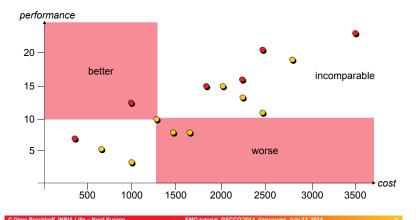
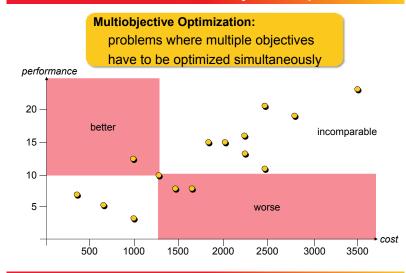


A Brief Introduction to Multiobjective Optimization

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

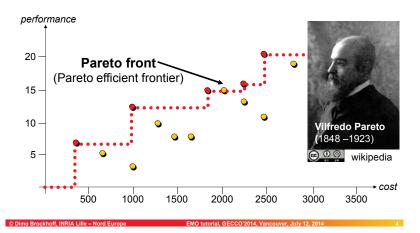


A Brief Introduction to Multiobjective Optimization



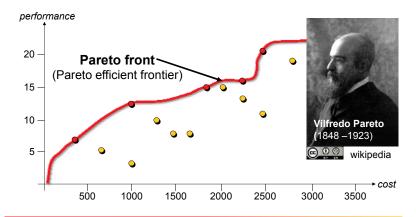
A Brief Introduction to Multiobjective Optimization

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



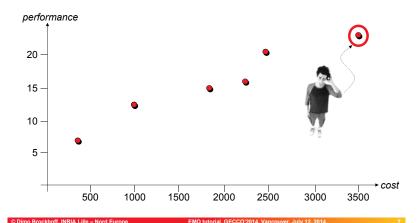
A Brief Introduction to Multiobjective Optimization

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



Selecting a Solution: Examples

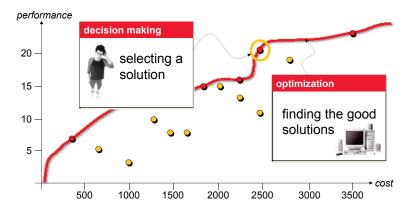
Possible • ranking: performance more important than cost Approaches:



A Brief Introduction to Multiobjective Optimization

Observations:
● there is no single optimal solution, but

● some solutions (•) are better than others (•)

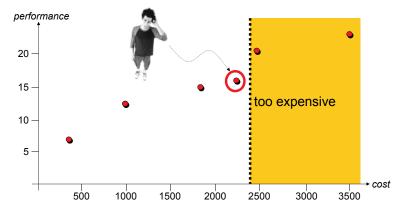


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Selecting a Solution: Examples

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

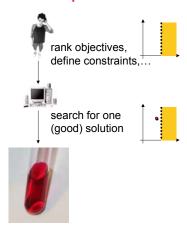


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When to Make the Decision

Before Optimization:



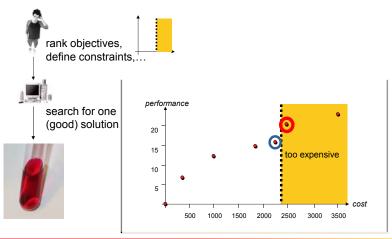
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After Optimization:

When to Make the Decision

Before Optimization:



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When to Make the Decision

Before Optimization:



_

search for a set of (good) solutions select one solution considering constraints, etc.



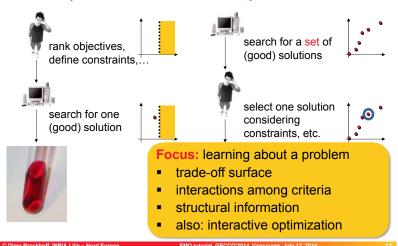
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When to Make the Decision

Before Optimization:

After Optimization:



Two Communities...





