Tutorial on Evolutionary Multiobjective Optimization GECCO 2007

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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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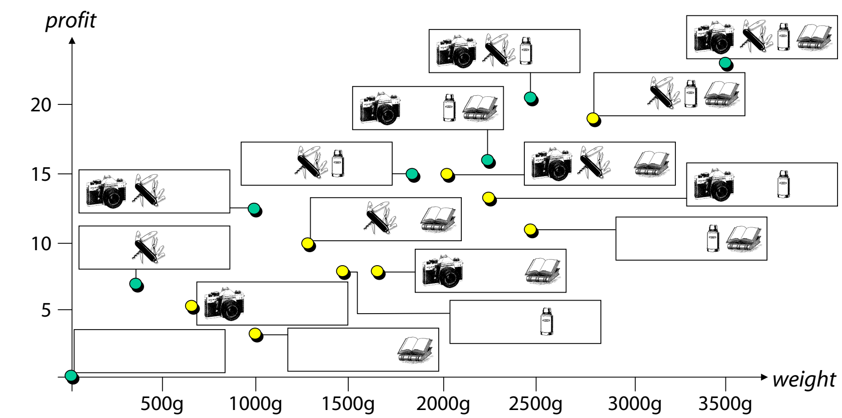
The Search Space



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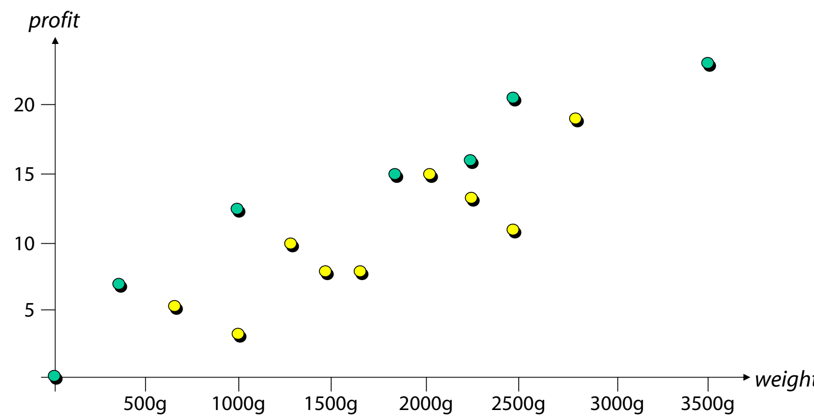
The Trade-off Front

Observations: ❶
❷ some solutions (●) are better than others (●)



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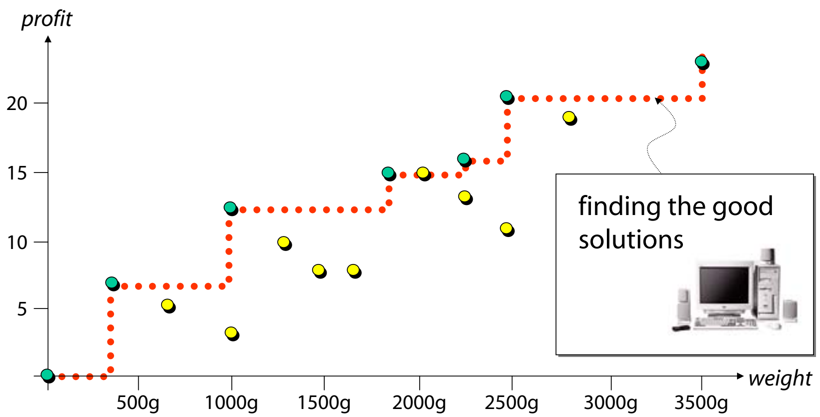
The Trade-off Front

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



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The Trade-off Front

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Observations: ❶ there is no single optimal solution, but
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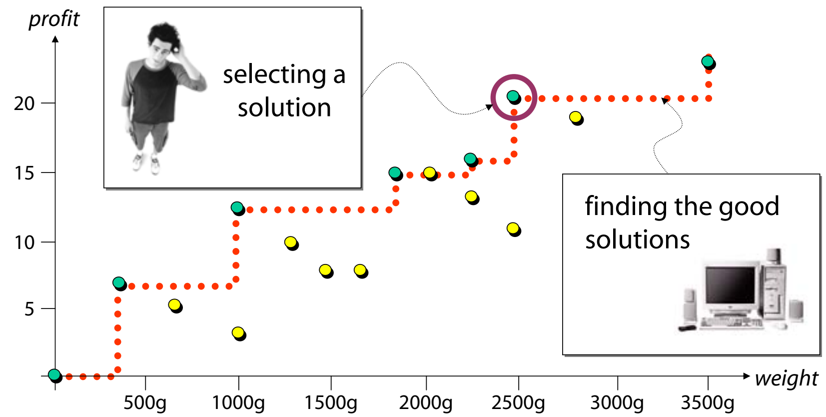

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Decision Making: Selecting a Solution

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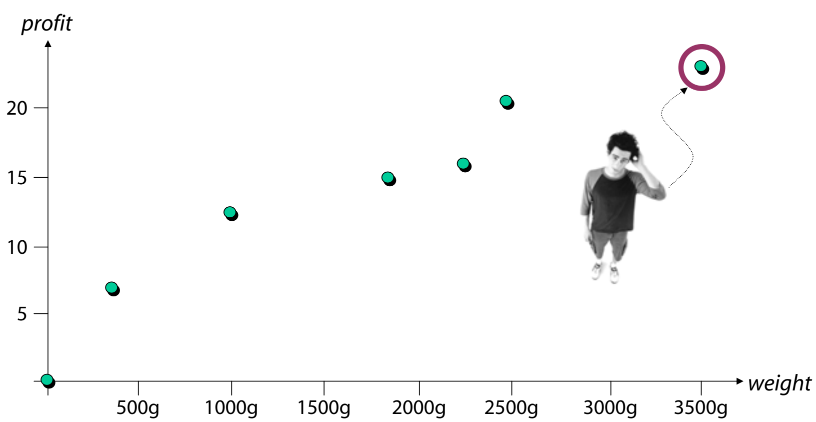
Approaches:
- profit more important than cost (ranking)



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Decision Making: Selecting a Solution

