Principles and Concepts

Performance Assessment and Benchmarking

Preference Articulation

Once Upon a Time...

... multiobjective EAs were mainly compared visually:

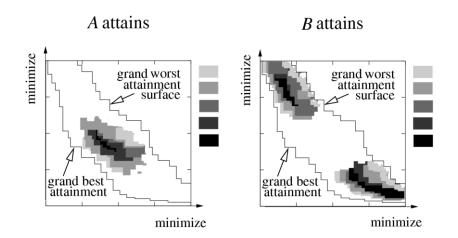


ZDT6 benchmark problem: IBEA, SPEA2, NSGA-II

Two Approaches for Empirical Studies

Attainment function approach

- applies statistical tests directly to the approximation set
- detailed information about how and where performance differences occur

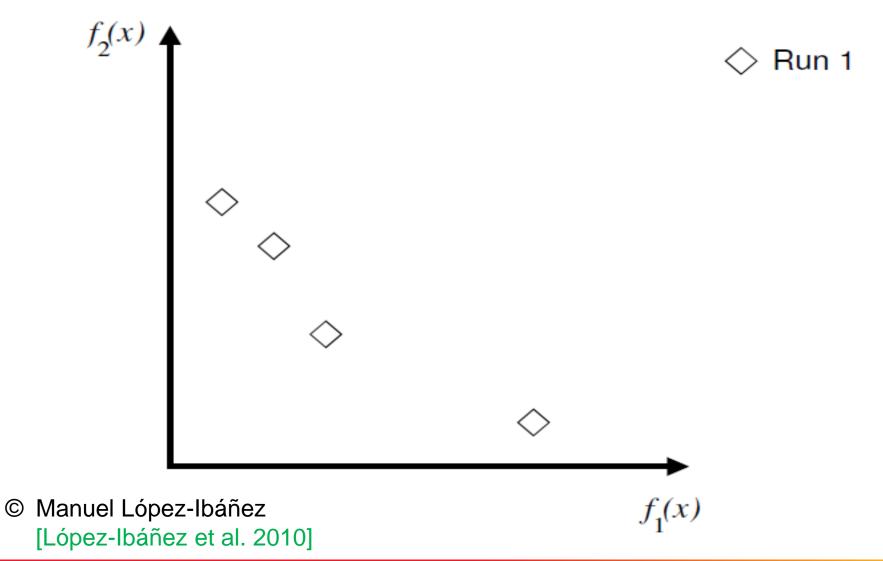


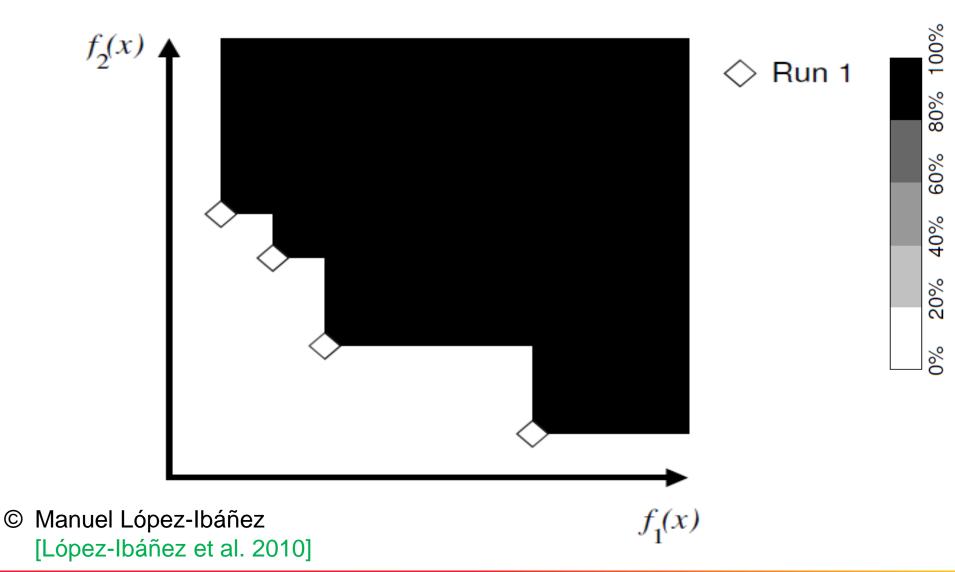
Quality indicator approach

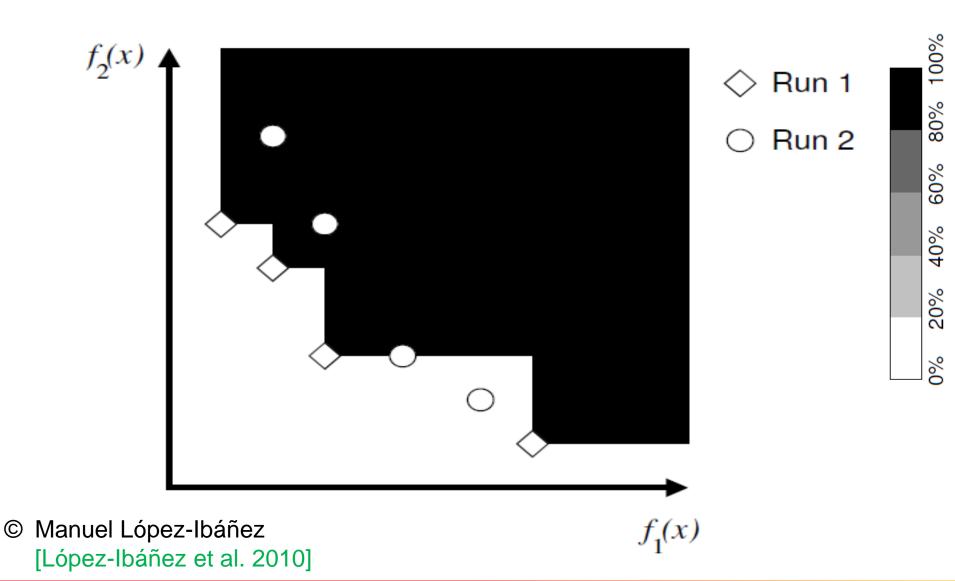
- reduces each approximation set to a single quality value
- applies statistical tests to the quality values

