Tutorial on Evolutionary Multiobjective Optimization GECCO 2008

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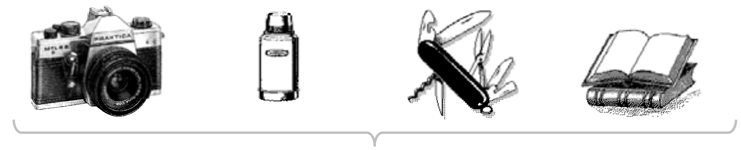
Introductory Example: The Knapsack Problem

weight = 750g profit = 5	weight = 1500g profit = 8	weight = 300g profit = 7	weight = 1000g profit = 3



Single objective:

choose subset that
- maximizes overall profit
- w.r.t. a weight limit

Multiobjective:

choose subset that
- maximizes overall profit
- minimizes overall weight

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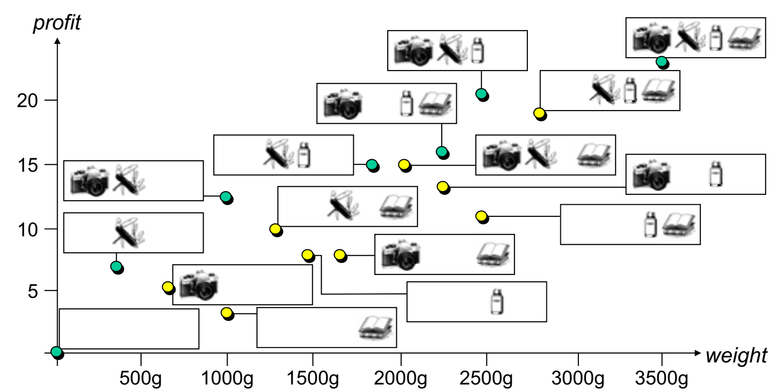
The Search Space



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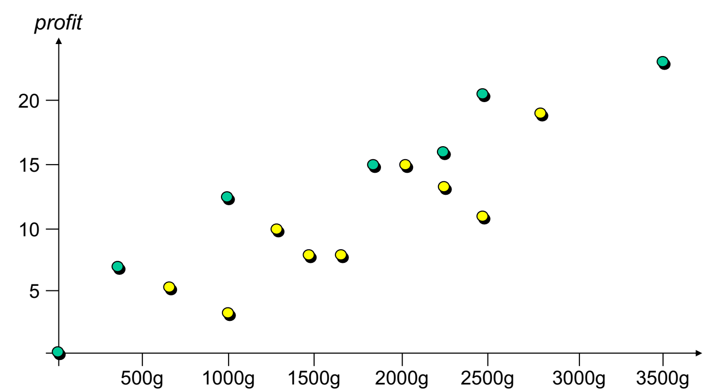
The Trade-off Front

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



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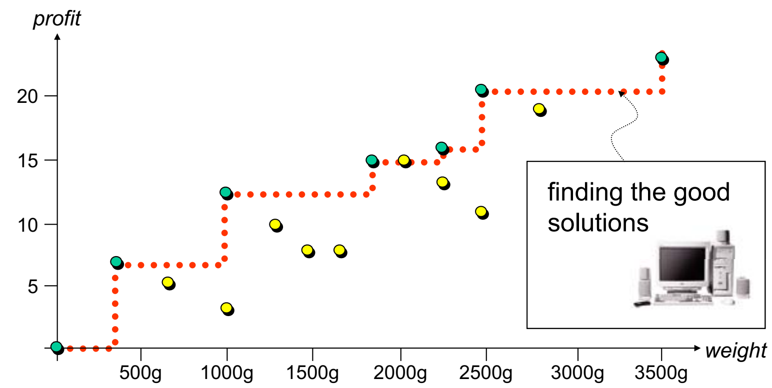

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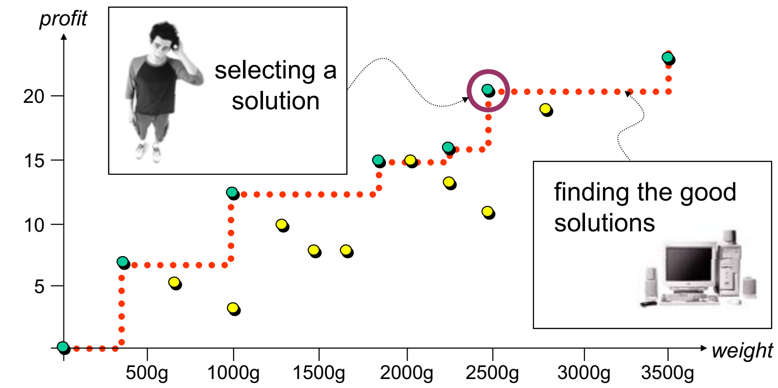

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Decision Making: Selecting a Solution

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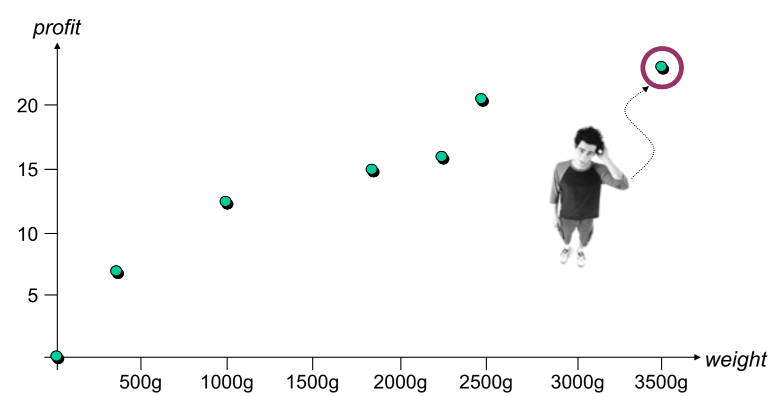
Approaches:
- profit more important than cost (ranking)



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Decision Making: Selecting a Solution

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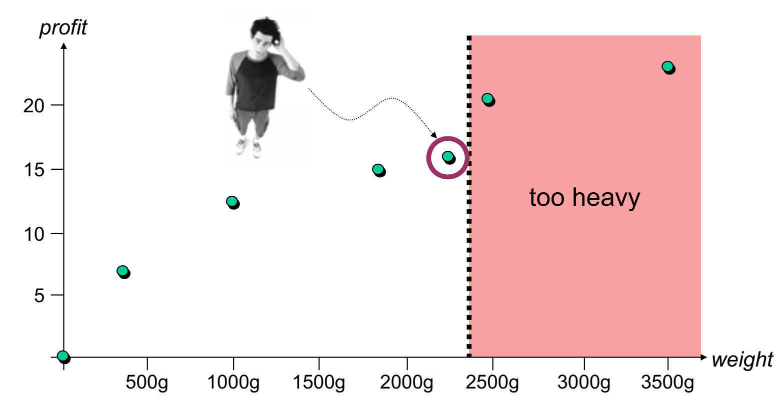
Tutorial on EMO

Approaches:
- profit more important than cost (ranking)
- weight must not exceed 2400g (constraint)



When to Make the Decision

Before Optimization:

ranks objectives,
defines constraints,…

searches for one
(green) solution

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When to Make the Decision

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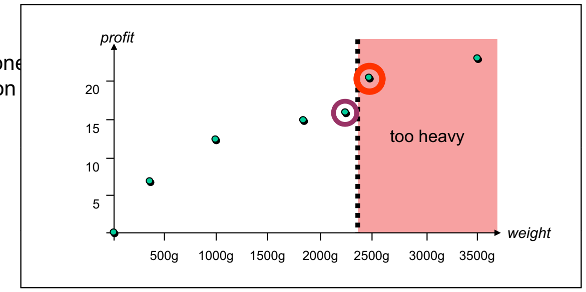

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When to Make the Decision

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Before Optimization:

ranks objectives,
defines constraints,…

searches for one
(green) solution

After Optimization:

searches for a set of
(green) solutions

selects one solution
considering constraints, etc.

