GECCO 2015 Tutorial on Evolutionary Multiobjective Optimization

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updated slides will be available at http://researchers.lille.inria.fr/~brockhof/



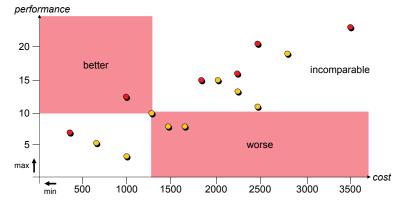


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GECCO'15 Companion, July 11-15, 2015, Madrid, Spain, ACM, ISBN 978-1-4503-3488-4/1507, DOI:10.1145/2739482.2756574

A Brief Introduction to Multiobjective Optimization

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



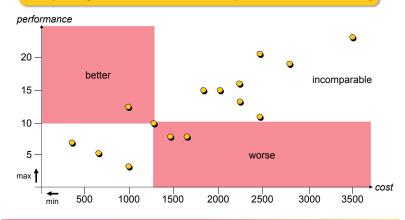
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A Brief Introduction to Multiobjective Optimization

Multiobjective Optimization

Multiple objectives that have to be optimized simultaneously



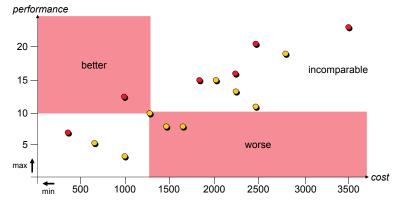
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A Brief Introduction to Multiobjective Optimization

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

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



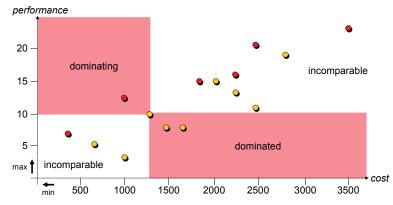
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A Brief Introduction to Multiobjective Optimization

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

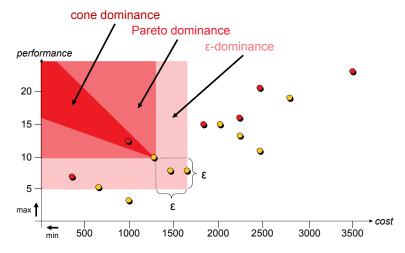
u Pareto dominates v ($u <_{par} v$): $u \leqslant_{par} v \land v \not\leqslant_{par} u$



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A Brief Introduction to Multiobjective Optimization

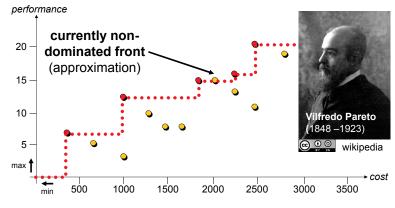


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A Brief Introduction to Multiobjective Optimization

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

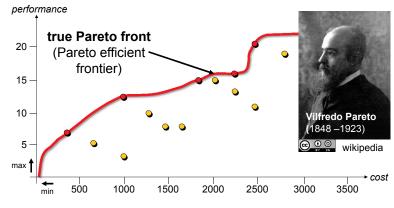


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A Brief Introduction to Multiobjective Optimization

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

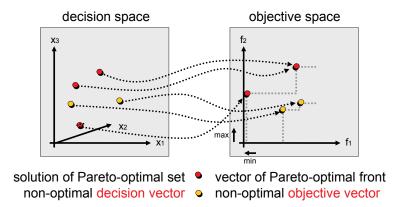
Pareto front: its image in the objective space



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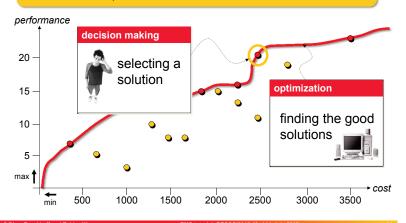
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40

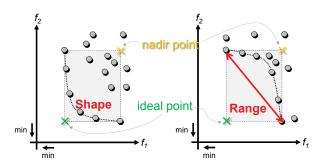
Optimization vs. Decision Making

Multiobjective Optimization

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



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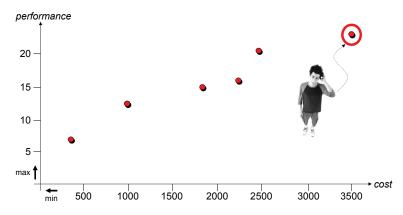


ideal point: best values nadir point: worst values

obtained for Pareto-optimal points

Selecting a Solution: Examples

Possible • ranking: performance more important than cost Approaches:

