# An Introduction to Evolutionary Multiobjective Optimization

#### **Dimo Brockhoff**

#### École des Ponts, December 3, 2009

#### copyright in part by Eckart Zitzler

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE



#### A hypothetical problem: all solutions plotted



#### A hypothetical problem: all solutions plotted







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



## **Decision Making: Selecting a Solution**

#### **Approaches:** • supply more important than cost (ranking)



# **Decision Making: Selecting a Solution**



#### **Before Optimization:**





#### **Before Optimization:**



© Dimo Brockhoff and Eckart Zitzler

#### When to Make the Decision



#### **After Optimization:**





### When to Make the Decision

#### **Before Optimization:**



#### **After Optimization:**





#### Focus: learning about a problem

- trade-off surface
- interactions among criteria
- structural information

# 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





MOM

**Multiple Criteria Decision Making** 

# 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



International Society on Multiple Criteria Decision Making





# 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



International Society on Multiple Criteria Decision Making



# **Evolutionary Multiobjective Optimization (EMO)**

#### **Definition: EMO**

#### **EMO** = **evolutionary algorithms** / randomized search algorithms

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





# The History of EMO At A Glance

1984	first EMO approaches					
1990	dominance-based population ranking dominance-based EMO algorithms with diversity preservation techniques					
1995	attainment function	S				
	elitist EMO algorithms	preferer	nce articulation	convergend	ce proofs	
2000	test problem design	quantita	quantitative performance assessment		mu	Itiobjectivization
	uncertainty and robustness	runnir	running time analyses		quality measure design	
	MCDI	MCDM + EMO		EMO algorithms based on set quality		
2009	high-dimensional objective s	statistical performance assessment				

© Dimo Brockhoff and Eckart Zitzler

INRIA Saclay and ETH Zurich An Introduction to EMO, École des Ponts, December 3, 2009

# The History of EMO At A Glance





http://delta.cs.cinvestav.mx/~ccoello/EMOO/EMOOstatistics.html

© Dimo Brockhoff and Eckart Zitzler

INRIA Saclay and ETH Zurich An Introduction to EMO, École des Ponts, December 3, 2009

#### The EMO conference series:



#### Many further activities:

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

© Dimo Brockhoff and Eckart Zitzler

# The Big Picture

**Basic Principles of Multiobjective Optimization** 

# Algorithm Design Principles and Concepts

Performance Assessment

# A Few Examples From Practice

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



© Dimo Brockhoff and Eckart Zitzler

# A General (Multiobjective) Optimization Problem

A multiobjective optimization problem is defined by a 5-tuple  $(X, Z, \mathbf{f}, \mathbf{g}, \leq)$  where

- X is the decision space,
- $Z = \mathbb{R}^n$  is the objective space,
- **f** = (f<sub>1</sub>,...,f<sub>n</sub>) is a vector-valued function consisting of n objective functions f<sub>i</sub>: X → ℝ,
- g = (g<sub>1</sub>,...,g<sub>m</sub>) is a vector-valued function consisting of m constraint functions g<sub>i</sub> : X → ℝ, and
- $\leq \subseteq Z \times Z$  is a binary relation on the objective space.

The goal is to identify a decision vector  $\mathbf{a} \in X$  such that (i) for all  $1 \le i \le m$ holds  $g_i(\mathbf{a}) \le 0$  and (ii) for all  $\mathbf{b} \in X$  holds  $\mathbf{f}(\mathbf{b}) \le \mathbf{f}(\mathbf{a}) \Rightarrow \mathbf{f}(\mathbf{a}) \le \mathbf{f}(\mathbf{b})$ .