- decision making often easier
- EAs well suited

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Outline

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1. **Introduction:** Why multiple objectives make a difference
2. **Basic Principles:** Terms one needs to know
3. **Algorithm Design:** Do it yourself
4. **Performance Assessment:** How to compare algorithms
5. **Applications Domains:** Where EMO is useful
6. **Further Information:** What else

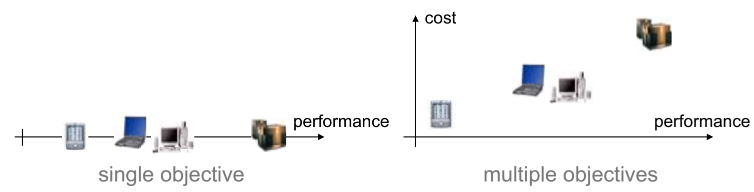
Optimization Problem: Definition

A general optimization problem is given by a quadruple *(X, Z, f, rel)* where

- *X* denotes the decision space containing the elements among which the best is sought; elements of *X* are called decision vectors or simply solutions;
- *Z* denotes the objective space, the space within which the decision vectors are evaluated and compared to each other; elements of *Z* are denoted as objective vectors;
- *f* represents a function $f: X \to Z$ that assigns each decision vector a corresponding objective vector; *f* is usually neither injective nor surjective;
- *rel* is a binary relation over *Z*, i.e., $rel \subseteq Z \times Z$, which represents a partial order over *Z*.

Objective Functions

- Usually, *f* consists of one or several functions $f_1, ..., f_n$ that assign each solution a real number. Such a function $f_i: X \to \Re$ is called an objective function, and examples are cost, size, execution time, etc.
- In the case of a single objective function (n=1), the problem is denoted as a single-objective optimization problem; a multiobjective optimization problem involves several (n ≥ 2) objective functions:

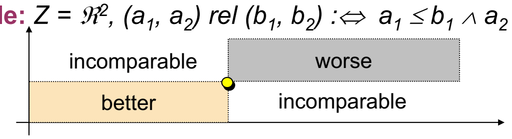


Comparing Objective Vectors

The pair *(Z, rel)* forms a partially ordered set, i.e., for any two objective vectors $a, b \in Z$ there can be four situations:

- *a* and *b* are equal: *a rel b* and *b rel a*
- *a* is better than *b*: *a rel b* and not *(b rel a)*
- *a* is worse than *b*: not *(a rel b)* and *b rel a*
- *a* and *b* are incomparable: neither *a rel b* nor *b rel a*

Example: $Z = \Re^2$, $(a_1, a_2)\ rel\ (b_1, b_2) :\Leftrightarrow a_1 \leq b_1 \wedge a_2 \leq b_2$



Often, *(Z, rel)* is a totally ordered set, i.e., for all $a, b \in Z$ either *a rel b* or *b rel a* or both holds (no incomparable elements).

Preference Structures

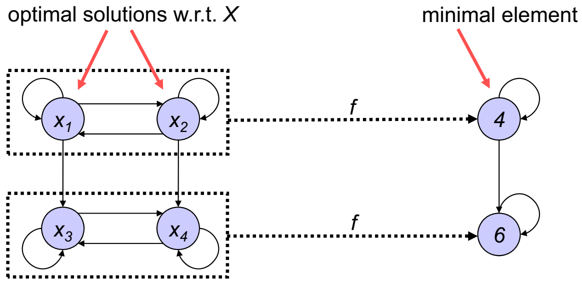
- The function *f* together with the partially ordered set *(Z, rel)* defines a preference structure on the decision space *X* that reflects which solutions the decision maker / user prefers to other solutions:

  $x_1\ prefrel\ x_2 :\Leftrightarrow f(x_1)\ rel\ f(x_2)$

- One says:
  - Two solutions x_1, x_2 are equal iff $x_1 = x_2$;
  - A solution x_1 is indifferent to a solution x_2 iff $x_1\ prefrel\ x_2$ and $x_2\ prefrel\ x_1$ and $x_1 \neq x_2$;
  - A solution x_1 is preferred to a solution x_2 iff $x_1\ prefrel\ x_2$;
  - A solution x_1 is strictly preferred to a solution x_2 iff $x_1\ prefrel\ x_2$ and not ($x_2\ prefrel\ x_1$);
  - A solution x_1 is incomparable to a solution x_2 iff neither $x_1\ prefrel\ x_2$ nor $x_2\ prefrel\ x_1$.

The Notion of Optimality

- A solution $x \in X$ is called optimal with respect to a set $S \subseteq X$ iff no solution $x' \in S$ is strictly preferred to x, i.e., for all $x' \in S$: x' *prefrel* $x \Rightarrow x$ *prefrel* x'.
- In other words, $f(x)$ is a minimal element of $f(S)$ regarding the partially ordered set (Z, rel).



Pareto Dominance

Assumption:

- n objective functions $f_i: X \rightarrow \Re$ where $Z = \Re^n$
- all objectives are to be maximized

Usually considered relation: weak Pareto dominance

- optimization problem: $(X, \Re^n, (f_1, \ldots, f_n), \succeq)$
- weak Pareto dominance:

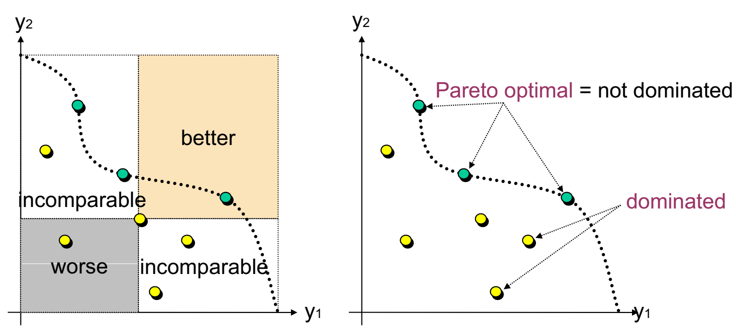
$$x_1 \succeq x_2 :\Leftrightarrow \forall 1 \leq i \leq n : f_i(x_1) \geq f_i(x_2)$$

- Pareto dominance: strict version of weak Pareto dominance

$$x_1 \succ x_2 :\Leftrightarrow x_1 \succeq x_2 \;\wedge\; x_2 \not\succeq x_1$$

