

GECCO 2019 Tutorial on Evolutionary Multiobjective Optimization

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updated slides will be available at
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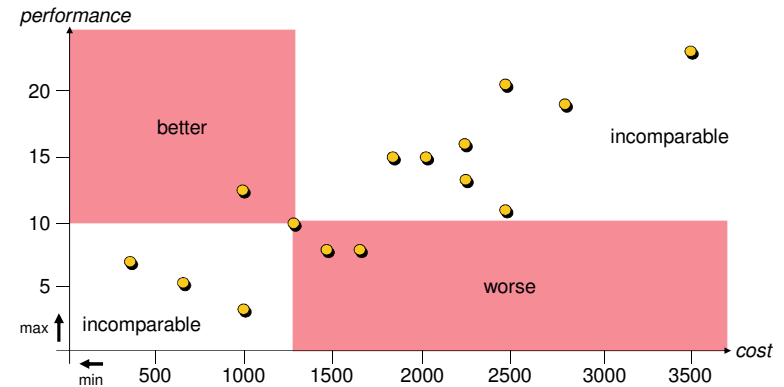


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ACM ISBN 978-1-4503-6748-6/19/07.
<https://doi.org/10.1145/3319619.3323396>

A Brief Introduction to Multiobjective Optimization

Multiobjective Optimization

Multiple objectives that have to be optimized simultaneously



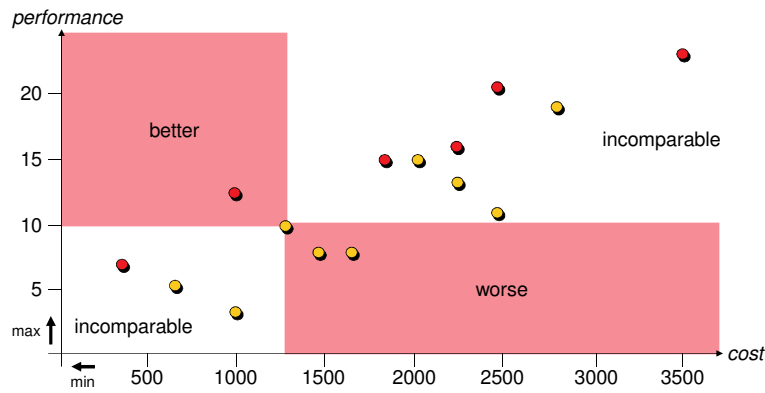
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A Brief Introduction to Multiobjective Optimization

Observations: ① there is no single optimal solution, but
② some solutions (●) are better than others (●)



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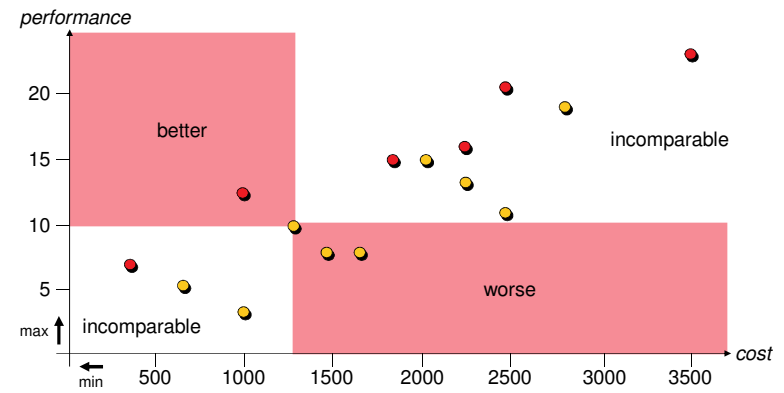
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A Brief Introduction to Multiobjective Optimization

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 ($u <_{par} v$): $u \leq_{par} v \wedge v \not\leq_{par} u$



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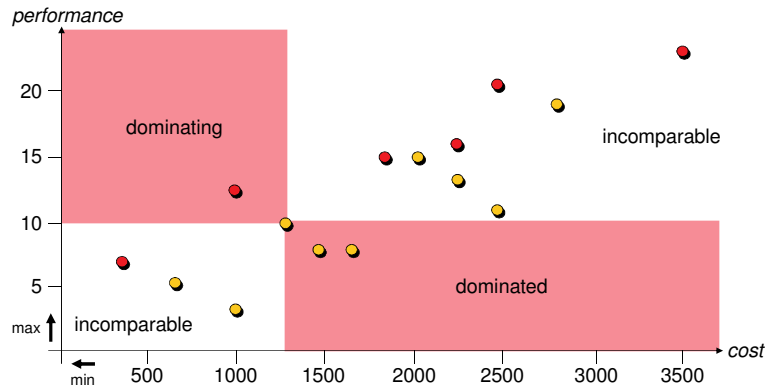
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A Brief Introduction to Multiobjective Optimization

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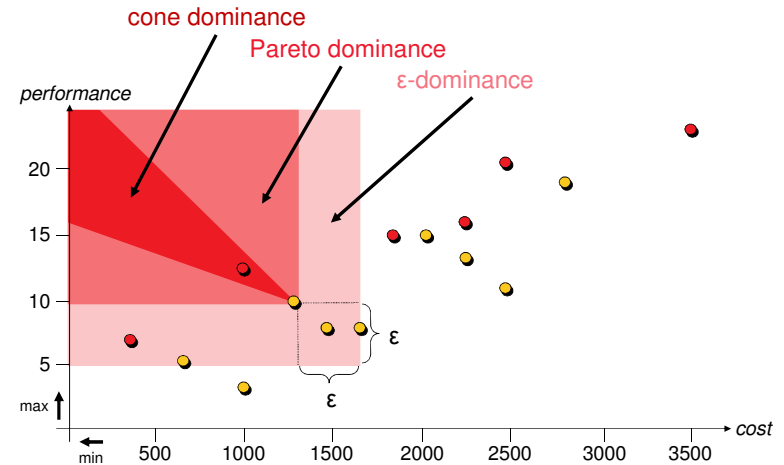


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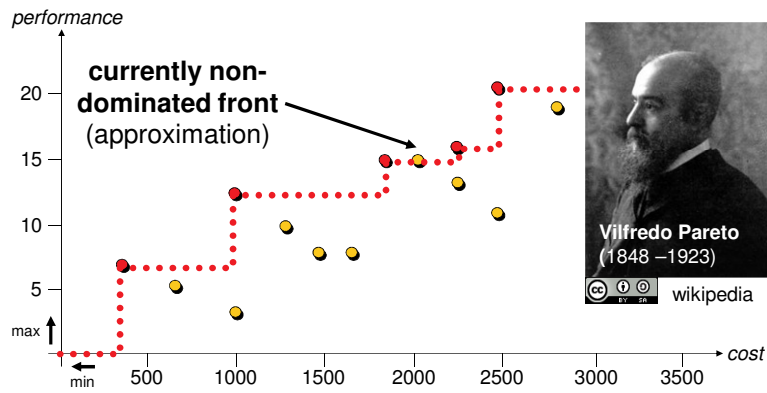
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A Brief Introduction to Multiobjective Optimization

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

Pareto front: its image in the objective space



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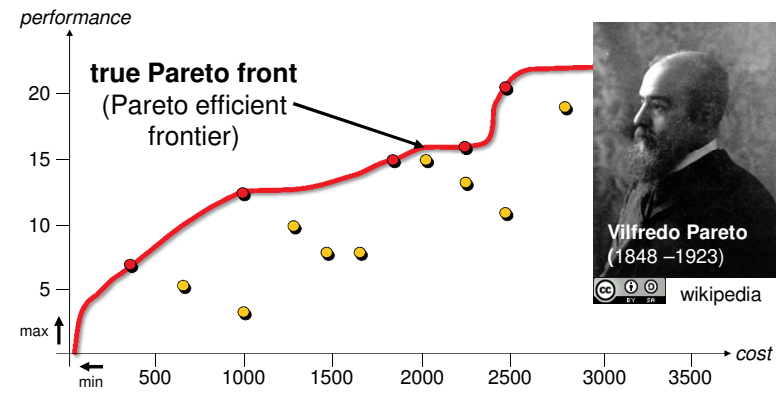
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A Brief Introduction to Multiobjective Optimization

