Metaheuristics for Multi-objective Optimization: A Unified View

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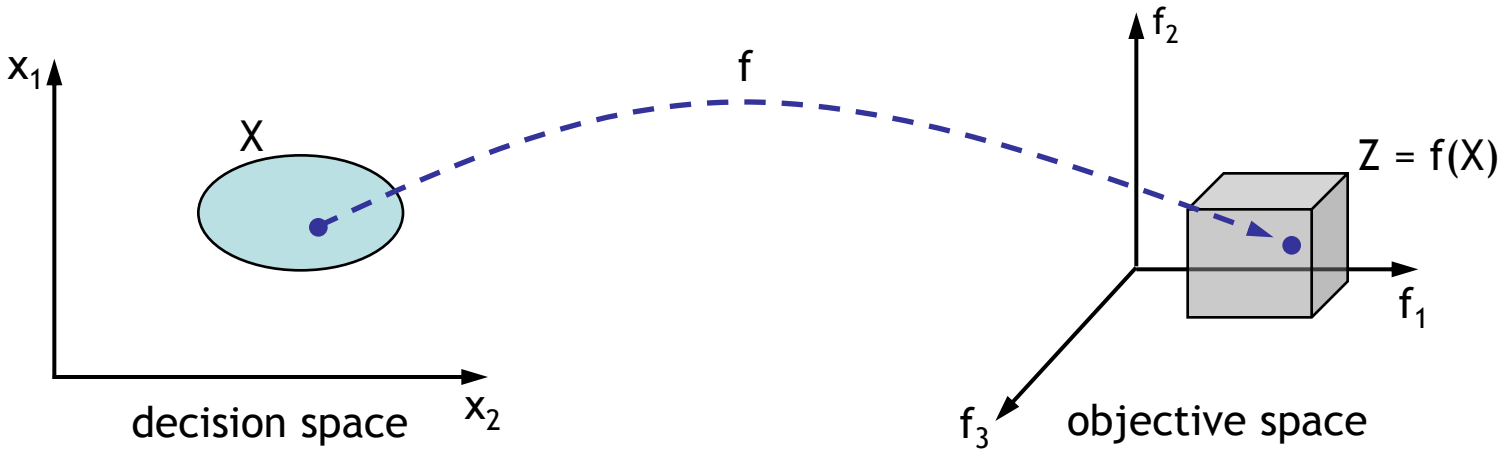
Outline

- Multi-objective optimization: definitions, problems, etc
- A unified view of multi-objective metaheuristics
- Landscapes and performance analysis
- Software framework for multi-objective optimization: ParadisEO-MOEO

Multiobjective Optimization Problem (MOP)

$$(MOP) = \begin{cases} \text{« min »} & f(x) = (f_1(x), f_2(x), \ldots, f_n(x)) \\ \text{s. t.} & x \in X \end{cases}$$

- $n \geq 2$ objective functions (f1, f2, …, fn)
- $x \in X$ is a decision vector
- X is the feasible set in the decision space
- Z is the feasible set in the objective space

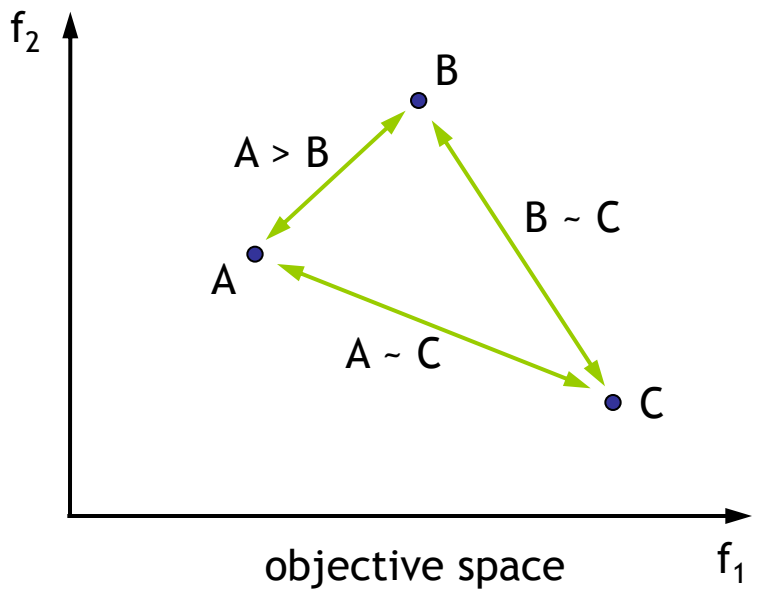


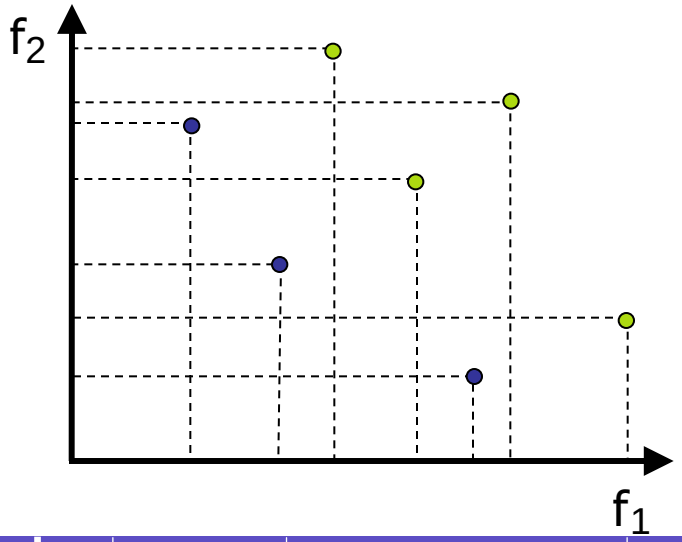
Pareto dominance [Pareto 1896]

An objective vector z Є Z dominates an objective vector z' Є Z iff

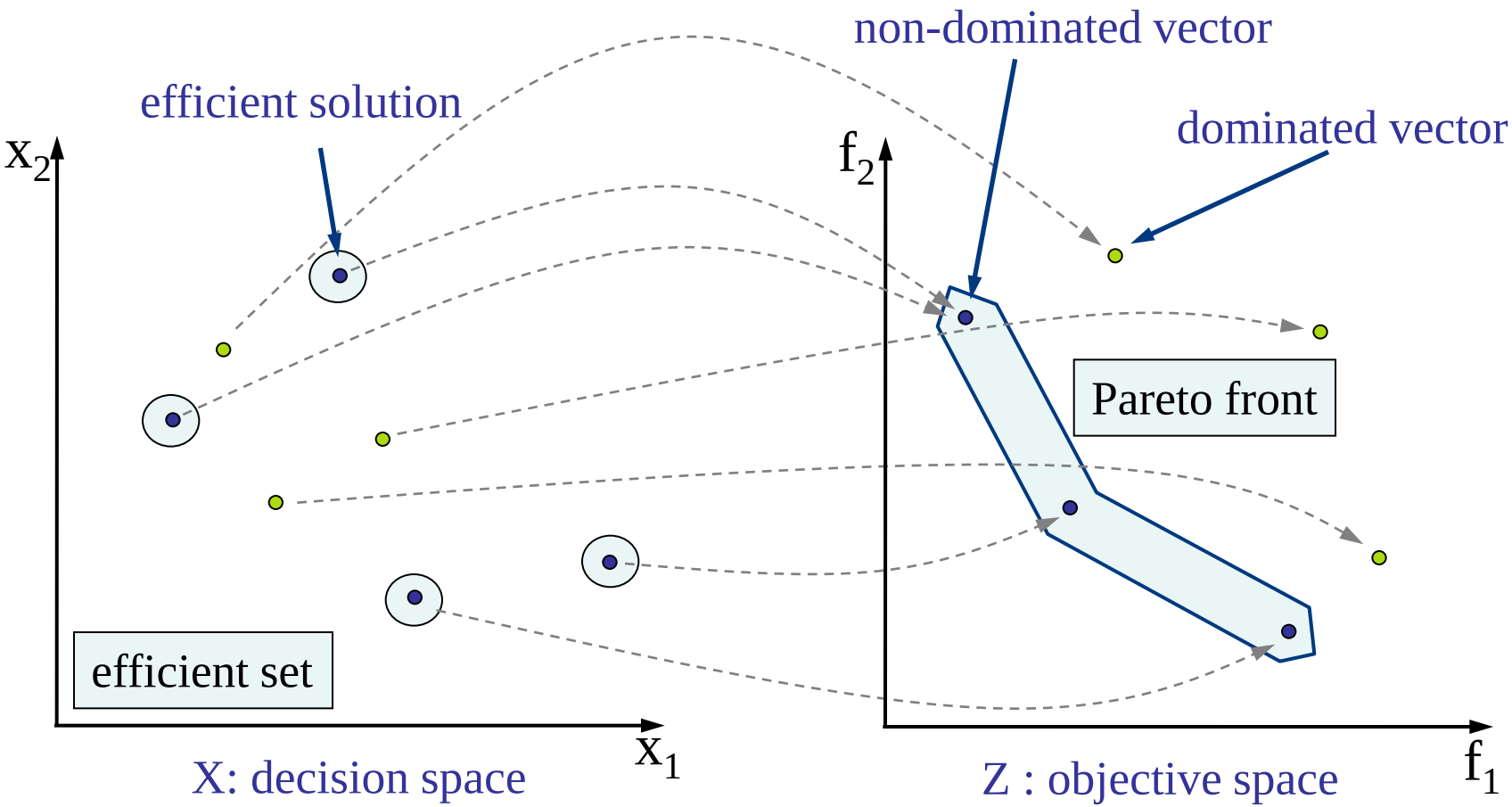
- $\forall i \in \{1,\ldots,n\}$, $z_i \leq z_i'$
- $\exists j \in \{1,\ldots,n\}$, $z_j < z_j'$

Non-dominated solution (eligible, efficient, non inferior, Pareto optimal)





Multi-objective Optimization Problem (MOP)