- beginning in 1950s/1960s
- bi-annual conferences since 1975
- background in economics, math, management science
- both optimization and decision making
- quite young field (first papers in mid 1980s)
- bi-annual conference since 2001
- background evolutionary computation (applied math, computer science, engineering, ...)
- focus on optimization algorithms

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...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

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4.4

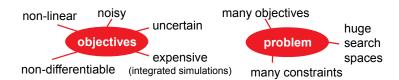
One of the Main Differences

Blackbox optimization



only mild assumptions

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



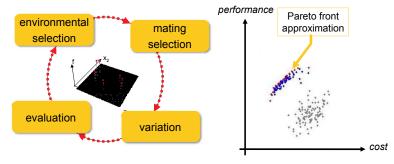
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The Other Main Difference

Evolutionary Multiobjective Optimization

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



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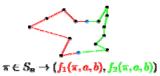
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Multiobjectivization

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]

Innovization

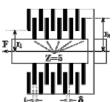
Often innovative design principles among solutions are found

example:

clutch brake design

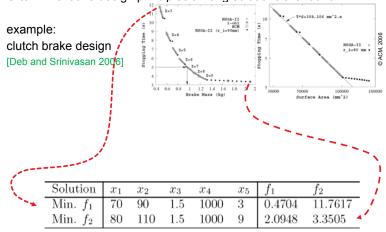
[Deb and Srinivasan 2006]

min. mass + stopping time



Innovization

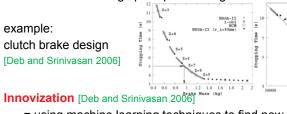
Often innovative design principles among solutions are found



Innovization

Often innovative design principles among solutions are found

example: clutch brake design [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:

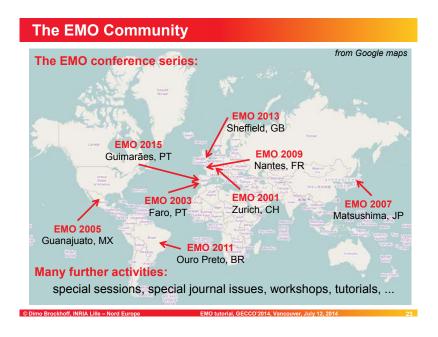
- SOM for supersonic wing design [Obayashi and Sasaki 2003]
- biclustering for processor design and KP [Ulrich et al. 2007]

The History of EMO At A Glance first EMO approaches 1984 dominance-based population ranking dominance-based EMO algorithms with diversity preservation techniques 1995 attainment functions elitist EMO algorithms preference articulation convergence proofs test problem design quantitative performance assessment multiobjectivization uncertainty and robustness running time analyses quality measure design MCDM + EMO quality indicator based EMO algorithms

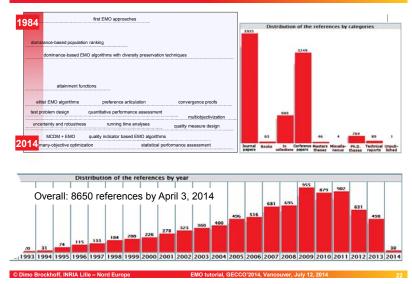
statistical performance assessment

2010

many-objective optimization



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

- indicator-based EMO
- preference articulation

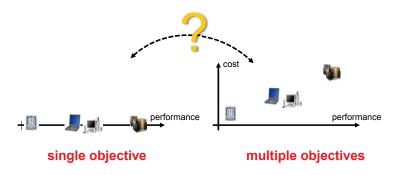
A Few Examples From Practice

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Starting Point

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

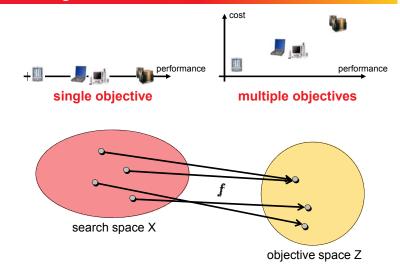


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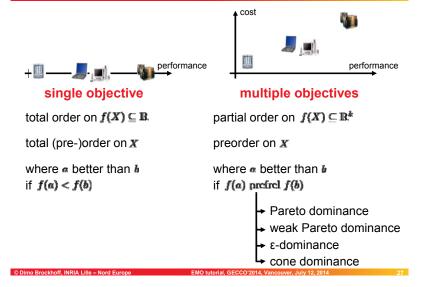
25