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

Pareto front: its image in the objective space

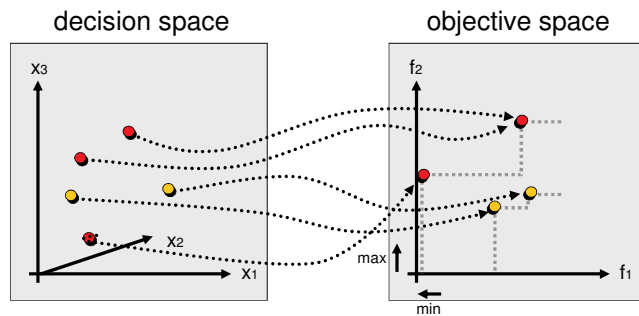


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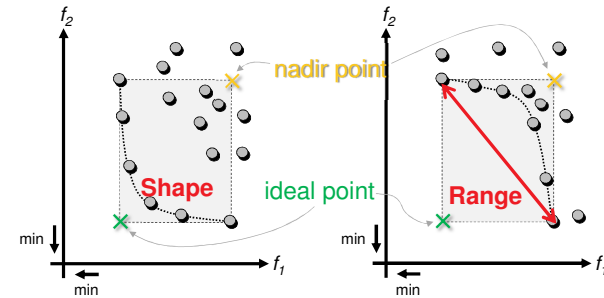
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A Brief Introduction to Multiobjective Optimization



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

A Brief Introduction to Multiobjective Optimization



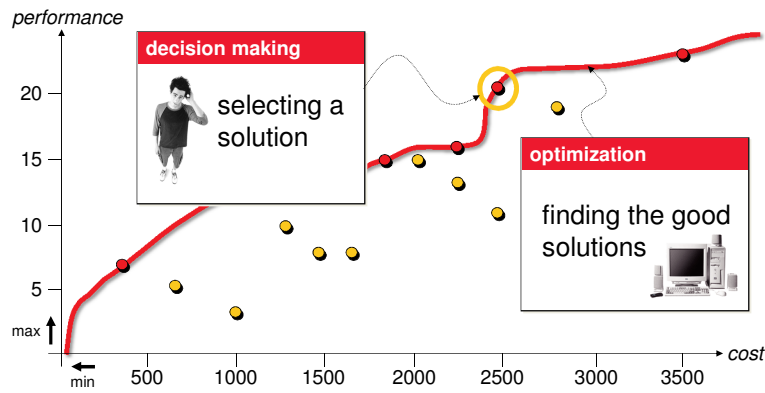
ideal point: best values
 nadir point: worst values

} obtained for Pareto-optimal points

Optimization vs. Decision Making

Multiobjective Optimization

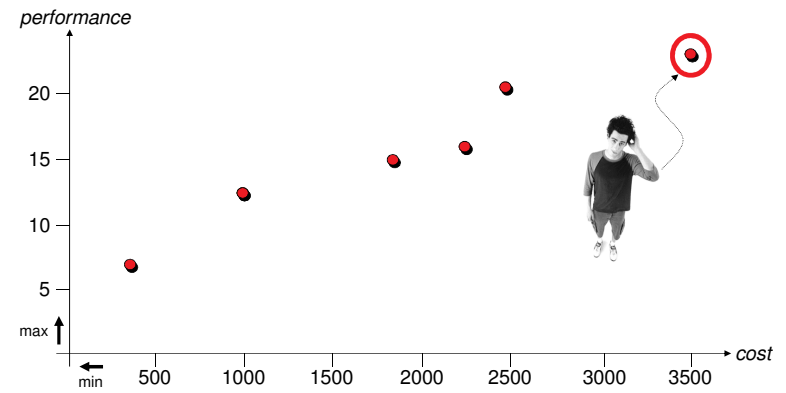
combination of optimization of a set and a decision for a solution



Selecting a Solution: Examples

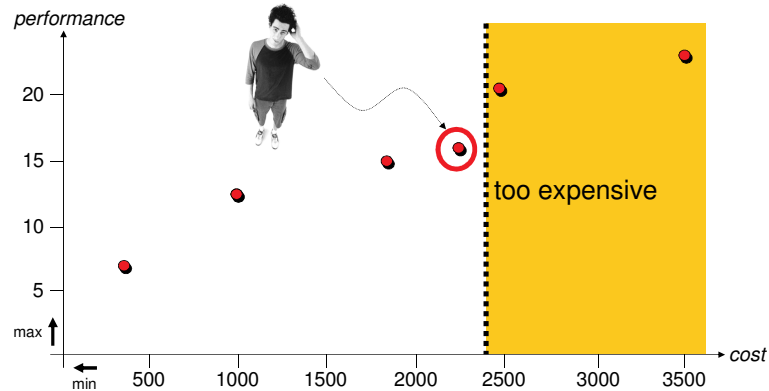
Possible Approaches:

- ① ranking: performance more important than cost



Selecting a Solution: Examples

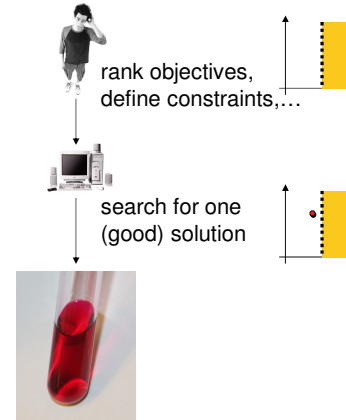
Possible Approaches: ① ranking: performance more important than cost
 ② constraints: cost must not exceed 2400



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When to Make the Decision

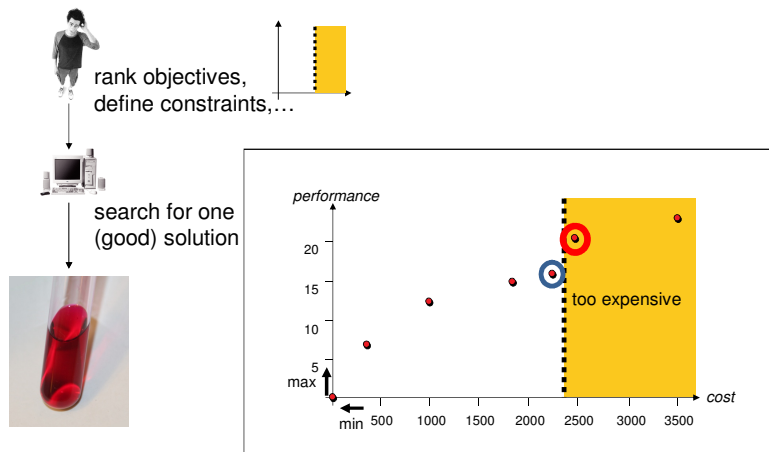
Before Optimization:



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When to Make the Decision

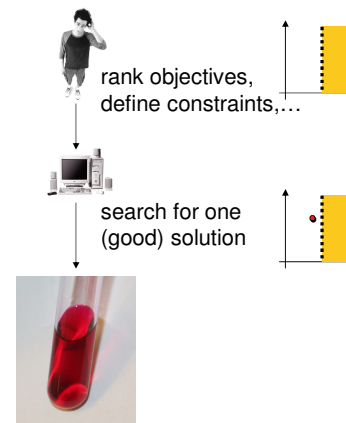
Before Optimization:



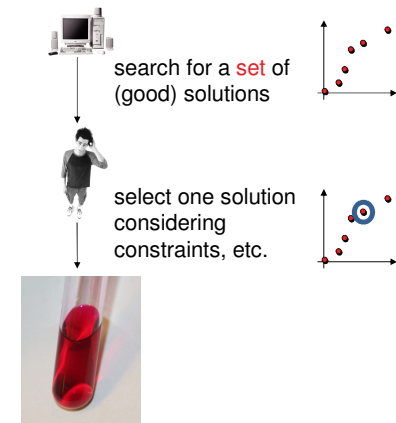
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When to Make the Decision

Before Optimization:



After Optimization:



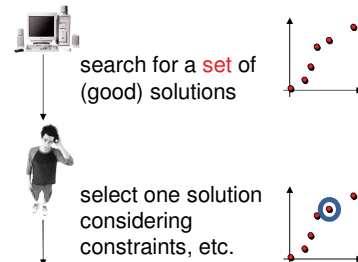
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When to Make the Decision

Before Optimization:



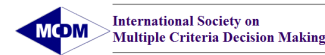
After Optimization:



Focus: learning about a problem

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

Two Communities...



- | | |
|--|--|
| <ul style="list-style-type: none"> 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 | <ul style="list-style-type: none"> 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

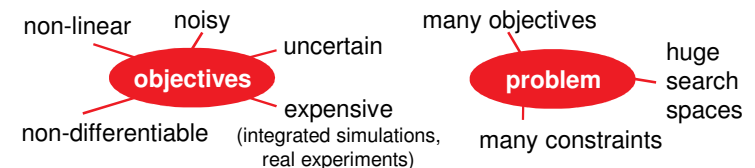
One of the Main Differences

Blackbox optimization

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

only mild assumptions

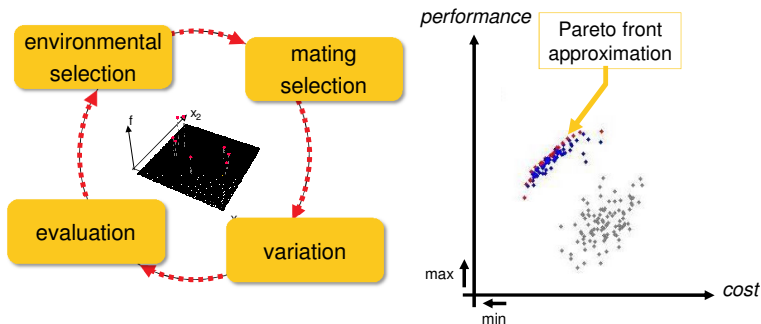
→ EMO therefore well-suited for real-world engineering problems



The Other Main Difference

Evolutionary Multiobjective Optimization

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

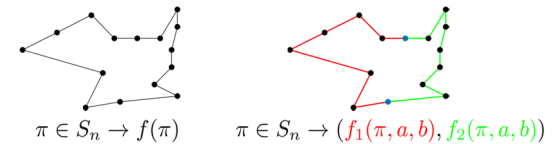


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Multiobjectivization

Some problems are easier to solve in a multiobjective scenario

example: TSP
[Knowles et al. 2001]



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]

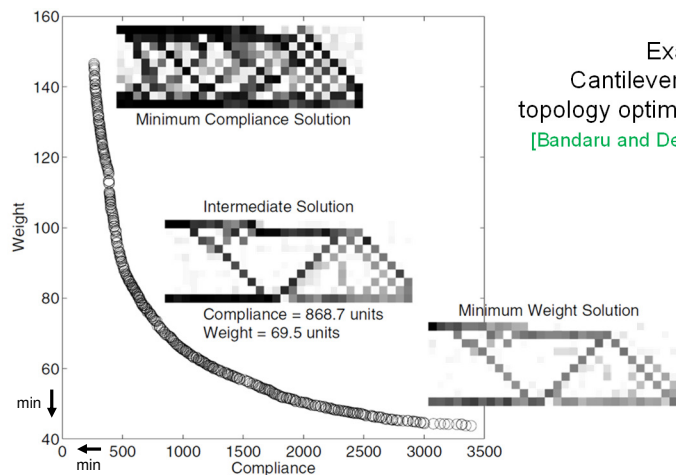
related to **constrained** and **multimodal** single-objective optimization

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

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Innovization

Often innovative design principles among solutions are found



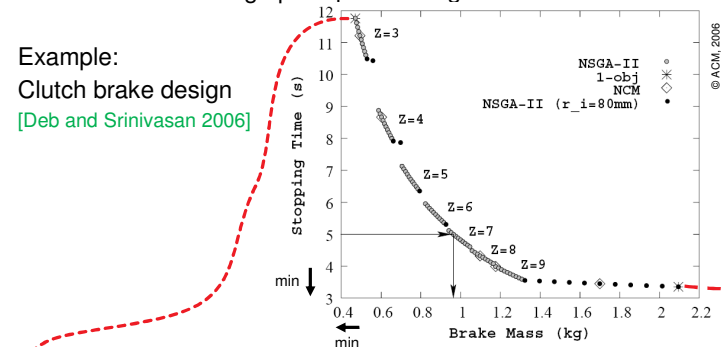
Example:
Cantilever beam
topology optimization
[Bandaru and Deb 2015]

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Innovization

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

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Innovization

Often innovative design principles among solutions are found

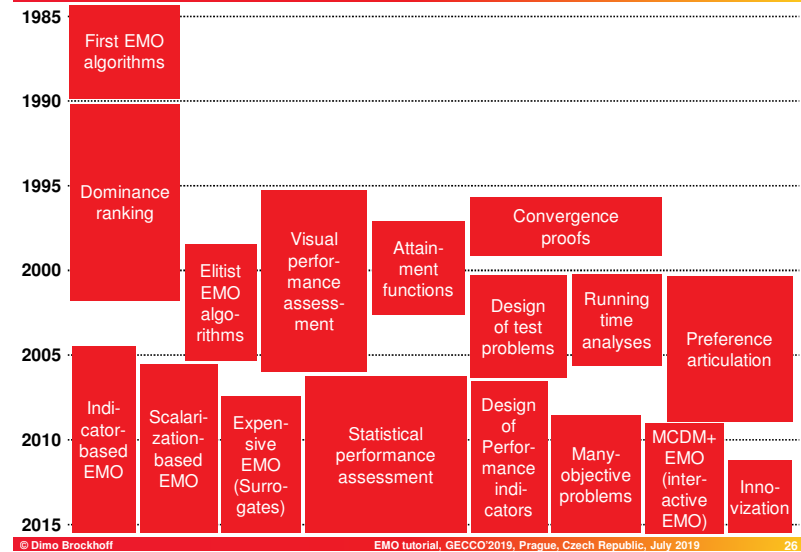
Innovization [Deb and Srinivasan 2006]

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

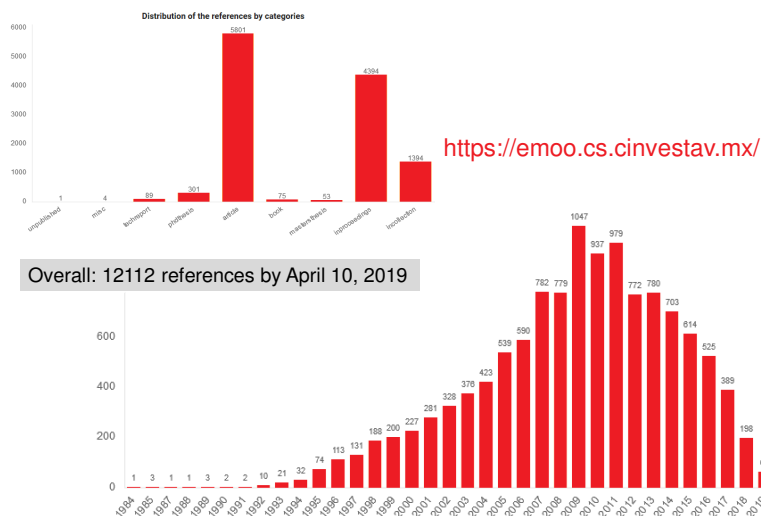
Other examples:

- 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]

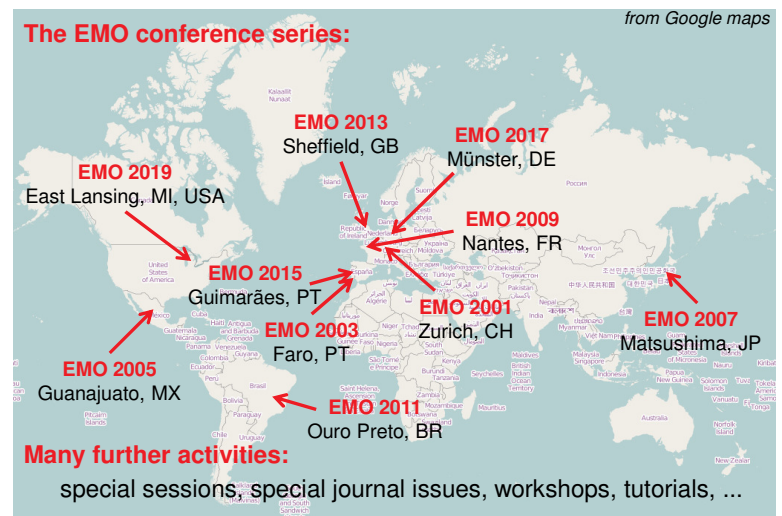
The History of EMO At A Glance



The History of EMO At A Glance



The EMO Community



Overview

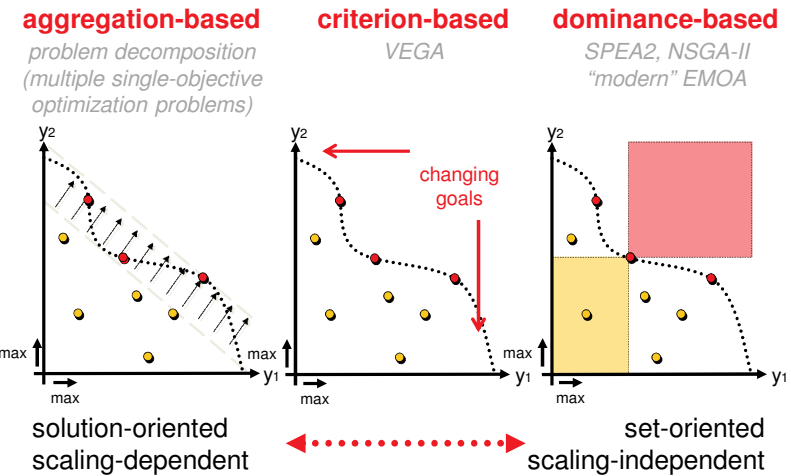
The Big Picture

Basic Algorithm Design Principles and Concepts

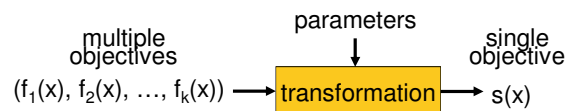
Performance Assessment and Benchmarking

Preference Articulation

Fitness Assignment: Principal Approaches

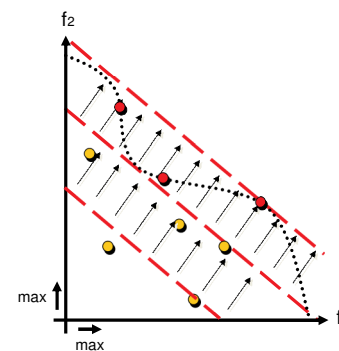
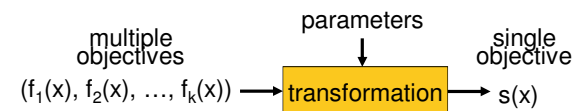


Solution-Oriented Problem Transformations



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

Solution-Oriented Problem Transformations

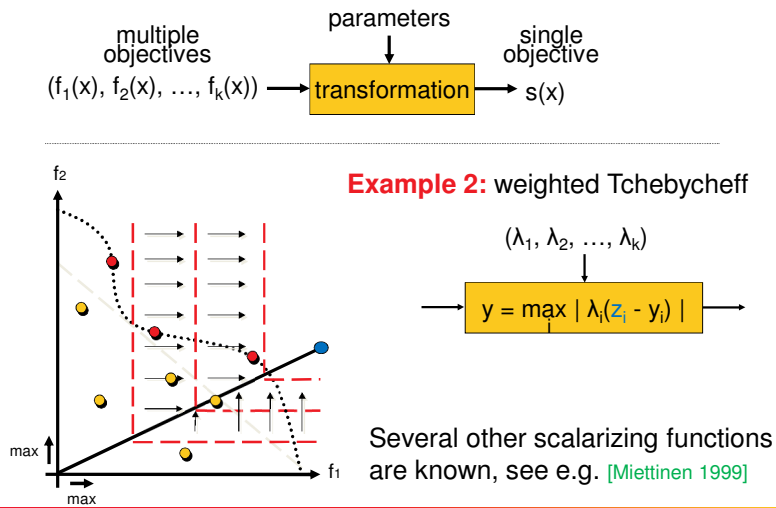


Example 1: weighted sum approach

$$(w_1, w_2, \dots, w_k) \rightarrow y = w_1 y_1 + \dots + w_k y_k \rightarrow$$

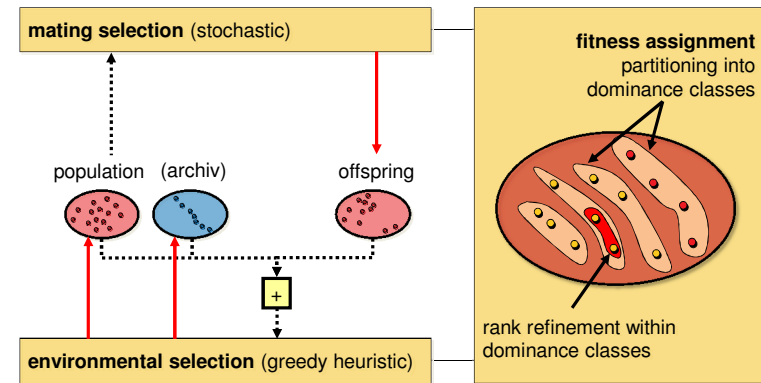
Disadvantage: not all Pareto-optimal solutions can be found if the front is not convex

Solution-Oriented Problem Transformations



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General Scheme of Most Set-Oriented EMO



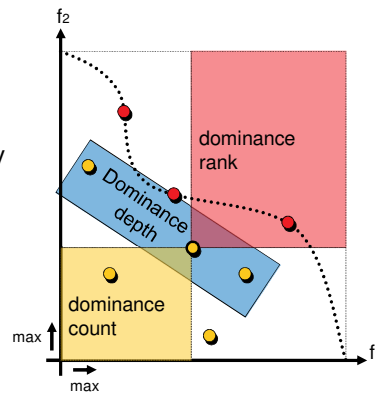
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Ranking of the Population Using Dominance

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

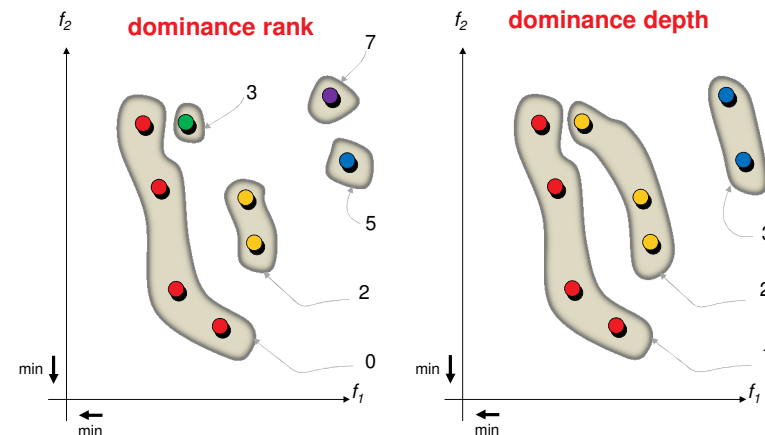
... is based on pairwise comparisons of the individuals only.