Multi-objective optimization problems

- **Academic problems**
  - Continuous optimization: ZDT, CTP, DTLZ,
  - Combinatorial optimization problems
    - Polynomially problems (assignment, spanning tree, shortest path)
    - NP-hard problems (TSP, QAP, knapsack, routing, scheduling)
- **Real-life applications**
  - Engineering design
  - Environment and energetics
  - Networks
  - Control
  - Bioinformatics and computational biology
  - Transportation and logistics

Resolution Approaches

Multiobjective optimization as a part of the decision making process:

A priori

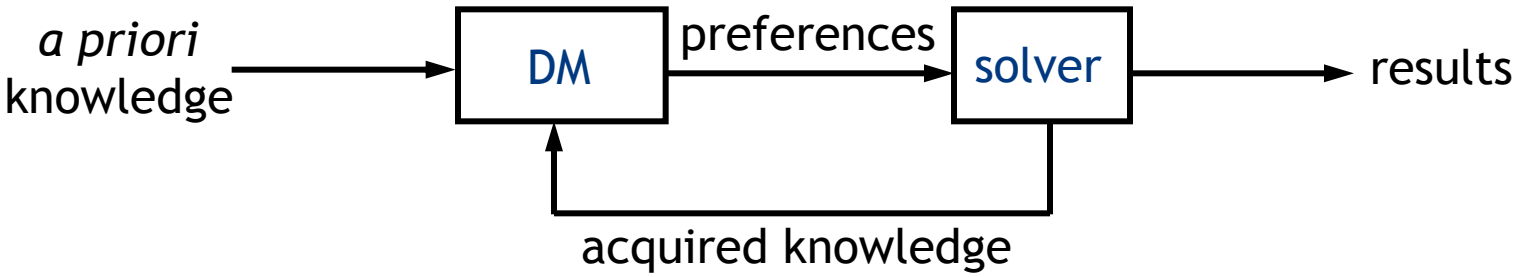
- Decision Maker (DM) before the resolution process

A posteriori

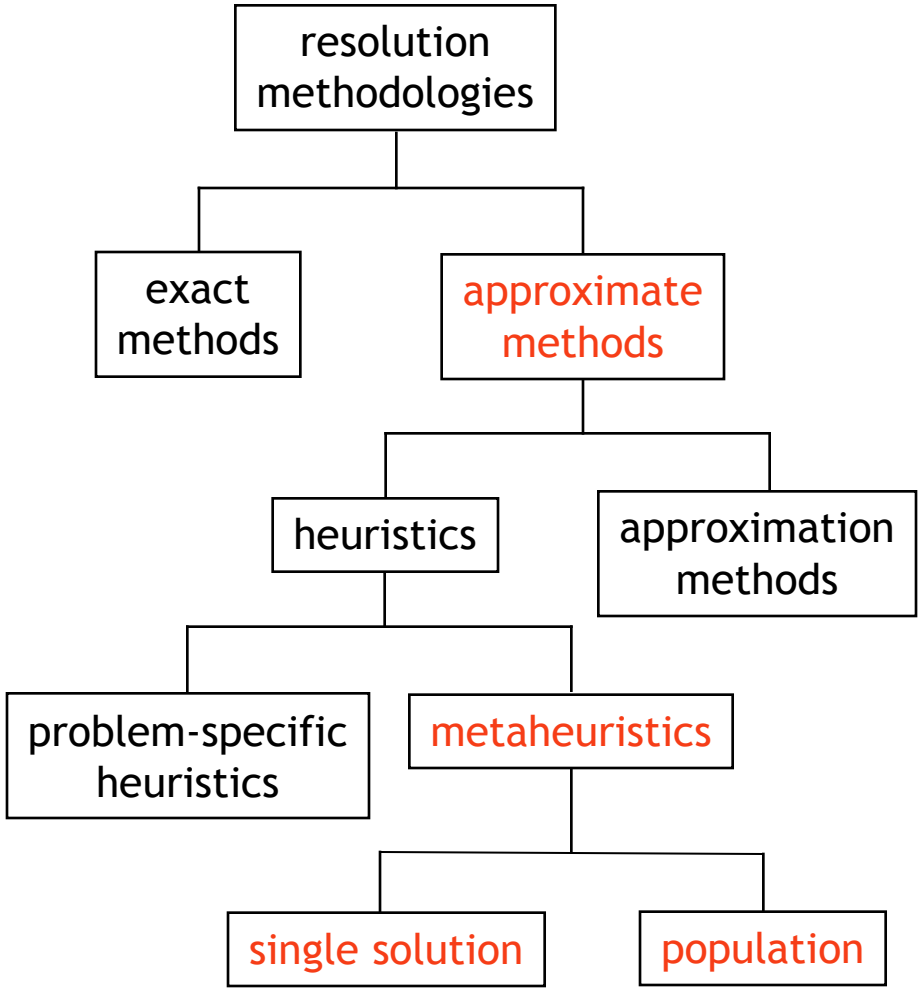
- Decision Maker (DM) after the resolution process

Interactive

- Decision Maker (DM) during the resolution process



Resolution Methodologies

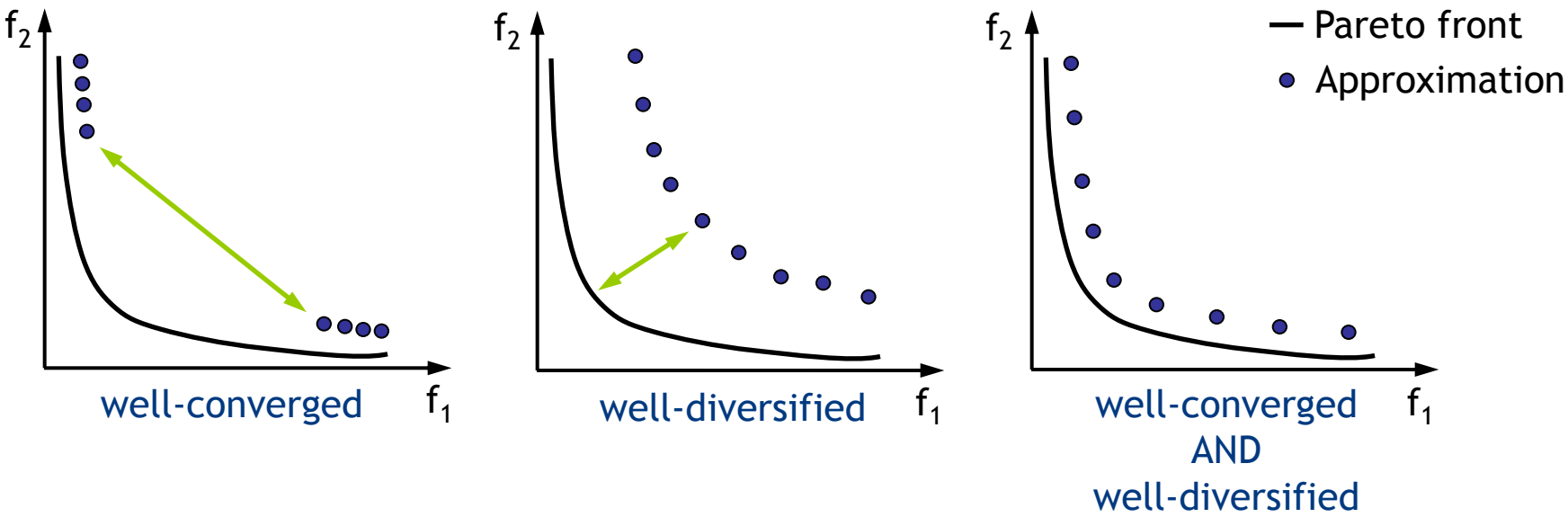


- Exact Methods
  - Problems of small size or specific structure
- Metaheuristics
  - Find a good approximation of the efficient set (or Pareto front)
  - Metaheuristics able to find multiple non-dominated solutions in a single run

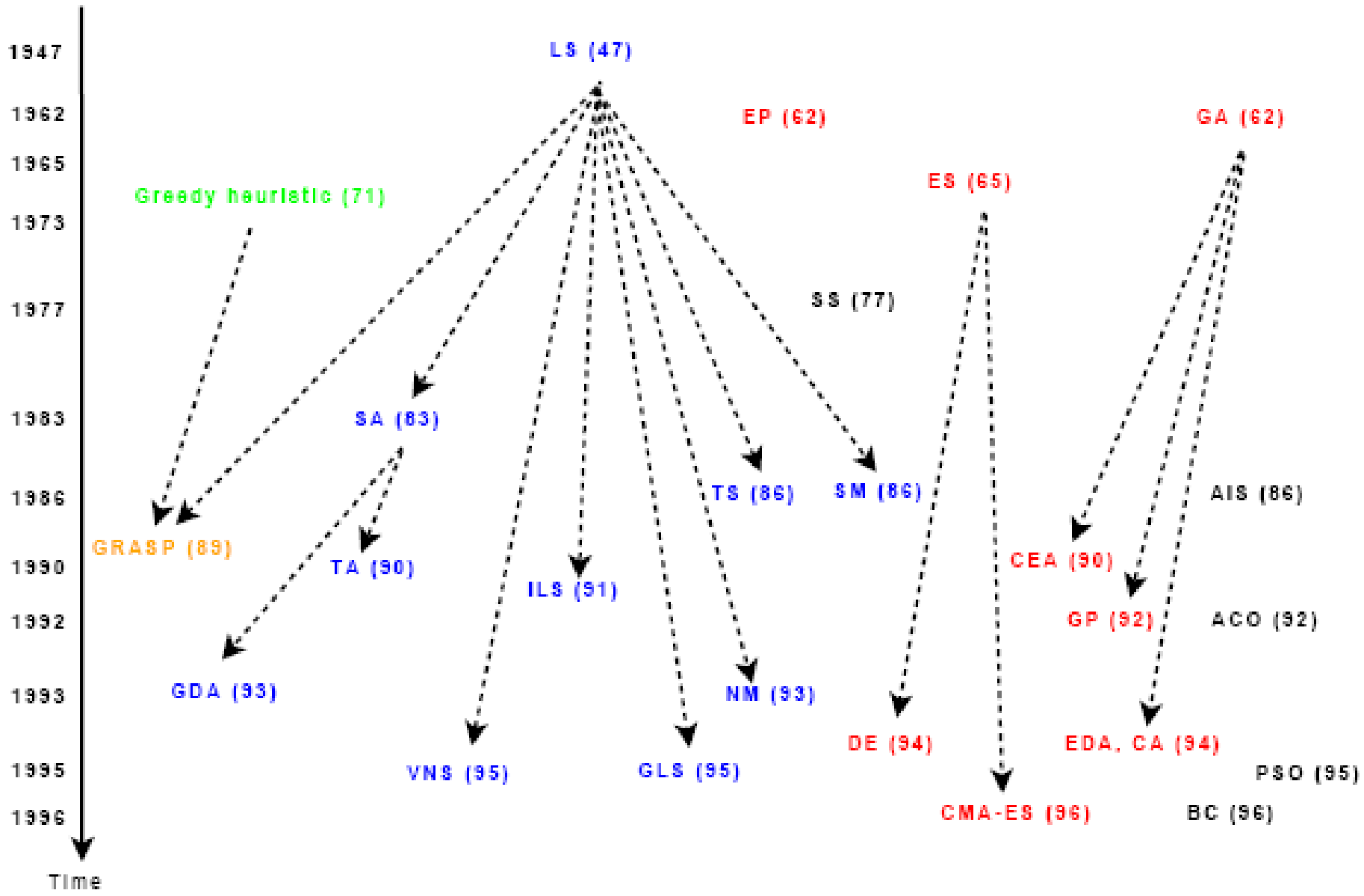
What is a Good Approximation?

