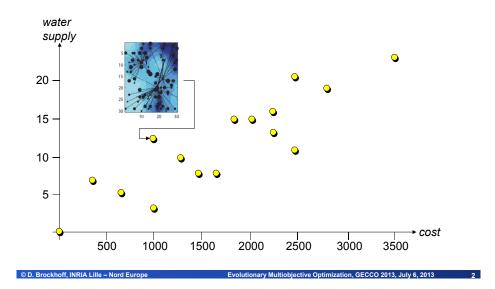
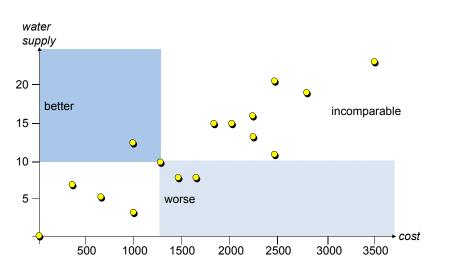


Principles of Multiple Criteria Decision

A hypothetical problem: all solutions plotted

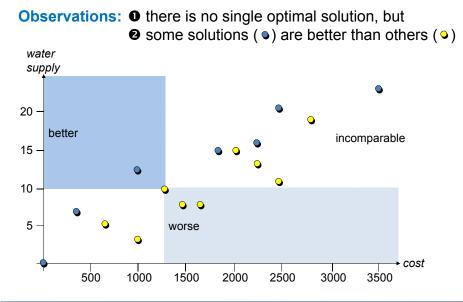


Principles of Multiple Criteria Decision



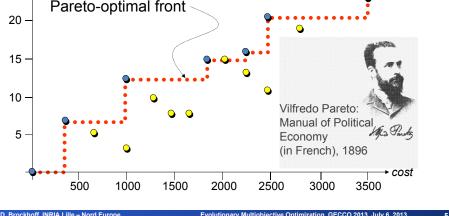
A hypothetical problem: all solutions plotted

Principles of Multiple Criteria Decision



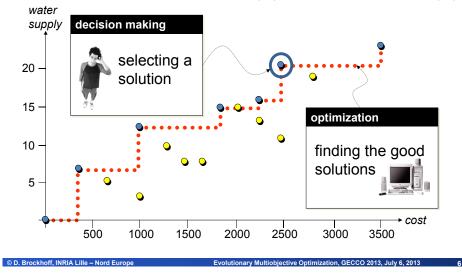
Principles of Multiple Criteria Decision

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



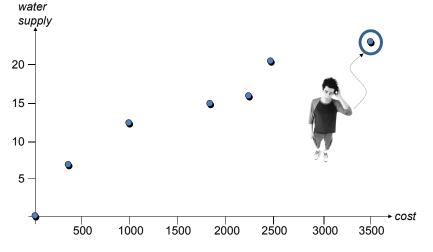
Principles of Multiple Criteria Decision

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

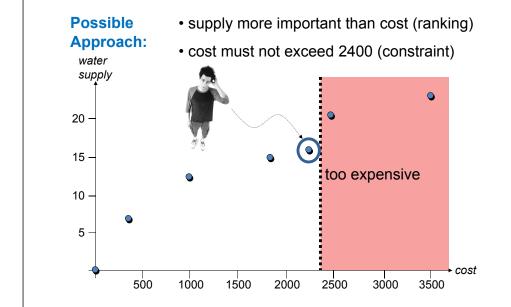


Decision Making: Selecting a Solution

• supply more important than cost (ranking)
Approach:

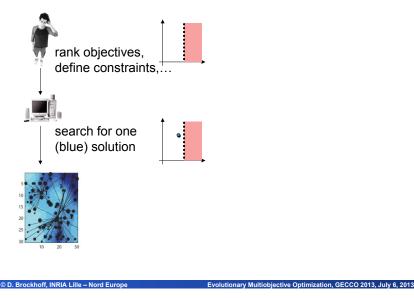


Decision Making: Selecting a Solution



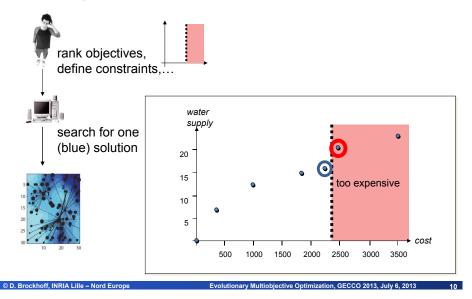
When to Make the Decision

Before Optimization:



When to Make the Decision

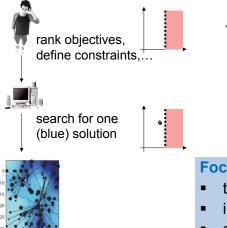
Before Optimization:



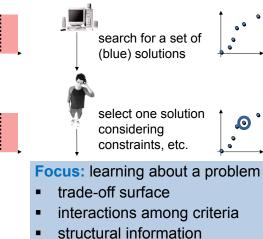
When to Make the DecisionSefore Optimization: $\widehat{\mathsf{optimization}}$ $\widehat{\mathsf{optimization}}$

When to Make the Decision

Before Optimization:



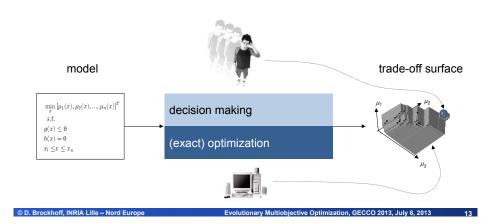
After Optimization:



Multiple Criteria Decision Making (MCDM)

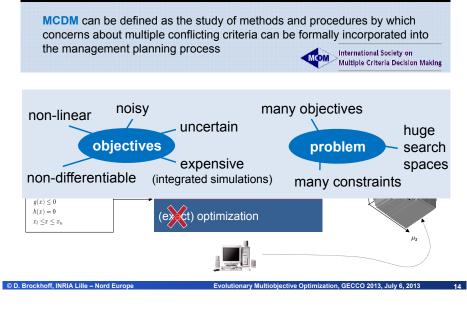
Definition: MCDM

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



Multiple Criteria Decision Making (MCDM)

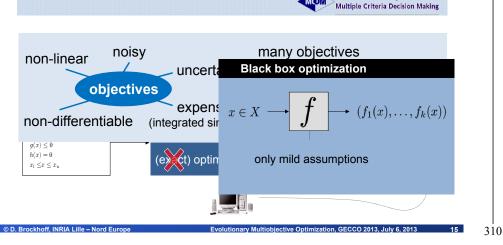
Definition: MCDM



Multiple Criteria Decision Making (MCDM)

Definition: MCDM

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

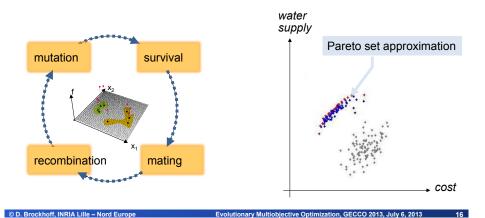


Evolutionary Multiobjective Optimization

Definition: EMO

EMO = evolutionary algorithms / randomized search algorithms

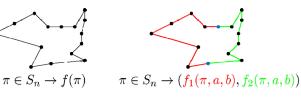
- applied to multiple criteria decision making (in general)
- used to approximate the Pareto-optimal set (mainly)



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], theoretical (runtime) analyses [Brockhoff et al. 2009]

by decomposition of the single objective

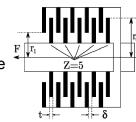
TSP [Knowles et al. 2001], minimum spanning trees [Neumann and Wegener 2006], protein structure prediction [Handl et al. 2008a], theoretical (runtime) analyses [Handl et al. 2008b]

Innovization

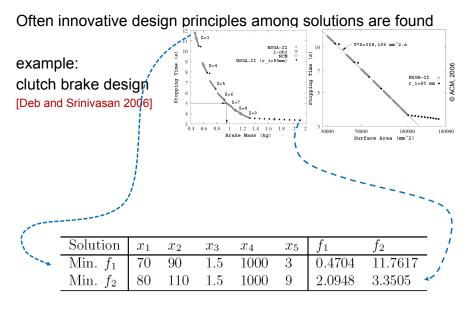
Often innovative design principles among solutions are found

example: clutch brake design [Deb and Srinivasan 2006]

min. mass + stopping time



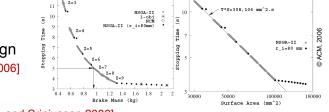
Innovization



Innovization

Often innovative design principles among solutions are found

example: clutch brake design [Deb and Srinivasan 2006]



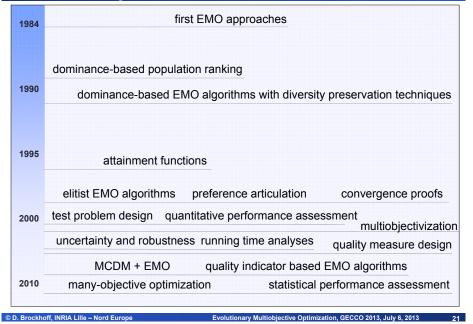
Innovization [Deb and Srinivasan 2006]

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

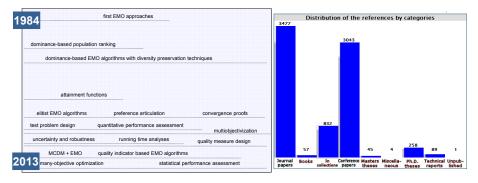
Other examples:

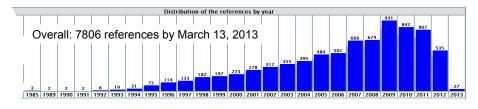
- SOM for supersonic wing design [Obayashi and Sasaki 2003]
- biclustering for processor design and KP [Ulrich et al. 2007]

The History of EMO At A Glance



The History of EMO At A Glance





The EMO Community

The EMO conference series:



Many further activities:

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

Overview

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The Big Picture

Basic Principles of Multiobjective Optimization

- algorithm design principles and concepts
- performance assessment

Selected Advanced Concepts

- indicator-based EMO
- preference articulation

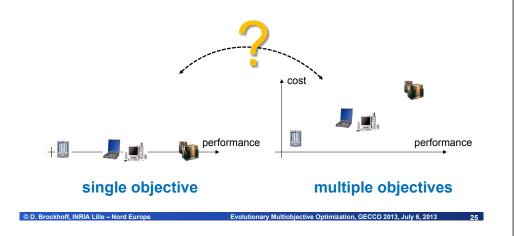
A Few Examples From Practice

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ary Multiobiective Optimization, GECCO 2013, July 6, 2013