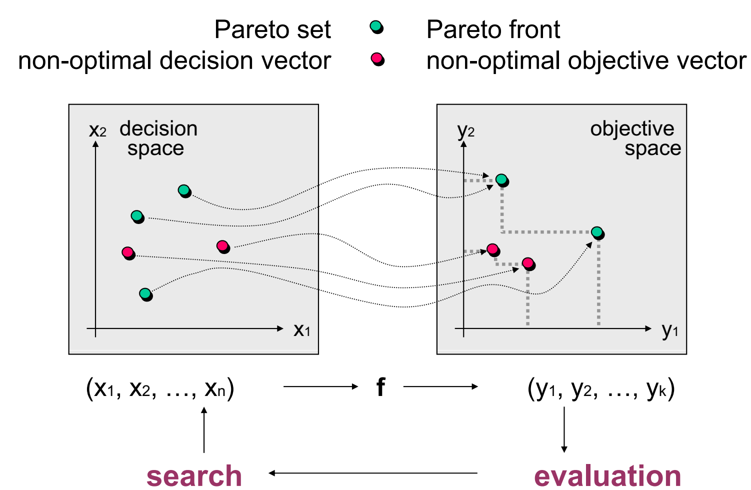
Illustration of Pareto Optimality

Maximize $(y_1, y_2, \ldots, y_k) = f(x_1, x_2, \ldots, x_n)$



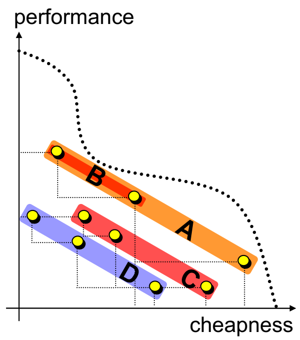
Pareto(-optimal) set = set of all Pareto-optimal solutions

Decision and Objective Space



Pareto Set Approximations

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



A is **better** than **B**
= not worse in all objectives and sets not equal

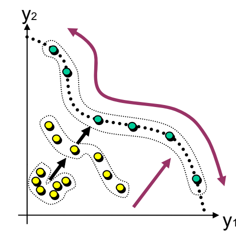
C **dominates** **D**
= better in at least one objective

A **strictly dominates** **C**
= better in all objectives

B is **incomparable** to **C**
= neither set weakly better

What Is the Optimization Goal?

- 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:
    - ❶ close to the Pareto front
    - ❷ well distributed

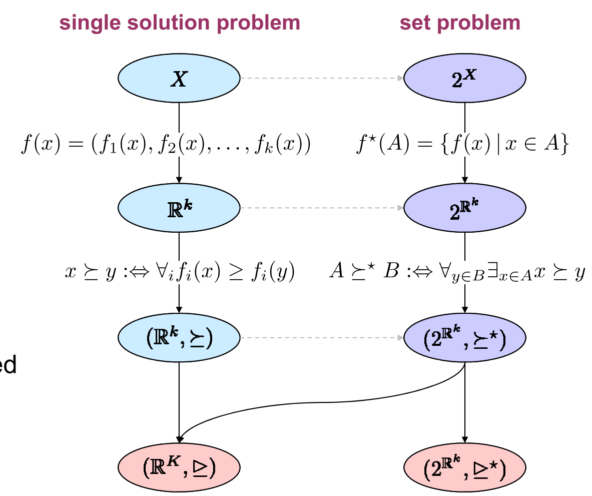


Problem Transformations and Set Problems

search space

objective space

(partially) ordered set

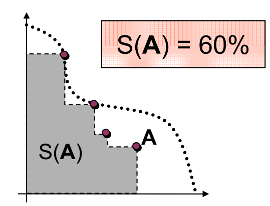


Preference Information

Preference information (here) = any additional information that refines the dominance relation on approximation sets (partial order → total order)

Example:

optimization goal
=
maximize size S of dominated objective space



Note: every algorithm implicitly or explicitly makes assumptions about the decision maker's preferences (limited memory, selection)

Outline

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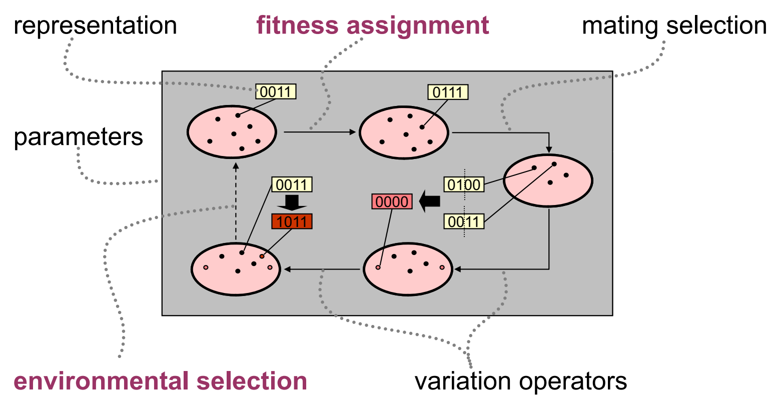
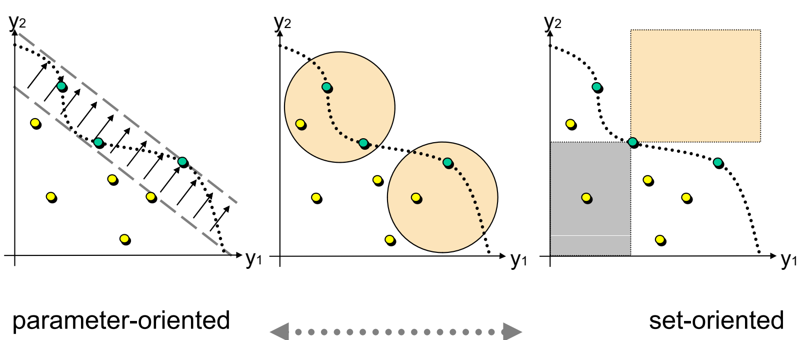
Design Choices



Ranking Solutions

aggregation-based	criterion-based	dominance-based
weighted sum	*VEGA*	*SPEA2*

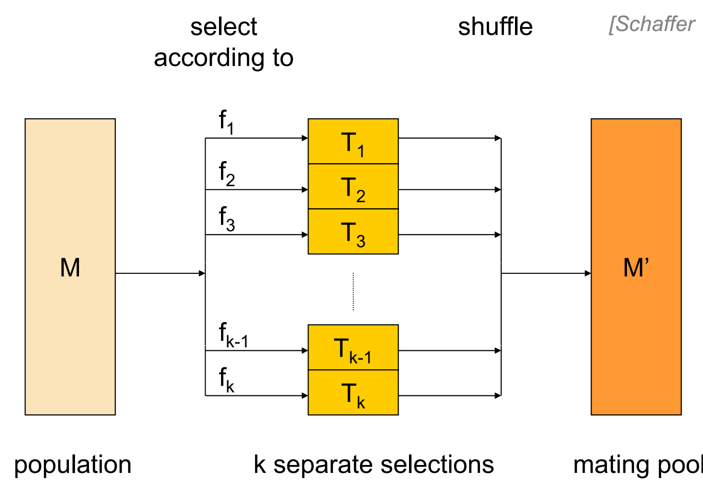


parameter-oriented
scaling-dependent

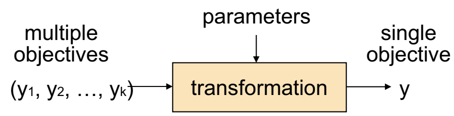
set-oriented
scaling-independent

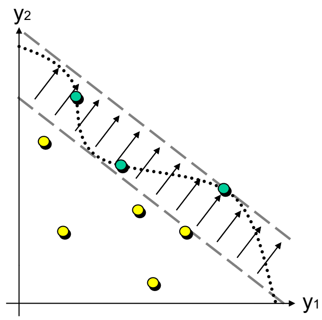
Example: VEGA

[Schaffer 1985]