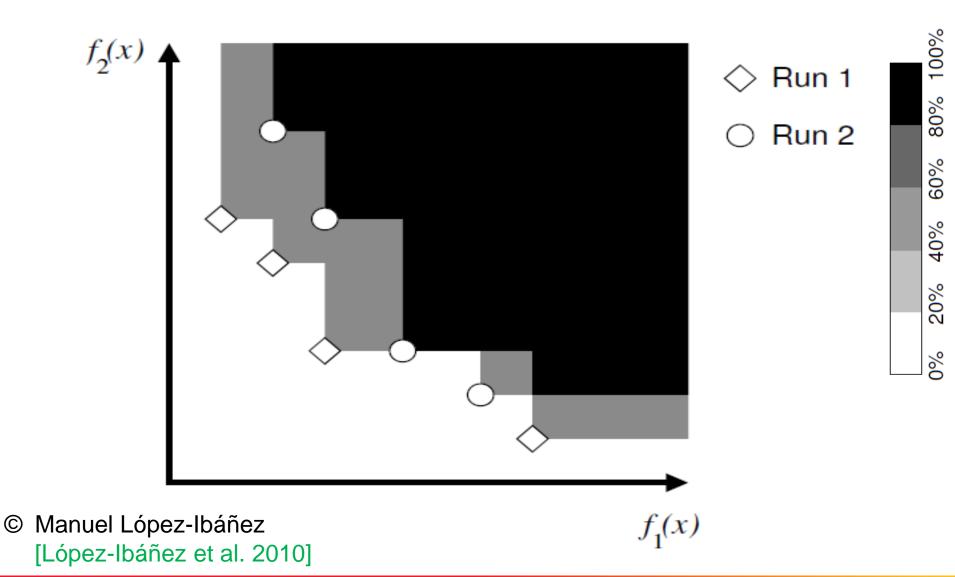
Indicator	\mathbf{A}	В
Hypervolume indicator	6.3431	7.1924
$\epsilon ext{-indicator}$	1.2090	0.12722
R_2 indicator	0.2434	0.1643
R_3 indicator	0.6454	0.3475

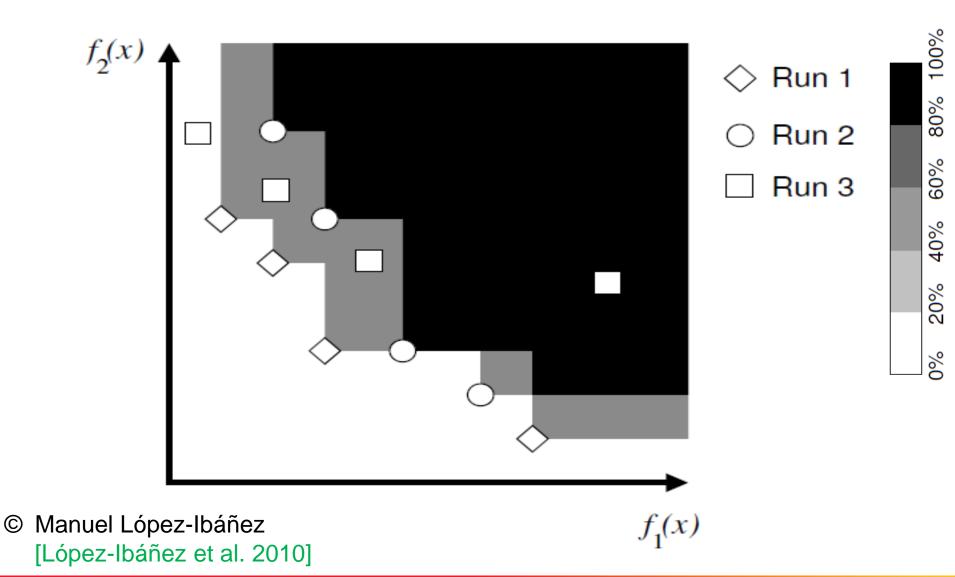
see e.g. [Zitzler et al. 2003]