Starting Point

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

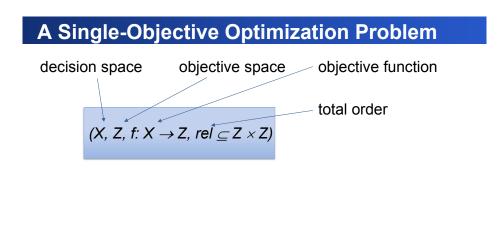


A General (Multiobjective) Optimization

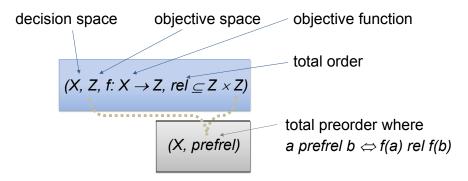
A multiobjective optimi	zation problem: $(X,Z,\mathbf{f},\mathbf{g},\leq)$	
X	search / parameter / decision space	
$Z = \mathbb{R}^n$	objective space	
$\mathbf{f} = (f_1, \dots, f_n)$	vector-valued objective function with	
	$f_i: X \mapsto \mathbb{R}$	
$\mathbf{g} = (g_1, \ldots, g_m)$	vector-valued constraint function with	
	$g_i: X \mapsto \mathbb{R}$	
$\leq \subseteq Z \times Z$	binary relation on objective space	
Goal: find decision vector(s) $\mathbf{a} \in X$ such that		

Goal: find decision vector(s) $\mathbf{a} \in X$ such that

- for all $1 \leq i \leq m : g_i(\mathbf{a}) \leq 0$ and
- **2** for all $\mathbf{b} \in X : \mathbf{f}(\mathbf{b}) \leq \mathbf{f}(\mathbf{a}) \Rightarrow \mathbf{f}(\mathbf{a}) \leq \mathbf{f}(\mathbf{b})$



A Single-Objective Optimization Problem



A Single-Objective Optimization Problem

Example: Leading Ones Problem

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

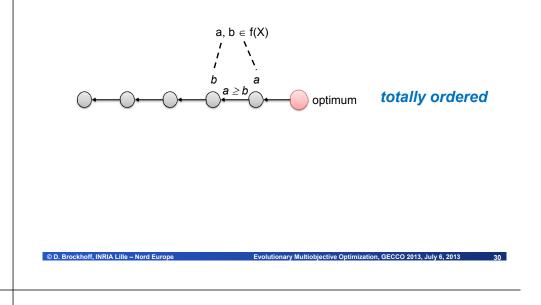
$$(X, prefrel)$$

$$(\{0,1\}^n, \{0,1,2,...,n\}, f_{LO}, \geq) \quad \text{where } f_{LO}(a) = \sum_i (\prod_{j \leq i} a_j)$$

Evolutionary Multiobiective Optimization, GECCO 2013, July 6, 2013

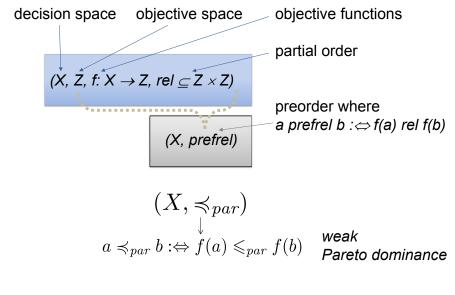
Simple Graphical Representation

Example: ≥ (total order)



Preference Relations

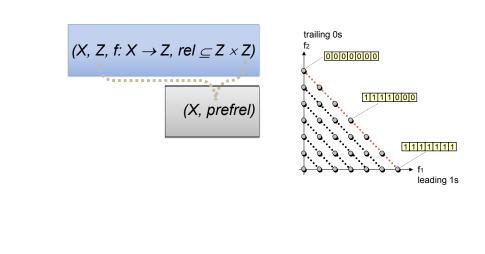
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Evolutionary Multiobjective Optimization, GECCO 20

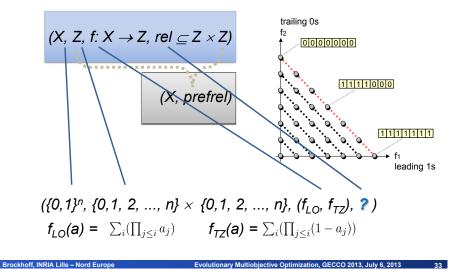
A Multiobjective Optimization Problem

Example: Leading Ones Trailing Zeros Problem

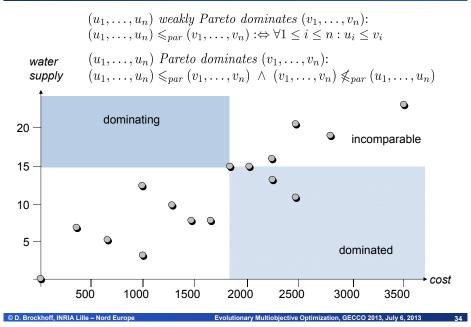


A Multiobjective Optimization Problem

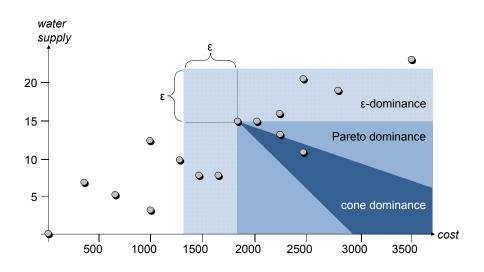
Example: Leading Ones Trailing Zeros Problem