- 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



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Illustration of Dominance-Based Partitioning



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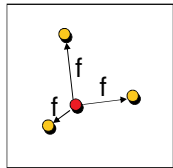
Refinement of Dominance Rankings

Goal: rank incomparable solutions within a dominance class

1 Diversity information

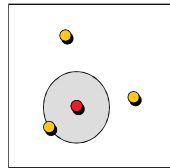
Kernel method

diversity =
function of the
distances



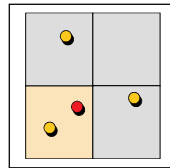
k-th nearest neighbor

diversity =
function of distance
to k-th nearest neighbor



Histogram method

diversity =
number of elements
within box(es)

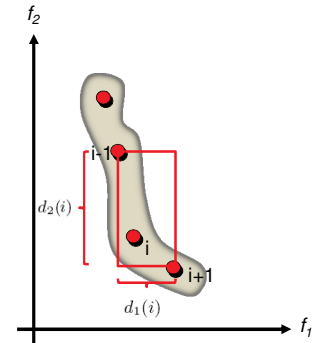


2 (Contribution to a) quality indicator

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



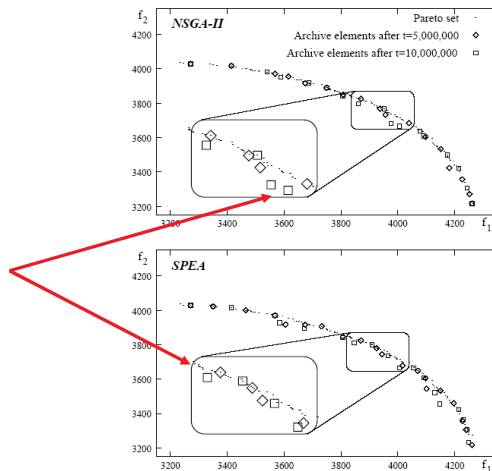
$$CD(i) = \frac{d_1(i)}{f_{1,\max} - f_{1,\min}} + \dots + \frac{d_m(i)}{f_{m,\max} - f_{m,\min}}$$

SPEA2 and NSGA-II: Deteriorative Cycles

Selection in SPEA2 and NSGA-II can result in

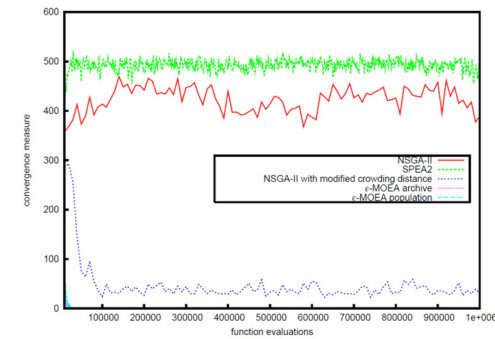
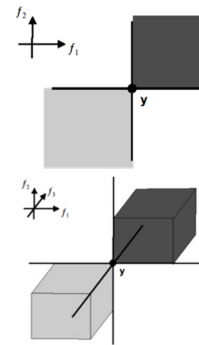
deteriorative cycles

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



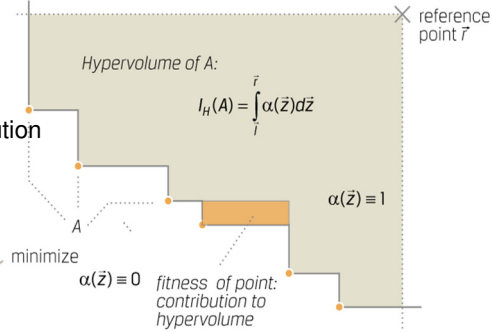
Hypervolume-Based Selection

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

use hypervolume indicator to guide the search: refines dominance

Main idea

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



But:

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

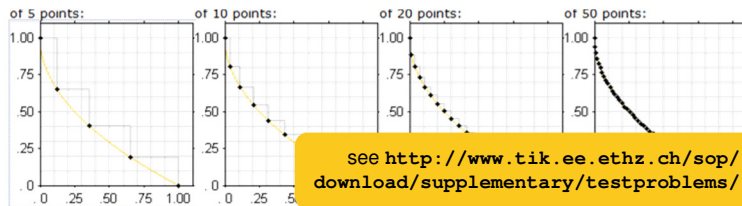
The Optimization Goal in Indicator-Based EMO

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. 2019]

[Friedrich et al. 2011]:

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

! (probably) does not hold for > 2 objectives

$$\begin{aligned} \text{OPT} & 1 + \frac{\log(\min\{A/a, B/b\})}{n} \\ \text{HYP} & 1 + \frac{\sqrt{A/a} + \sqrt{B/b}}{n-4} \\ \text{logHYP} & 1 + \frac{\sqrt{\log(A/a) \log(B/b)}}{n-2} \end{aligned}$$

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?

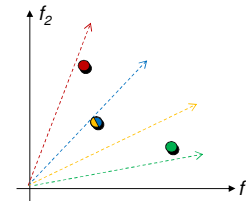
further open questions on indicator-based EMO available at
<http://simco.gforge.inria.fr/doku.php?id=openproblems>

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 \neq 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]

Overview

The Big Picture

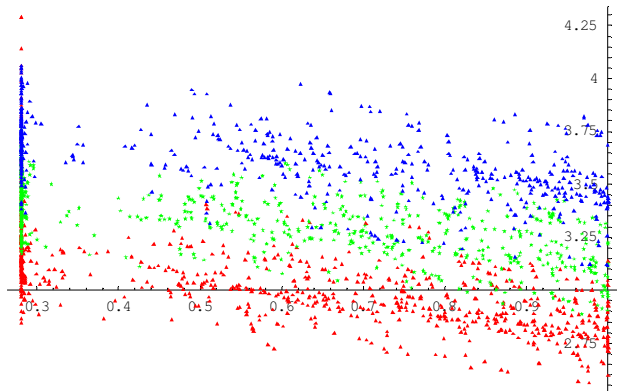
Basic Algorithm Design Principles and Concepts

Performance Assessment and Benchmarking

Preference Articulation

Once Upon a Time...