Approximating an efficient set is itself a bi-objective problem

- Min the distance to the Pareto front
  - ➔ well-converged efficient set approximation
- Max the diversity in the objective space (and/or decision space)
  - ➔ well-diversified efficient set approximation



Genealogy of Metaheuristics



The number of multi-objective metaheuristics is growing exponentially !

- Very active research in the last two decades
- For each metaheuristic (e.g. EA, PSO, LS, TS, SA, ACO) :
  - Hundreds of different designs
  - Hundreds of different implementations

- Give you the Catalog of the proposed algorithms : I don't like it
  - May be bigger than a dictionary

- May have:
  - MO Evolutionary Algorithm 1 # MO Evolutionary Algorithm 2
  - MO Evolutionary Algorithm = MO Scatter Search 1 = MO PSO 1
  - MO Local Search 1 # MO Local Search 2
  - MO Iterated Local Search = MO GRASP

Just some algorithms: Compare with all those algorithms !

WBGA COMPETants MACS MO-CMA-ES MOMGA MOSS MOGLS RDGA PAES PESA PESA2 MODE VEGA MOPSO moRBC NPGA MO-PACO MOTS IBMOLS E-MOEA Micro-GA MIDEA MOGP MOACO NSGA NSGA-II MONACO PLS-1 PLS-2 SPEA SPEA-2 MOEA TAPaS MOSA NPGA RM-MEDA SSPMO SACO SEEA ACOAMO DMLS FASTPGA MOGA MEA IBEA MOES MOSA-2 ANT-Q P-ACO MOLS MOAQ DMOEA RWGA MOACOM MOEA-D

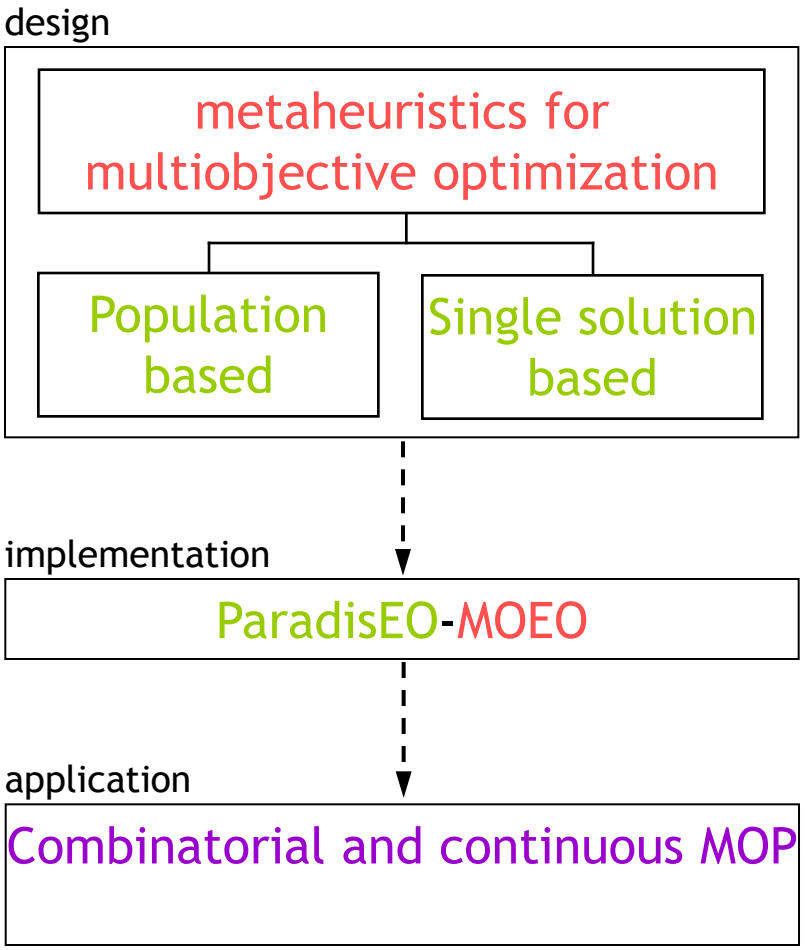
Motivations

➔ A unified view

- Design and Implementation

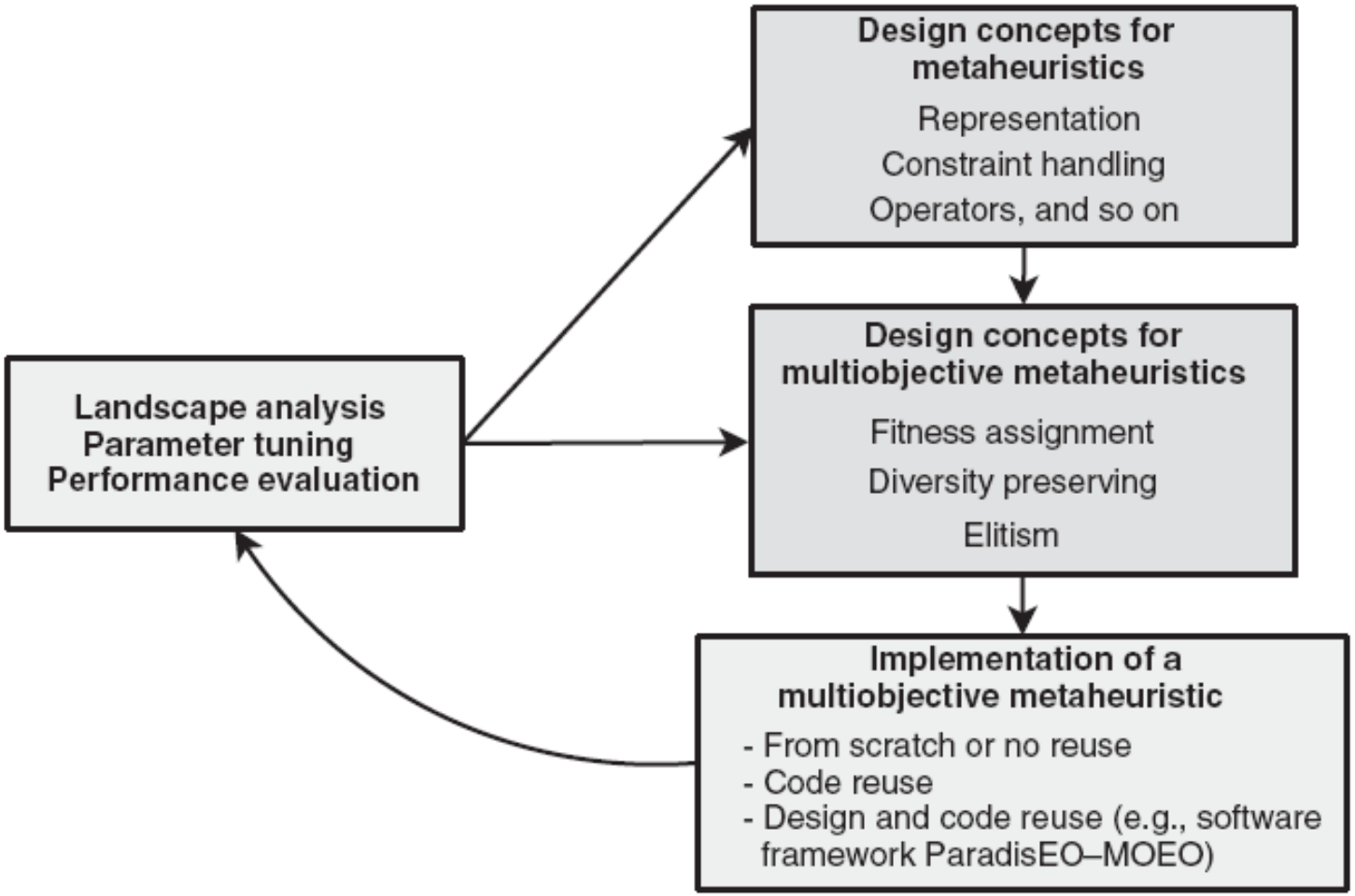
  problem-dependent
  Multi-objective-specific
  metaheuristic-specific

- Fine-grained decomposition of search mechanisms
- Common terminology and classification
  - Comparison of approaches (experimental analysis)
  - New approaches



A unified design view

Development process of a multi-objective metaheuristic



Design issues of multi-objective metaheuristics

- **Fitness assignment**
  - Guide the search towards Pareto optimal solutions for a better convergence.

- **Diversity preserving**
  - Generate a diverse set of Pareto solutions in the objective space and/or the decision space.