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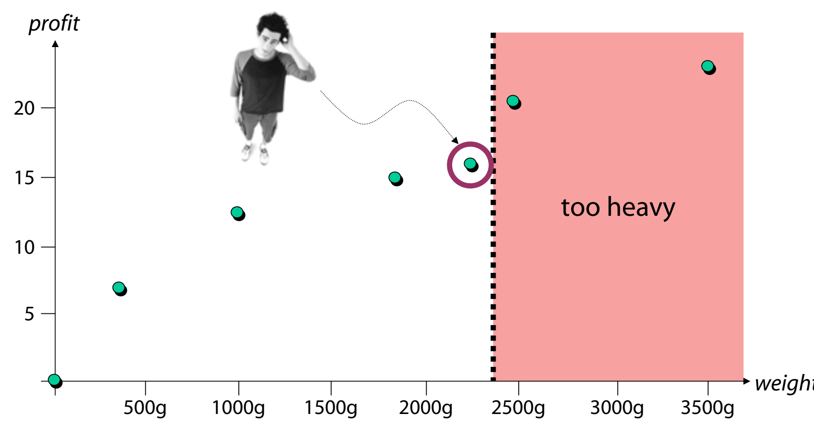
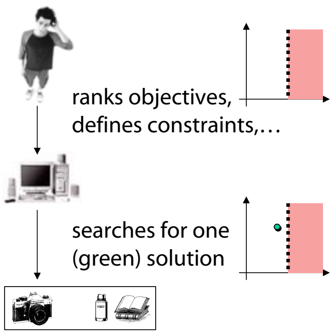
Approaches:
- profit more important than cost (ranking)
- weight must not exceed 2400g (constraint)



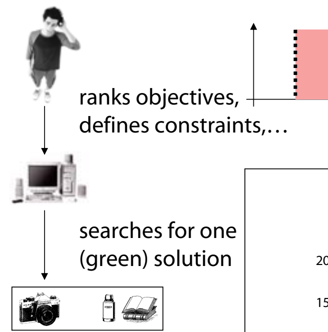
When to Make the Decision

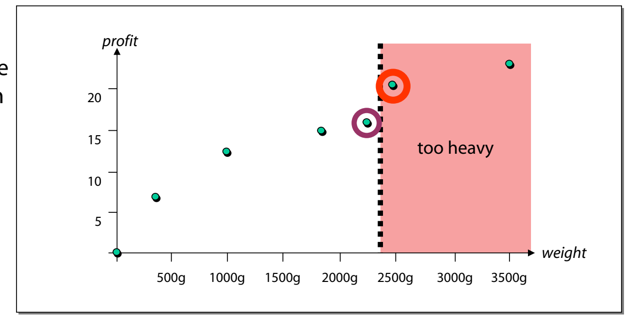
Before Optimization:



When to Make the Decision

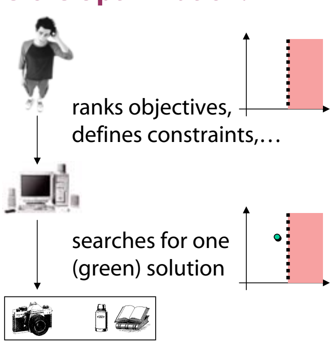
Before Optimization:



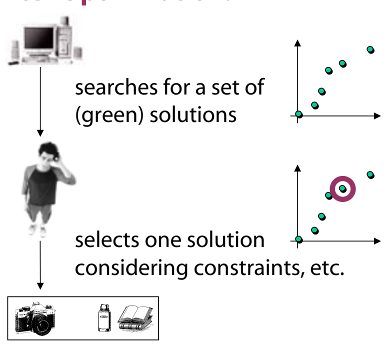


When to Make the Decision

Before Optimization:



After Optimization:



- decision making often easier
- EAs well suited

Outline

1. **Introduction:** Why multiple objectives make a difference
2. **Basic Principles:**
3. **Algorithm Design:** Do it yourself
4. **Performance Assessment:**
5. **Applications Domains:** Where EMO is useful
6. **Further Information:**

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Optimization Problem: Definition

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

- *X* denotes the decision space containing the elements among which the best is sought; elements of 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 $f: X \rightarrow Z$
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*.

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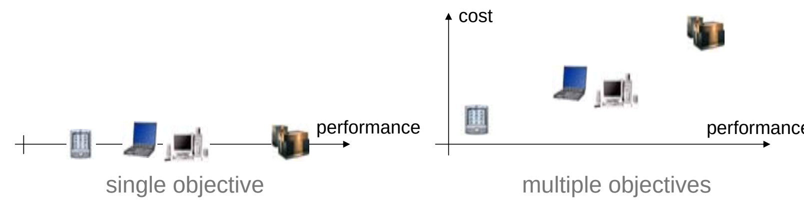
Objective Functions

- Usually, consists of one or several functions $_1, ..., f_n$
assign each solution a real number. Such a function
$f_i: X \rightarrow \Re$
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:



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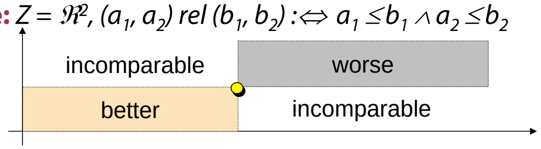
Comparing Objective Vectors

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

- *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).

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Preference Structures

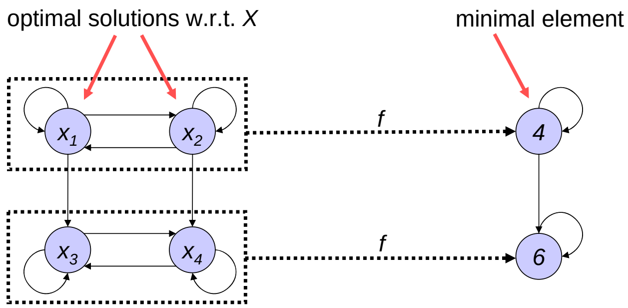
- The function *f* together with the partially ordered set *(Z, rel)*
a preference structure on the decision space *X*
solutions the decision maker / user prefers to other solutions:

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

- One says:
  - Two solutions x_1, x_2 are equal iff $= x_2$;
  - A solution is indifferent to a solution iff and *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 ( );
  - A solution x_1 is incomparable to a solution iff neither x_2 nor x_2 *prefrel* x_1.