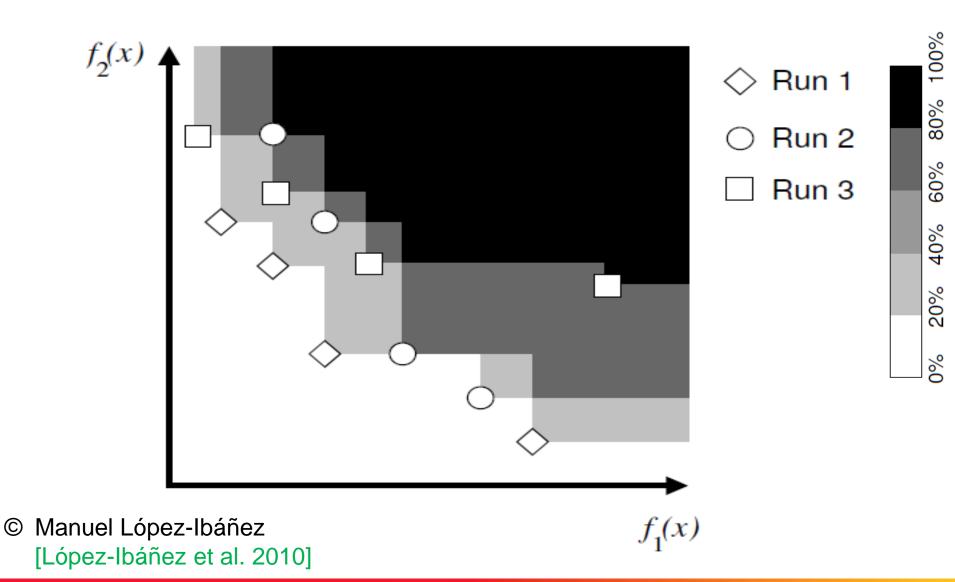












Empirical Attainment Functions: Definition

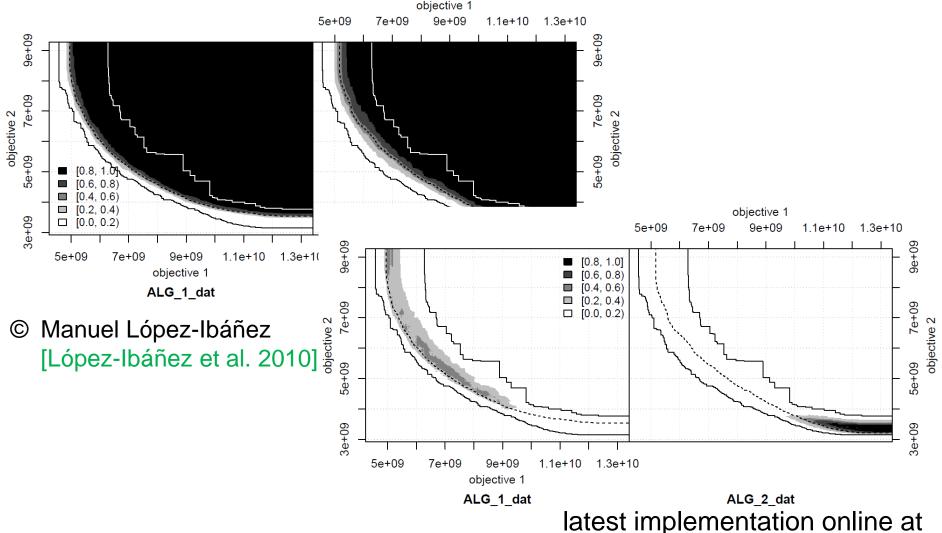
The Empirical Attainment Function $\alpha(z)$ "counts" how many solution sets \mathcal{X}_i attain or dominate a vector z at time T:

$$\alpha_T(z) = \frac{1}{N} \sum_{i=1}^{N} \mathbf{1}_{\{\chi_i \leq_T z\}}$$

with $extstyle _{T}$ being the weak dominance relation between a solution set and an objective vector at time T.

Note that $\alpha_T(z)$ is the empirical cumulative distribution function of the achieved objective function distribution at time T in the single-objective case ("fixed budget scenario").

Empirical Attainment Functions in Practice

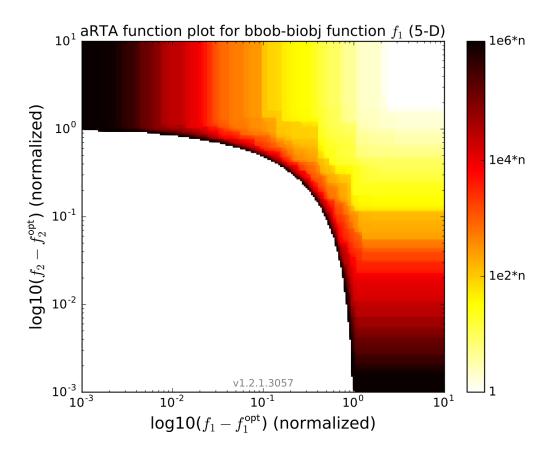


http://eden.dei.uc.pt/~cmfonsec/software.html R package: http://lopez-ibanez.eu/eaftools

see also [López-Ibáñez et al. 2010, Fonseca et al. 2011]

Plotting Average Runtimes

Note: success probability can be naturally replaced by the average runtime of an artificially restarted algorithm (aRT):



code available at http://github.com/numbbo/coco/ see also [Brockhoff et al. 2017]

Quality Indicator Approach

Idea:

- transfer multiobjective problem into a set problem
- define an objective function ("quality indicator") on sets
- use the resulting total (pre-)order (on the quality values)

Question:

Can any total (pre-)order be used or are there any requirements concerning the resulting preference relation?

⇒ Underlying dominance relation should be reflected!

$$A \leq B :\Leftrightarrow \forall_{y \in B} \exists_{x \in A} x \leq_{par} y$$

Refinements and Weak Refinements

● refines a preference relation iff

$$A \preceq B \land B \not\preceq A \Rightarrow A \preceq B \land B \not\preceq A$$
 (better \Rightarrow better)

- ⇒ fulfills requirement
- $\mathbf{2} \overset{\mathrm{ref}}{\preccurlyeq}$ weakly refines a preference relation \preccurlyeq iff

$$A \preccurlyeq B \land B \npreceq A \Rightarrow A \stackrel{\text{ref}}{\preccurlyeq} B$$
 (better \Rightarrow weakly better)

 \Rightarrow does not fulfill requirement, but $\stackrel{\mathrm{ref}}{\preccurlyeq}$ does not contradict \preccurlyeq

! sought are total refinements... [Zitzler et al. 2010]