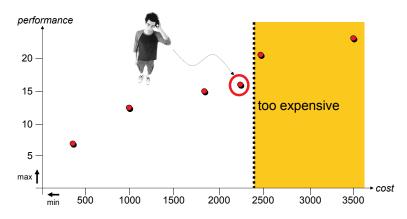


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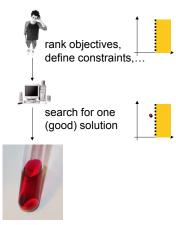
Selecting a Solution: Examples

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



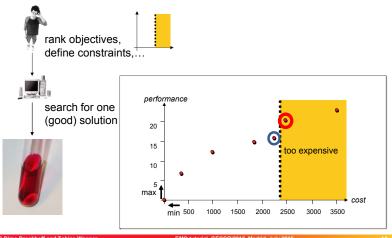
When to Make the Decision

Before Optimization:



When to Make the Decision

Before Optimization:

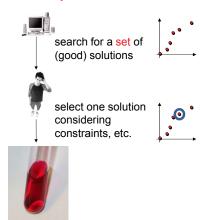


When to Make the Decision

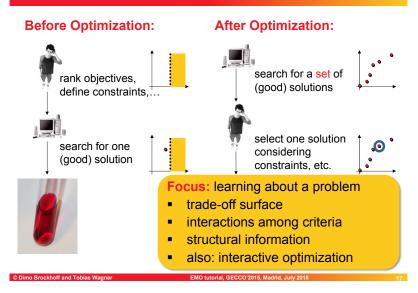
Before Optimization:

rank objectives, define constraints,... search for one (good) solution

After Optimization:



When to Make the Decision



...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

Two Communities...





- 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

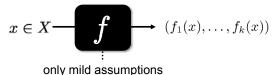
- quite young field (first papers in mid 1980s)
- bi-annual conference since 2001
- background in computer science, applied math and engineering
- focus on optimization algorithms

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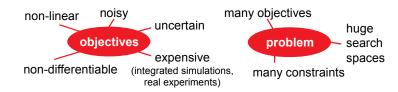
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One of the Main Differences

Blackbox optimization



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



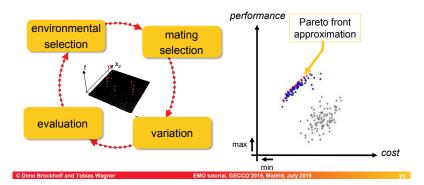
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The Other Main Difference

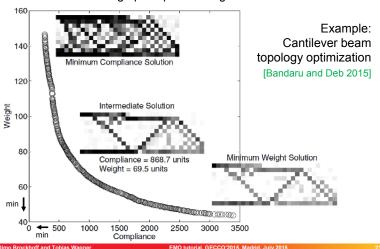
Evolutionary Multiobjective Optimization

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



Innovization

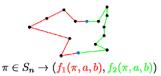
Often innovative design principles among solutions are found



Multiobjectivization

Some problems are easier to solve in a multiobjective scenario





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]

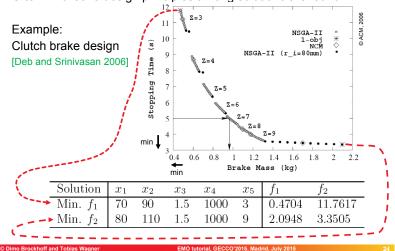
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Innovization

Often innovative design principles among solutions are found



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:

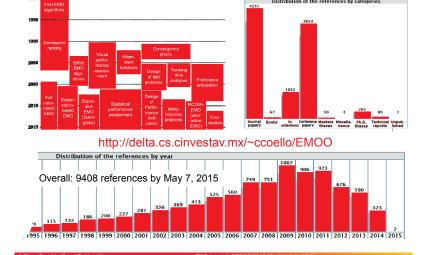
- SOM for supersonic wing design [Obayashi and Sasaki 2003]
- Biclustering for processor design and knapsack [Ulrich et al. 2007]
- Successful case studies in engineering (noise barrier design, polymer extrusion, friction stir welding)
 [Deb et al. 2014]