The Notion of Optimality

- A solution $x \in X$ $S \subseteq X$
  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 $f_i: X \rightarrow \Re$ $Z = \Re^n$
- all objectives are to be maximized

Usually considered relation: weak Pareto dominance

- $(X, \Re^n, (f_1, ..., f_n), \;) \preceq$
- weak Pareto dominance:

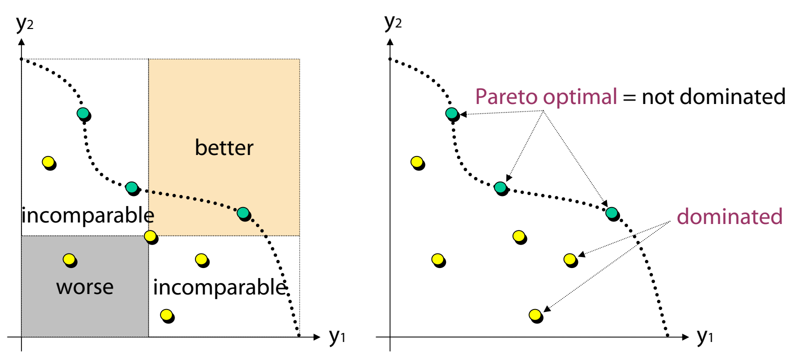
$$x_1 \preceq x_2 :\Leftrightarrow \forall 1 \leq i \leq n : f_i(x_1) \geq f_i(x_2)$$

- Pareto dominance: strict version of weak Pareto dominance

$$x_1 \prec x_2 :\Leftrightarrow x_1 \preceq x_2 \;\wedge\; x_2 \not\preceq x_1$$

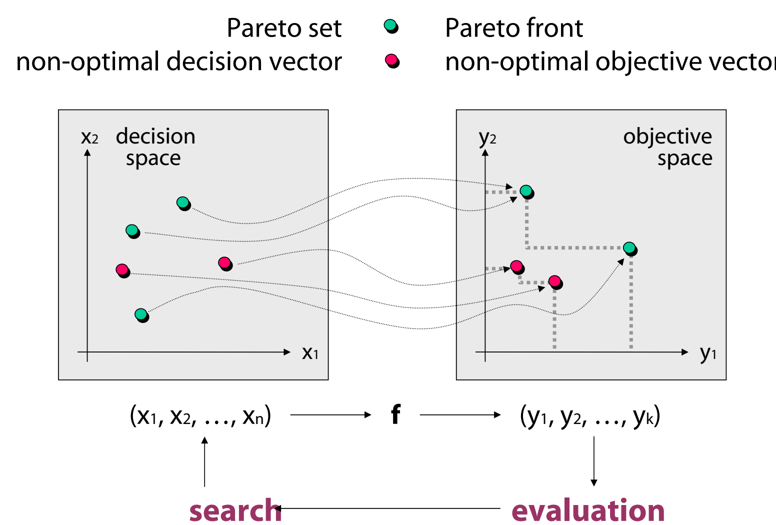
Illustration of Pareto Optimality

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



Pareto(-optimal) set

Decision and Objective Space



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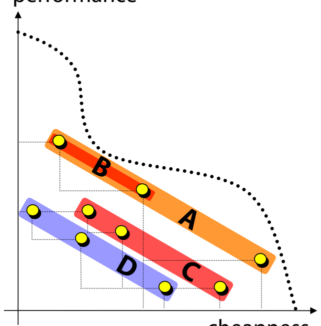
Pareto Set Approximations

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

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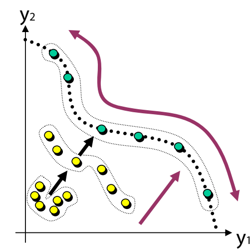
What Is the Optimization Goal?

- 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



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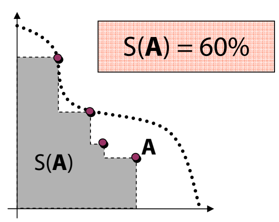
Preference Information

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:
about the decision maker's preferences
(limited memory, selection)

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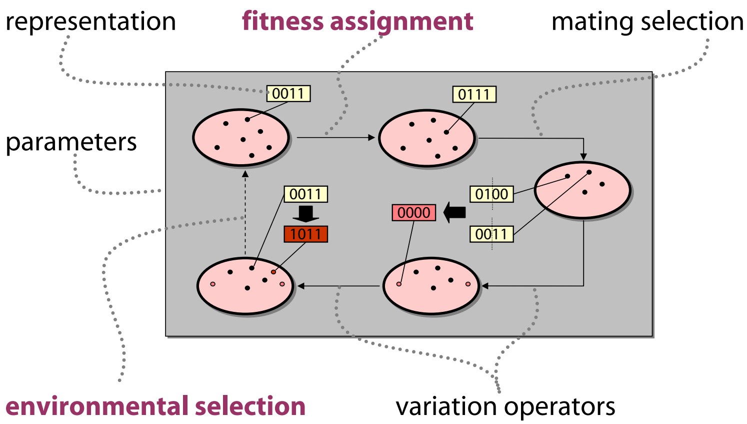
Design Choices



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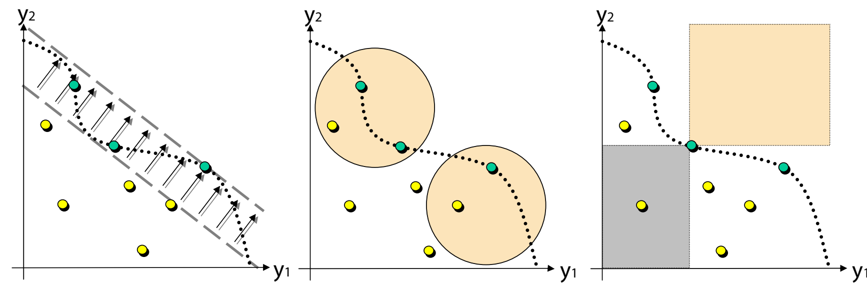
Ranking Solutions

aggregation-based *weighted sum*

criterion-based *VEGA* *SPEA2*

dominance-based



parameter-oriented
scaling-dependent

set-oriented
scaling-independent

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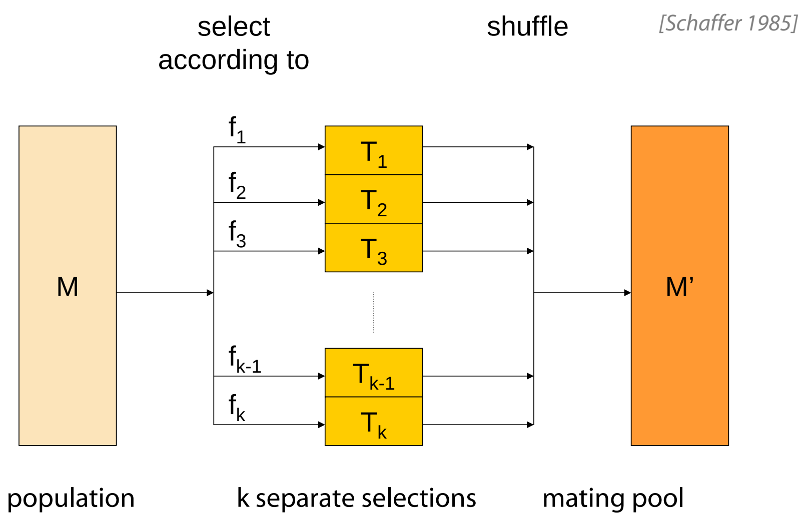
Example: VEGA