Aggregation-Based Ranking





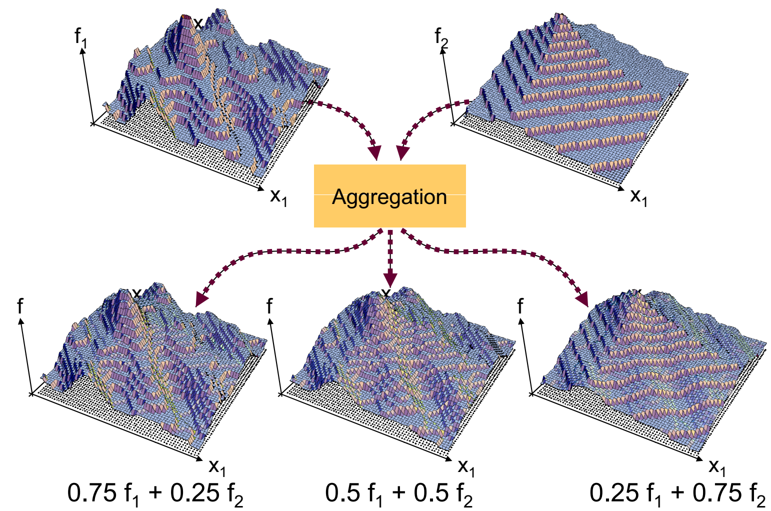
Example: weighting approach

$(w_1, w_2, \ldots, w_k)$

$y = w_1 y_1 + \ldots + w_k y_k$

Note: weights need to be varied during the run...

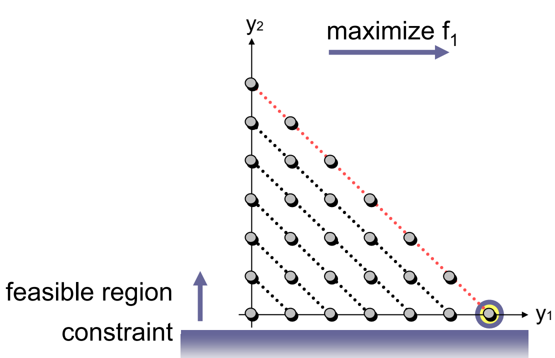
Example: Weighted Sum



Example: Multistart Constraint Method

Underlying concept:

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



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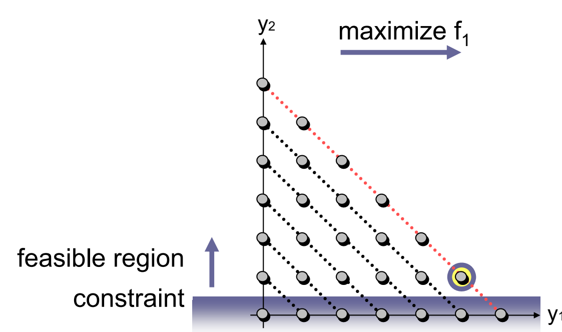

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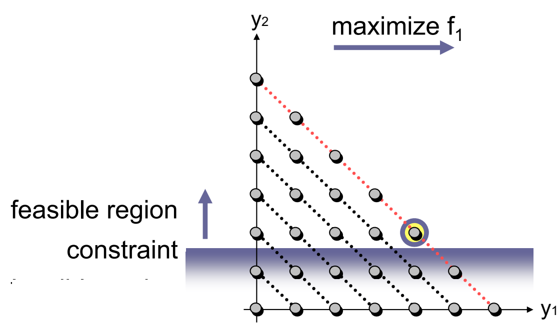
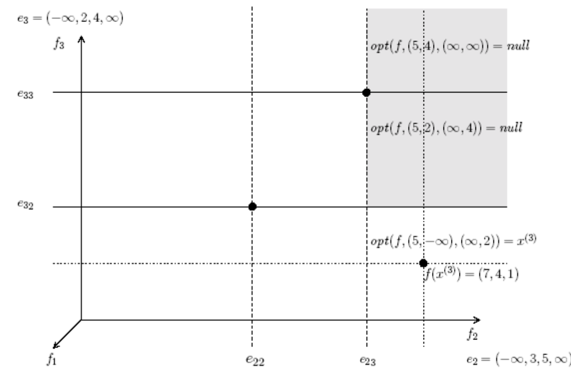


Example: Multistart Constraint Method (Cont'd)

Extension to n objectives: ECEA *[Laumanns et al. 2006]*

- f_1 is the objective to optimize
- The boxes are defined by constraints on f_2 and f_3



Dominance-Based Ranking

Types of information:

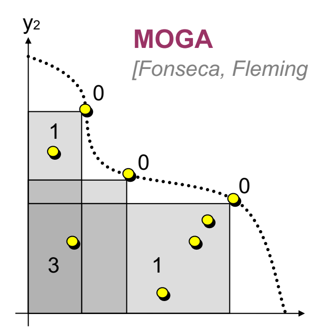
- **dominance rank** — by how many individuals is an individual dominated?
- **dominance count** — how many individuals does an individual dominate?
- **dominance depth** — at which front is an individual located?

Examples:

- *MOGA, NPGA* — dominance rank
- *NSGA/NSGA-II* — dominance depth
- *SPEA/SPEA2* — dominance count + rank

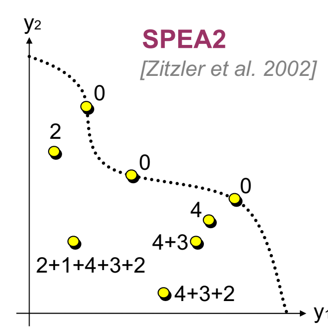
Example: MOGA and SPEA2

MOGA
[Fonseca, Fleming 1993]



R (raw fitness) = #dominating solutions

SPEA2
[Zitzler et al. 2002]