Pareto Dominance

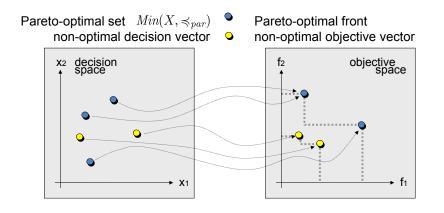


Different Notions of Dominance

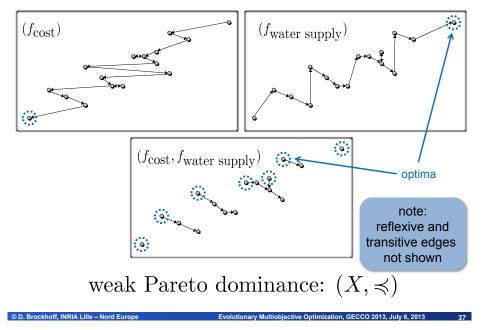


The Pareto-optimal Set

The minimal set of a preordered set (Y, \leq) is defined as $Min(Y, \leq) := \{a \in Y \mid \forall b \in Y : b \leq a \Rightarrow a \leq b\}$



Visualizing Preference Relations

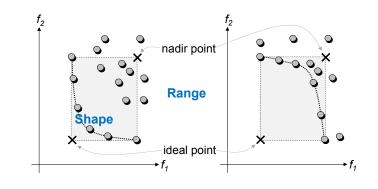


Remark: Properties of the Pareto Set

Computational complexity:

multiobjective variants can become NP- and #P-complete

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



Approaches To Multiobjective Optimization

A multiobjective problem is as such underspecified ...because not any Pareto-optimum is equally suited!

Additional preferences are needed to tackle the problem:

Solution-Oriented Problem Transformation:

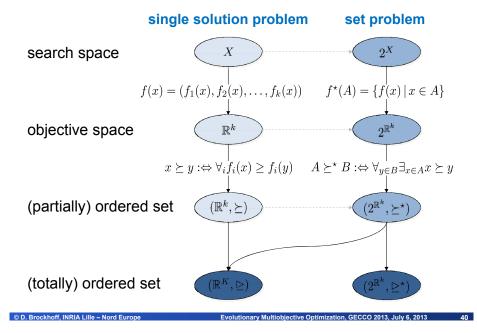
Induce a total order on the decision space, e.g., by aggregation.

Set-Oriented Problem Transformation:

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

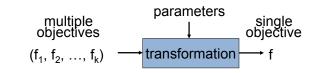
Preferences are needed in any case, but the latter are weaker!

Problem Transformations and Set Problems



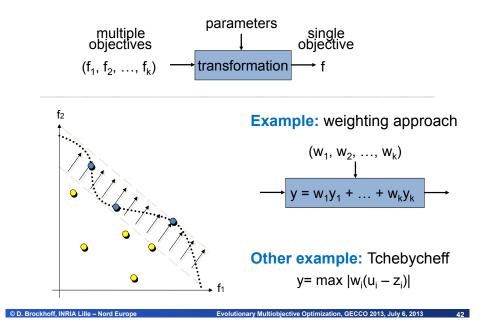
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Solution-Oriented Problem Transformations



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

Aggregation-Based Approaches



Set-Oriented Problem Transformations

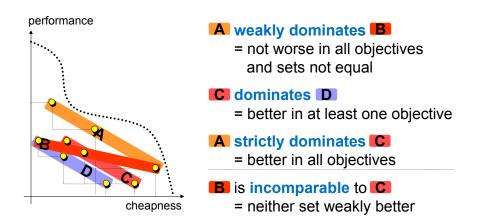
For a multiobjective optimization problem $(X, Z, \mathbf{f}, \mathbf{g}, \leq)$, the associated *set problem* is given by $(\Psi, \Omega, F, \mathbf{G}, \leq)$ where

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

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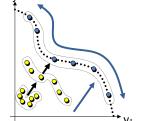
Pareto Set Approximations

Pareto set approximation (algorithm outcome) = set of (usually incomparable) solutions



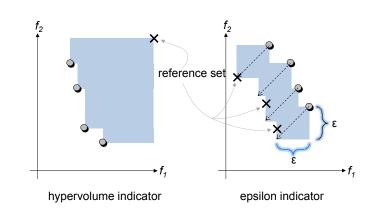
What Is the Optimization Goal (Total Order)?

- Find all Pareto-optimal solutions?
 - Impossible in continuous search spaces
 - How should the decision maker handle 10000 solutions?
- Find a representative subset of the Pareto set?
 - Many problems are NP-hard
 - ▶ What does representative actually mean?
- Find a good approximation of the Pareto set?
 - What is a good approximation?
 - How to formalize intuitive understanding:
 - close to the Pareto frontwell distributed



Quality of Pareto Set Approximations

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



General Remarks on Problem

Idea:

Transform a preorder into a total preorder

Methods:

- Define single-objective function based on the multiple criteria (shown on the previous slides)
- Define any total preorder using a relation (not discussed before)

Question:

Is any total preorder ok resp. are there any requirements concerning the resulting preference relation?