[Schaffer 1985]



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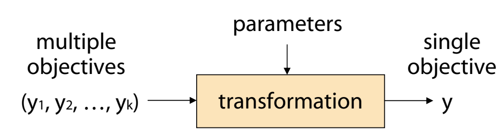
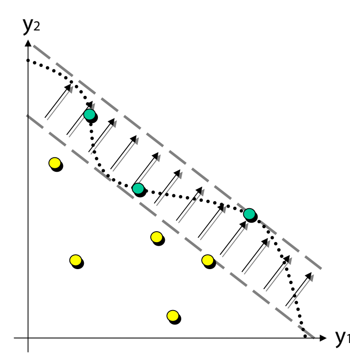
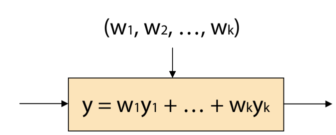
Aggregation-Based Ranking





Example: weighting approach



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

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Example: Weighted Sum

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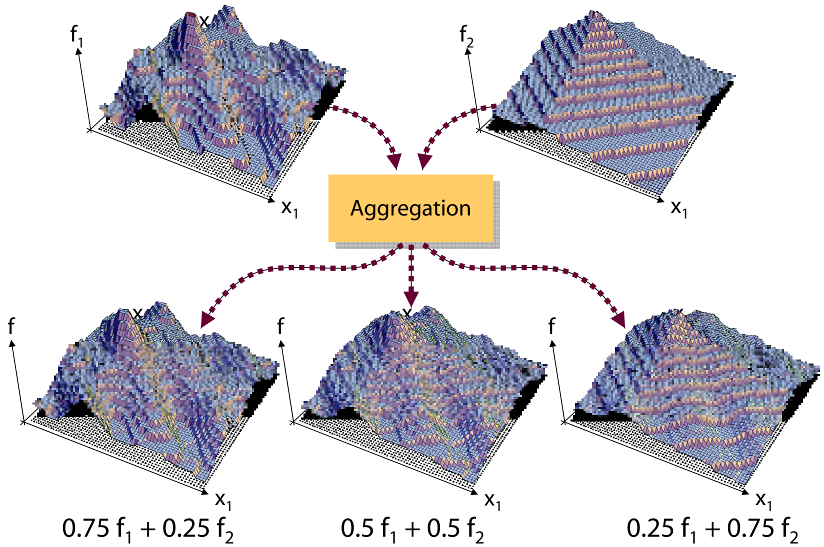

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Example: Multistart Constraint Method

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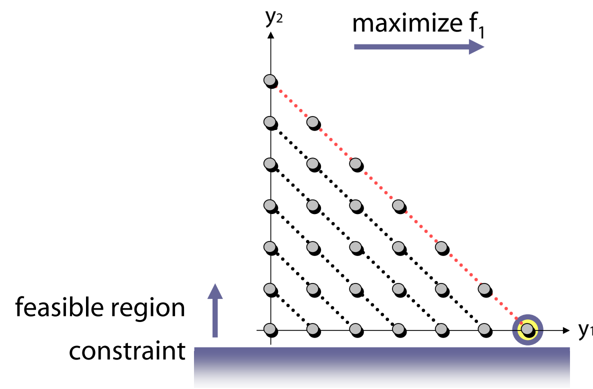
Underlying concept:

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



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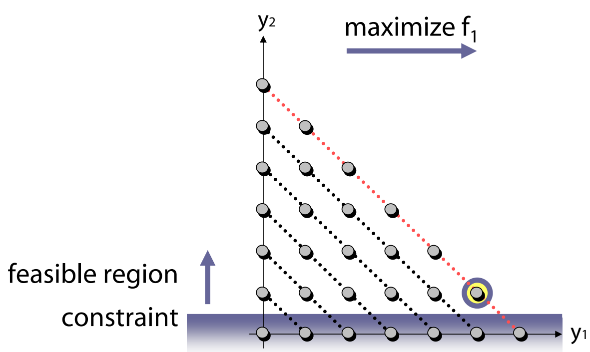

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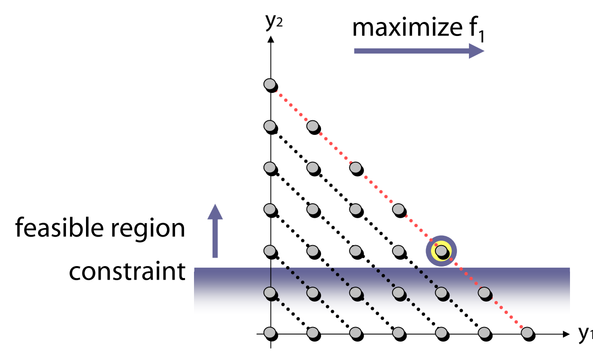
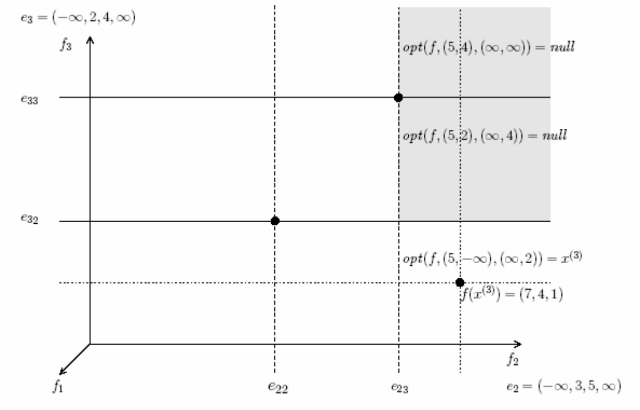


Example: Multistart Constraint Method (Cont'd)

[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?