S (strength) = #dominated solutions

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

Refining Rankings

ranks	pure dominance rank
1	0
2	0
3	0
4	1
5	1
6	2
7	2
8	2
9	3

no selection pressure within equivalence classes

refined ranking

❶ density information based on Euclidean distance

0.245
0.311
0.329

0
1
2

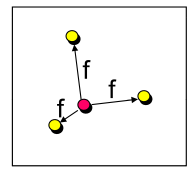
❷ modified dominance relation

Methods Based On Euclidean Distance

Density estimation techniques: *[Silverman 1986]*

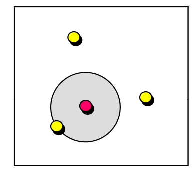
Kernel
MOGA

density estimate = sum of f values where f is a function of the distance



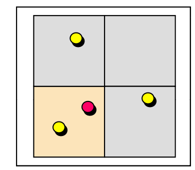
Nearest neighbor
SPEA2

density estimate = volume of the sphere defined by the nearest neighbor



Histogram
PAES

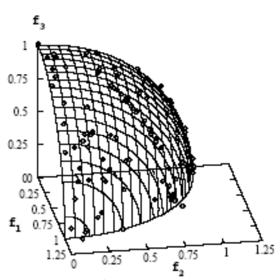
density estimate = number of solutions in the same box



Computation Effort Versus Accuracy

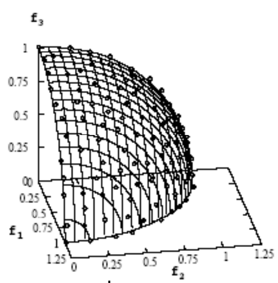
Two Nearest Neighbor Variants

Objective-Wise
NSGA-II



faster
good for 2 objectives
[Deb et al. 2002]

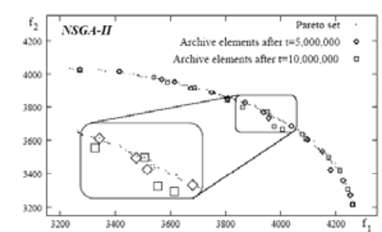
Euclidean Distance
SPEA2

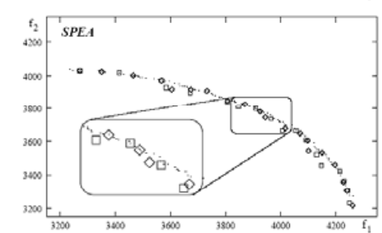


slower
good for 3 objectives and more
[Zitzler et al. 2002]

The Problem of Deterioration

Observation:
The use of Euclidean distance can lead to deterioration





Knapsack problem
[Laumanns et al. 2002]

Refinement of Dominance Relations

Integration of Goals, Priorities, Constraints:
[Fonseca, Fleming 1998]

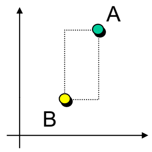
A is preferable over B $\Leftrightarrow$ $(\boldsymbol{u}_p^{\frown\boldsymbol{u}}\ {}_p\!< \boldsymbol{v}_p^{\frown\boldsymbol{u}}) \vee \{(\boldsymbol{u}_p^{\frown\boldsymbol{u}} = \boldsymbol{v}_p^{\frown\boldsymbol{u}})$
$\wedge [(\boldsymbol{v}_p^{\smile\boldsymbol{u}} \not\leq \boldsymbol{g}_p^{\smile\boldsymbol{u}}) \vee (\boldsymbol{u}_{1,\cdots,p-1} \underset{\boldsymbol{g}_{1,\cdots,p-1}}{\prec} \boldsymbol{v}_{1,\cdots,p-1})]\}$

Continuous dominance "relations": *[Zitzler et al. 2003]*

$I_{\varepsilon+}(A,B) = \min_i f_i(A) - f_i(B)$

$I_{\varepsilon+}(A,B) \geq 0$ and $I_{\varepsilon+}(B,A) < 0 \Leftrightarrow$ A dominates B

(binary additive epsilon quality indicator)



Example: IBEA

Question: How to continuous dominance "relations" for fitness assignment? *[Zitzler, Künzli 2004]*

Given: function I (binary quality indicator) with

A dominates B $\Leftrightarrow$ I(A, B) < I(B, A)

Idea: measure for "loss in quality" if A is removed

Fitness: $F'(\boldsymbol{x}^1) = \sum_{\boldsymbol{x}^2 \in P \setminus \{\boldsymbol{x}^1\}} I(\{\boldsymbol{x}^2\}, \{\boldsymbol{x}^1\})$

...corresponds to continuous extension of dominance rank
...blurrs influence of dominating and dominated individuals

Example: IBEA (Cont'd)

Fitness assignment: O(n²)

Fitness: $$F(\boldsymbol{x}^1) = \sum_{\boldsymbol{x}^2 \in P \setminus \{\boldsymbol{x}^1\}} -e^{-I(\{\boldsymbol{x}^2\}, \{\boldsymbol{x}^1\})/\kappa}$$

- parameter κ is problem- and indicator-dependent
- no additional diversity preservation mechanism

Mating selection: O(n)

- binary tournament selection, fitness values constant

Environmental selection: O(n²)

- iteratively remove individual with lowest fitness
- update fitness values of remaining individuals after each deletion

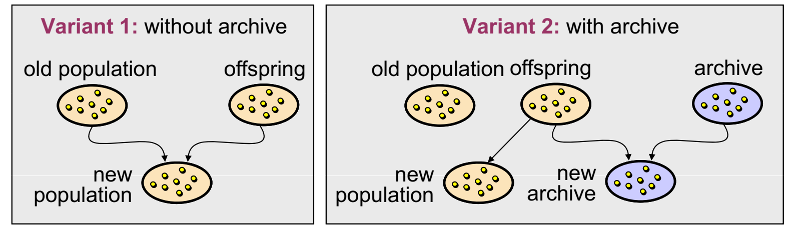
Further Design Aspects

- **Constraint handling:**
  How to integrate constraints into fitness assignment?
- **Archiving / environmental selection:**
  How to keep a good approximation?
- **Hybridization:**
  How to integrate, e.g., local search in a multiobjective EA?
- **Preference articulation:**
  How to focus the search on interesting regions?
- **Robustness and uncertainty:**
  How to account for variations in the objective function values?
- **Data structures:**
  How to support, e.g., fast dominance checks?

Constraint Handling & Multiple Objectives

	penalty functions	**constraints as objectives**	**modified dominance**
	Add penalty term to fitness	Introduce additional objective(s)	extend to infeasible solutions
overall constraint violation	*[Michalewicz 1992]*	*[Wright, Loosemore 2001]*	*[Deb 2001]*
constraints treated separately	?	*[Coello 2000]*	*[Fonseca, Fleming 1998]*

Archiving / Environmental Selection



deterministic truncation

archive = only nondominated solutions

Additional selection criteria:

- Density information / other preferences
- Time
- Chance

Outline

1. **Introduction:** Why multiple objectives make a difference
2. **Basic Principles:** Terms one needs to know
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4. **Performance Assessment:** How to compare algorithms
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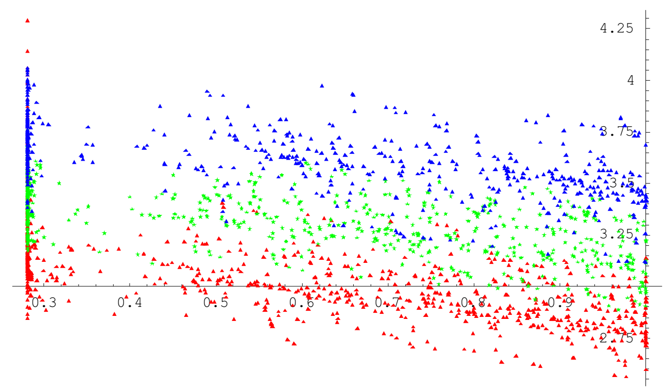
Once Upon a Time...