- **Elitism:**
  - Preservation and use of elite solutions.
  - Allows a robust, fast and a monotically improving performance of a metaheuristic

Fitness Assignment

- Scalar approaches
  - Transformation to mono-objective problem(s)
- Criterion-based approaches
  - Each objective is treated separately
- Dominance-based approaches
  - The concept of dominance is used
- Indicator-based approaches
  - Use performance indicators to drive the search

Scalar approaches

- Aggregation methods

$$f(x) = \sum_{i=1}^{n} \lambda_i f_i(x), \;\; x \in S$$

- Weighted metrics

$$(MOP(\lambda, z)) \begin{cases} min(\sum_{j=1}^{n} \lambda_j |f_j(x) - z_j|^p)^{\frac{1}{p}} \\ \text{s.c. } x \in S \end{cases}$$

- Goal programming
- ε-constraint approach
- Achievement functions

$$(MCOP(\overline{z})) \begin{cases} min(\sum_{j=1}^{n} \lambda_j \delta_j \\ \text{s.c. } f_j(x) - \delta_j \leq \overline{z}_j, j \; in[1,n] \\ \delta_j \geq 0, j \; in[1,n] \\ x \in S \end{cases}$$

$$(MOP(\lambda, z)) \begin{cases} \min \; max_{j \in [1,n]}[w_j(f_j(x) - \overline{z}_j)] + \rho \sum_{j=1}^{n} (f_j(x) - \overline{z}_j) \\ \text{s.c. } x \in S \end{cases} \tag{1.16}$$

- Goal attainment

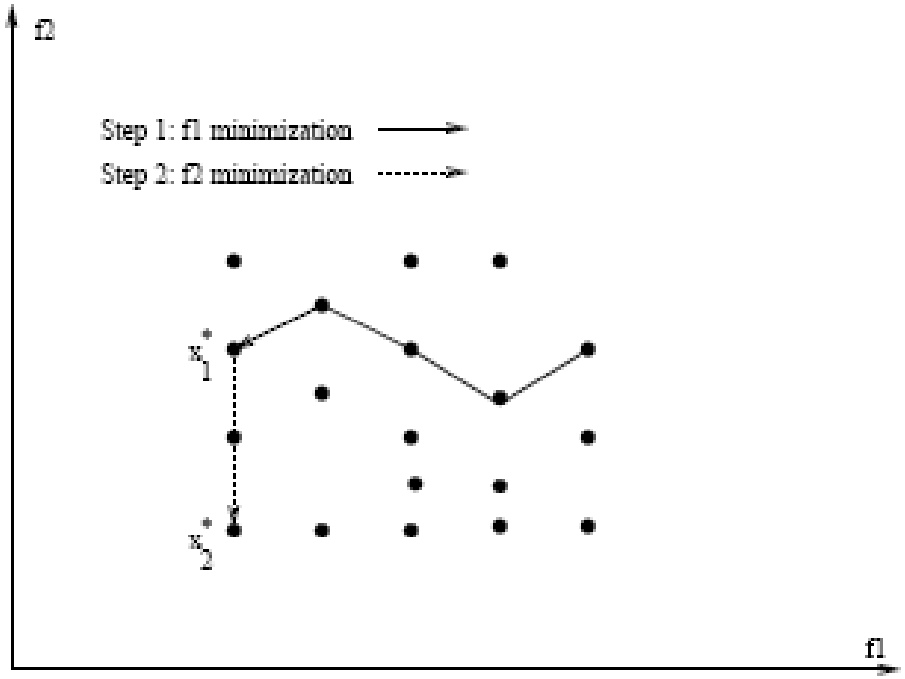
$$\begin{cases} min \; \alpha \\ \text{s.c. } x \in S \\ f_i(x) \leq z*_i + \alpha\lambda_i, \; i = 1, .., n \\ \sum_{i=1}^{n} \lambda_i = 1 \end{cases}$$

Aggregation Metaheuristics

- Weights: Static, Multiple, Dynamic, Adaptive
- Genetic algorithms [Hajela et Lin 92]
  - Individual representation: solution + λ
  - Goal: generating various Pareto solutions
- Simulated annealing [Serafini 92]
  - Acceptance probability
- Tabu search [Dahl et al. 95]
- Hybrid metaheuristics [Talbi 98]
  - Greedy algorithm + Simulated annealing [Tuyttens 98]
  - Genetic algorithm (Local search) [Ishibuchi et Murata 98]
    - Selection with different weights
    - Local search on the produced individual (same weights)

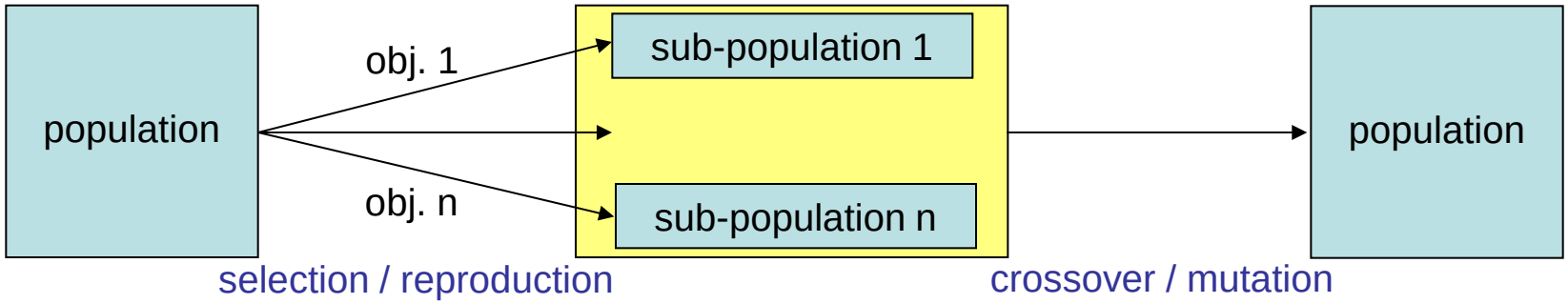
Criterion-based Approaches: Sequential

- Sequential approach: Objectives are handled in sequential
- Lexicographic selection (priority order)
    - Tabu search, Genetic algorithms [Fourman 85]
    - Evolutionary strategies [Kursawe 91], …



Criterion-based Approaches: Parallel

- Parallel approach: Objectives are handled in parallel
- Parallel selection (VEGA) [Schaffer 85]



- Multi-sexual reproduction [Lis & Eiben 96]
  - One class per objective
  - Reproduction (crossover) over several individuals
- Ant colonies (pheromone/objective)

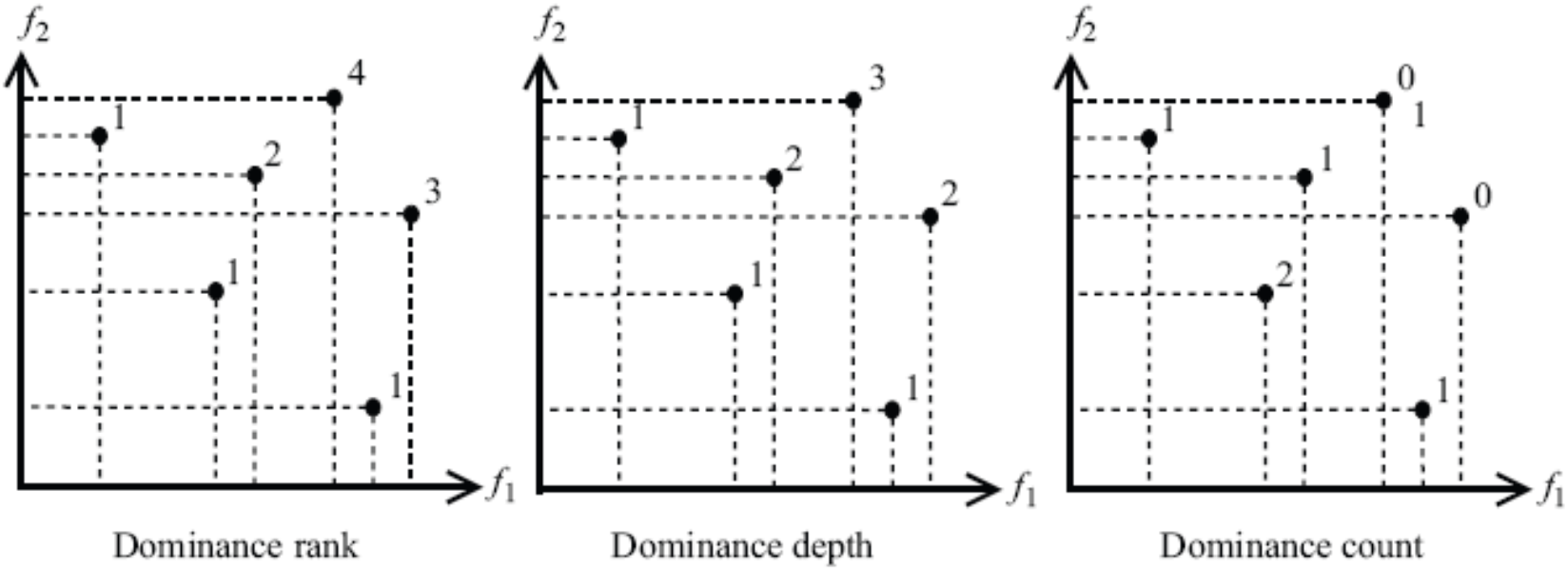
➔ Tends to ignore compromised solutions

Dominance-based Approaches

- Dominance relation used during the fitness assignment process:
  - Pareto dominance
  - Weak dominance
  - Strict dominance
  - ε-dominance [Helbig & Pateva 1994]
  - g-dominance [Molina et al. 2009]
  - Guided domination
  - Fuzzy dominance
  - …

Fitness assignment: Pareto ranking

- Pareto-based fitness assignment strategies
  - Dominance rank (*e.g.* used in MOGA)
    - Number of solutions which dominates the solution
  - Dominance depth (*e.g.* used in NSGA and NSGA-II)
  - Dominance count (*e.g.* combined with dominance rank in SPEA and SPEA2)
    - Number of solutions dominated by the solution



Indicator-Based Fitness Assignment

[Zitzler & Künzli 04]

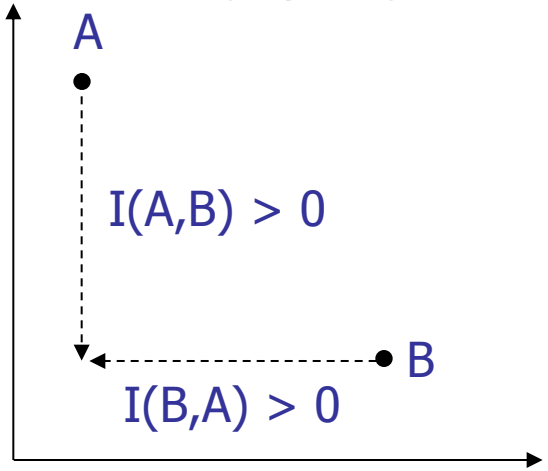
Solutions compared on the basis of a binary quality indicator I

Fitness (A) = usefulness of A according to the optimization goal (I)

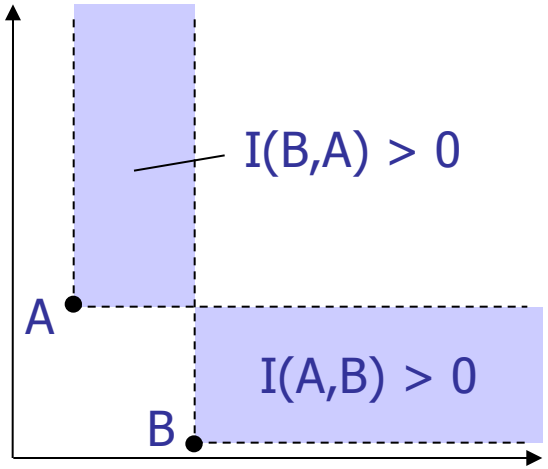
$$arg\ min_{A \in \Omega} I(A, R)$$

where Ω represents the space of all efficient set approximations.