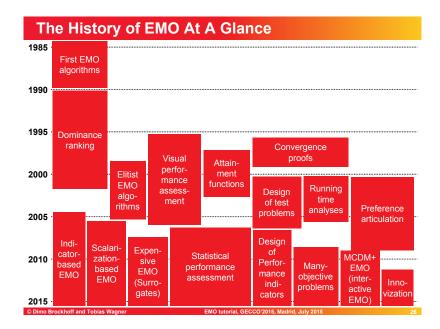
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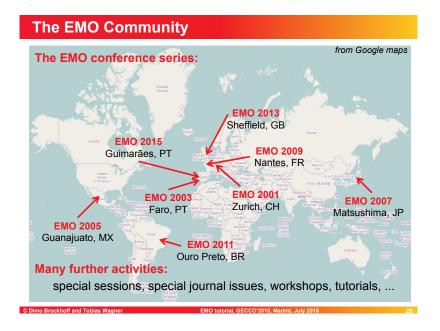
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25

The History of EMO At A Glance







Overview

The Big Picture

Basic Principles of Multiobjective Optimization

- algorithm design principles and concepts
- performance assessment

Selected Advanced Concepts

- preference articulation
- surrogate-based EMO

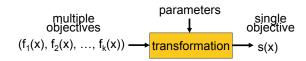
A Few Examples From Practice

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Solution-Oriented Problem Transformations



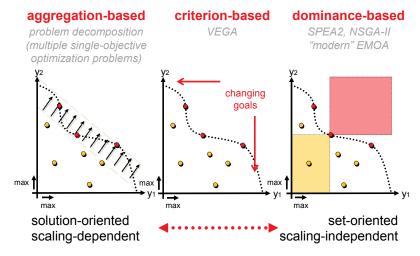
A scalarizing function s is a function $s:Z\to\mathbb{R}$ that maps each objective vector $u=(u_1,\ldots,u_n)\in Z$ to a real value $s(u)\in\mathbb{R}$

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31

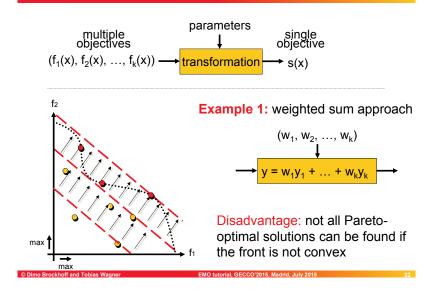
Fitness Assignment: Principal Approaches



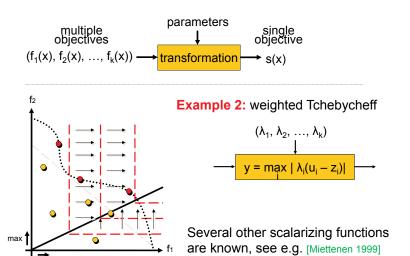
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Solution-Oriented Problem Transformations

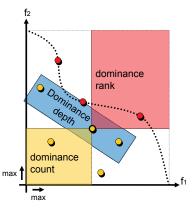


Solution-Oriented Problem Transformations



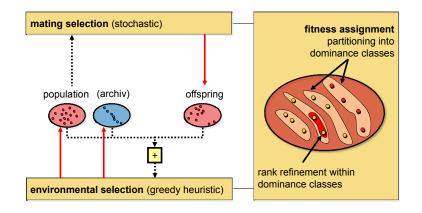
Ranking of the Population Using Dominance

- ... 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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General Scheme of Most Set-Oriented EMO

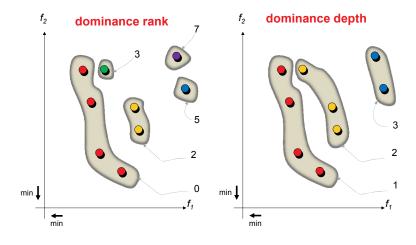


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Illustration of Dominance-Based Partitioning



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Refinement of Dominance Rankings

Goal: rank incomparable solutions within a dominance class

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)