... multiobjective EAs were mainly compared visually:



ZDT6 benchmark problem: IBEA, SPEA2, NSGA-II

Performance Assessment: Approaches

❶ **Theoretically (by analysis):** difficult

- Limit behavior (unlimited run-time resources)
- Running time analysis

❷ **Empirically (by simulation):** standard

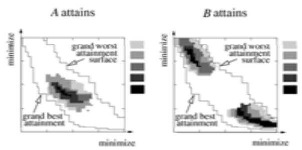
Problems: randomness, multiple objectives

Issues: quality measures, statistical testing, visualization, benchmark problems, parameter settings, …

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



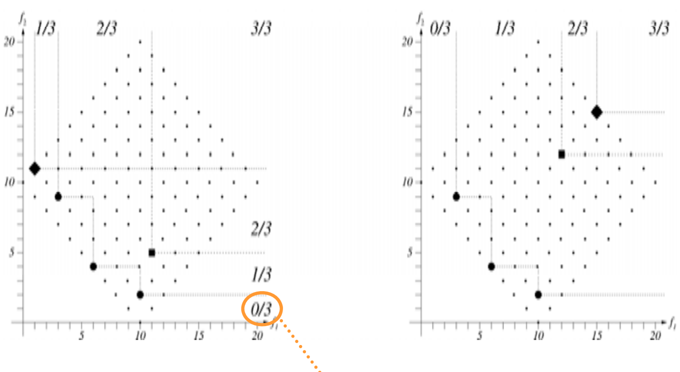
Quality indicator approach:

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

Indicator	A	B
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

Empirical Attainment Functions

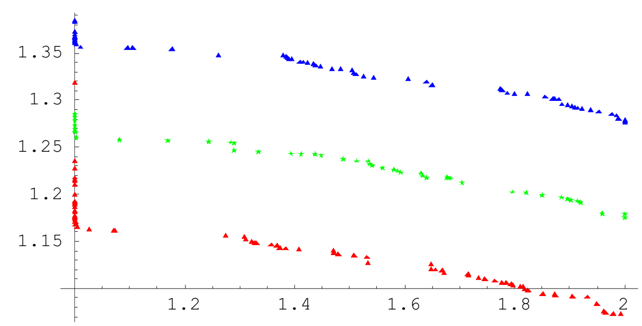
three runs of two multiobjective optimizers



frequency of attaining regions

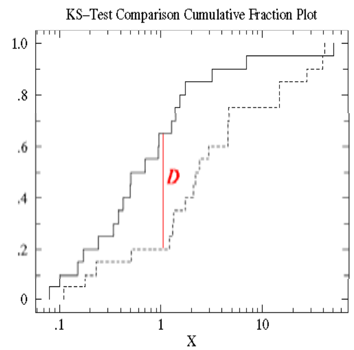
Attainment Plots

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



Attainment Function Analysis

- A Kolmogorov-Smirnov test examines the maximum difference between two cumulative distribution functions
- A KS-like test can be used to probe differences between the empirical attainment functions of a pair of optimizers, *A* and *B*
- The null hypothesis is that the attainment functions of *A* and *B* are identical
- The alternative hypothesis is that the distributions differ somewhere



[Fonseca et al. 2001]

Statistical Assessment

ZDT6

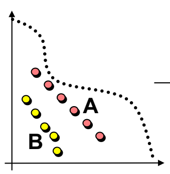
- IBEA – NSGA-II
  - significant difference (p=0)
- IBEA – SPEA2
  - significant difference (p=0)
- SPEA2 – NSGA-II
  - significant difference (p=0)

Knapsack

- IBEA – NSGA-II
  - no significant difference
- IBEA – SPEA2
  - no significant difference
- SPEA2 – NSGA-II
  - no significant difference

Quality Indicator Approach

Goal: compare two Pareto set approximations A and B



→

	A	B
hypervolume	*432.34*	*420.13*
distance	*0.3308*	*0.4532*
diversity	*0.3637*	*0.3463*
spread	*0.3622*	*0.3601*
cardinality	*6*	*5*

→ "**A** better"

Comparison method C = quality measure(s) + Boolean function

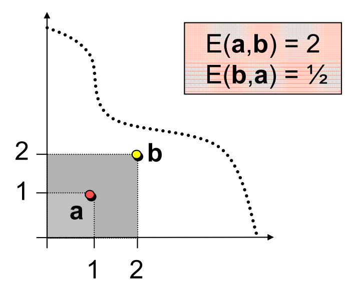
$$A, B \xrightarrow[\text{reduction}]{\text{quality measure}} R^n \xrightarrow[\text{interpretation}]{\text{Boolean function}} \text{statement}$$

reduction **interpretation**

Example: ε-Quality Indicator

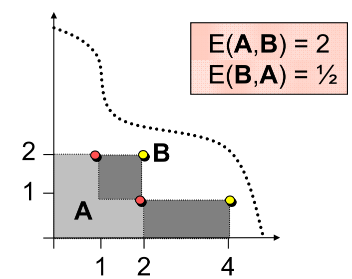
Two solutions:

$E(\mathbf{a},\mathbf{b}) = \max_{1 \le i \le n} \min_{\varepsilon} \varepsilon \cdot f_i(\mathbf{a}) \ge f_i(\mathbf{b})$



Two approximations:

$E(\mathbf{A},\mathbf{B}) = \max_{\mathbf{b} \in \mathbf{B}} \min_{\mathbf{a} \in \mathbf{A}} E(\mathbf{a},\mathbf{b})$



Unary quality indicator: I(A) = E(A,R) where R is a reference set

[Zitzler et al. 2003]