Examples of binary quality indicators:



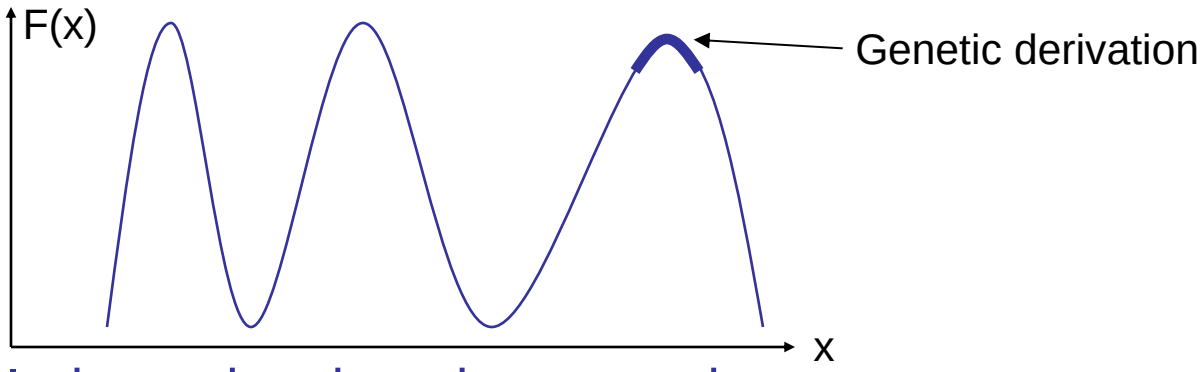
Additive epsilon indicator ($I_{\epsilon+}$)



Hypervolume indicator (I_{HD})

Diversity

Multi-modal optimization: locating every optima of the problem

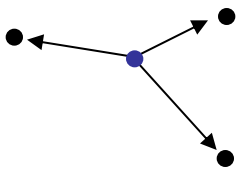


- Independent iterative executions
- Sequential niching
  - Iterative execution with a penalization of the optima already found
- Parallel niching (sharing, crowding)
  - Only one execution

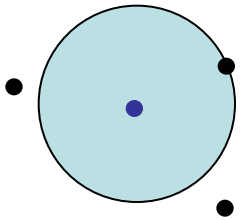
Diversity: Statistical density estimation

- Kernel methods (sharing)
  - Neighborhood of a solution in term of a function taking a distance as argument
- Nearest neighbour techniques
  - Distance of a solution to its kth nearest neighbour
- Histograms
  - Space divided onto neighbourhoods by an hypergrid

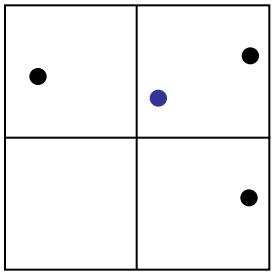
➔ decision / objective space



kernel



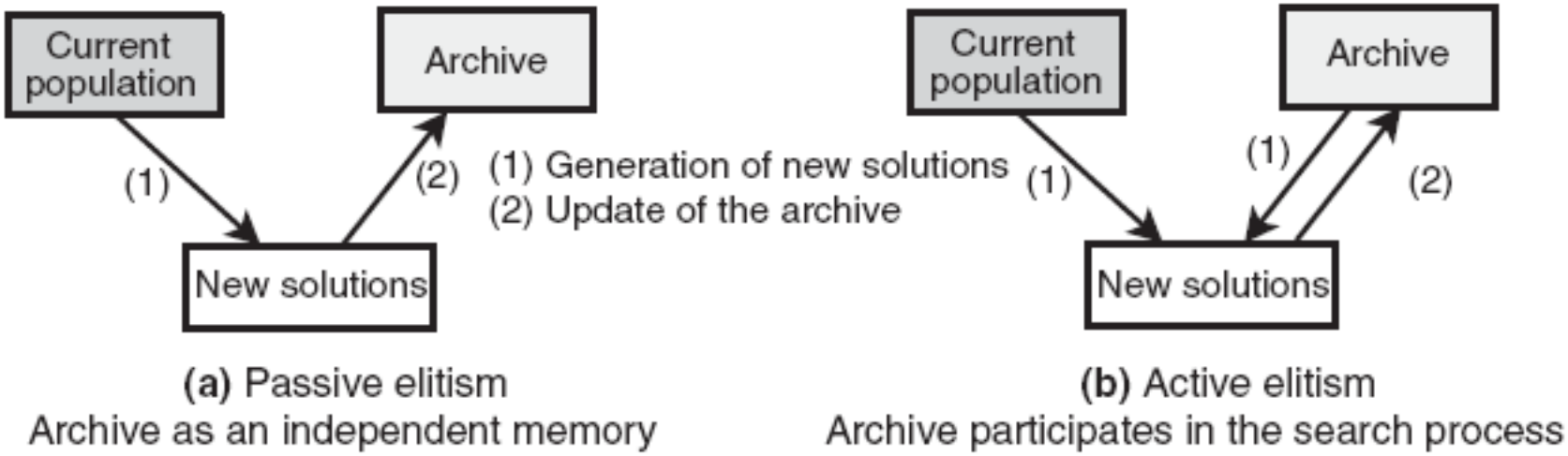
nearest neighbor



histogram

Elitism

- Archive
  - External set storing non dominated solutions
  - Update criteria: size, convergence, diversity
- The archive can be involved in the search process:
  - Elitist selection



(a) Passive elitism
Archive as an independent memory

(b) Active elitism
Archive participates in the search process

Elitism

- No archive
  - Current approximation contained in the main population
- Unbounded archive
  - All nondominated solutions
- Bounded archive
  - A reasonable number of nondominated solutions
- Fixed-size archive
  - cf. SPEA2 [Zitzler et al. 2001]

A Model for Evolutionary Algorithms

Main issues

- Problem-dependent components

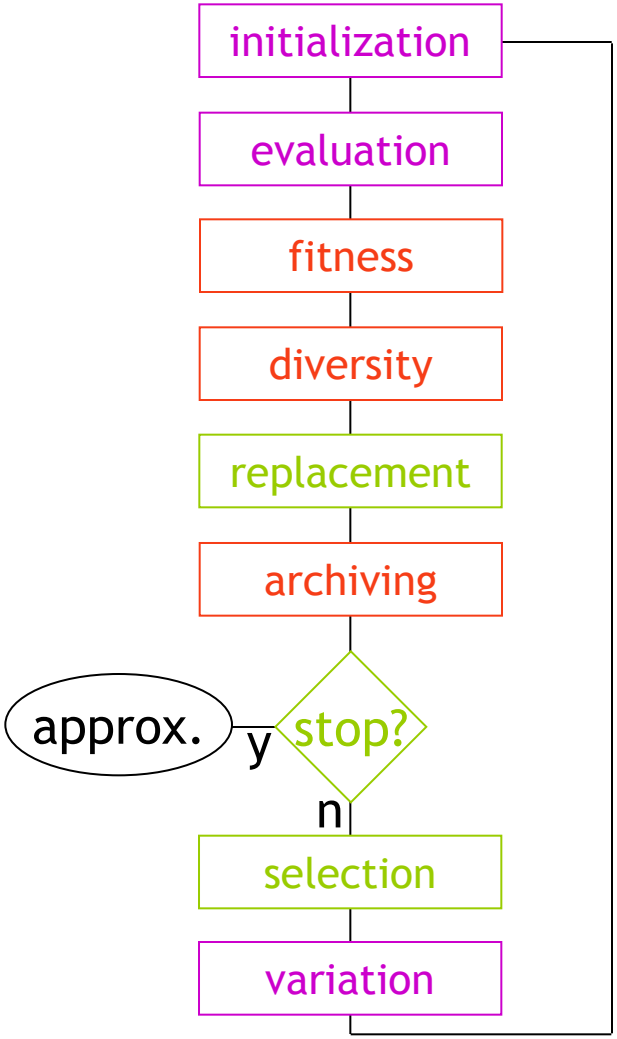
  representation, initialization, evaluation, variation (recombination, mutation)

- Multi-objective specific components

  fitness assignment, diversity preservation, archiving

- Metaheuristic specific components

  selection, replacement, stopping condition



EMO Algorithms as Instances of the Model

Components	NSGA-II [Deb et al. 02]	SPEA2 [Zitzler et al. 01]	IBEA [Zitzler and Künzli 04]	SEEA [Liefooghe et al. 10]
fitness assignment	**dominance-depth**	**dom-count + dom-rank**	**quality indicator**	none
diversity preservation	crowding distance	k^{th} nearest neighbor	none	none
archiving	none	**fixed-size archive**	none	**unbounded**
selection	binary tournament	elitist selection	binary tournament	elitist selection
replacement	elitist replacement	generational replacement	elitist replacement	generational replacement
stopping condition	number of generations	number of generations	number of generations	user-defined

