Principles of Multiple Criteria Decision

A hypothetical problem: all solutions plotted

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

Possible Approach: 1. supply more important than cost (ranking)

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**Principles of Multiple Criteria Decision**

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

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**Decision Making: Selecting a Solution**

Possible Approach: 1. supply more important than cost (ranking) 2. cost must not exceed 2400 (constraint)

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When to Make the Decision

**Before Optimization:**
- rank objectives, define constraints, ...
- search for one (blue) solution

**After Optimization:**
- search for a set of (blue) solutions
- select one solution considering constraints, etc.

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.

- **Model**: \( f(x) = f_1(x) \ldots f_n(x) \)
  - \( x \in \mathcal{X} \)
  - \( f_i : \mathcal{X} \rightarrow \mathbb{R} \)
- **Trade-off Surface**: \( \mathcal{S} \)
- **Decision Making**: (exact) optimization
- **Problem**: huge search spaces
- **Objectives**: non-linear, noisy, uncertain, many objectives, many constraints

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)

- **Black box optimization**: \( x \in \mathcal{X} \rightarrow (f_1(x), \ldots, f_n(x)) \)
- **Mutation**: survival
- **Recombination**: mating
- **Cost**: water supply
- **Pareto set approximation**
**Multiobjectivization**

Some problems are easier to solve in a multiobjective scenario

example: TSP

$\pi \in S_n \rightarrow f(\pi)$

TSP 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]

TSP, 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

min. mass + stopping time

= 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

1984
- first EMO approaches
- dominance-based population ranking
- dominance-based EMO algorithms with diversity preservation techniques

1990
- attainment functions
- elitist EMO algorithms
- preference articulation
- convergence proofs
- test problem design
- quantitative performance assessment
- uncertainty and robustness
- running time analyses
- quality measure design
- many-objective optimization
- statistical performance assessment

2000
- multiobjectivization
- MCDM + EMO
- quality indicator based EMO algorithms
- convergence proofs
- preference articulation
- uncertainty and robustness
- running time analyses
- quality measure design
- statistical performance assessment

2007
- quality indicator based EMO algorithms
- many-objective optimization
- statistical performance assessment

2011
- high-dimensional objective spaces
- many-objective optimization

Overall: 6105 references by June 15th, 2011

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

The EMO Community

The EMO conference series:

- EMO2001 Zurich, Switzerland
- EMO2003 Faro, Portugal
- EMO2005 Guanajuato, Mexico
- EMO2007 Matsushima, Japan
- EMO2009 Nantes, France
- EMO2011 Ouro Peto, Brazil

45 / 87 56 / 100 59 / 115 65 / 124 39 / 72 42 / 83

Many further activities:
- special sessions, special journal issues, workshops, tutorials, ...

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
Starting Point

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

A General (Multiobjective) Optimization

A multiobjective optimization problem is defined by a 5-tuple \((X, Z, f, g, \preceq)\) where

- \(X\) is the decision space,
- \(Z = \mathbb{R}^n\) is the objective space,
- \(f = (f_1, \ldots, f_n)\) is a vector-valued function consisting of \(n\) objective functions \(f_i : X \rightarrow \mathbb{R}\),
- \(g = (g_1, \ldots, g_m)\) is a vector-valued function consisting of \(m\) constraint functions \(g_j : X \rightarrow \mathbb{R}\), and
- \(\preceq \subseteq Z \times Z\) is a binary relation on the objective space.