(Contribution to a) quality indicator

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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

$$d_2(i) = \begin{cases} 1 & \text{i+1} \\ d_1(i) & \text{i+1} \end{cases}$$

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

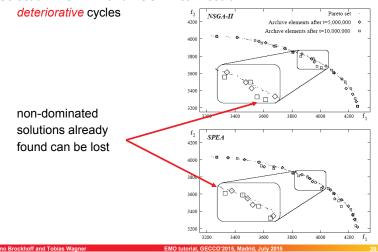
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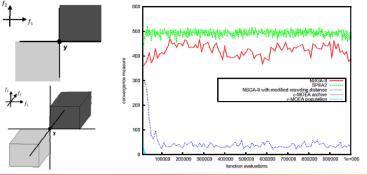
SPEA2 and NSGA-II: Deteriorative Cycles

Selection in SPEA2 and NSGA-II can result in



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

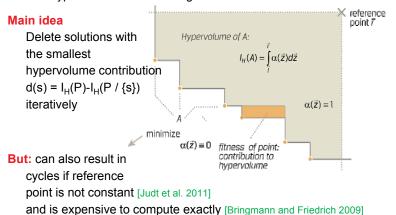


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Hypervolume-Based Selection

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



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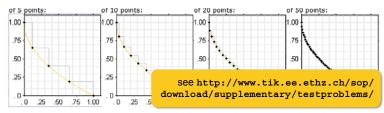
The Optimization Goal in Indicator-Based EMO

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]



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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 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

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42

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

[Friedrich et al. 2011]:

optimal μ -distributions for the hypervolume correspond to e-approximations of the front $\begin{array}{ccc} & & & \text{OPT} & 1 + \frac{\sqrt{8 \sqrt{\ln \ln(1/\epsilon)} D/\epsilon}}{n} \\ & & & 1 + \frac{\sqrt{A/a} + \sqrt{B}}{n} \\ & & & 1 + \frac{\sqrt{A/a} + \sqrt{B}}{n-4} \\ & & & & \frac{\log HYP}{n-2} & 1 + \frac{\sqrt{\log(A/a) \log(B/\epsilon)}}{n-2} \\ \end{array}$

! (probably) does not hold for > 2 objectives

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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]
- 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?

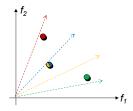
further open questions on indicator-based EMO available at http://simco.gforge.inria.fr/doku.php?id=openproblems

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



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]
- 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]

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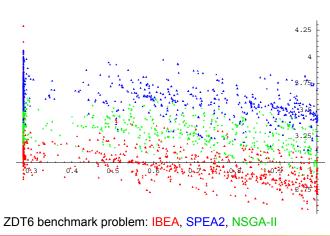
Selected Advanced Concepts

- preference articulation
- surrogate-based EMO

A Few Examples From Practice

Once Upon a Time...

... multiobjective EAs were mainly compared visually:



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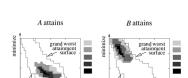
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Two Approaches for Empirical Studies

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	В
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]

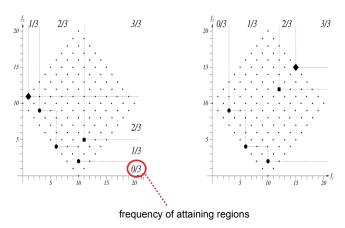
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Empirical Attainment Functions

three runs of two multiobjective optimizers



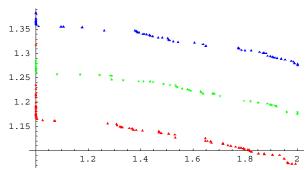
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51

Attainment Plots

50% attainment surface for IBEA, SPEA2, NSGA2 (ZDT6)



latest implementation online at http://eden.dei.uc.pt/~cmfonsec/software.html

see [Fonseca et al. 2011]

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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!

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

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Refinements and Weak Refinements

 \bullet refines a preference relation \preceq iff

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

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

$$A \preccurlyeq B \land B \nleq A \Rightarrow A \overset{\text{ref}}{\preccurlyeq} B$$
 (better \Rightarrow weakly better)

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

! sought are total refinements...