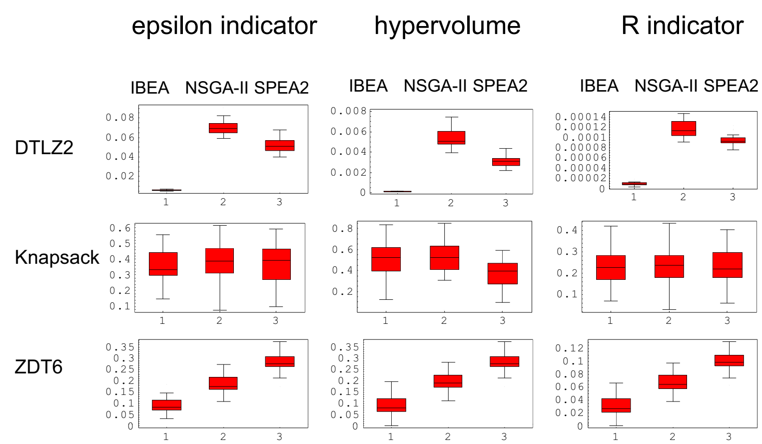
Power of Unary Quality Indicators

Important: compliance with dominance relations *[Zitzler et al. 2003]*

indicator	name / reference	Boolean function	compatibility	completeness
I_{HC}	enclosing hypercube indicator / Section III-B.1	$I_2^{HC}(A) < I_1^{HC}(B)$	$\succ\succ$	-
I_O	objective vector indicator / Section III-B.1	$I_i^O(A) < I_i^O(B)$	$\succ\succ$	-
I_H	hypervolume indicator / [7]	$I_H(A) > I_H(B)$	$\not\triangleright$	$\triangleright$
I_W	average best weight combination / [19]	$I_W(A) < I_W(B)$	$\not\triangleright$	$\succ\succ$
I_D	distance from reference set / [20]	$I_D(A) < I_D(B)$	$\not\triangleright$	$\succ\succ$
$I_{\epsilon 1}$	unary ϵ-indicator / Section III-B.2	$I_{\epsilon 1}(A) < I_{\epsilon 1}(B)$	$\not\triangleright$	$\succ\succ$
I_{PF}	fraction of Pareto-optimal front covered / [22]	$I_{PF}(A) > I_{PF}(B)$	$\not\triangleright$	-
I_P	number of Pareto points contained / Section III-B.2	$I_P(A) > I_P(B)$	$\not\triangleright$	-
I_{ER}	error ratio / [13]	$I_{ER}(A) > 0$	$\not\succ$	-
I_{CD}	chi-square-like deviation indicator / [14]	$I_{CD}(A) < I_{CD}(B)$	-	-
I_S	spacing / [23]	$I_S(A) < I_S(B)$	-	-
I_{ONVG}	overall nondominated vector generation / [13]	$I_{ONVG}(A) > I_{ONVG}(B)$	-	-
I_{GD}	generational distance / [13]	$I_{GD}(A) < I_{GD}(B)$	-	-
I_{ME}	maximum Pareto front error / [13]	$I_{ME}(A) < I_{ME}(B)$	-	-
I_{MS}	maximum spread / [21]	$I_{MS}(A) > I_{MS}(B)$	-	-
I_{MD}	minimum distance between two solutions / [24]	$I_{MD}(A) > I_{MD}(B)$	-	-
I_{CE}	coverage error / [24]	$I_{CE}(A) < I_{CE}(B)$	-	-
I_{DU}	deviation from uniform distribution / [25]	$I_{DU}(A) < I_{DU}(B)$	-	-
I_{OS}	Pareto spread / [26]	$I_{OS}(A) > I_{OS}(B)$	-	-
I_A	accuracy / [26]	$I_A(A) > I_A(B)$	-	-
I_{NDC}	number of distinct choices / [26]	$I_{NDC}(A) > I_{NDC}(B)$	-	-
I_{CL}	cluster / [26]	$I_{CL}(A) < I_{CL}(B)$	-	-

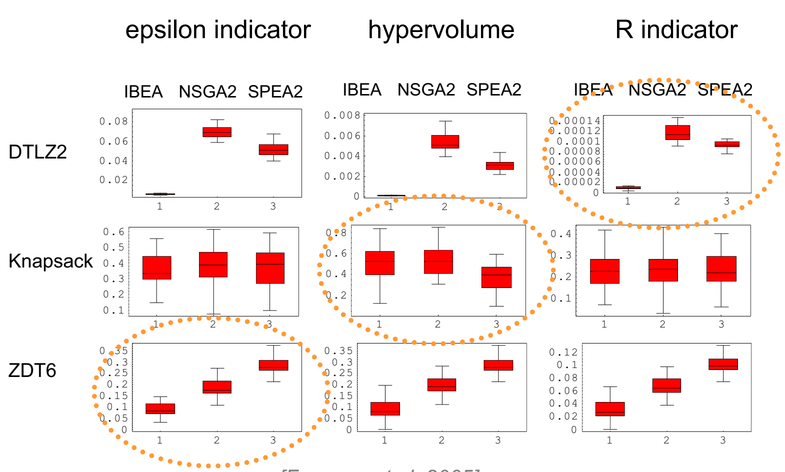
strictly better | not weakly better | not better | weakly better

Example: Box Plots



[Fonseca et al. 2005]

Example: Box Plots



[Fonseca et al. 2005]

Statistical Assessment (Kruskal Test)

ZDT6
Epsilon

is better than

	IBEA	NSGA2	SPEA2
IBEA		~0	~0
NSGA2	1		~0
SPEA2	1	1	

Overall p-value = 6.22079e-17.
Null hypothesis rejected (alpha 0.05)

DTLZ2
R

is better than

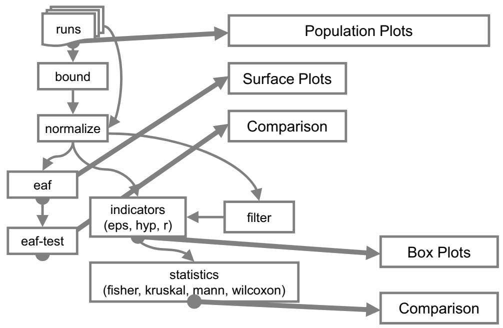
	IBEA	NSGA2	SPEA2
IBEA		~0	~0
NSGA2	1		1
SPEA2	1	~0	

Overall p-value = 7.86834e-17.
Null hypothesis rejected (alpha 0.05)

Knapsack/Hypervolume: H0 = No significance of any differences

Performance Assessment Tools

- Reference set calculation
- Attainment function calculation
- Indicators
- Statistical testing procedures



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

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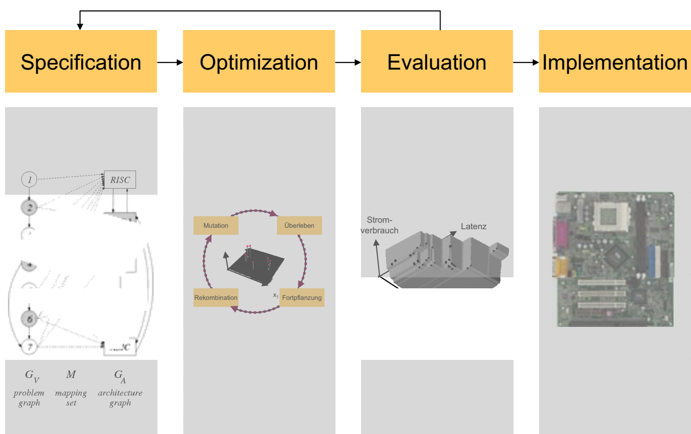
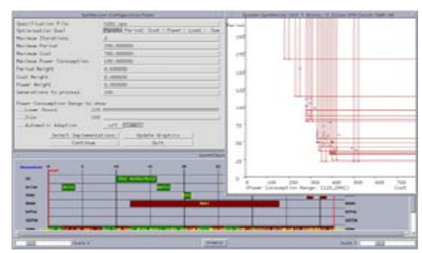
Design Space Exploration



Examples: computer design, biological experiment design, etc.