 \Rightarrow Underlying dominance relation *rel* should be reflected

Refinements and Weak Refinements

$$\mathbf{0} \stackrel{\text{ref}}{\prec} \mathbf{refines}$$
 a preference relation \prec iff

$$A \preccurlyeq B \land B \preccurlyeq A \Rightarrow A \preccurlyeq^{ref} B \land B \preccurlyeq^{ref} A$$
 (better \Rightarrow better

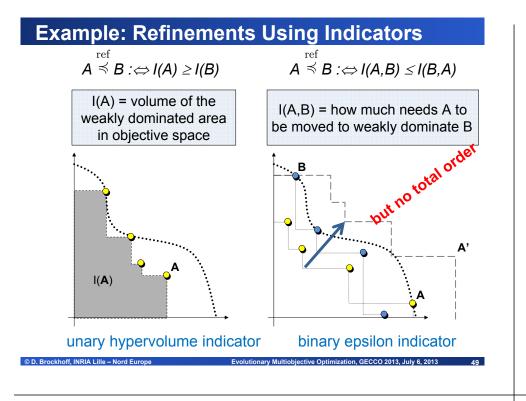
- \Rightarrow fulfills requirement
- **2** $\stackrel{\text{ref}}{\prec}$ weakly refines a preference relation \prec iff

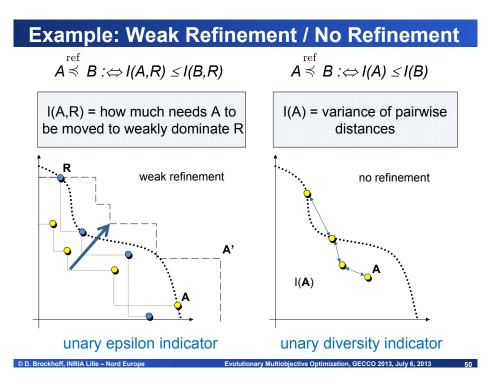
 $A \preccurlyeq B \land B \preccurlyeq A \Rightarrow A \stackrel{\text{ref}}{\preccurlyeq} B$ (better \Rightarrow weakly better)

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

...sought are total refinements...

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Overview

The Big Picture

Basic Principles of Multiobjective Optimization

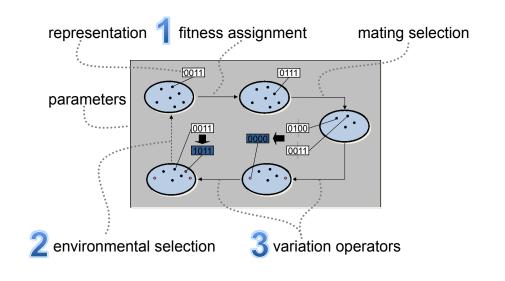
- algorithm design principles and concepts
- performance assessment

Selected Advanced Concepts

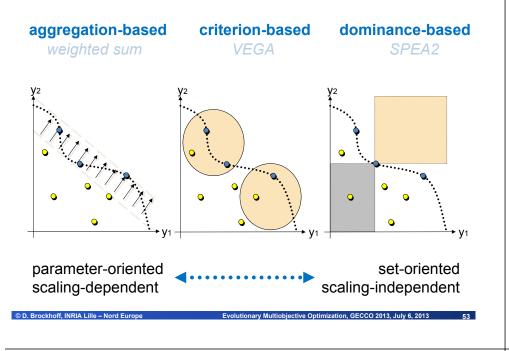
- indicator-based EMO
- preference articulation

A Few Examples From Practice

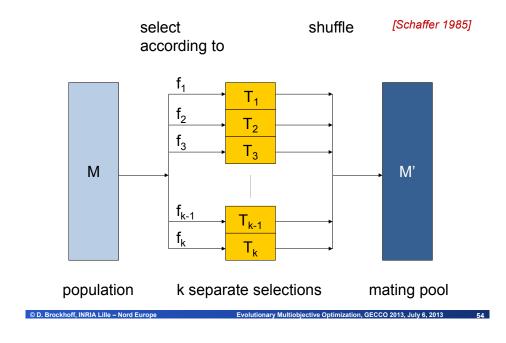
Algorithm Design: Particular Aspects



Fitness Assignment: Principal Approaches



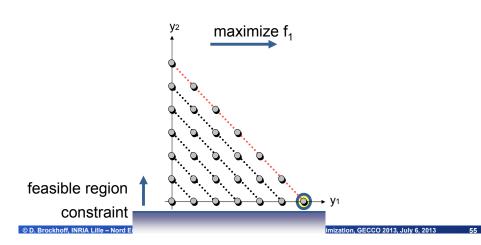
Criterion-Based Selection: VEGA



Aggregation-Based: Multistart Constraint Method

Underlying concept:

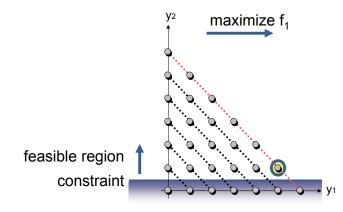
- Convert all objectives except of one into constraints
- Adaptively vary constraints



Aggregation-Based: Multistart Constraint Method

Underlying concept:

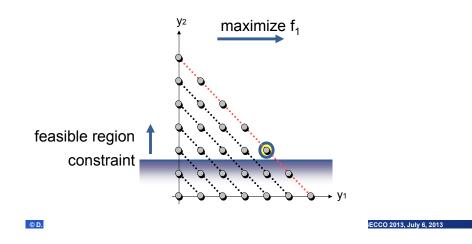
- Convert all objectives except of one into constraints
- Adaptively vary constraints



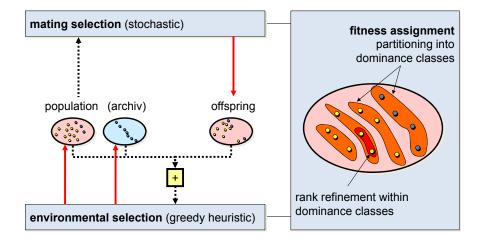
Aggregation-Based: Multistart Constraint Method

Underlying concept:

- Convert all objectives except of one into constraints
- Adaptively vary constraints



General Scheme of Dominance-Based EMO



Note: good in terms of set quality = good in terms of search?