Starting Point

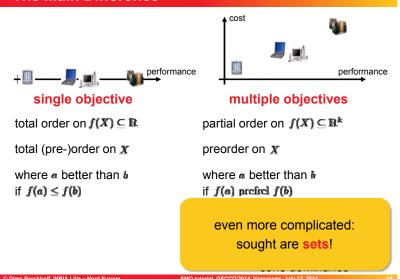


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The Main Difference

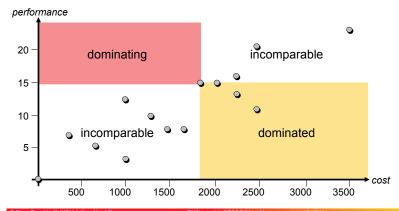


The Main Difference



Most Common Example: Pareto Dominance

u weakly Pareto dominates v ($u \leqslant_{par} v$): $\forall 1 \le i \le k : f_i(u) \le f_i(v)$ $u \text{ Pareto dominates } v \text{ } (u <_{par} v) : \quad u \leqslant_{par} v \ \land \ v \not\leqslant_{par} u$



500 1000

performance

20

15

10 -

5 -

2500

ε-dominance

Pareto dominance

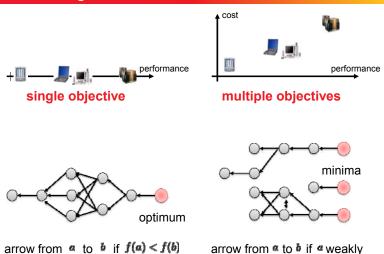
cone dominance

3500

3000

00

Visualizing Preference Relations



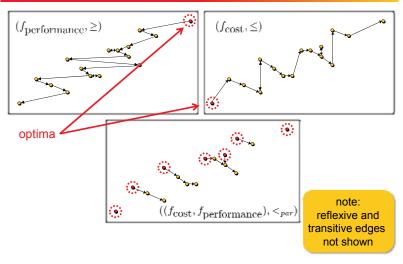
dominates 6

Visualizing Preference Relations

1500

2000

Different Notions of Dominance



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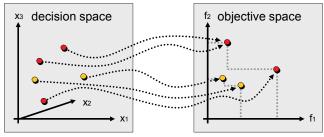
Pareto-optimal Set and Pareto(-optimal) Front

The minimal set of a preordered set (Y, \leq) is defined as

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

Pareto-optimal set $Min(X, \leqslant_{par})$ non-optimal decision vector

Pareto-optimal frontnon-optimal objective vector



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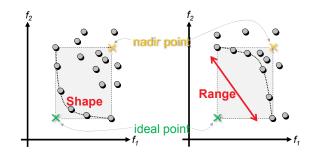
33

Other Related Definitions

Computational complexity for discrete problems:

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])



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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:

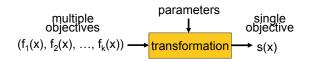
Classical approach: Induce a total order on the decision space, e.g., by aggregation

Set-Oriented Problem Transformation:

Recent view on EMO: First transform problem into a set problem and then define an objective function on sets [Zitzler et al. 2010]

Preferences are needed in bases cases, but the latter are weaker!

Solution-Oriented Problem Transformations



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

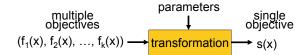
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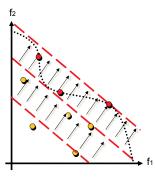
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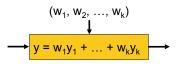
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Solution-Oriented Problem Transformations





Example 1: weighted sum approach

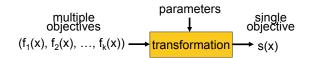


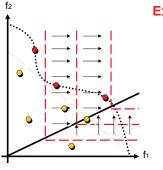
Disadvantage: not all Paretooptimal solutions can be found if the front is not convex

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Solution-Oriented Problem Transformations





Example 2: weighted Tchebycheff

$$(\lambda_{1}, \lambda_{2}, ..., \lambda_{k})$$

$$\downarrow$$

$$y = \max_{i} |\lambda_{i}(u_{i} - z_{i})|$$

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

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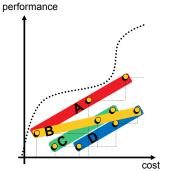
Set-Oriented Problem Transformations

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

- Ψ = 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 f to sets, i.e.,
 F(Λ) := {f(a) : a ∈ Λ} for Λ ∈ Ψ,
- $\mathbf{G} = (G_1, \dots, G_m)$ 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 $A \geq B : \Leftrightarrow \forall \mathbf{b} \in B \exists \mathbf{a} \in A : \mathbf{a} \leq \mathbf{b}$.