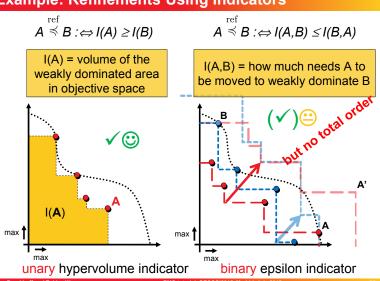
[Zitzler et al. 2010]

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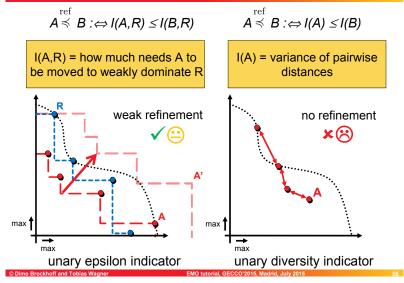
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Example: Refinements Using Indicators

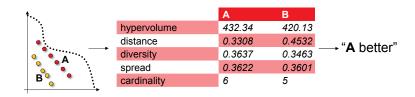


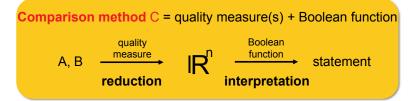
Example: Weak Refinement / No Refinement



Quality Indicator Approach

Goal: compare two Pareto set approximations A and B





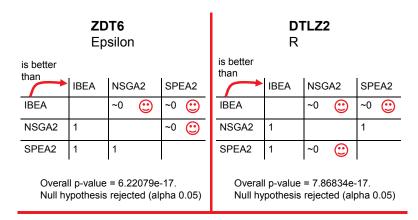
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Statistical Assessment (Kruskal Test)



Knapsack/Hypervolume: H_0 = No significance of any differences

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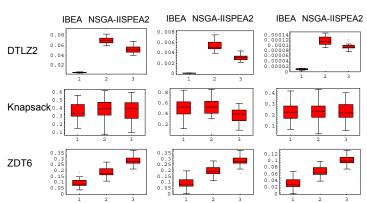
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Example: Box Plots

hypervolume

R indicator



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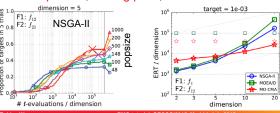
Set Quality Indicators

Open Questions:

- are there other unary indicators that are (weak) refinements?
- how to compute indicators efficiently (enough for practice)?
 - especially for >3 objective functions
- how to achieve good indicator values?

Automated Benchmarking

- State-of-the-art in single-objective optimization: Blackbox Optimization Benchmarking (BBOB) with Coco platform
- Multiobjective BBOB on the way to release
- 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 Expected Runtimes (ERT) to reach target precision
- provides data profiles, scaling plots, etc.



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Overview

The Big Picture

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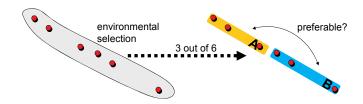
Articulating User Preferences During Search

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



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63

Incorporation of Preferences During Search

Basic Principles of Multiobjective Optimization

performance assessment

Selected Advanced Concepts

preference articulationsurrogate-based EMO

A Few Examples From Practice

algorithm design principles and concepts

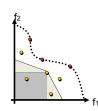
Nevertheless...

- 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]



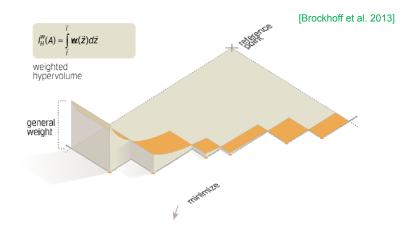
Use quality indicators, e.g.:

- 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]

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Example: Weighted Hypervolume Indicator

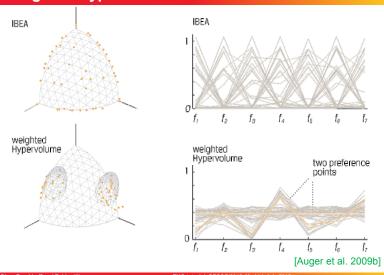


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65

Weighted Hypervolume in Practice

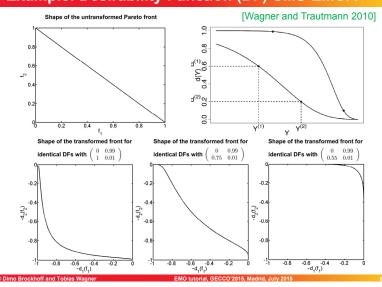


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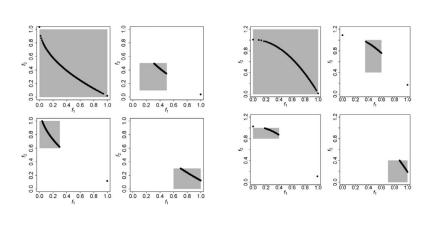
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88