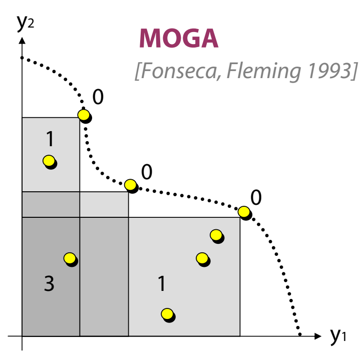
Examples:

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

Example: MOGA and SPEA2

MOGA

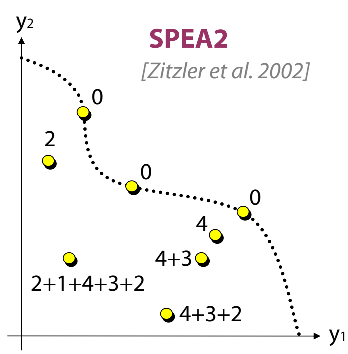
[Fonseca, Fleming 1993]



R (raw fitness) =
#dominating solutions

SPEA2

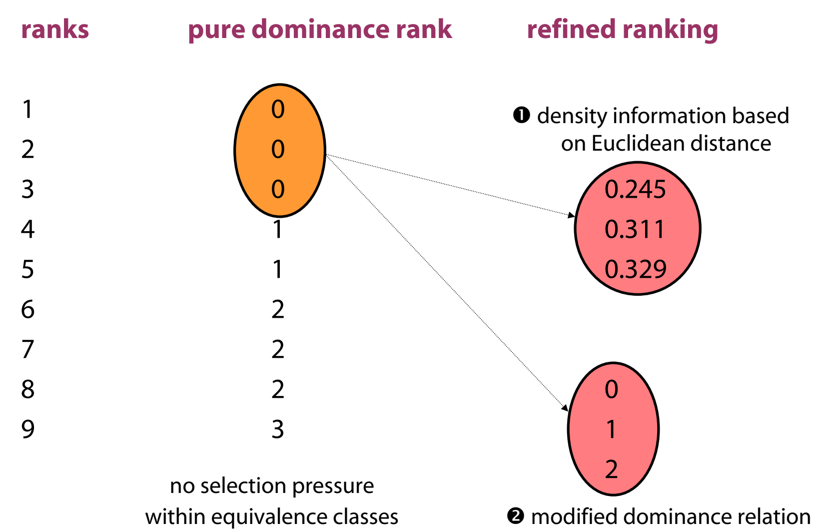
[Zitzler et al. 2002]



S (strength) =
#dominated solutions

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

Refining Rankings



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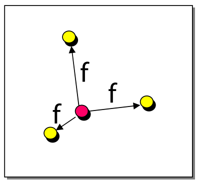
Methods Based On Euclidean Distance

Density estimation techniques: *[Silverman 1986]*

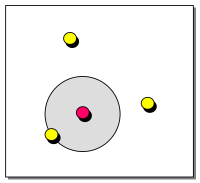
Kernel
MOGA

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



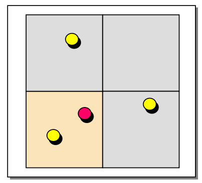
Nearest neighbor

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



Histogram
PAES

density estimate
=
number of solutions in the same box



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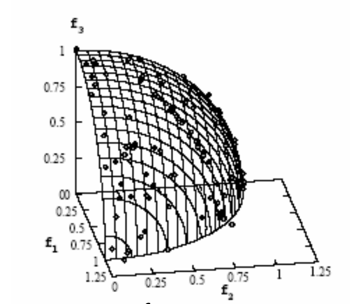
Computation Effort Versus Accuracy

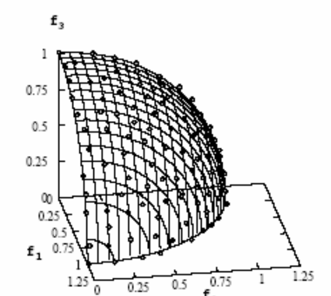
Two Nearest Neighbor Variants

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]

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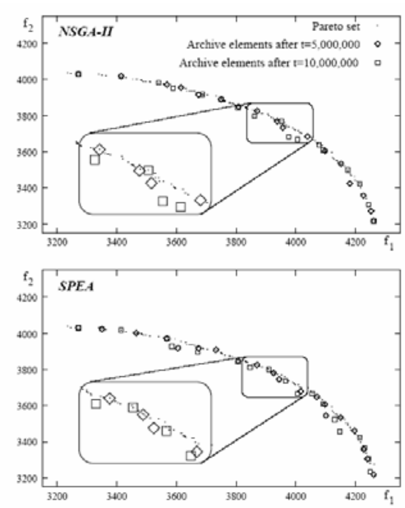
The Problem of Deterioration

Observation:
The use of Euclidean distance can lead to deterioration



Knapsack problem
[Laumanns et al. 2002]

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Refinement of Dominance Relations

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

A is preferable over B ⇔

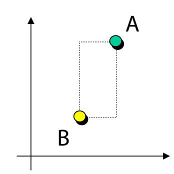
$$(\boldsymbol{u}_p^{\frown u} \; _p < \boldsymbol{v}_p^{\frown u}) \vee \{(\boldsymbol{u}_p^{\frown u} = \boldsymbol{v}_p^{\frown u}) \wedge [(\boldsymbol{v}_p^{\smile u} \not\leq \boldsymbol{g}_p^{\smile u}) \vee (\boldsymbol{u}_{1,\cdots,p-1} \underset{\boldsymbol{g}_{1,\cdots,p-1}}{\prec} \boldsymbol{v}_{1,\cdots,p-1})]\}$$

Continuous dominance "relations":

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

$I_{\varepsilon+}(A,B) \geq 0$ 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

Künzli 2004]

function I (binary quality indicator) with

A dominates B ⇔ 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(n^2)

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(n^2)