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

A Single-Objective Optimization Problem

\((X, Z, f: X \rightarrow Z, \preceq \subseteq Z \times Z)\)

A Single-Objective Optimization Problem

\((X, Z, f: X \rightarrow Z, \preceq \subseteq Z \times Z)\)

total preorder where \(a \text{ pref} f(b) \iff f(a) \preceq f(b)\)
A Single-Objective Optimization Problem

**Example:** Leading Ones Problem

\[(X, Z, f: X \to Z, \text{rel} \subseteq Z \times Z)\]

\[(X, \text{prefrel})\]

\[\langle 0,1 \rangle^n, \{0,1,2,\ldots,n\}, f_{LO} \geq \]

where \(f_{LO}(a) = \sum_i (\prod_{j \leq i} a_j)\)

**Preference Relations**

Decision space \(X\), objective space \(Z\), objective functions \(f: X \to Z\), partial order \(\text{rel} \subseteq Z \times Z\), preorder where \(a \text{ prefrel } b \iff f(a) \text{ rel } f(b)\)

\[(X, \text{prefrel})\]

\[\langle 0,1 \rangle^n, \{0,1,2,\ldots,n\}, f_{LO}, f_{LO} \geq \]

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A Multiobjective Optimization Problem

**Example:** Leading Ones Trailing Zeros Problem

\[(X, Z, f: X \to Z, \text{rel} \subseteq Z \times Z)\]

\[(X, \text{prefrel})\]

\[\langle 0,1 \rangle^n, \{0,1,2,\ldots,n\}, f_{LO} \geq \]

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A Multiobjective Optimization Problem

**Example:** Leading Ones Trailing Zeros Problem

\[(X, Z, f: X \to Z, \text{rel} \subseteq Z \times Z)\]

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A Multiobjective Optimization Problem

Example: Leading Ones Trailing Zeros Problem

\( (X, Z, f: X \to Z, \text{rel} \subseteq Z \times Z) \)

\( (X, \text{prefrel}) \)

\[ \{(0,1)^n, \{0,1,2,\ldots,n\} \times \{0,1,2,\ldots,n\}, (f_{\text{LO}}, f_{\text{TZ}}), f_{\text{LO}}(a) = \sum_i (\prod_{j \leq i} a_j), f_{\text{TZ}}(a) = \sum_i (\prod_{j \leq i} (1 - a_j)) \]
Different Notions of Dominance

The Pareto-optimal Set

Visualizing Preference Relations

Remark: Properties of the Pareto Set

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

**Pareto-optimal set** \( \text{Min}(X, \preceq_{\text{par}}) \)
non-optimal decision vector
non-optimal objective vector

**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], MST [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

<table>
<thead>
<tr>
<th>Single Solution Problem</th>
<th>Set Problem</th>
</tr>
</thead>
<tbody>
<tr>
<td>Search space</td>
<td>$\mathcal{X}$</td>
</tr>
<tr>
<td>Parameters</td>
<td>$\mathbb{R}^k$</td>
</tr>
<tr>
<td>objective space</td>
<td>$\mathbb{R}^k$</td>
</tr>
<tr>
<td>$f(x) = (f_1(x), f_2(x), \ldots, f_k(x))$</td>
<td></td>
</tr>
<tr>
<td>$f^*(A) = {f(x) \mid x \in A}$</td>
<td></td>
</tr>
<tr>
<td>(partially) ordered set</td>
<td>($\mathbb{R}^k, \preceq$)</td>
</tr>
<tr>
<td>(totally) ordered set</td>
<td>($\mathbb{R}^k, \succeq$)</td>
</tr>
</tbody>
</table>

Solution-Oriented Problem Transformations

<table>
<thead>
<tr>
<th>multiple objectives $f_1, f_2, \ldots, f_k$</th>
<th>parameters $w_1, w_2, \ldots, w_k$</th>
<th>single objective $f$</th>
</tr>
</thead>
</table>

Transformation

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

Example: weighting approach

$y = w_1y_1 + \ldots + w_ky_k$

Other example: Tchebycheff

$y = \max w_i(u_i - z_i)$
Set-Oriented Problem Transformations

For a multiobjective optimization problem \((X, Z, f, g, \leq)\), the associated set problem is given by \((\Psi, \Omega, F, G, \leq)\) 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 \(f\) to sets, i.e., \(F(A) := \{f(a) : a \in A\} \text{ for } A \in \Psi\),
- \(G = (G_1, \ldots, G_m)\) is the extension of \(g\) to sets, i.e., \(G_i(A) := \max\{g_i(a) : a \in A\} \text{ for } 1 \leq i \leq m \text{ and } A \in \Psi\),
- \(\leq\) extends \(\leq\) to sets where \(A \leq B \iff \forall b \in B \exists a \in A : a \leq b\).