Example: Desirability Function (DF)-SMS-EMOA



DF-SMS-EMOA in Practice



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Example: R2-EMOA

Concept

Integration of preferences by varying the scalarizing functions

Position of ideal point

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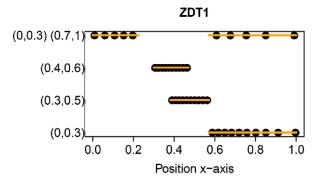
69

Example: R2-EMOA

Concept

Integration of preferences by varying the scalarizing functions

Restriction of the weight space



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70

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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A Few Examples From Practice

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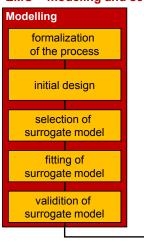
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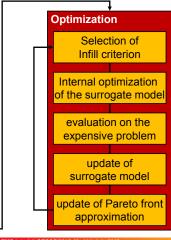
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Surrogate-Based EMO

EMO + modeling and sequential experimental design





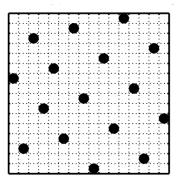
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Initial design

Latin Hypercube Sampling (LHS)

- Space-filling coverage of the decision space
- Maximum resolution for each parameter



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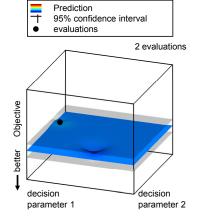
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Selection of Surrogate Model

Design and Analysis of Computer Experiments (DACE)

[Sacks et al. 1989]

- based on kriging models
- local modeling of the available evaluations
- possibility of adaptive refinement

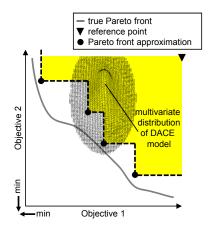


Aim

refinement of the Pareto front approximation

Selection of infill criterion

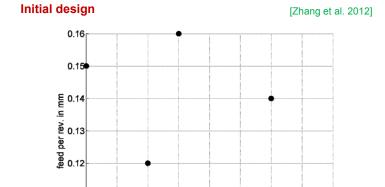
- maximization of the dominated hypervolume
- improvements through experiments in the currently nondominated area
- see [Wagner et al. 2010] for a survey and first theoretical results



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Practical application (drilling of Inconel 708)



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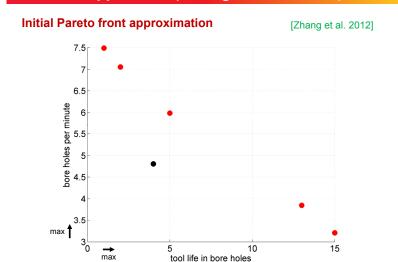
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Practical application (drilling of Inconel 708)



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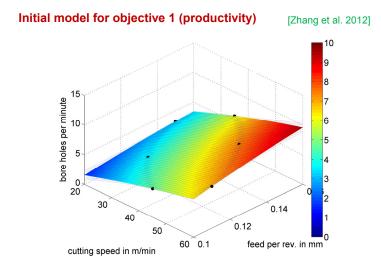
Practical application (drilling of Inconel 708)

35

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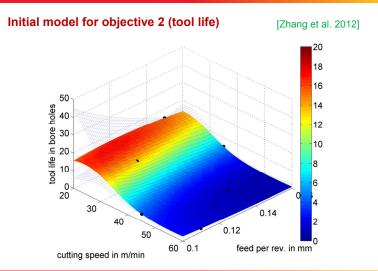
cutting speed in m/min

30



79

Practical application (drilling of Inconel 708)

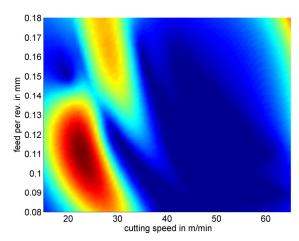


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Optimization of Infill criterion



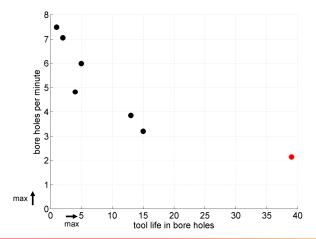
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Practical application (drilling of Inconel 708)

Updated Pareto front approximation

[Zhang et al. 2012]