A Model for Dominance-based Local Search (DMLS)

Main issues

- Problem dependent components

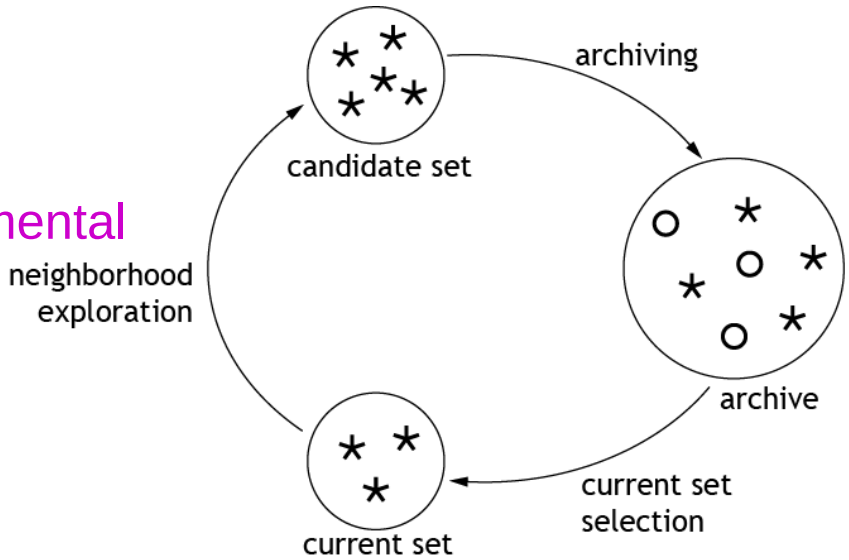
  representation, initialization, evaluation, neighborhood, incremental evaluation

- Multi-objective specific components

  dominance relation, archiving

- Metaheuristic specific components

  current set selection, neighborhood exploration, stopping condition



DMLS Algorithms as Instances of the Model

Components	PLS-1 [Paquete et al. 04]	PLS-2 [Talbi et al. 01]	PAES [Knowles & Corne00]	moRBC [Aguire & Anaka 05]
dominance relation	Pareto	Pareto	Pareto	Pareto
archiving	unbounded	unbounded	bounded hypergrid	bounded crowding
current set selection	partial 1 random sol.	exhaustive all solutions	partial μ solutions	partial 1 solution
neighborhood exploration	exhaustive all neighbors	exhaustive all neighbors	partial λ random neighbors	partial 1 dominating neighbor
stopping condition	natural all sol. visited	natural all sol. visited	user-defined	natural all sol. visited

Landscapes and Performance Analysis

Performance indicators

- **Unary / Binary indicators**

$$I : \Omega \longrightarrow \mathbb{R}$$

$$I : \Omega \times \Omega \longrightarrow \mathbb{R}$$

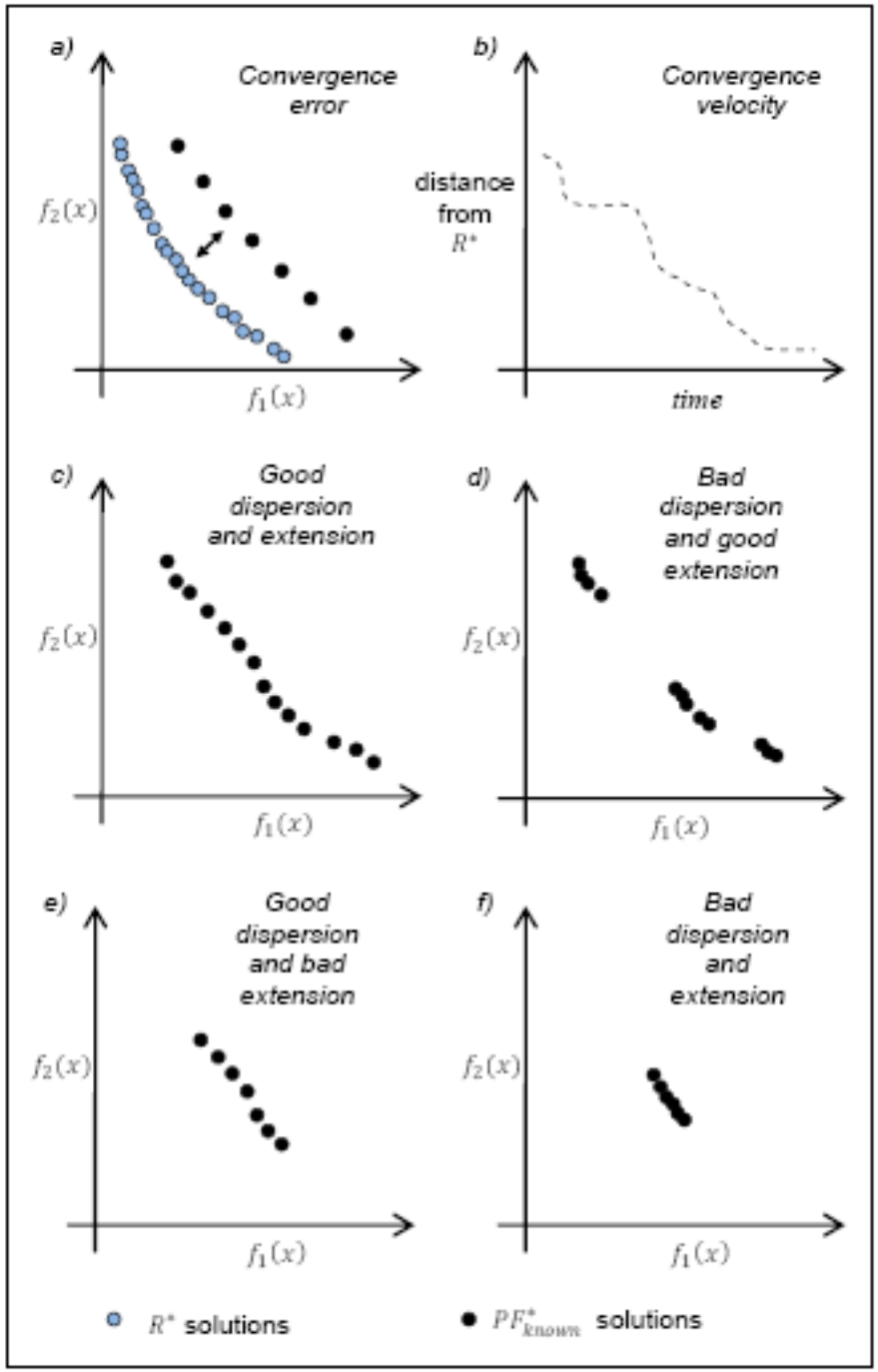
- **Known Pareto optimal set / Unknown**

- **Cardinality, Distance, Volume**

- **Parameter less / additional parameters**: reference point, ideal point, Nadir point, reference set, …

Performance indicators: Properties

- **Monotonicity**
- **Objective scale independence**
- **Computational complexity**
- **Classification**:
  - Convergence
  - Diversity (dispersion, extension)
  - Hybrid


a)
Convergence error
$f_2(x)$
$f_1(x)$
b)
Convergence velocity
distance from R^*
time
c)
Good dispersion and extension
$f_2(x)$
$f_1(x)$
d)
Bad dispersion and good extension
$f_2(x)$
$f_1(x)$
e)
Good dispersion and bad extension
$f_2(x)$
$f_1(x)$
f)
Bad dispersion and extension
$f_2(x)$
$f_1(x)$
R^* solutions
PF^*_{known} solutions

PO known

- Absolute efficiency (convergence)
  - Proportion of Pareto solutions within PO*

$$AE = \frac{|PO^* \cap PO|}{|PO|}$$

- Distance (PO*, PO)
  - Worst distance

$$WD = \max\left(d(PO^*, y)\right), y \in PO$$

  - Mean distance

$$MD = \frac{\sum_{y \in PO} d(PO^*, y)}{|PO|}$$

$$d(PO^*, y) = \min\left(d(x, y)\right), x \in PO^*$$

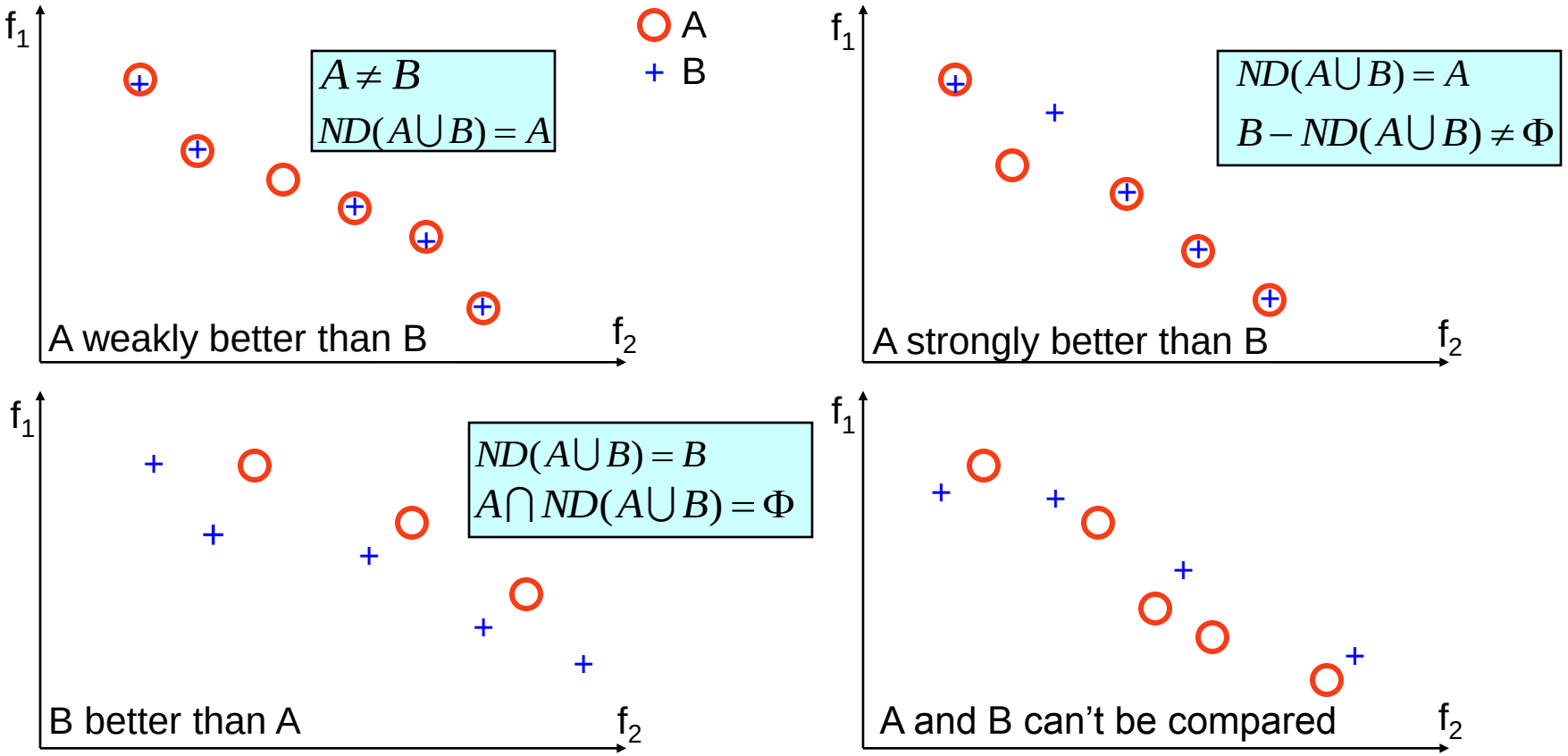
$$d(x, y) = \sum_{i=1}^{n} \lambda_i \left| f_i(x) - f_j(y) \right|$$