Pareto Set Approximations

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



- weakly dominates B
 - = not worse in all objectives and sets not equal
- **c** dominates **D** = better in at least one objective
- = better in all objectives
- B is incomparable to C = neither set weakly better

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What Is the Optimization Goal of a Set Problem?

- 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 front
 - well distributed

Most common: use of quality indicators

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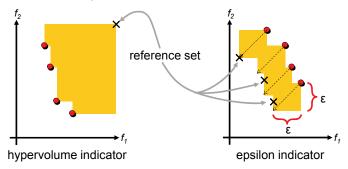
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41

Quality of Pareto Set Approximations

A (unary) quality indicator I is a function $I: \Psi = 2^X \mapsto \mathbb{R}$ that assigns a Pareto set approximation a real value.

well-known examples:

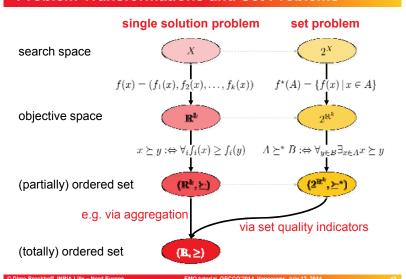


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40

Problem Transformations and Set Problems



General Remarks on Problem Transformations

Main Goal:

Transform a preorder into a total preorder on X

Methods:

- Define single-objective function based on the multiple criteria (e.g. via aggregation)
- Define total preorder on sets by using a quality indicator (e.g. via hypervolume indicator)

Question:

Is any total preorder okay or are there any requirements concerning the resulting preference relation?

⇒ Underlying dominance relation should be reflected!

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Refinements and Weak Refinements

● ▼ refines a preference relation ▼ iff

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

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

$$A \preccurlyeq B \land B \nleq A \Rightarrow A \stackrel{\text{ref}}{\preccurlyeq} B$$

(better ⇒ weakly better)

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

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

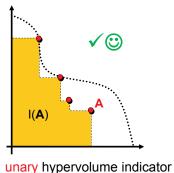
Example: Refinements Using Indicators

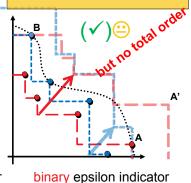
$$A \stackrel{\mathrm{ref}}{\leq} B : \Leftrightarrow I(A) \geq I(B)$$

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

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





The Big Picture

Overview

Basic Principles of Multiobjective Optimization

performance assessment

Selected Advanced Concepts indicator-based EMO preference articulation

A Few Examples From Practice

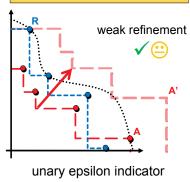
algorithm design principles and concepts

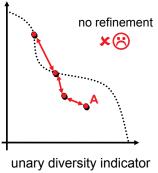
Example: Weak Refinement / No Refinement

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

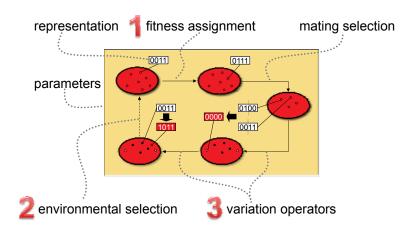
 $A \preceq B : \Leftrightarrow I(A) \leq I(B)$