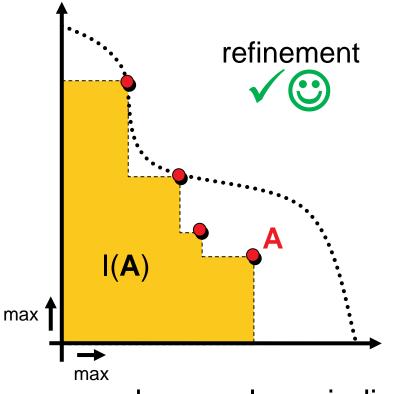
Example: Refinements Using Indicators

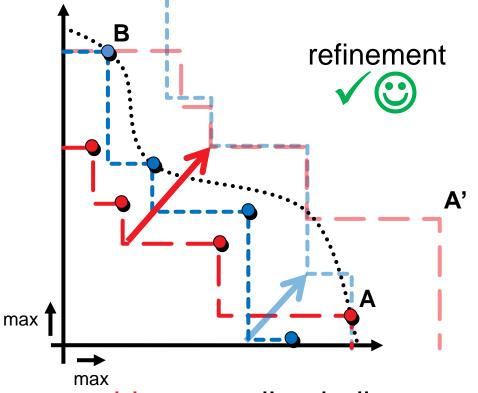
$$A \stackrel{\mathrm{ref}}{\preccurlyeq} B : \Leftrightarrow I(A) \geq I(B)$$

 $A \stackrel{\mathrm{ref}}{\prec} B :\Leftrightarrow I(A,B) \leq I(B,A)$

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

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





binary epsilon indicator

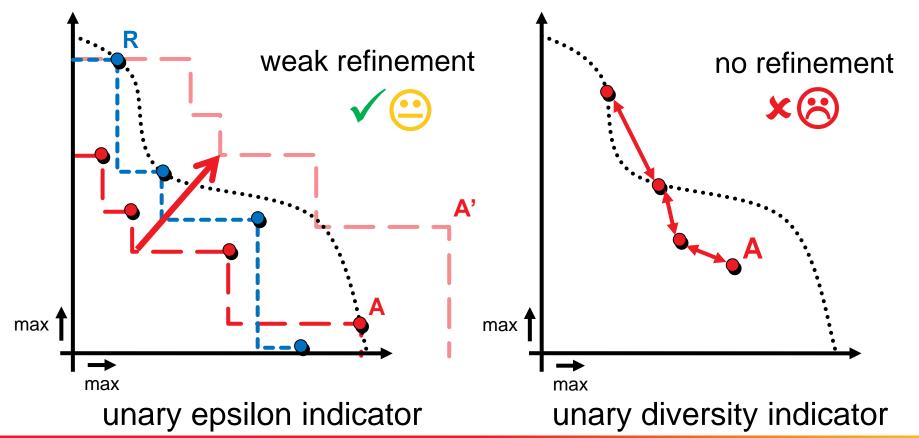
unary hypervolume indicator

Example: Weak Refinement / No Refinement

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

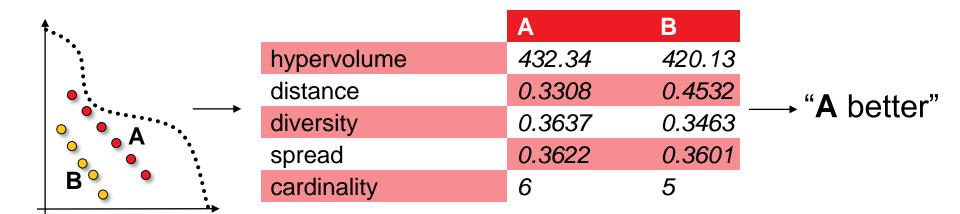
 $A \stackrel{\mathrm{ref}}{\prec} B : \Leftrightarrow I(A) \leq I(B)$

I(A,R) = how much needs A to be moved to weakly dominate R I(A) = variance of pairwise distances



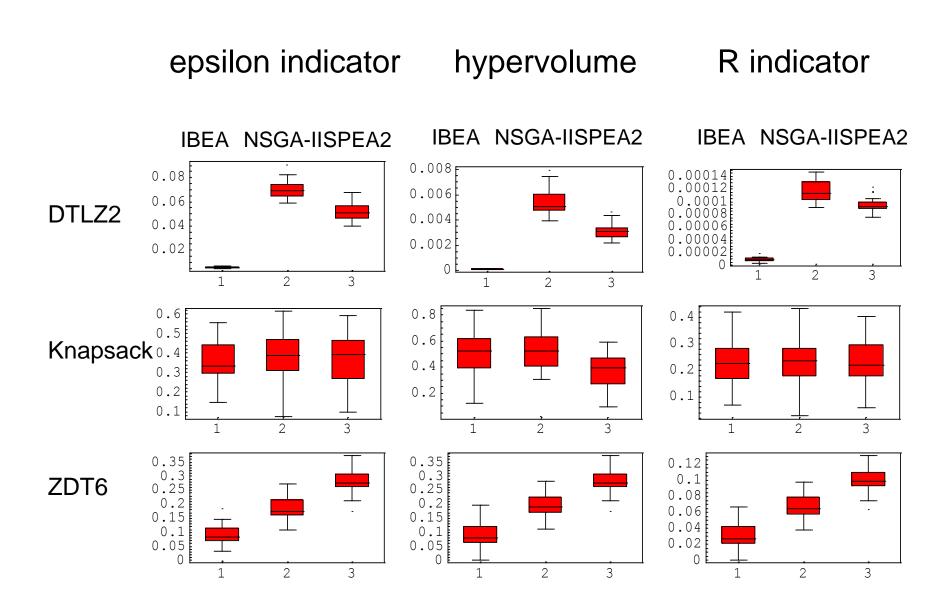
Quality Indicator Approach

Goal: compare two Pareto set approximations A and B



Comparison method C = quality measure(s) + Boolean function

Example: Box Plots



Statistical Assessment (Kruskal Test)

ZDT6 Epsilon

than					
man	IBEA	NSGA2		SPEA2	
IBEA		~0	<u></u>	~0	©
NSGA2	1			~0	<u></u>
SPEA2	1	1			