- Uniformity

$$DIV = \frac{WD}{MD}$$

PO unknown

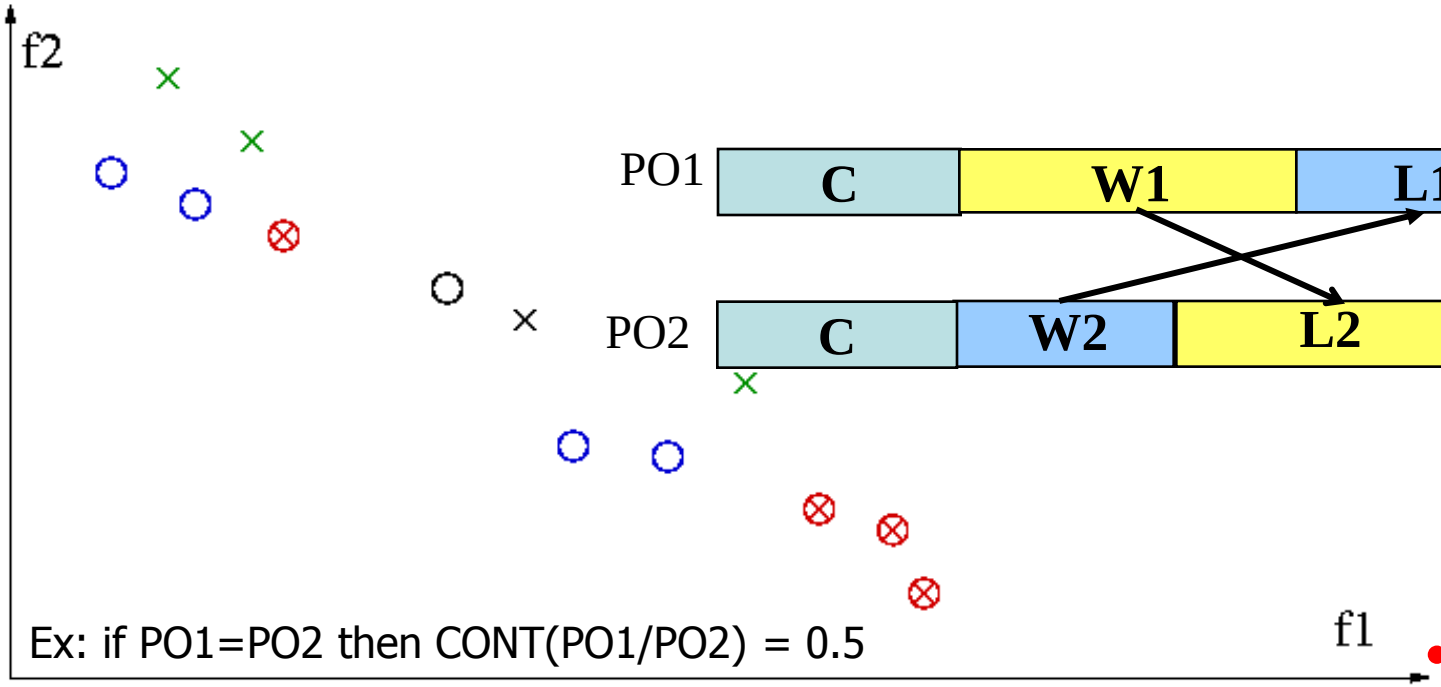
- Relative efficiency: number of solutions from A dominated by B

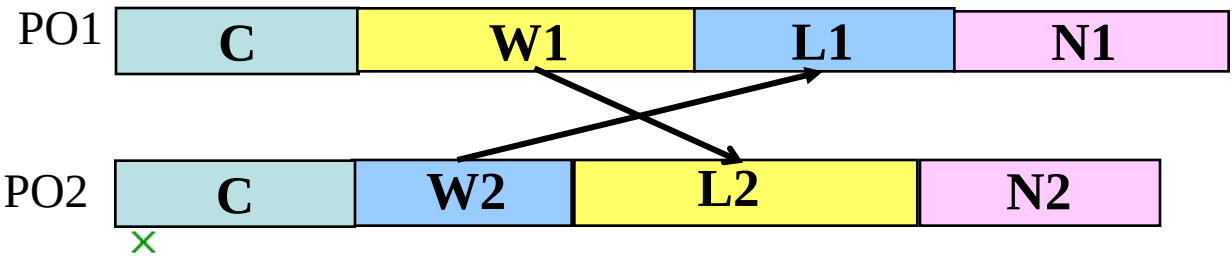


PO unknown: Convergence

Contribution: Evaluating the quality of the solutions from a set towards another one

$$Cont(PO_1/PO_2)=\frac{\|C\|/2+\|W_1\|+\|N_1\|}{\|C\|+\|W_1\|+\|N_1\|+\|W_2\|+\|N_2\|}$$





C=4

W1=4 - N1=1

W2=0 - N2=1

- Cont(O,X)=0,7
- Cont(X,O)=0,3

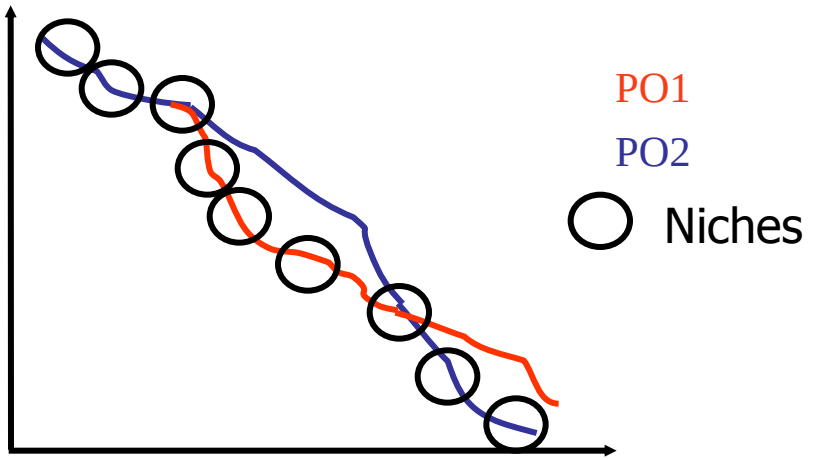
Ex: if PO1=PO2 then CONT(PO1/PO2) = 0.5

if PO1>PO2 then CONT(PO1/PO2) = 1

PO unknown: Diversity

- Entropy: builds a niche around every solution of ND(PO_1 U PO_2)=PO*
  - E(PO_1,PO_2) : diversity of the solutions of PO_1 in comparison of those in the niches of PO*

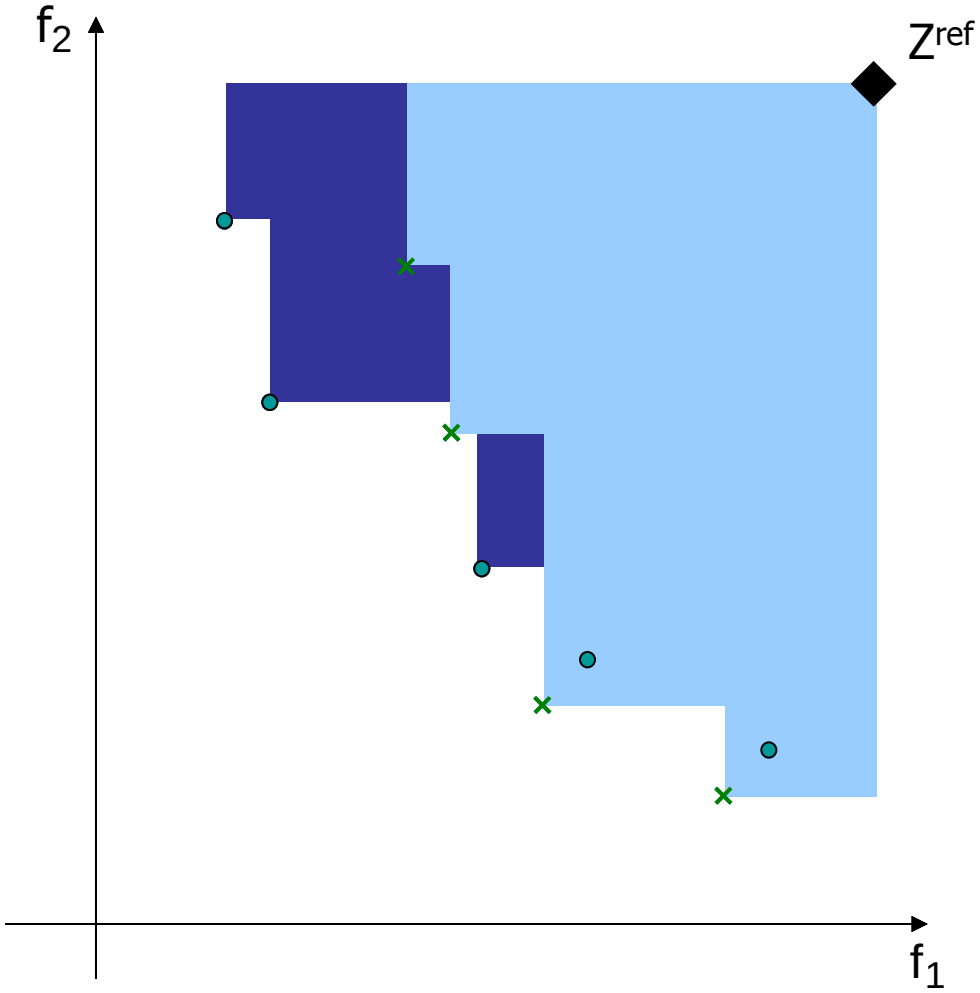
$$E(PO_1,PO_2)=\frac{-1}{\ln(\gamma)}\sum_{i=1}^{|PO^*|}\left(\frac{1}{Ni}\frac{n_i}{\|PO_1\|}\ln\frac{n_i}{\|PO_1\|}\right)$$