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





Algorithm Design: Particular Aspects



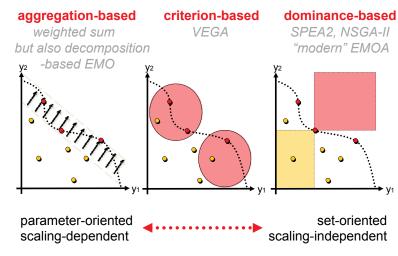
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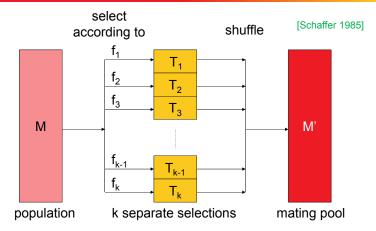
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Fitness Assignment: Principal Approaches



Criterion-Based Selection: VEGA



Drawback: only allows to find extremes of the Pareto front

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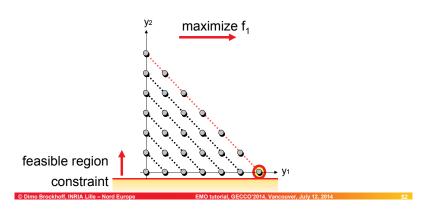
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51

Aggregation-Based: Multistart Constraint Method

Underlying concept:

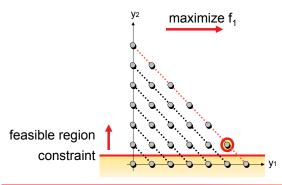
- Convert all objectives except of one into constraints
- Adaptively vary constraints



Aggregation-Based: Multistart Constraint Method

Underlying concept:

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

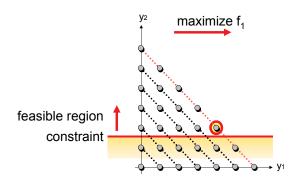


Underlying concept:

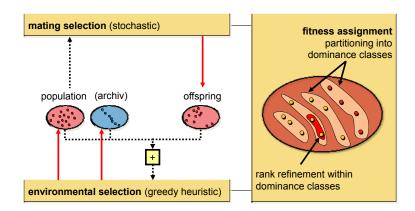
Convert all objectives except of one into constraints

Aggregation-Based: Multistart Constraint Method

Adaptively vary constraints



General Scheme of Most Dominance-Based EMO



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

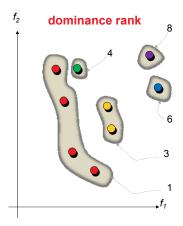
Ranking of the Population Using Dominance

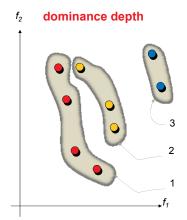
- ... goes back to a proposal by David Goldberg in 1989.
- ... is based on pairwise comparisons of the individuals only.
- dominance rank: by how many individuals is an individual dominated? MOGA, NPGA
- dominance count: how many individuals does an individual dominate? SPEA, SPEA2

dominance depth: at which front is an individual located? NSGA, NSGA-II, most of the recently proposed algorithms

dominance dominance count

Illustration of Dominance-based Partitioning





Refinement of Dominance Rankings

Goal: rank incomparable solutions within a dominance class

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

Kernel method density = function of the distances



density = function of distance to k-th neighbor



k-th nearest neighbor Histogram method

density = number of elements within box



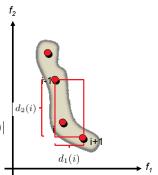
Quality indicator (good for set quality): soon...

Example: NSGA-II Diversity Preservation

Density Estimation

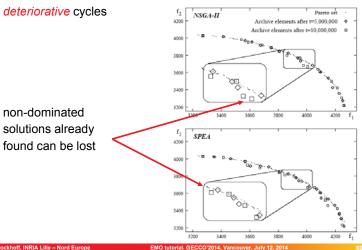
crowding distance:

- sort solutions wrt. each objective
- crowding distance to neighbors: $d(i) - \sum_{\text{obj. } m} |f_m(i-1) - f_m(i+1)|$



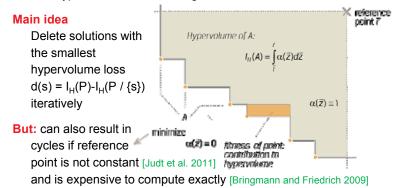
SPEA2 and NSGA-II: Cycles in Optimization

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!