# **A Single-Objective Optimization Problem**



# **A Single-Objective Optimization Problem**



# **A Single-Objective Optimization Problem**

#### **Example:** Leading Ones Problem



where 
$$f_{LO}(a) = \sum_{i} (\prod_{j \le i} a_j)$$

#### **Simple Graphical Representation**

**Example:**  $\geq$  (total order)



## **Preference Relations**

decision space objective space objective functions  

$$\begin{array}{c} (X, Z, f: X \rightarrow Z, rel \subseteq Z \times Z) \\ (X, prefrel) \end{array}$$
preorder where  
a prefrel b : $\Leftrightarrow$  f(a) rel f(b)

$$\begin{array}{ll} (X,\preccurlyeq_{par}) & \downarrow \\ \downarrow & & \\ a \preccurlyeq_{par} b : \Leftrightarrow f(a) \leqslant_{par} f(b) & \text{weak} \\ & \text{Pareto dominance} \end{array}$$

#### **Example:** Leading Ones Trailing Zeros Problem



© Dimo Brockhoff and Eckart Zitzler

#### **Example:** Leading Ones Trailing Zeros Problem



 $(\{0,1\}^n,$ 

#### **Example:** Leading Ones Trailing Zeros Problem



 $({0,1}^n, {0,1,2,...,n} \times {0,1,2,...,n},$ 

#### **Example:** Leading Ones Trailing Zeros Problem



© Dimo Brockhoff and Eckart Zitzler

INRIA Saclay and ETH Zurich An Introduction to EMO, École des Ponts, December 3, 2009

#### **Example:** Leading Ones Trailing Zeros Problem



#### **Pareto Dominance**



© Dimo Brockhoff and Eckart Zitzler

## **Different Notions of Dominance**



## **The Pareto-optimal Set**

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

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



### **Visualizing Preference Relations**


#### **Remark: Properties of the Pareto-optimal Set**

#### **Computational complexity:**

multiobjective variants can be become NP- and #P-complete

Size: Pareto set can be exponential in the input length (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**



© Dimo Brockhoff and Eckart Zitzler

### **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  $s(u_1, \ldots, u_n) \in \mathbb{R}$ .

© Dimo Brockhoff and Eckart Zitzler

#### **Aggregation-Based Approaches**





**Example:** weighting approach

$$(W_1, W_2, \dots, W_k)$$

$$\downarrow$$

$$\downarrow$$

$$y = W_1y_1 + \dots + W_ky_k$$

**Other example:** Tchebycheff  $y = \max w_i(u_i - z_i)$ 

## **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,
- $\Omega = 2^Z$  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  $A \leq B : \Leftrightarrow \forall \mathbf{b} \in B \exists \mathbf{a} \in A : \mathbf{a} \leq \mathbf{b}.$

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



#### A 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



# 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 front
    - **2** well 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 Transformations**

#### 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**

 $\bullet \stackrel{\rm ref}{\prec} refines a preference relation \prec iff$ 

$$A \preccurlyeq B \land B \preccurlyeq A \Rightarrow A \preccurlyeq B \land B \preccurlyeq A$$

(better 
$$\Rightarrow$$
 better)

## $\Rightarrow$ fulfills requirement

**2**  $\stackrel{\mathrm{ref}}{\prec}$  weakly refines a preference relation  $\stackrel{\mathrm{ref}}{\prec}$  iff

$$A \preccurlyeq B \land B \preccurlyeq A \Rightarrow A \preccurlyeq B$$

(better  $\Rightarrow$  weakly better)

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

#### ...sought are total refinements...

© Dimo Brockhoff and Eckart Zitzler

## **Example: Refinements Using Set Quality Measures**

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

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



#### unary hypervolume indicator





binary epsilon indicator

### **Example: Weak Refinement and No Refinement**



© Dimo Brockhoff and Eckart Zitzler

# The Big Picture

**Basic Principles of Multiobjective Optimization** 

# **Algorithm Design Principles and Concepts**

Performance Assessment

# A Few Examples From Practice

### **Algorithm Design: Particular Aspects**



## **Fitness Assignment: Principal Approaches**

#### aggregation-based

weighted sum

criterion-based VEGA

#### dominance-based SPEA2



scaling-dependent

© Dimo Brockhoff and Eckart Zitzler

#### **Criterion-Based Selection: VEGA**



© Dimo Brockhoff and Eckart Zitzler

INRIA Saclay and ETH Zurich An Introduction to EMO, École des Ponts, December 3, 2009

## **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



### A General Scheme of a Dominance-Based MOEA



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

© Dimo Brockhoff and Eckart Zitzler

## **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



### **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



k-th nearest neighbor

density = function of distance to k-th neighbor



Histogram method

density = number of elements within box



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),<br/>then add up weights of dominating solutions