Pareto Set Approximations

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
- \(A\) strictly dominates \(C\) = better in all objectives
- \(B\) is incomparable to \(C\) = neither set weakly better

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:
    1. close to the Pareto front
    2. well distributed

Quality of Pareto Set Approximations

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

- hypervolume indicator
- epsilon indicator
**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?
⇒ Underlying dominance relation $\preceq$ should be reflected

---

**Example: Refinements Using Indicators**

1. $\preceq$ **refines** a preference relation $\preceq$ iff
   
   $A \preceq B \land B \not\preceq A \Rightarrow A \preceq B \land B \not\preceq A$  
   (better $\Rightarrow$ better)

   ⇒ fulfills requirement

2. $\preceq$ **weakly refines** a preference relation $\preceq$ iff
   
   $A \preceq B \land B \not\preceq A \Rightarrow A \preceq\preceq B$  
   (better $\Rightarrow$ weakly better)

   ⇒ does not fulfill requirement, but $\preceq$ does not contradict $\preceq$

   …sought are total refinements…

---

**Example: Weak Refinement / No Refinement**

1. $\preceq$ **ref** $A \preceq B : \Leftrightarrow I(A,R) \leq I(B,R)$

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

2. $\preceq$ **ref** $A \preceq B : \Leftrightarrow I(A) \leq I(B)$

   $I(A) =$ variance of pairwise distances
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A Few Examples From Practice

Algorithm Design: Particular Aspects

1. fitness assignment
2. environmental selection
3. variation operators

Fitness Assignment: Principal Approaches

aggregation-based
criterion-based
dominance-based

weighted sum
VEGA
SPEA2

Criterion-Based Selection: VEGA

select according to
shuffle

[Schaffer 1985]
**General Scheme of Dominance-Based EMO**

- **mating selection** (stochastic)
- **fitness assignment**
  - partitioning into dominance classes
- **environmental selection** (greedy heuristic)
- **population** (archiv)
- **offspring**

**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**

- **dominance rank**
- **dominance depth**

**Refinement of Dominance Rankings**

**Goal**: rank incomparable solutions within a dominance class

1. Density information (good for search, but usually no refinements)
2. Quality indicator (good for set quality): soon...

- **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
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

\[ S \text{ (strength)} = \#\text{dominated solutions} \]
\[ R \text{ (raw fitness)} = \sum \text{strengths of dominators} \]

Example: SPEA2 Diversity Preservation

**Density Estimation**

- k-th nearest neighbor method:
  - Fitness = \( R + \frac{1}{(2 + D_k)} \)
  - \( D_k \) = distance to the k-th nearest individual
  - Usually used: \( k = 2 \)

Example: NSGA-II Diversity Preservation

**Density Estimation**

- Crowding distance:
  - sort solutions wrt. each objective
  - crowding distance to neighbors:
    \[ d(i) = \sum_{m} |f_m(i-1) - f_m(i+1)| \]

Example: SPEA2 and NSGA-II: Cycles in Optimization

Selection in SPEA2 and NSGA-II can result in *deteriorative cycles*

- non-dominated solutions already found can be lost
Hypervolume-Based Selection

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

Main idea
Delete solutions with the smallest hypervolume loss
\[ d(s) = I(P) - I(P / \{ s \}) \]
iteratively

But: can also result in cycles [Judt et al. 2011]
and is expensive [Bringmann and Friedrich 2009]