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

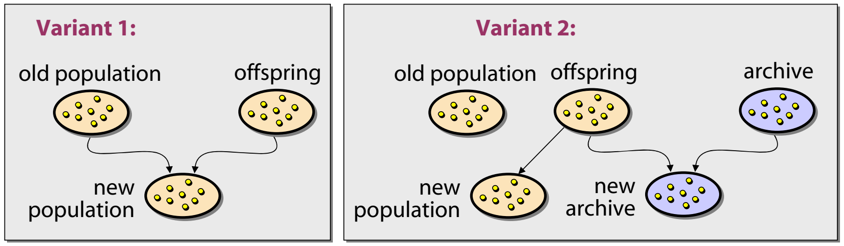
Further Design Aspects

- **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 Add penalty term to fitness	**constraints as objectives** Introduce additional objective(s)	**modified dominance** 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:**
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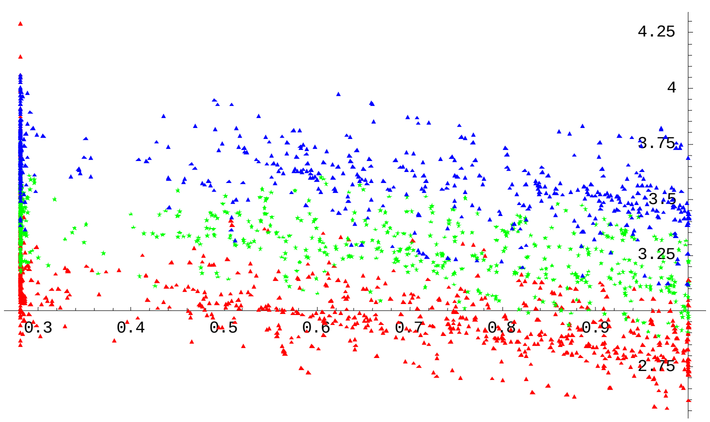
Once Upon a Time...

... 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, …

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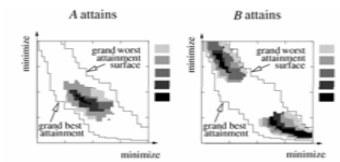
Two Approaches for Empirical Studies

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

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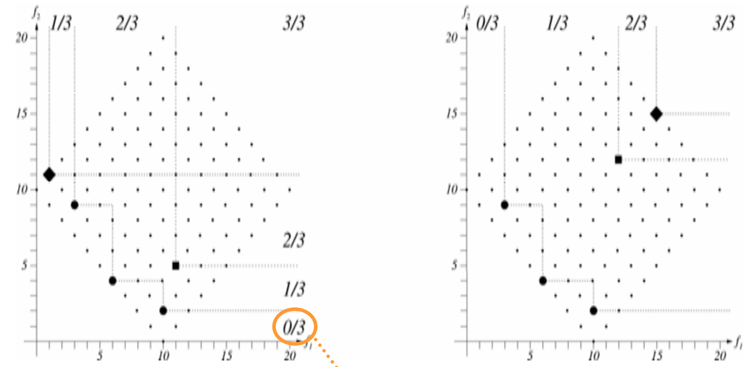
Empirical Attainment Functions

three runs of two multiobjective optimizers



frequency of attaining regions

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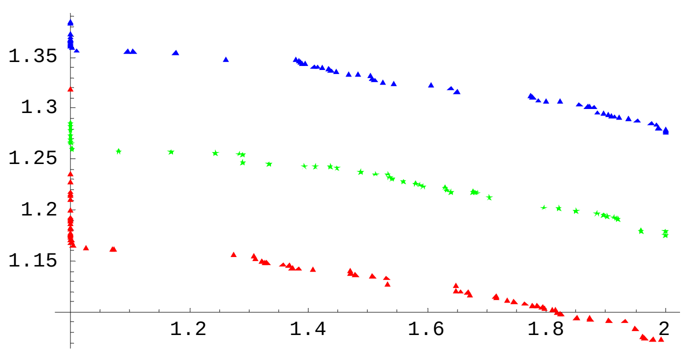
Attainment Plots

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



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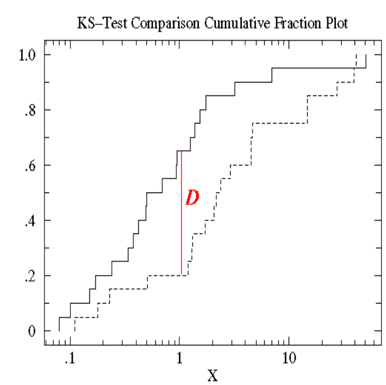
Attainment Function Analysis

- 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* *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]

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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

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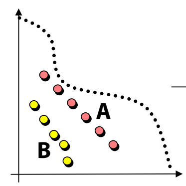
Quality Indicator Approach

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 —quality measure→ $\mathbb{R}^n$ —Boolean function→ statement

reduction **interpretation**

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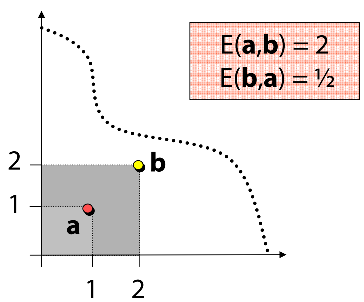
Example: ε-Quality Indicator

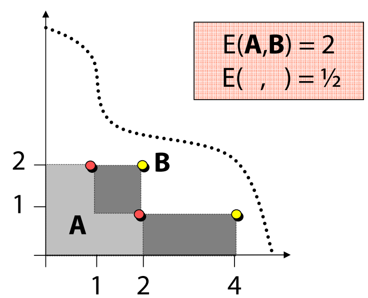
Two solutions:

E(**a**,**b**) =
max$_{1 \leq i \leq n}$ min$_\varepsilon$ ε · f$_i$( ) ≥ f$_i$( )



Two approximations:

E(**A**,**B**) =
max$_{\mathbf{b} \in \mathbf{B}}$ $_{\mathbf{a} \in \mathbf{A}}$ **a b**



Unary quality indicator:

[Zitzler et al. 2003]

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Power of Unary Quality Indicators

Important: *[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]	$I_H(A) > I_H(B)$	$\ntriangleright$	$\triangleright$
I_W	average best weight combination / [19]	$I_W(A) < I_W(B)$	$\ntriangleright$	$\succ\succ$
I_D	distance from reference set / [20]	$I_D(A) < I_D(B)$	$\ntriangleright$	$\succ\succ$
$I_{\epsilon 1}$	unary ϵ-indicator / Section III-B.2	$I_{\epsilon 1}(A) < I_{\epsilon 1}(B)$	$\ntriangleright$	$\succ\succ$
I_{PF}	fraction of Pareto-optimal front covered / [22]	$I_{PF}(A) > I_{PF}(B)$	$\ntriangleright$	-
I_P	number of Pareto points contained / Section III-B.2	$I_P(A) > I_P(B)$	$\ntriangleright$	-
I_{ER}	error ratio / [13]	$I_{ER}(A) > 0$	$\nsucc$	-
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