Moreover: HypE [Bader and Zitzler 2011]

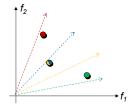
Sampling + Contribution if more than 1 solution deleted

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 "neighbored scalarizing function" for mating
- keep the best solutions for each scalarizing function
- eventually replace neighbors
- 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 singleobjective 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 [Igel et al. 2007] [Voß et al. 2010]
- set-based variation [Bader et al. 2009]
- set-based fitness landscapes [Verel et al. 2011]

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A Few Examples From Practice

Two Approaches for Empirical Studies

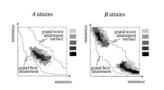
Attainment function approach:

Applies statistical tests directly to the samples of approximation

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

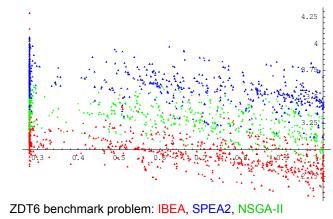


Indicator	A	В
Hypervolume indicator	6.3431	7.1924
ϵ -indicator	1.2090	0.12722
R_2 indicator	0.2434	0.1643
R_3 indicator	0.6454	0.3475

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

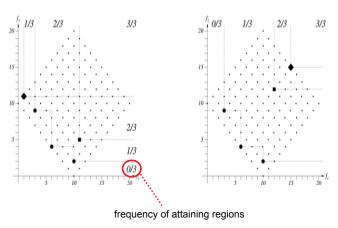
Once Upon a Time...

... multiobjective EAs were mainly compared visually:



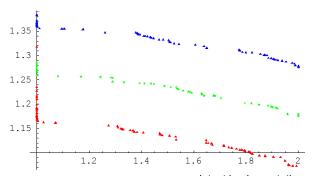
Empirical Attainment Functions

three runs of two multiobjective optimizers



Attainment Plots

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



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

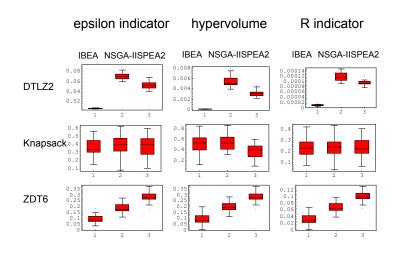
see [Fonseca et al. 2011]

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69

Example: Box Plots

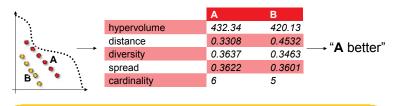


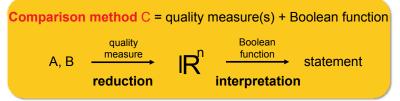
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Quality Indicator Approach

Goal: compare two Pareto set approximations A and B



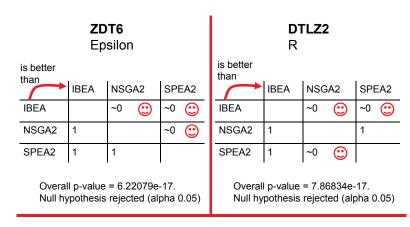


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70

Statistical Assessment (Kruskal Test)

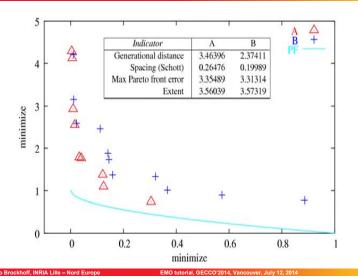


Knapsack/Hypervolume: H_0 = No significance of any differences

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Problems With Non-Compliant Indicators



Set Quality Indicators

Open Questions:

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

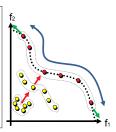
What Are Good Set Quality Measures?

There are three aspects [Zitzler et al. 2000]

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

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

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



Wrong! [Zitzler et al. 2003]

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

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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!

Indicator Single-objective Multiobjective Problem Problem

Optimal µ-Distribution:

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

optimal µ-distribution for I.

Optimal µ-Distributions for the Hypervolume

Hypervolume indicator refines dominance relation

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

(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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Articulating User Preferences During Search

What we thought: EMO is preference-less

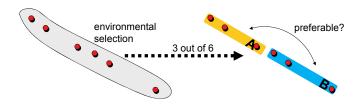
given by the Divi.