Example Applications

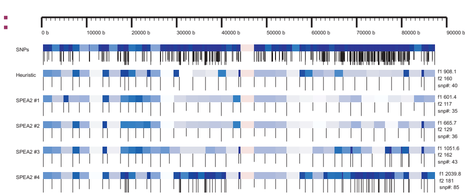


Architecture exploration:
- min. cost
- max. performance
- min. power consumption

[Eisenring, Thiele, Zitzler 2000]

Genetic marker selection:
- min. cost
- max. sensitivity

[Hubley, Zitzler, Roach 2003]



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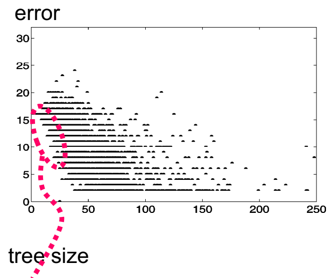
Application: Genetic Programming

GECCO 2008
Tutorial on EMO

Problem: Trees grow rapidly
- Premature convergence
- Overfitting of training data

Common approaches:
- Constraint (tree size limitation)
- Penalty term (parsimony pressure)
- Objective ranking (size post-optimization)
- Structure-based (ADF, etc.)

Multiobjective approach:
Optimize both error and size



Keep and optimize small trees (potential building blocks)

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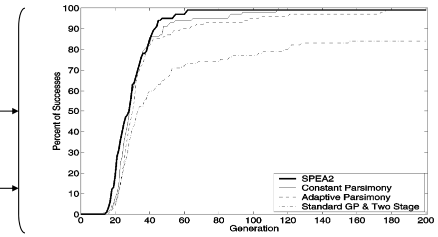
Multiobjective GP: Results

GECCO 2008
Tutorial on EMO

Multiobjective approach (SPEA2) can find

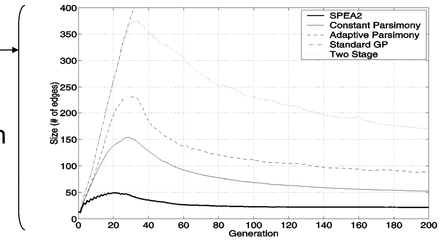
- a correct solution with higher probability
- a correct solution slightly faster



- more compact (correct) solutions

than alternative approaches on even-parity problem.

[Bleuler et al. 2001]



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Outline

GECCO 2008
Tutorial on EMO

1. **Introduction:** Why multiple objectives make a difference
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4. **Performance Assessment:** Once upon a time
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The Concept of PISA

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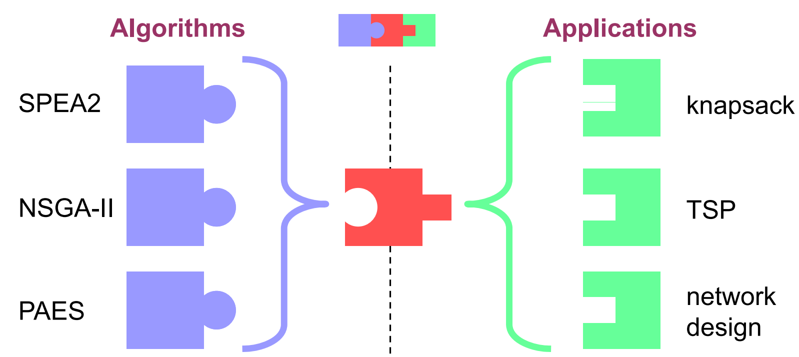
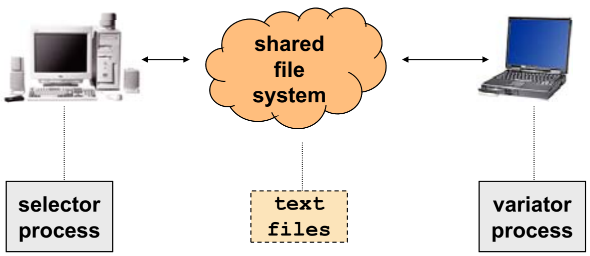


text-based
Platform and programming language independent **I**nterface for **S**earch **A**lgorithms *[Bleuler et al.: 2003]*

PISA: Implementation



application independent:

- mating / environmental selection
- individuals are described by IDs and objective vectors

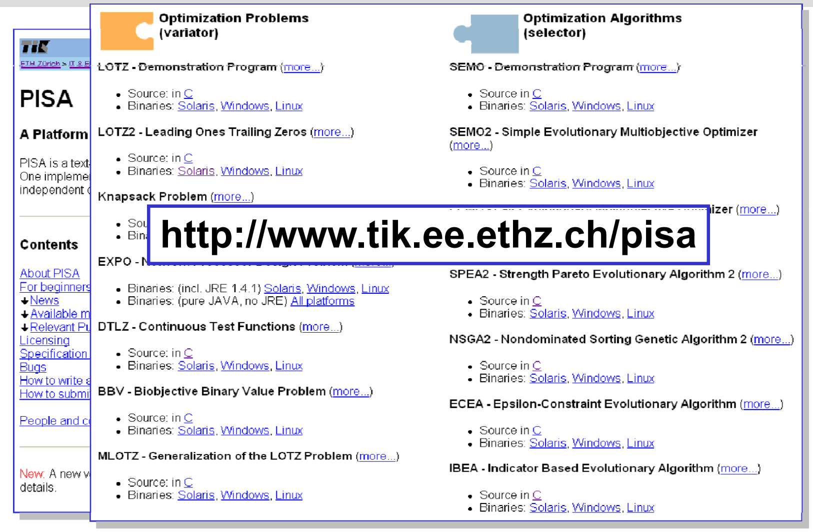
handshake protocol:

- state / action
- individual IDs
- objective vectors
- parameters

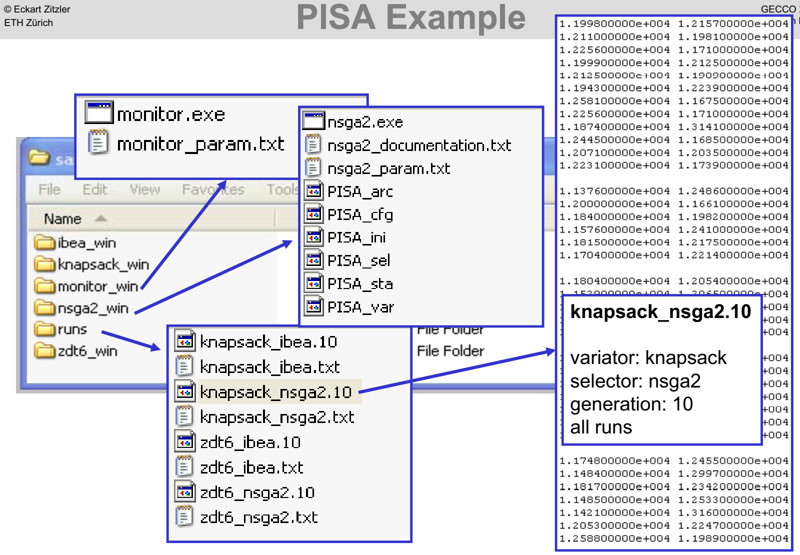
application dependent:

- variation operators
- stores and manages individuals

PISA Website



PISA Example



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 (EMO 2009 to be held in Nantes, France)

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, 2002

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