... multiobjective EAs were mainly compared visually:

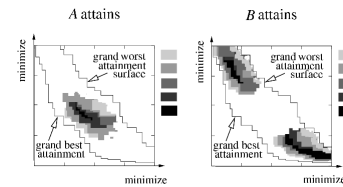


ZDT6 benchmark problem: IBEA, SPEA2, NSGA-II

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	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

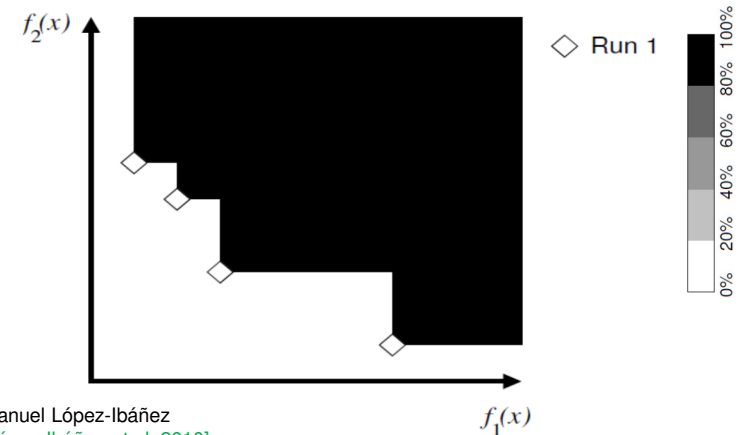
see e.g. [Zitzler et al. 2003]

Empirical Attainment Functions



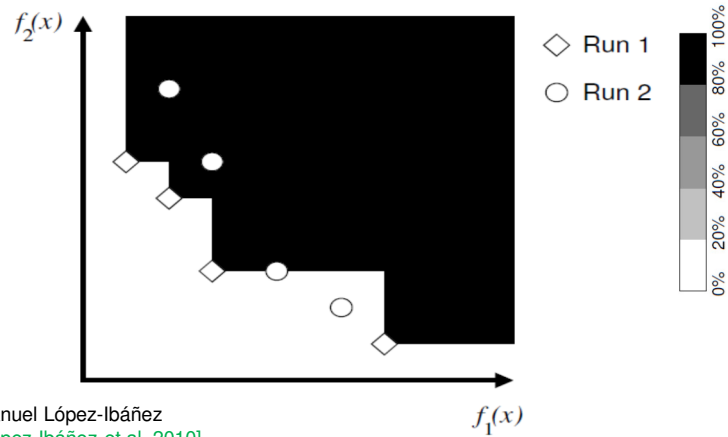
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[López-Ibáñez et al. 2010]

Empirical Attainment Functions



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Empirical Attainment Functions



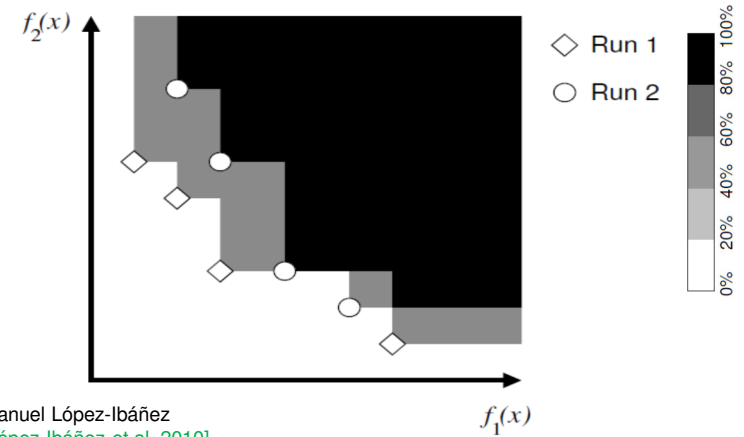
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Empirical Attainment Functions



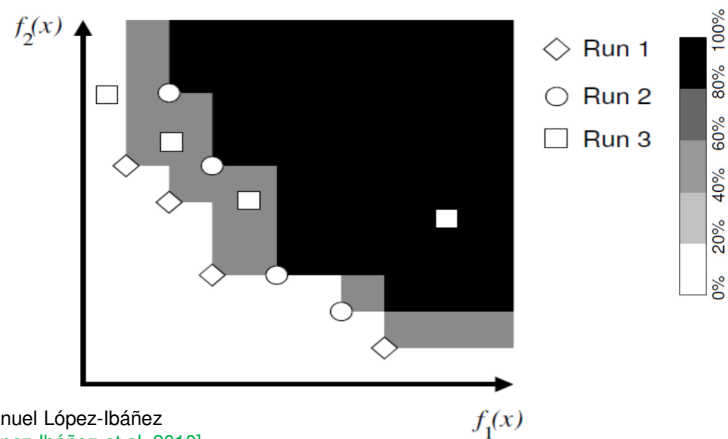
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Empirical Attainment Functions



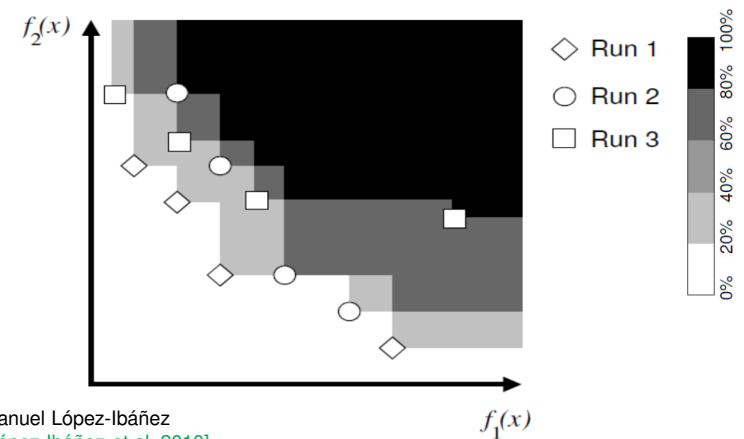
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Empirical Attainment Functions



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Empirical Attainment Functions: Definition

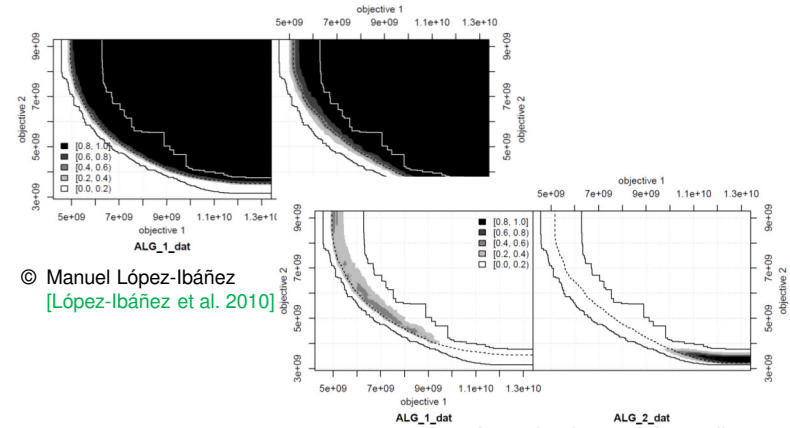
The Empirical Attainment Function $\alpha(z)$ "counts" how many solution sets X_i attain or dominate a vector z at time T :

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

with \preceq_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").

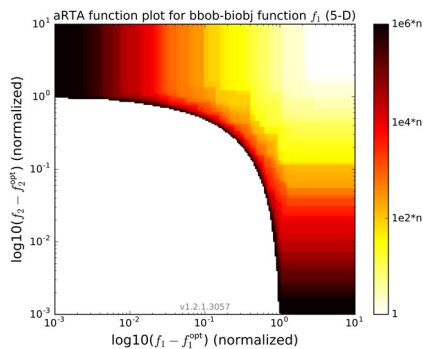
Empirical Attainment Functions in Practice



latest implementation online at
<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!

$$A \preceq B : \Leftrightarrow \forall y \in B \exists x \in A x \leq_{par} y$$

Refinements and Weak Refinements

- 1 $\stackrel{\text{ref}}{\preceq}$ **refines** a preference relation \preceq iff

$$A \preceq B \wedge B \not\preceq A \Rightarrow A \stackrel{\text{ref}}{\preceq} B \wedge B \not\stackrel{\text{ref}}{\preceq} A \quad (\text{better} \Rightarrow \text{better})$$

\Rightarrow fulfills requirement

- 2 $\stackrel{\text{ref}}{\preceq}$ **weakly refines** a preference relation \preceq iff

$$A \preceq B \wedge B \not\preceq A \Rightarrow A \stackrel{\text{ref}}{\preceq} B \quad (\text{better} \Rightarrow \text{weakly better})$$

\Rightarrow does not fulfill requirement, but $\stackrel{\text{ref}}{\preceq}$ does not contradict \preceq

! sought are total refinements...