Overall p-value = 6.22079e-17. Null hypothesis rejected (alpha 0.05)

DTLZ2

is better

than	IBEA	NSGA2		SPEA2	
IBEA		~0	<u></u>	~0	<u></u>
NSGA2	1			1	
SPEA2	1	~0	<u></u>		

Overall p-value = 7.86834e-17. Null hypothesis rejected (alpha 0.05)

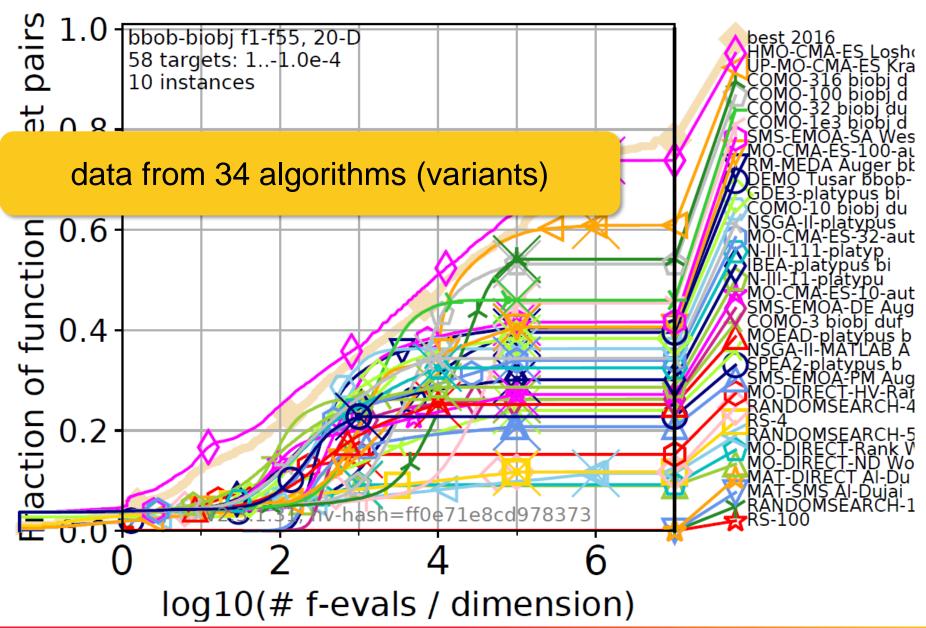
Knapsack/Hypervolume: $H_0 = No$ significance of any differences

ic hattar

Automated Benchmarking

- State-of-the-art in single-objective optimization: Blackbox
 Optimization Benchmarking (BBOB) with COCO platform
 https://github.com/numbbo/coco
- Release of a bi-objective test suite at BBOB-2016 workshop
- New bi-objective mixed-integer suite this year
- Focus on target-based runlengths
 - gives (nearly) anytime, interpretable results
 - defines problem=(test function instance, single-objective goal e.g. min. indicator difference to reference set, target precision)
 - reports average runtimes (aRT) to reach target precision
- COCO provides data profiles, scaling plots, scatter plots, tables, statistical tests, etc. automatically

Exemplary BBOB Workshop Results



A Few Recommendations

- always display everything you have
- look at single runs
- do each experiment at least twice

(= look at the *variance* of your results)

- as quality indicators, use hypervolume, R2, or epsilon indicator
- see also the tutorial slides by Nikolaus Hansen on this topic (not restricted to single-objective optimization!)

Overview

The Big Picture

Basic Algorithm Design Principles and Concepts

Performance Assessment and Benchmarking

Preference Articulation

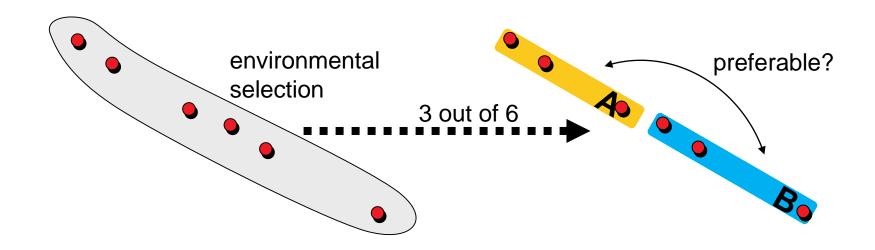
Articulating User Preferences During Search

What we thought: EMO is preference-less

Search before decision making: Optimization is performed without any preference information given. The result of the search process is a set of (ideally Pareto-optimal) candidate solutions from which the final choice is made by the DM.

[Zitzler 1999]

What we learnt: EMO just uses weaker preference information



Incorporation of Preferences During Search

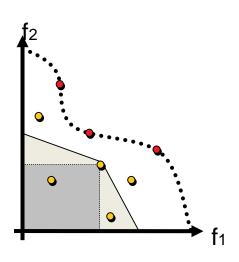
Nevertheless...

- the more (known) preferences incorporated the better
- in particular if search space is large

[Branke and Deb 2004] [Branke 2008] [Bechikh et al. 2015]

Refine/modify dominance relation, e.g.:

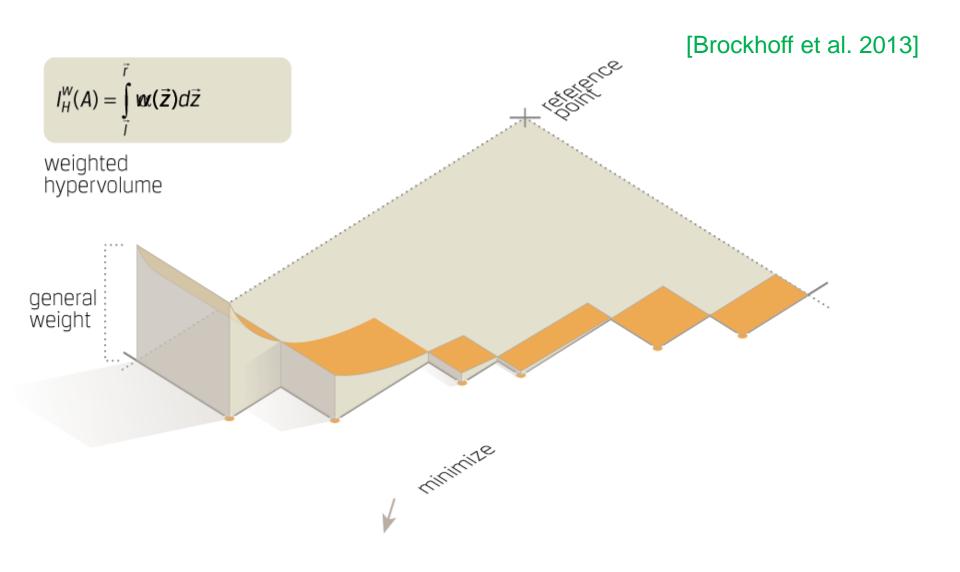
- using goals, priorities, constraints
 [Fonseca and Fleming 1998a,b]
- using different types of dominance cones [Branke and Deb 2004]



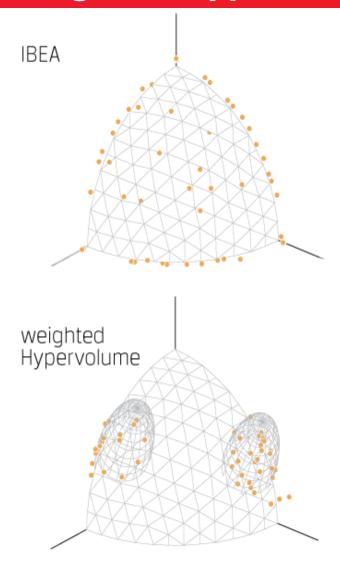
2 Use quality indicators, e.g.:

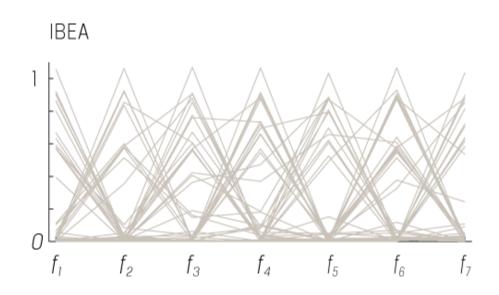
- based on reference points and directions [Deb and Sundar 2006,
 Deb and Kumar 2007]
- based on the hypervolume indicator
 [Brockhoff et al. 2013] [Wagner and Trautmann 2010]
- based on the R2 indicator [Trautmann et al. 2013]