Ranking of the Population Using Dominance

- ... goes back to a proposal by David Goldberg in 1989.
- \ldots is based on pairwise comparisons of the individuals only.
- dominance rank: by how many individuals is an individual dominated?
 MOGA, NPGA
- dominance count: how many individuals does an individual dominate? SPEA, SPEA2
- dominance depth: at which front is an individual located? NSGA, NSGA-II

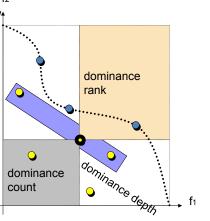
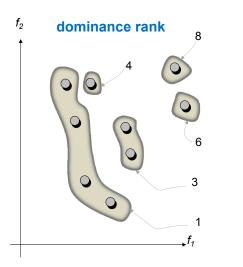
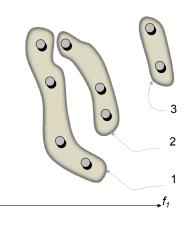


Illustration of Dominance-based Partitioning

 f_2



dominance depth

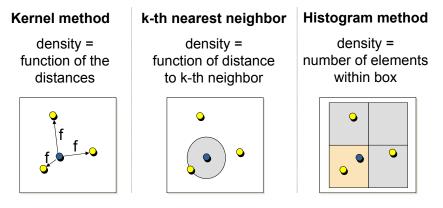


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Refinement of Dominance Rankings

Goal: rank incomparable solutions within a dominance class

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

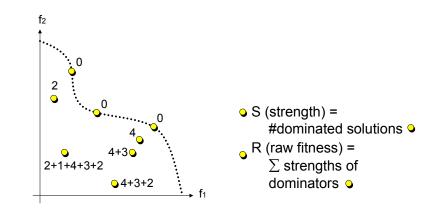


Quality indicator (good for set quality): soon...

Example: SPEA2 Dominance Ranking

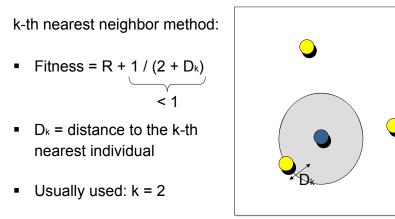
Basic idea: the less dominated, the fitter...

Principle: first assign each solution a weight (strength), then add up weights of dominating solutions



Example: SPEA2 Diversity Preservation

Density Estimation



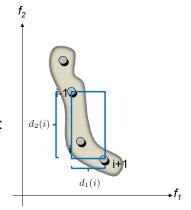
Example: NSGA-II Diversity Preservation

Density Estimation

crowding distance:

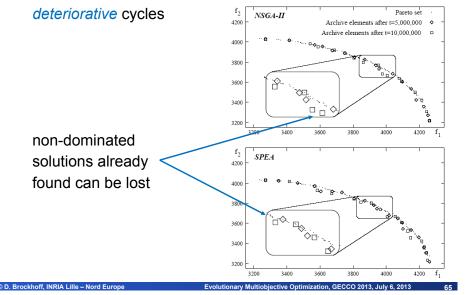
- sort solutions wrt. each objective
- crowding distance to neighbors:

$$d(i) - \sum_{\text{obj. }m} |f_m(i-1) - f_m(i+1)|$$



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SPEA2 and NSGA-II: Cycles in Optimization

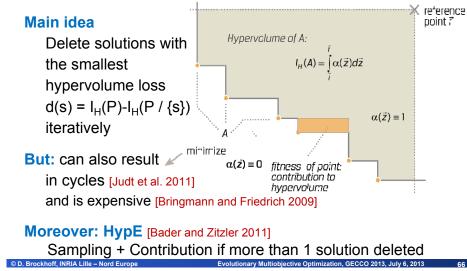


Selection in SPEA2 and NSGA-II can result in

Hypervolume-Based Selection

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

use hypervolume indicator to guide the search: refinement!

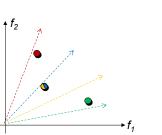


Decomposition-Based Selection: MOEA/D

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

Ideas:

- Optimize N scalarizing functions in parallel
- Use only best solutions of "neighbored scalarizing function" for mating
- keep the best solutions for each scalarizing function
- use external archive for nondominated solutions
- several improved versions recently



Scalarizing Approaches

Open Questions:

- how to choose "the right" scalarization even if the direction in objective space is given by the DM?
- combinations/adaptation of scalarization functions
- independent optimization vs. cooperation between single-objective optimization

Variation in EMO

- At first sight not different from single-objective optimization
- Most algorithm design effort on selection until now
- But: convergence to a set ≠ convergence to a point

Open Question:

how to achieve fast convergence to a set?

Related work:

- multiobjective CMA-ES [lgel et al. 2007] [Voß et al. 2010]
- set-based variation [Bader et al. 2009]
- set-based fitness landscapes [Verel et al. 2011]

Overview

The Big Picture

Basic Principles of Multiobjective Optimization

- algorithm design principles and concepts
- performance assessment

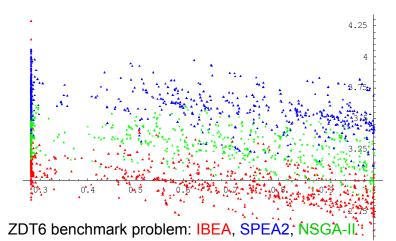
Selected Advanced Concepts

- indicator-based EMO
- preference articulation

A Few Examples From Practice

Once Upon a Time...