[Zitzler et al. 2010]

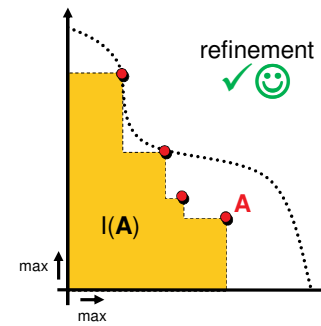
Example: Refinements Using Indicators

$$A \stackrel{\text{ref}}{\preceq} B \Leftrightarrow I(A) \geq I(B)$$

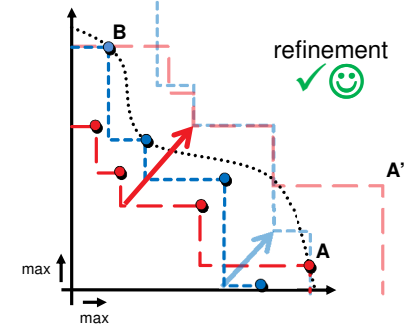
$$A \stackrel{\text{ref}}{\preceq} B \Leftrightarrow I(A, B) \leq I(B, A)$$

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

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



unary hypervolume indicator



binary epsilon indicator

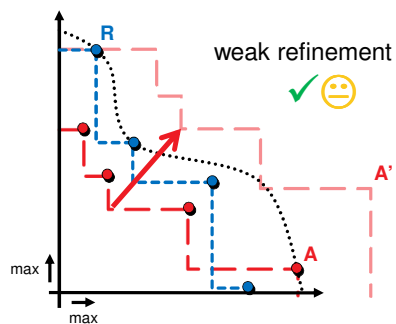
Example: Weak Refinement / No Refinement

$$A \stackrel{\text{ref}}{\preceq} B \Leftrightarrow I(A, R) \leq I(B, R)$$

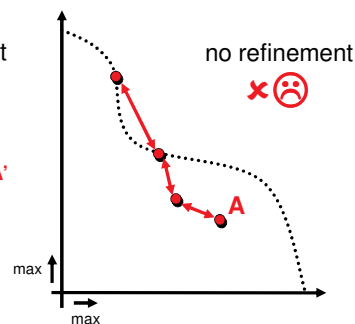
$$A \stackrel{\text{ref}}{\preceq} B \Leftrightarrow I(A) \leq I(B)$$

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

$I(A)$ = variance of pairwise distances



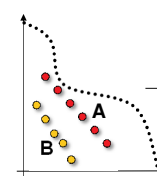
unary epsilon indicator



unary diversity indicator

Quality Indicator Approach

Goal: compare two Pareto set approximations A and B



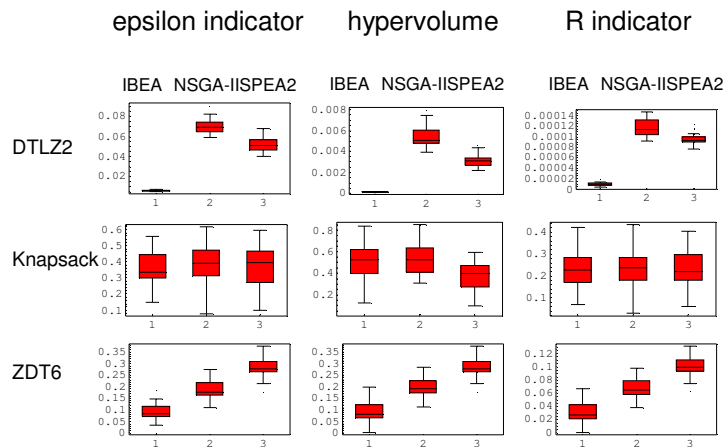
	A	B
hypervolume	432.34	420.13
distance	0.3308	0.4532
diversity	0.3637	0.3463
spread	0.3622	0.3601
cardinality	6	5

→ "A better"

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



Example: Box Plots



Statistical Assessment (Kruskal Test)

ZDT6 Epsilon				DTLZ2 R			
is better than							
IBEA		~0 😊	~0 😊	IBEA		~0 😊	~0 😊
NSGA2	1		~0 😊	NSGA2	1		1
SPEA2	1	1		SPEA2	1	~0 😊	

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

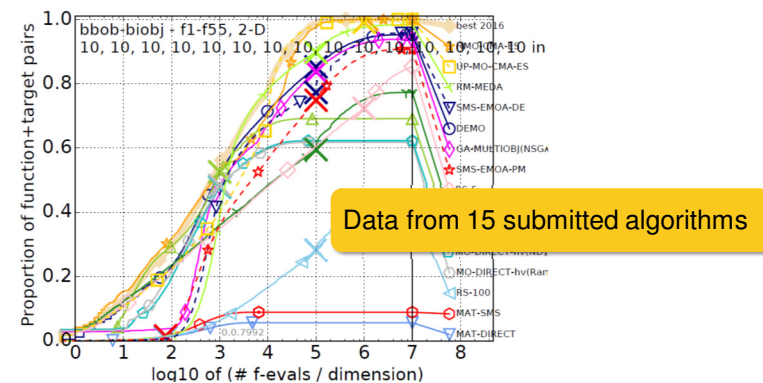
Overall p-value = 7.86834e-17.
Null hypothesis rejected (alpha 0.05)

Knapsack/Hypervolume: H_0 = No significance of any differences

Automated Benchmarking

- State-of-the-art in single-objective optimization: **Blackbox Optimization Benchmarking (BBOB)** with COCO platform
<https://github.com/numbbbo/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-2016 Results



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Incorporation of Preferences During Search

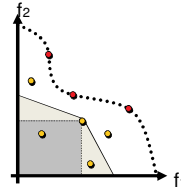
Nevertheless...

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

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

1 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]