Moreover: HypE [Bader and Zitzler 2011]
Sampling + Contribution if more than 1 solution deleted

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

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

Empirical Attainment Functions

Three runs of two multiobjective optimizers

Attainment Plots

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

Quality Indicator Approach

Goal: compare two Pareto set approximations A and B

<table>
<thead>
<tr>
<th>Indicator</th>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hypervolume</td>
<td>6.3433</td>
<td>7.1924</td>
</tr>
<tr>
<td>e-indicator</td>
<td>1.2000</td>
<td>0.12772</td>
</tr>
<tr>
<td>R2 indicator</td>
<td>0.2434</td>
<td>0.1646</td>
</tr>
<tr>
<td>R3 indicator</td>
<td>0.6454</td>
<td>0.3475</td>
</tr>
</tbody>
</table>

Comparison method $C = \text{quality measure(s)} + \text{Boolean function}$
Example: Box Plots

Statistical Assessment (Kruskal Test)

What Are Good Set Quality Measures?

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 achieve good indicator values?

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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 $\mu$ plays a role!

Multiobjective Problem $\xrightarrow{\text{Indicator}}$ Single-objective Problem

Optimal $\mu$-Distribution:
A set of $\mu$ solutions that maximizes a certain unary indicator $I$ among all sets of $\mu$ solutions is called optimal $\mu$-distribution for $I$.  

Optimal $\mu$-Distributions for the Hypervolume

Hypervolume indicator refines dominance relation $\implies$ most results on optimal $\mu$-distributions for hypervolume

Optimal $\mu$-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 $\mu$-distributions for the hypervolume correspond to $\varepsilon$-approximations of the front

\[
\begin{align*}
\text{OPT} & : 1 + \frac{\log(\min(A/n, B/n))}{n} \\
\text{HYP} & : 1 + \frac{A/n + \sqrt{B/n}}{n - 4} \\
\log\text{HYP} & : 1 + \frac{\log(A/n) \log(\log(5/n))}{n - 2}
\end{align*}
\]
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A Few Examples From Practice

Articulating User Preferences During Search

What we thought: EMO is preference-less

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]

- 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

- \( C(x) = \sum w(x) \cdot \text{hypervolume} \)

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**Weighted Hypervolume in Practice**

![Weighted Hypervolume in Practice](image)

[Auger et al. 2009b]

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A Few Examples From Practice

**Application: Design Space Exploration**

![Application: Design Space Exploration](image)

**Truss Bridge Design**

[Bader 2010]
Application: Design Space Exploration

**Truss Bridge Design** [Bader 2010]

**Network Processor Design** [Thiele et al. 2002]

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

Conclusions: EMO as Interactive Decision Support

- modeling
- adjustment
- analysis
- visualization
- preference articulation
- decision making
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.mat.ufmg.br/emo2011/

Books:
- and more…

Announcement

Journal of Multi Criteria Decision Analysis

Special Issue
“Evolutionary Multiobjective Optimization: Methodologies and Applications”
guest editors: Dimo Brockhoff and Kalyanmoy Deb
submission deadline: **July 31, 2011**
http://emoatmcdm.gforge.inria.fr/specialissue.php

Questions?

Additional Slides
Instructor Biography

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After obtaining his diploma in computer science (Dipl. Inform.) from University of Dortmund, Germany in 2005, Dimo received his PhD (Dr. sc. ETH) from ETH Zurich, Switzerland in 2009. Between June 2009 and November 2010 he was a postdoctoral researcher at INRIA Saclay Ile-de-France in Orsay, France. Since November 2010 he has been a postdoctoral researcher at LIX, École Polytechnique within the CNRS-Microsoft chair "Optimization for Sustainable Development (OSD)" in Palaiseau, France. His research interests are focused on evolutionary multiobjective optimization (EMO), in particular on many-objective optimization and theoretical aspects of indicator-based search.

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[Online Date Wednesday, February 23, 2005]


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