... multiobjective EAs were mainly compared visually:



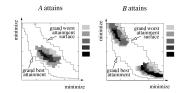
Two Approaches for Empirical Studies

Attainment function approach:

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

Quality indicator approach:

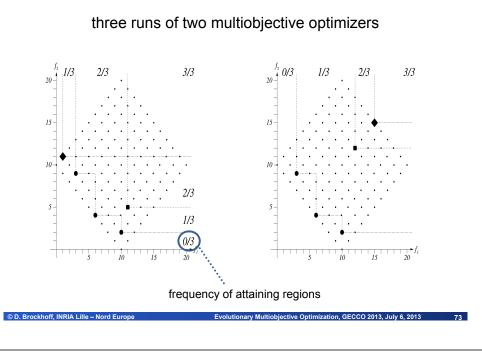
- First, reduces each approximation set to a single value of quality
- Applies statistical tests to the samples of quality values



Indicator	A	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

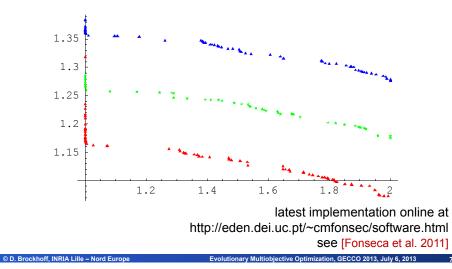
see e.g. [Zitzler et al. 2003]

Empirical Attainment Functions



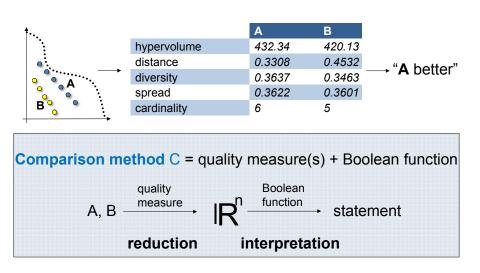
Attainment Plots

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

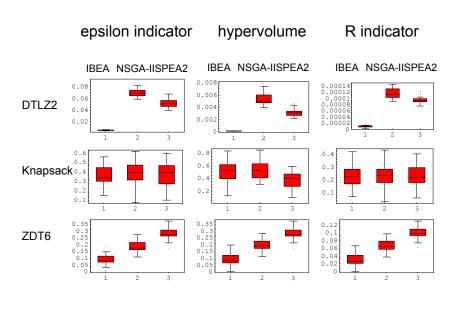


Quality Indicator Approach

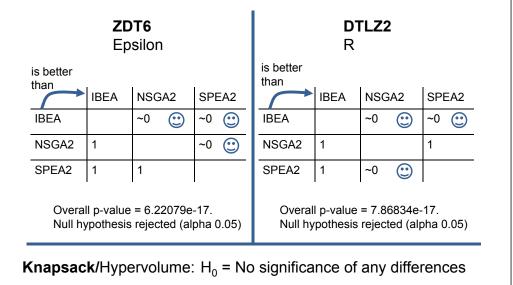
Goal: compare two Pareto set approximations A and B



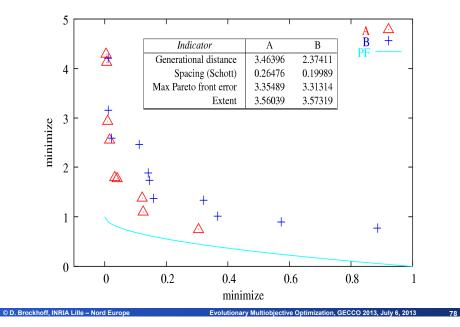
Example: Box Plots



Statistical Assessment (Kruskal Test)



Problems With Non-Compliant Indicators



What Are Good Set Quality Measures?

There are three aspects [Zitzler et al. 2000]

comparing oriertent optimization techniques experimentany aways involves the notion of performance. In the case of multiobjective optimization, the definition of quality is substantially more complex than for single-objectives optimization problems, because the optimization goal itself consists of multiple objectives:

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

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

Wrong! [Zitzler et al. 2003]

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

Set Quality Indicators

Open Questions:

- how to design a good benchmark suite?
- are there other unary indicators that are (weak) refinements?
- how to achieve good indicator values?

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Overview

The Big Picture

Basic Principles of Multiobjective Optimization

- algorithm design principles and concepts
- performance assessment

Selected Advanced Concepts

- indicator-based EMO
- preference articulation

A Few Examples From Practice

Indicator-Based EMO: Optimization Goal

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

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

Multiobjective Indicator Single-objective Problem

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

[Friedrich et al. 2011]:

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

OPT	$1 + \frac{\log(\min\{A/a, B/b\})}{n}$
НҮР	$1 + \frac{\sqrt{A/a} + \sqrt{B/b}}{n-4}$
$\log HYP$	$1 + \frac{\sqrt{\log(A/a)\log(B/b)}}{n-2}$

(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]
- how to do indicator-based subset selection quickly?
- 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

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A Few Examples From Practice

Articulating User Preferences During Search

[Zitzler 1999]

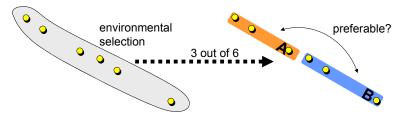
What we thought: EMO is preference-less

is made by the DM.

given by the DW. 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

Decision making during search: The DM can articulate preferences during

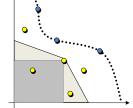
What we learnt: EMO just uses weaker preference information



Incorporation of Preferences During Search

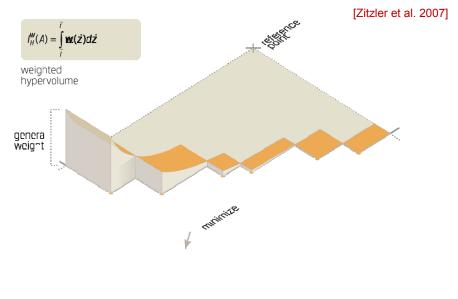
Nevertheless...