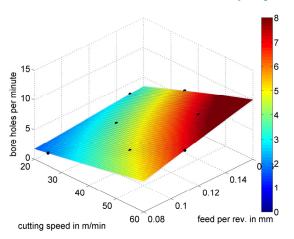


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Practical application (drilling of Inconel 708)

Updated model for objective 1 (productivity) [Zhang et al. 2012]



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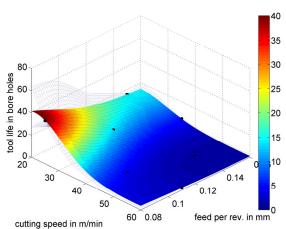
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83

Practical application (drilling of Inconel 708)

Updated model for objective 2 (tool life)

[Zhang et al. 2012]



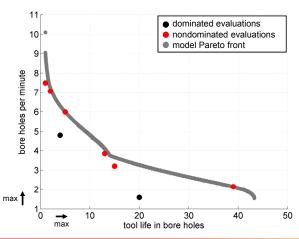
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Practical application (drilling of Inconel 708)

Final Pareto front approximation

[Zhang et al. 2012]

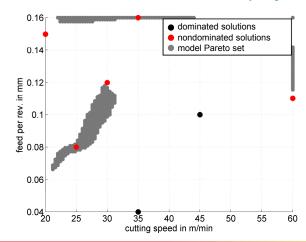


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Practical application (drilling of Inconel 708)

Final Pareto set approximation (Innovization) [Zhang et al. 2012]



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86

Overview

The Big Picture

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- algorithm design principles and concepts
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Selected Advanced Concepts

- preference articulation
- surrogate-based EMO

A Few Examples From Practice

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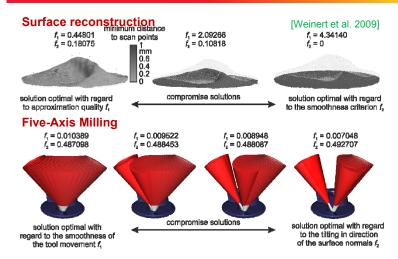
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88

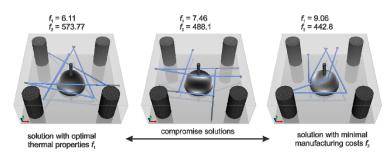
Applications of EMO



Applications of EMO

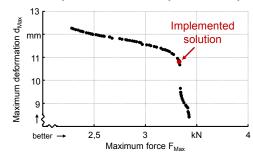
Mold Temperature Cooling Systems

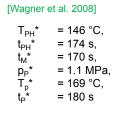
[Weinert et al. 2009]



Applications of EMO

Hot Compaction of Thermoplastic Composites

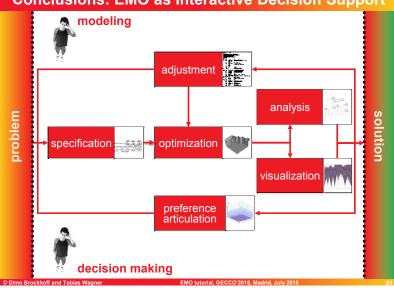






Position	T _M [°C]	F _{Max} [kN]	d _{Max} [mm]
1A	54	2.4	10.7
2B	84	2.8	9.8
3C	121	3.3	8.8
4D	147	3.3	8.3
5E	100	3.2	9.3

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 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...



Additional Slides

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?

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Instructor Biography: Dimo Brockhoff

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 he has been a junior researcher (now CR1) at INRIA Lille - Nord Europe in Villeneuve d'Ascq, France. 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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Instructor Biography: Tobias Wagner

Tobias Wagner

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After obtaining his diploma in computer science (Dipl.-Inform.) from the University of Dortmund, Germany in 2006, Tobias Wagner received his PhD in mechanical engineering (Dr.-Ing.) from the Technische Universität Dortmund, Germany in 2013. Between June 2006 and Sepember 2013 he held a scientific assistant position at the Institute of Machining Technology (ISF). Since October 2013 he works as a nonpermanent academic councilor at the ISF. His research is focused on surrogate-assisted single- and multi-objective optimization and sequential design techniques. With regard to EMO, he is particularly interested in the use of performance indicators and preference information within sequential design techniques.

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101

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EMO tutorial, GECCO'2015, Madrid, July 2015

103

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102

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