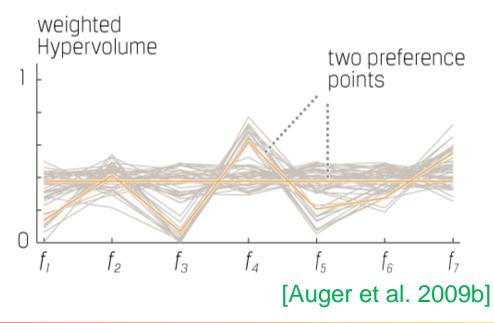
Example: Weighted Hypervolume Indicator



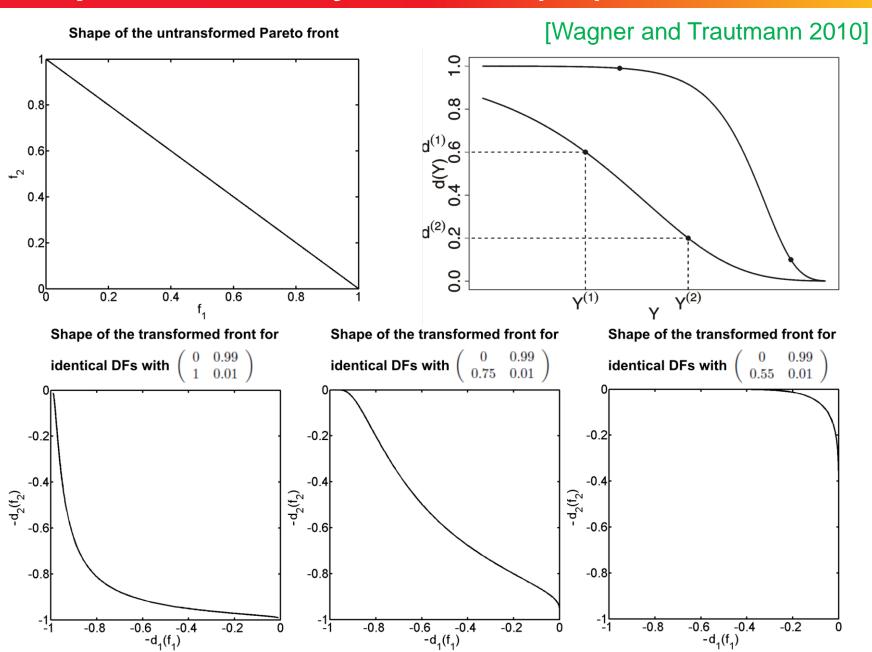
Weighted Hypervolume in Practice



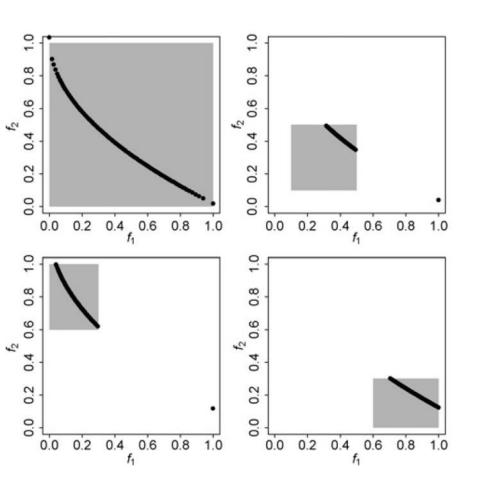


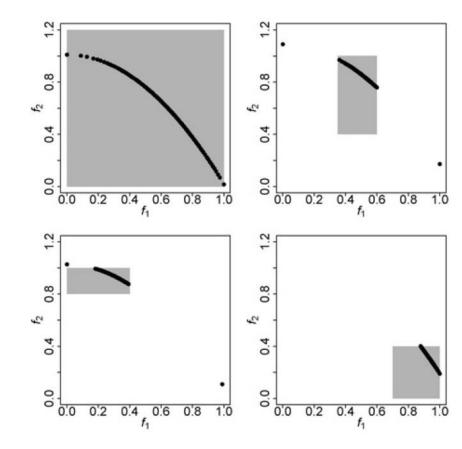


Example: Desirability Function (DF)-SMS-EMOA



DF-SMS-EMOA in Practice



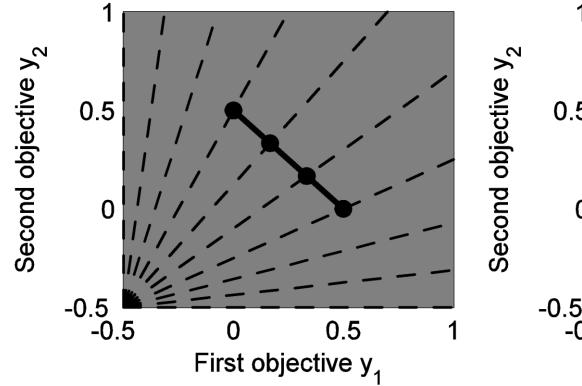


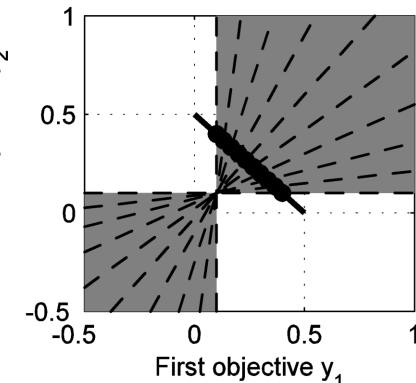
Example: R2-EMOA

Concept

Integration of preferences by varying the scalarizing functions

Position of ideal point



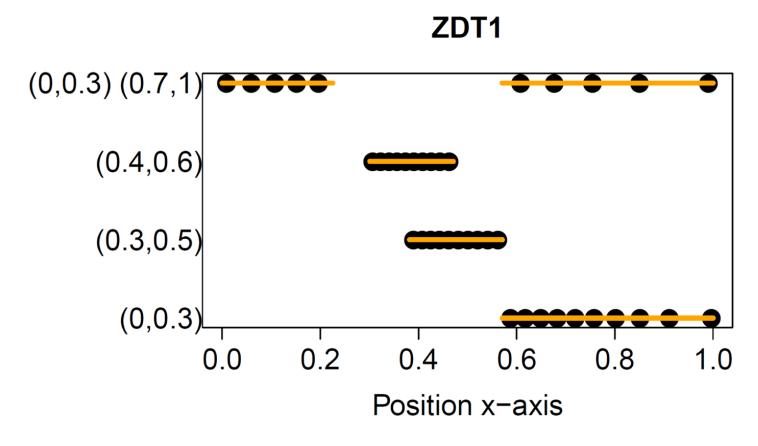


Example: R2-EMOA

Concept

Integration of preferences by varying the scalarizing functions

Restriction of the weight space



Interactive Approaches

Successive Preference Articulation = Interactive EMO

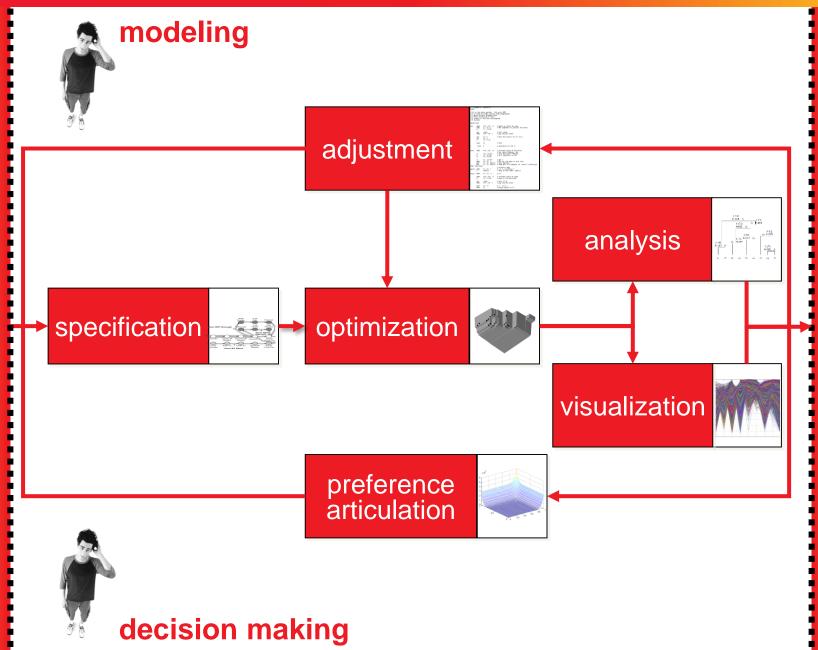
- recent interest of both EMO and MCDM community
- important in practice