- the more (known) preferences incorporated the better
- in particular if search space is too large [Branke 2008], [Rachmawati and Srinivasan 2006], [Coello Coello 2000]
- Refine/modify dominance relation, e.g.:
 - using goals, priorities, constraints [Fonseca and Fleming 1998a,b]
 - using different types of cones [Branke and Deb 2004]



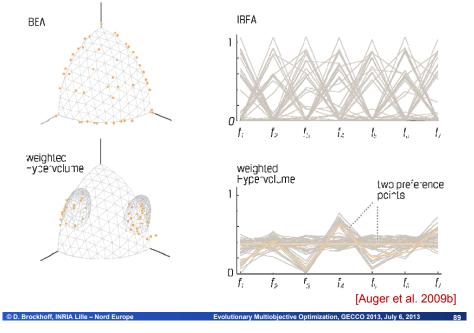
- **2** Use quality indicators, e.g.:
 - based on reference points and directions [Deb and Sundar 2006, Deb and Kumar 2007]
 - based on binary quality indicators [Zitzler and Künzli 2004]
 - based on the hypervolume indicator (now) [Zitzler et al. 2007]

Example: Weighted Hypervolume Indicator



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Weighted Hypervolume in Practice



Overview

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The Big Picture

Basic Principles of Multiobjective Optimization

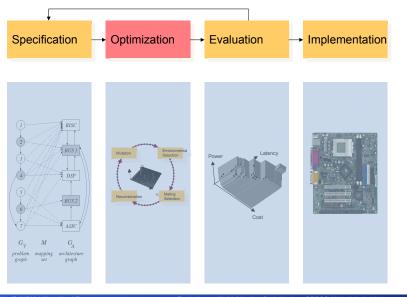
- algorithm design principles and concepts
- performance assessment

Selected Advanced Concepts

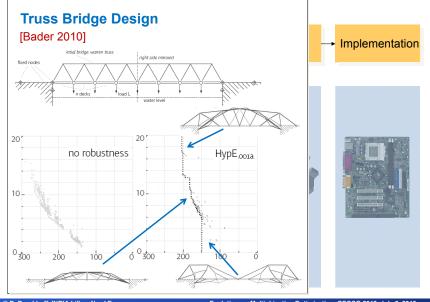
- indicator-based EMO
- preference articulation

A Few Examples From Practice

Application: Design Space Exploration

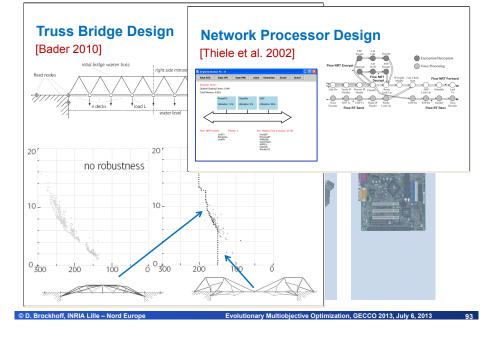


Application: Design Space Exploration

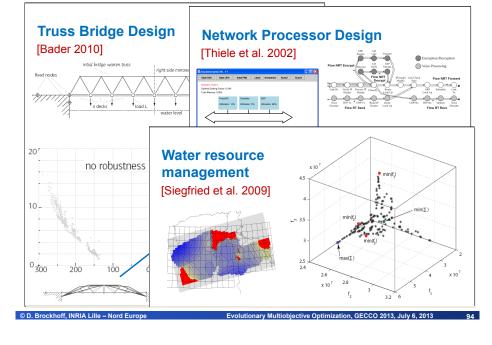


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Application: Design Space Exploration



Application: Design Space Exploration

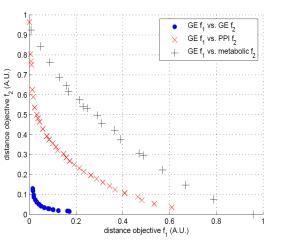


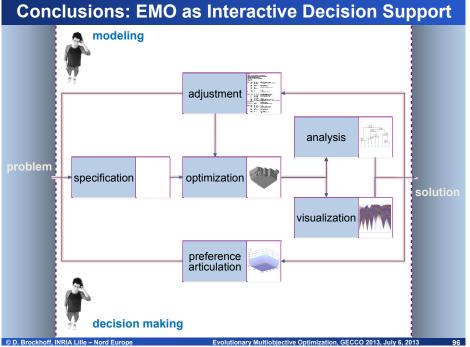
Application: Trade-Off Analysis

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

Find group of genes wrt different data types:

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





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The EMO Community

Links:

- EMO mailing list: http://w3.ualg.pt/lists/emo-list/
- EMO bibliography: http://www.lania.mx/~ccoello/EMOO/
- EMO conference series: http://www.shef.ac.uk/emo2013/

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 [many open questions!]

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and more...

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



Additional Slides

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 (CR2) at INRIA Lille - Nord Europe in Villeneuve d'Ascq, France . His research interests are focused on evolutionary multiobjective optimization (EMO), in particular on many-objective optimization, benchmarking, and theoretical aspects of indicator-based search.

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