S (strength) =
 #dominated solutions

• R (raw fitness) =  $\sum$  strengths of dominators •

#### **Density Estimation**

k-th nearest neighbor method:

- D<sub>k</sub> = distance to the k-th nearest individual
- Usually used: k = 2



#### **Hypervolume-Based Selection**

Problem of many secondary selection criterions: no refinement

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



# **Sampling New Points: Covariance Matrix Adaptation**

#### Concept

- use single-objective mutation of CMA-ES for each individual [ihr2007a]
- Sample multivariate normal distribution  $m+\sigma N(0,C)$
- m,  $\sigma$ , and C are updated every generation depending on success



## **Articulating User Preferences During Search**

#### What we thought: EMO is preference-less

given by the Divi.

**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



[Zitzler 1999]

### **Example: Weighted Hypervolume Indicator**



## Weighted Hypervolume in Practice



# The Big Picture

# **Basic Principles of Multiobjective Optimization**

# Algorithm Design Principles and Concepts

# **Performance Assessment**

# 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	Α	В
Hypervolume indicator	6.3431	7.1924
$\epsilon$ -indicator	1.2090	0.12722
$R_2$ indicator	0.2434	0.1643
$R_3$ indicator	0.6454	0.3475

### **Empirical Attainment Functions**

three runs of two multiobjective optimizers



frequency of attaining regions

#### **Attainment Plots**

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


## **Quality Indicator Approach**

Goal: compare two Pareto set approximations A and B



Comparison method C = quality measure(s) + Boolean function A, B  $\xrightarrow{\text{quality}}_{\text{measure}}$   $R^n \xrightarrow{\text{Boolean}}_{\text{function}}$  statement interpretation

#### **Example: Box Plots**



[Fonseca et al. 2005]

© Dimo Brockhoff and Eckart Zitzler

#### **Example: Box Plots**



### Statistical Assessment (Kruskal Test)

<b>ZDT6</b> Epsilon					DTLZ2 R					
is better than					is better than					
$ \longrightarrow $	IBEA	NSGA2	SPE	EA2	$ \frown $	IBEA	NSGA2		SPEA2	
IBEA		~0 🕐	~0	$\odot$	IBEA		~0		~0	
NSGA2	1		~0	$\odot$	NSGA2	1			1	
SPEA2	1	1			SPEA2	1	~0			
Overall p-value = 6.22079e-17. Null hypothesis rejected (alpha 0.05)					Overall p-value = 7.86834e-17. Null hypothesis rejected (alpha 0.05)					

**Knapsack/**Hypervolume: H0 = No significance of any differences

© Dimo Brockhoff and Eckart Zitzler

### **Problems With Non-Compliant Indicators**



## What Are Good Set Quality Measures?

#### There are three aspects [Zitzler et al. 2000]

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 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

© Dimo Brockhoff and Eckart Zitzler

# The Big Picture

**Basic Principles of Multiobjective Optimization** 

# Algorithm Design Principles and Concepts

Performance Assessment

# **A Few Examples From Practice**

## **EMO Provides Information About a Problem**



#### The question:

Why at all should one try to approximate the entire Pareto-optimal set?

#### An answer:

Because it provides useful information about the problem...

#### **Application: Design Space Exploration**



© Dimo Brockhoff and Eckart Zitzler

INRIA Saclay and ETH Zurich An Introduction to EMO, École des Ponts, December 3, 2009

## **Application: Design Space Exploration**



© Dimo Brockhoff and Eckart Zitzler

INRIA Saclay and ETH Zurich An Introduction to EMO, École des Ponts, December 3, 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



## **Application: Approximation Set Analysis**

#### Multiple disk clutch brake design [Deb, Srinivasan 2006]



## **Conclusions: EMO as Interactive Decision Support**



© Dimo Brockhoff and Eckart Zitzler

INRIA Saclay and ETH Zurich An Introduction to EMO, École des Ponts, December 3, 2009

# The EMO Community

#### Links:

- EMO mailing list: http://w3.ualg.pt/lists/emo-list/
- EMO bibliography: *http://www.lania.mx/~ccoello/EMOO/*

#### **Events:**

Conference on Evolutionary Multi-Criterion Optimization

#### **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, 2<sup>nd</sup> Ed. 2006
- and more...

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