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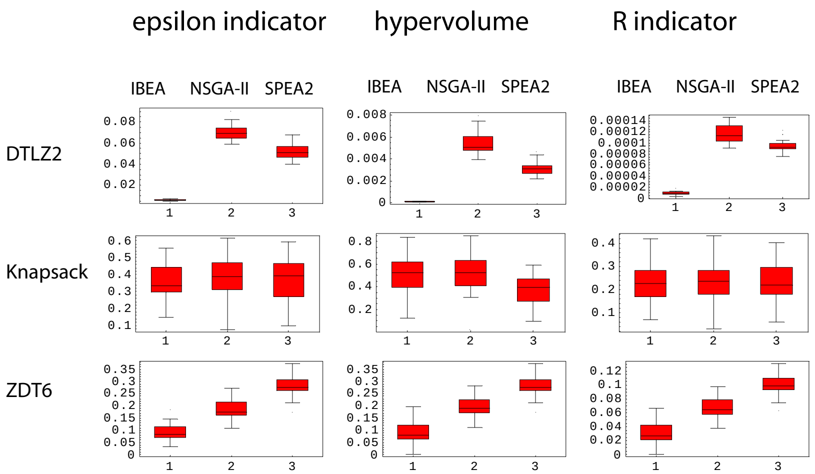
Example: Box Plots



[Fonseca et al. 2005]

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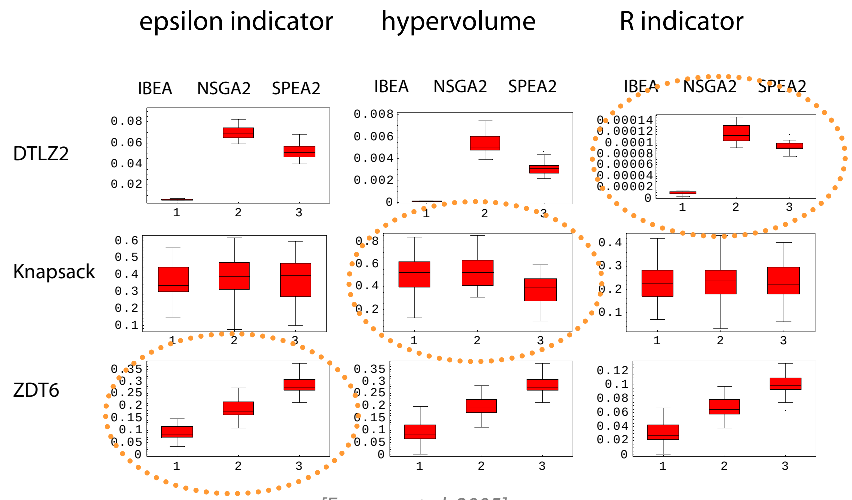
Example: Box Plots



[Fonseca et al. 2005]

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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

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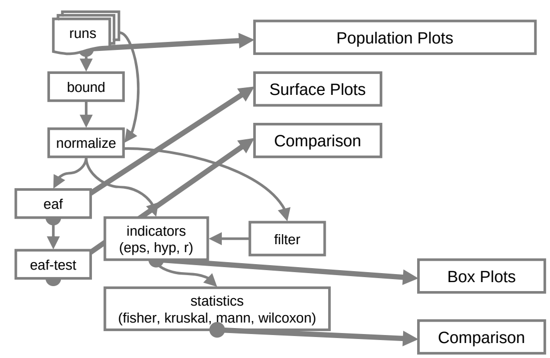
Performance Assessment Tools

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



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

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Outline

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1. **Introduction:**
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Design Space Exploration

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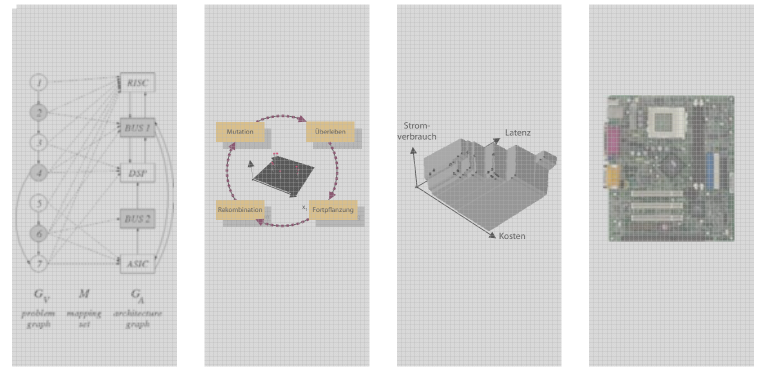
Specification → Optimization → Evaluation → Implementation



Examples: computer design, biological experiment design, etc.

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Example Applications

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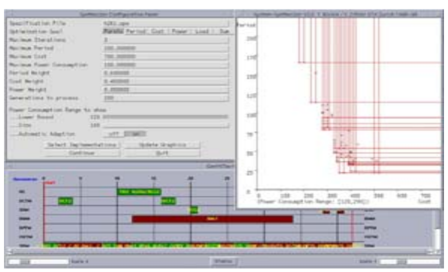
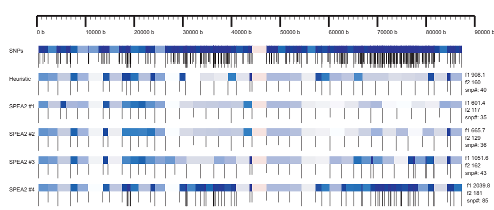


Architecture exploration:
- min. cost
- max. performance
- min. power consumption

[Eisenring, Thiele, Zitzler 2000]

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

[Hubley, Zitzler, Roach 2003]



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Application: Genetic Programming

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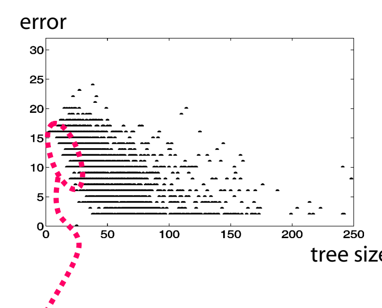
Problem: Trees grow rapidly
- Premature convergence
- Overfitting of training data