[Zitzler 1999]

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.

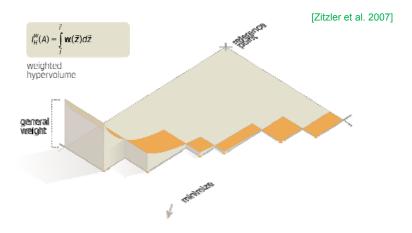
Decision making during search: The DM can articulate preferences during

What we learnt: EMO just uses weaker preference information



BEA

Example: Weighted Hypervolume Indicator



Incorporation of Preferences During Search

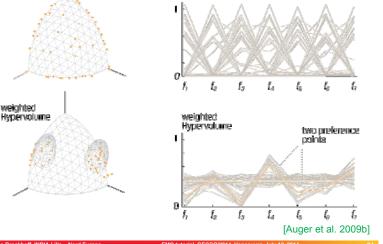
Nevertheless...

- 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]
- 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]

Weighted Hypervolume in Practice



IBEA

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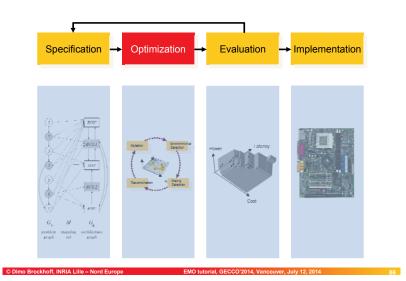
- indicator-based EMO
- preference articulation

A Few Examples From Practice

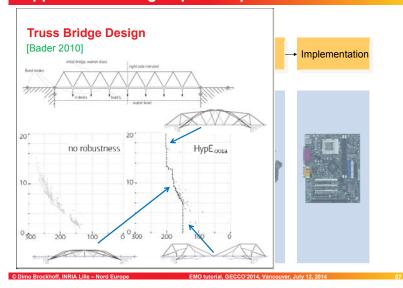
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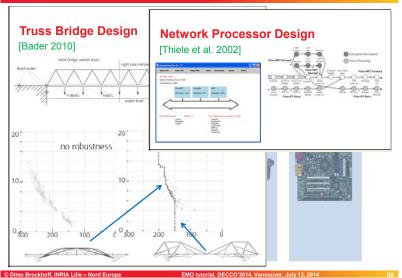
Application: Design Space Exploration



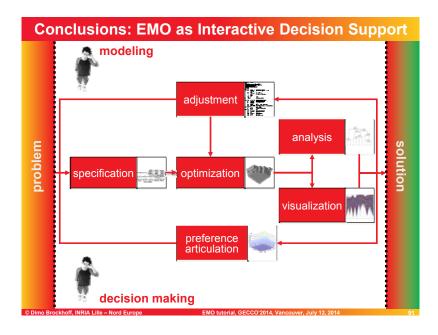
Application: Design Space Exploration



Application: Design Space Exploration



Truss Bridge Design [Bader 2010] Network Processor Design [Thiele et al. 2002] Water resource management [Siegfried et al. 2009]

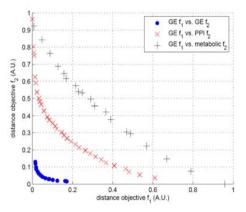


Application: Trade-Off Analysis

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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00

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/

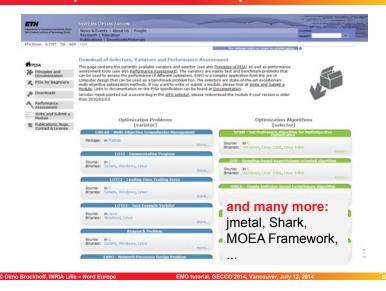
Books:

- 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...

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



Additional Slides

Perspectives

Challenging Open (Research) Directions

- Benchmarking
 - comparison with classical approaches
 - where are real strengths of EMO (how much better?)
 - algorithm recommendations for practice
- Many-objective Optimization
- growing EMO and MCDM to one field

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 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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97

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99

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98

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