Examples

- first interactive EMO: [Tanino et al. 1993]
- good overview: [Jaszkiewicz and Branke 2008]
- more recent work: [Brockhoff et al. 2014] [Branke et al. 2014]

Issues/Open Questions

- realistic scenarios/ value functions
- evaluation of interactive algorithms [López-Ibáñez and Knowles 2015]



problem

The EMO Community

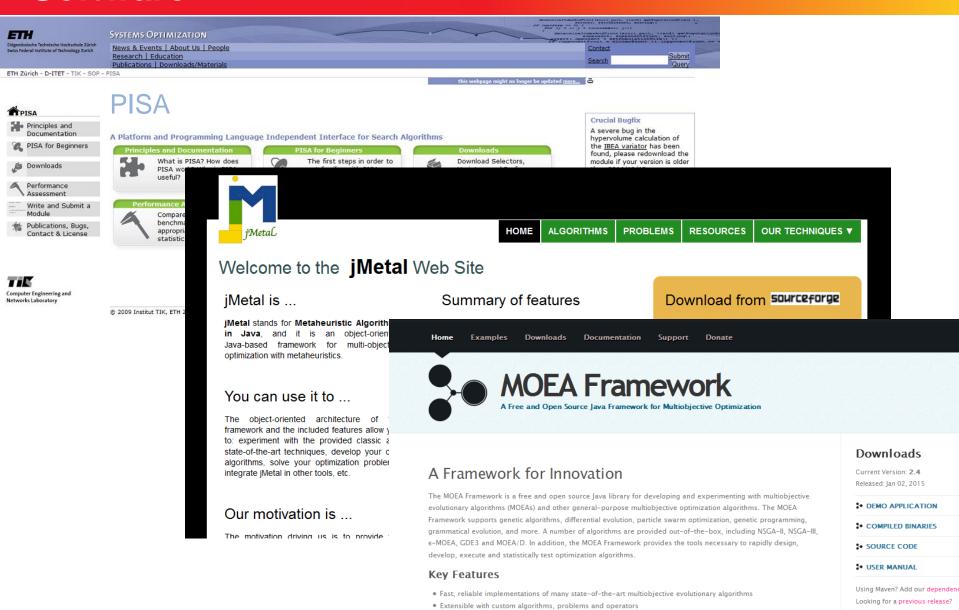
Links:

- 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: https://emoo.cs.cinvestav.mx/
- EMO conference series: https://www.emo2019.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



EMO tutorial, GECCO'2019, Prague, Czech Republic, July 2019

· Supports master-slave, island-model, and hybrid parallelization

· Permissive open source license

· Fully documented source code

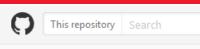
. Modular design for constructing new optimization algorithms from existing components

License

Licensed under the GNU Lesser

General Public License

Software



github.com/numbbo/coco/

numbbo / coco

<> Code

① Issues 115

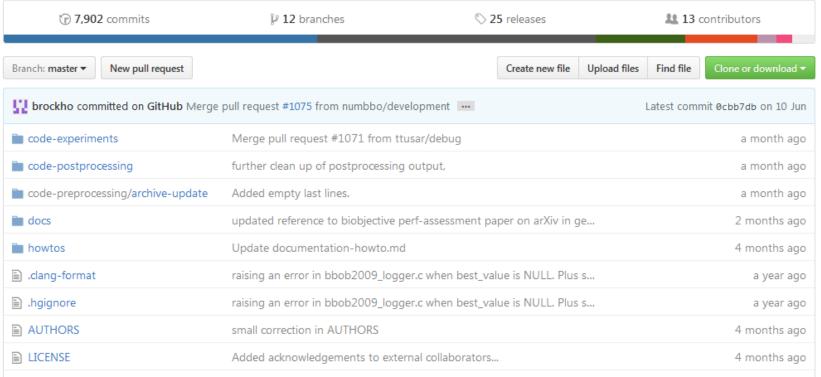
Pull requests 1

♣ Pulse

II Graphs

Settings \$

Numerical Black-Box Optimization Benchmarking Framework http://coco.gforge.inria.fr/ — Edit



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
- . Modular design for constructing new optimization algorithms from existing components
- · Permissive open source license
- Fully documented source code

Using Maven? Add our dependent Looking for a previous release?

License

Licensed under the GNU Lesser General Public License.

Perspectives

Challenging Open (Research) Directions

- from algorithms to toolkits
 - libraries of modules for each task (selection, variation, etc.)
 - problem-specific algorithm configuration/ parameter tuning
- benchmarking
 - comparison with classical approaches
 - design/selection of practically relevant problems
 - algorithm/toolkit recommendations for practice
- integration of EMO and MCDM into one field
- interactive preference articulation and learning
- interactive problem design
- integration of problem-specific knowledge

Questions?

Additional Slides

Instructor Biography: Dimo Brockhoff

Dimo Brockhoff

RandOpt team
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France



After obtaining his diploma in computer science (Dipl.-Inform.) from University of Dortmund, Germany in 2005, Dimo Brockhoff received his PhD (Dr. sc. ETH) from ETH Zurich, Switzerland in 2009. Between June 2009 and October 2011 he held postdoctoral research positions---first at Inria Saclay Ile-de-France in Orsay and then at Ecole Polytechnique in Palaiseau, both in France. Since November 2011, Dimo has been a permanent researcher at Inria: from 2011 till 2016 with the Inria Lille - Nord Europe research center and since October 2016 with the Saclay - Ile-de-France research center, co-located with CMAP, Ecole Polytechnique. His most recent research interests are focused on evolutionary multiobjective optimization (EMO) and other (single-objective) blackbox optimization techniques, in particular with respect to benchmarking, theoretical aspects, and expensive optimization.

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