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

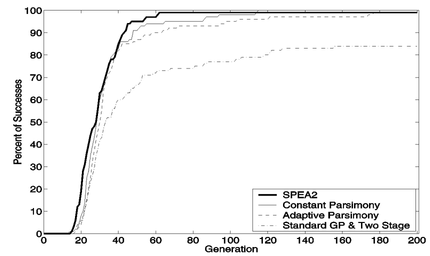


Keep and optimize small trees
(potential building blocks)

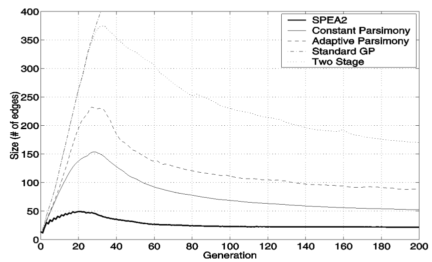
Multiobjective GP: Results

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

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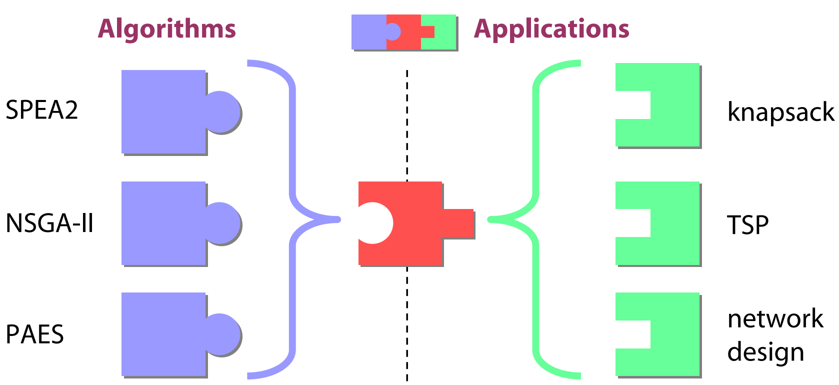
The Concept of PISA



text-based

Platform and programming language independent **I**nterface

[Bleuler et al.: 2003]

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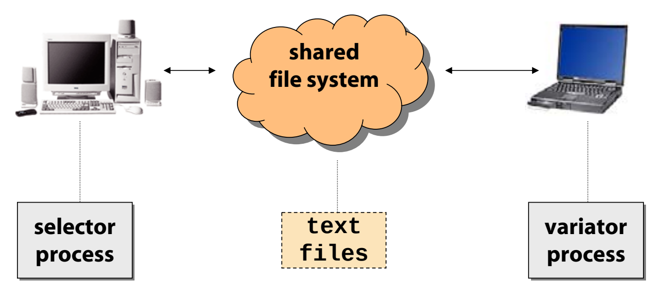
PISA: Implementation



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

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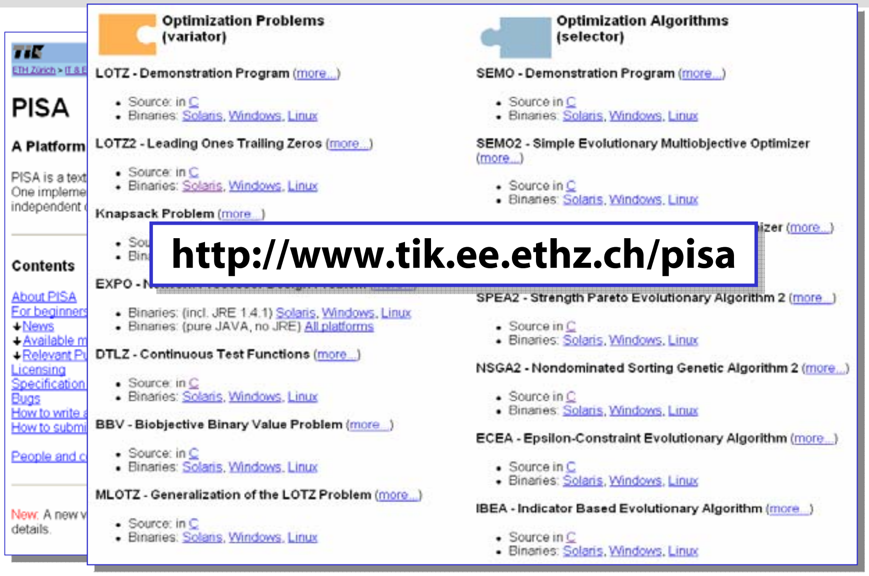
PISA Website



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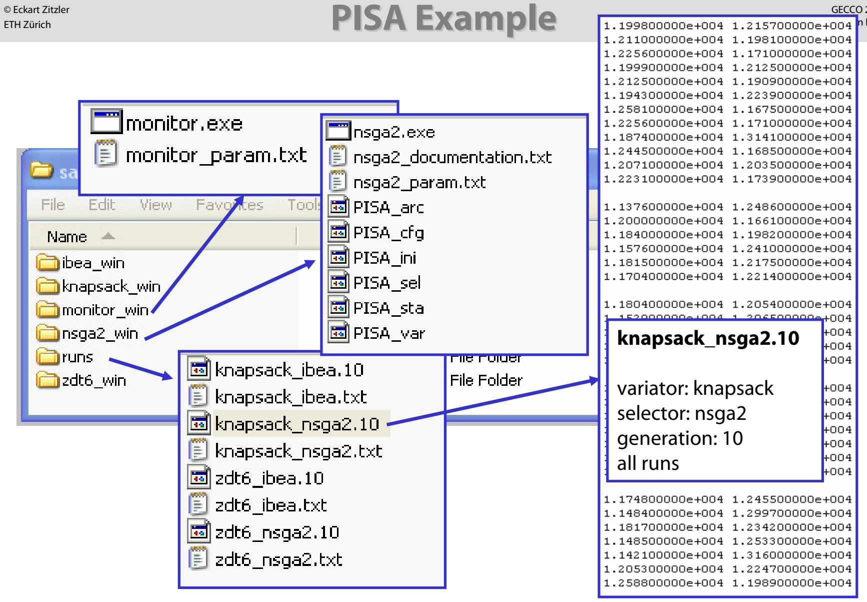
PISA Example



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The EMO Community

Links:

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

Events:

- Conference on Evolutionary Multi-Criterion Optimization (EMO 2009 to be held in 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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