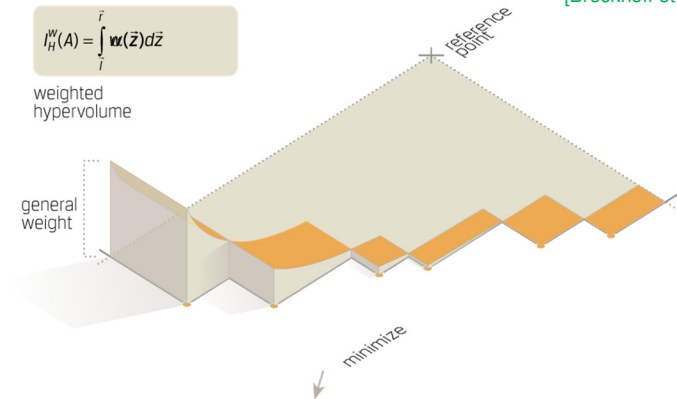


2 Use quality indicators, e.g.:

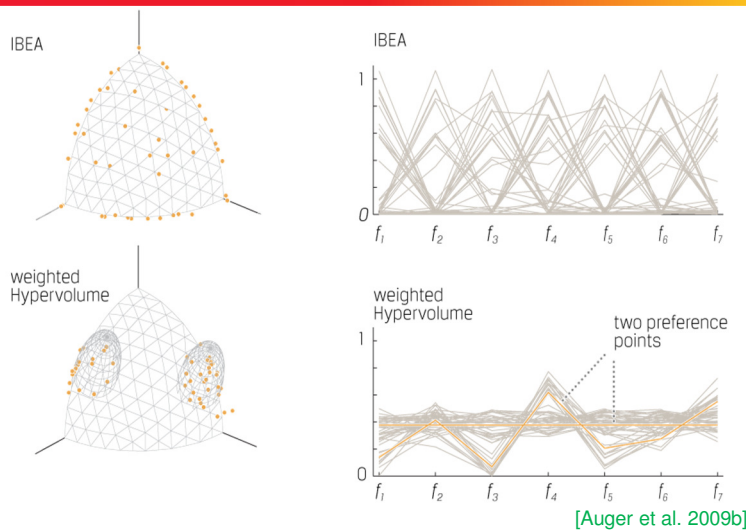
- based on reference points and directions [Deb and Sundar 2006, Deb and Kumar 2007]
- based on the hypervolume indicator [Brockhoff et al. 2013] [Wagner and Trautmann 2010]
- based on the R2 indicator [Trautmann et al. 2013]

Example: Weighted Hypervolume Indicator

[Brockhoff et al. 2013]



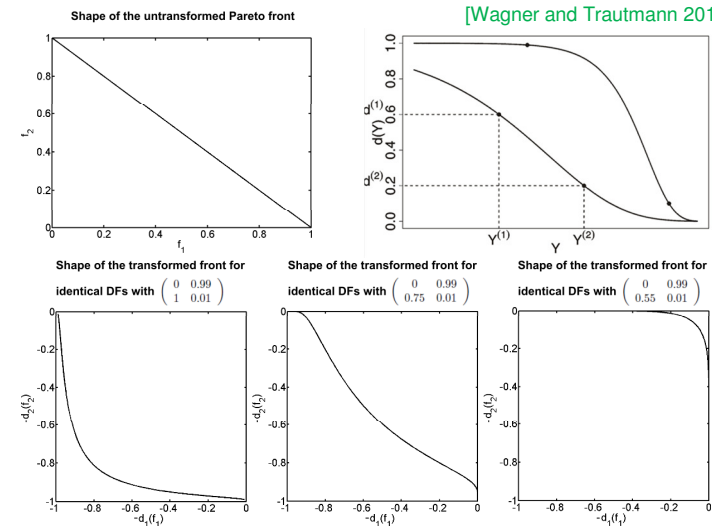
Weighted Hypervolume in Practice



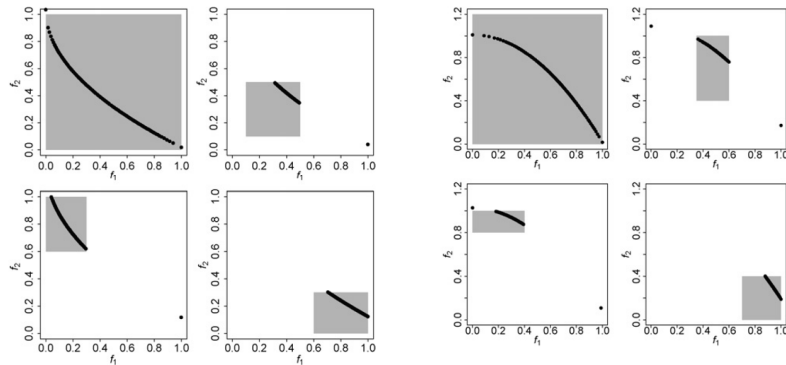
[Auger et al. 2009b]

Example: Desirability Function (DF)-SMS-EMOA

[Wagner and Trautmann 2010]



DF-SMS-EMOA in Practice



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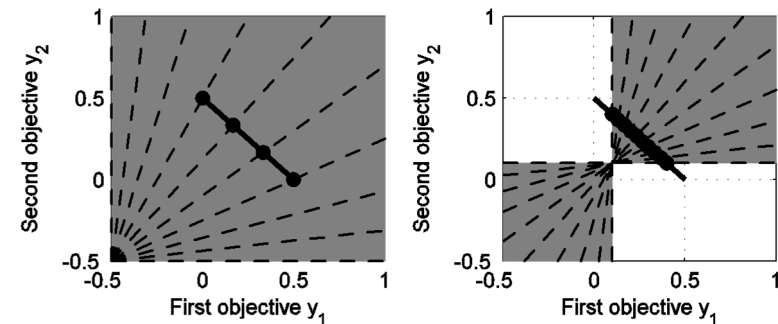
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Example: R2-EMOA

Concept

Integration of preferences by varying the scalarizing functions

Position of ideal point



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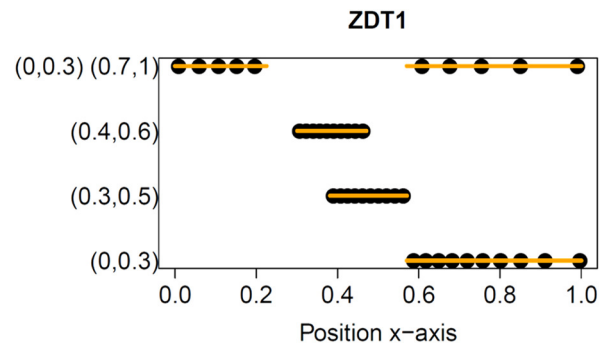
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Example: R2-EMOA

Concept

Integration of preferences by varying the scalarizing functions

Restriction of the weight space



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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

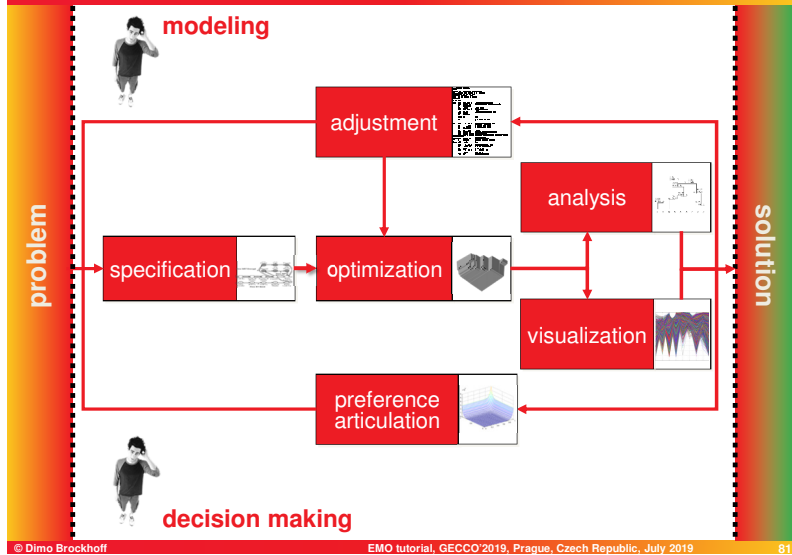
- realistic scenarios/ value functions
- evaluation of interactive algorithms [López-Ibáñez and Knowles 2015]

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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.dep.uminho.pt/EMO2015/>

Books:

- Multi-Objective Optimization using Evolutionary Algorithms** Kalyanmoy Deb, Wiley, 2001
- Evolutionary Algorithms for Solving Multi-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...

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Software

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Software

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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?

Instructor Biography: Dimo Brockhoff

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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.

Additional Slides

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Acknowledgements

I would like to thank in particular Eckart Zitzler and Tobias Wagner who contributed significantly to the content of these slides over the years.

Many thanks go also to Carlos Fonseca and Manuel López-Ibáñez for pointing out some mistakes during my PPSN 2016 presentation on the same topic that should be corrected in these slides.