PO unknown: Hybrid

- S-metric / Hypervolume *[Zitzler 99]*

Size of the objective space enclosed by PO* and a reference point Z^{ref}



Other indicators

- **Generational distance** (convergence)

$$I^t_{GD}(A,R) = \frac{(\sum_{u \in A} (min_{v \in R} \parallel F(u) - F(v) \parallel^2])^{1/2}}{|R|}$$

- **Extent** (diversity)

$$I_{ex}(A) = (\sum_{i=1}^{n} (max_{u,u' \in A} \parallel f_i(u) - f_i(u') \parallel))^{1/2}$$

- **Spread** (diversity)

$$I_S = \frac{\sum_{u \in A} |\{u' \in A : \parallel F(u) - F(u') \parallel > \sigma\}|}{|A| - 1}$$

- **E-indicator** (convergence)

$$I_{\epsilon+}(A,B) = min_{\epsilon \in \mathbb{R}}\{\forall z \in B, \exists z' \in A : z'_i - \epsilon \leq z_i, \forall 1 \leq i \leq n\}$$

Performance indicators

Indicator	Goal	Monotone	Complexity	Parameter	[],Min-Max
Contribution	Conv.	Mon.	$O(\|A\|.\|R\|)$	Ref. set	$[0,1]$, Max
Gen. Dist.	Conv.	No	$O(\|A\|.\|R\|)$	Ref. set	$[0,\infty)$, Min
$\epsilon - indicator$	Conv.	Mon.	$O(n.\|A\|.\|R\|)$	Ref. set	$[0,\infty)$, Min
I_p	Conv.	Mon.	$O(\|A\|.\|PO\|)$	Opt. set	$[0,1]$,Max
$I_a d$	Conv.	No	$O(\|A\|.\|PO\|)$	Opt. set	$[0,\infty)$, Min
Spread	Div.	No	$O(\|A\|^2)$	-	$[0,1]$,Min
Extent	Div.	No	$O(\|A\|^2)$	-	$[0,\infty)$, Max
B. Entropy	Div.	No	$O((\|R\|+\|A\|).\mu^n)$	Ref. set,μ	$[0,1]$, Max
U. Entropy	Div.	No	$O((\|A\|.\mu^n)$	μ	$[0,1]$, Max
Hypervolume	Hybrid	Strict	$O(\|A\|^n)$	Ref. point	$[0,\infty)$, Max
R-metrics	Hybrid	Mon.	$O(n.\|\Lambda\|.\|A\|.\|R\|)$	Ref. set Ideal point	$[0,\infty)$, Min

Landscapes

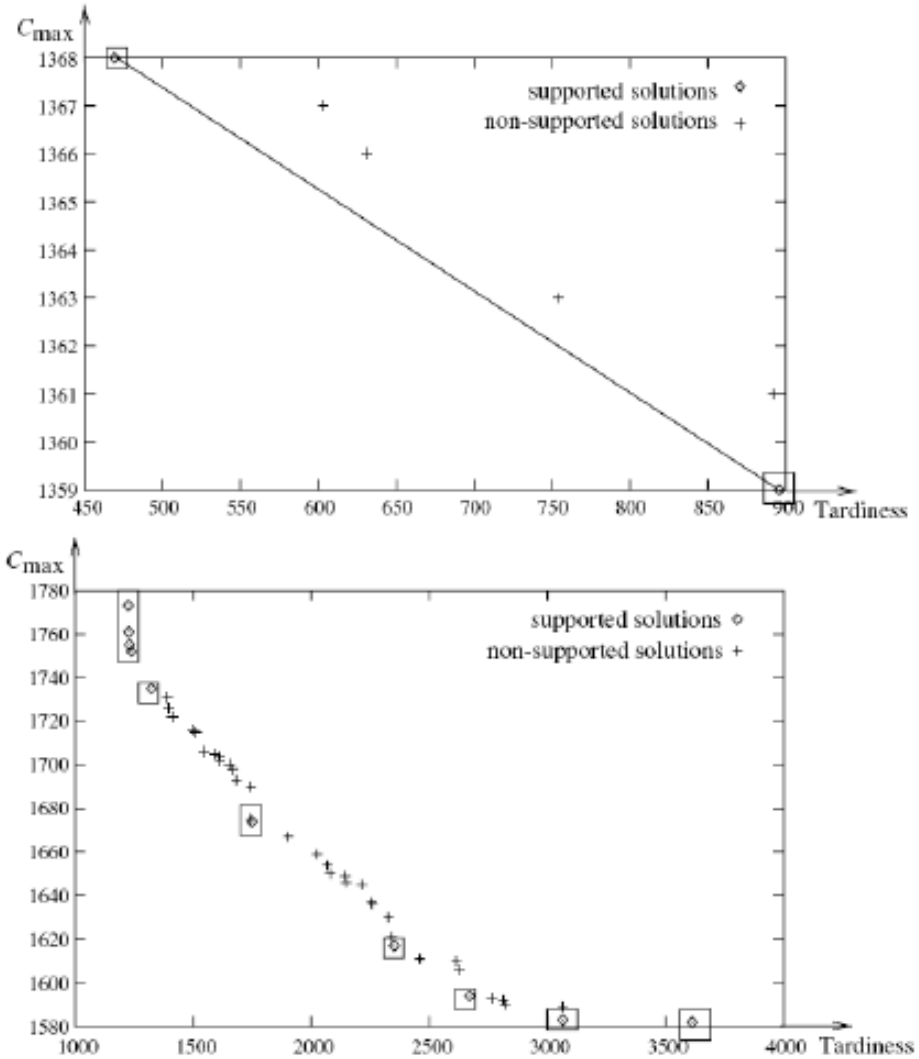
How to describe a Pareto front?

- Convexity / Concave Pareto fronts
- Multi-modality and deceptive attractors
- Isolated optimum (Flat space)
- Continuous / Discontinuous
- Uniform distribution

Benchmarks: ZDT

- *Convexity versus non-convexity of the Pareto optimal front (ZDT1 versus ZDT2).*
- *Discontinuities and gaps in the Pareto-optimal front (ZDT1 or ZDT2 versus ZDT3).*
- *Multiple locally Pareto optimal fronts towards the globally Pareto optimal front (ZDT1 versus ZDT4).*
- *Isolation and deception of the globally Pareto optimal front (ZDT1 versus ZDT5).*
- *Non-uniform density of solutions across the Pareto optimal front (ZDT2 versus ZDT6).*

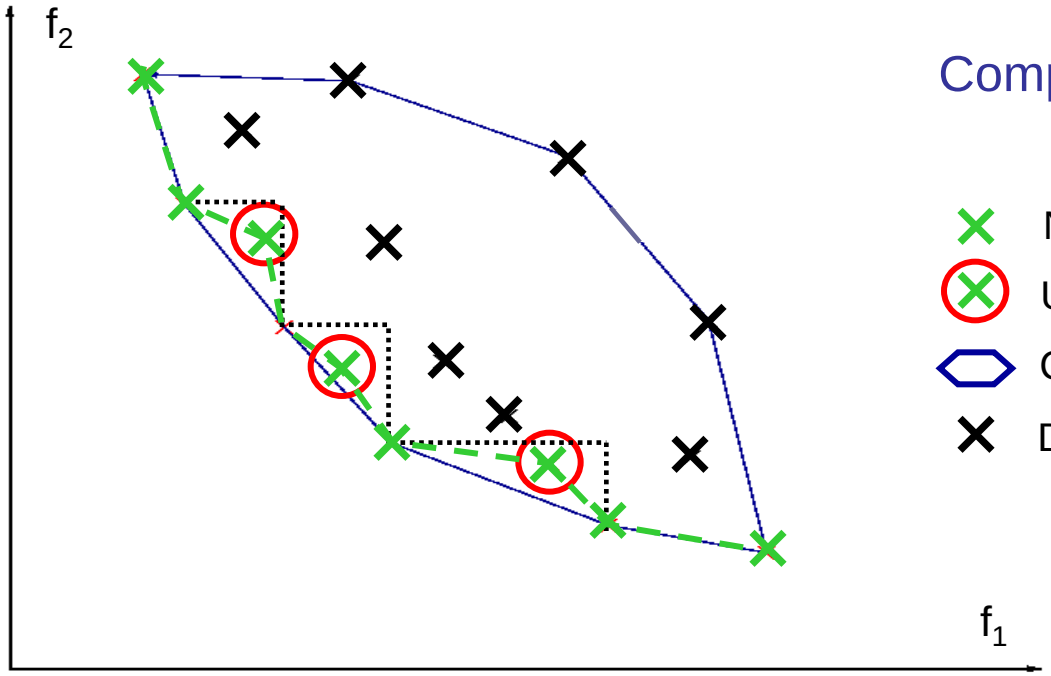
Supported / Non supported



Landscapes

Aggregation: supported solutions only

Convexity: Proportion of Pareto solutions belonging to the convex hull



Complexity: O(n.log(n))

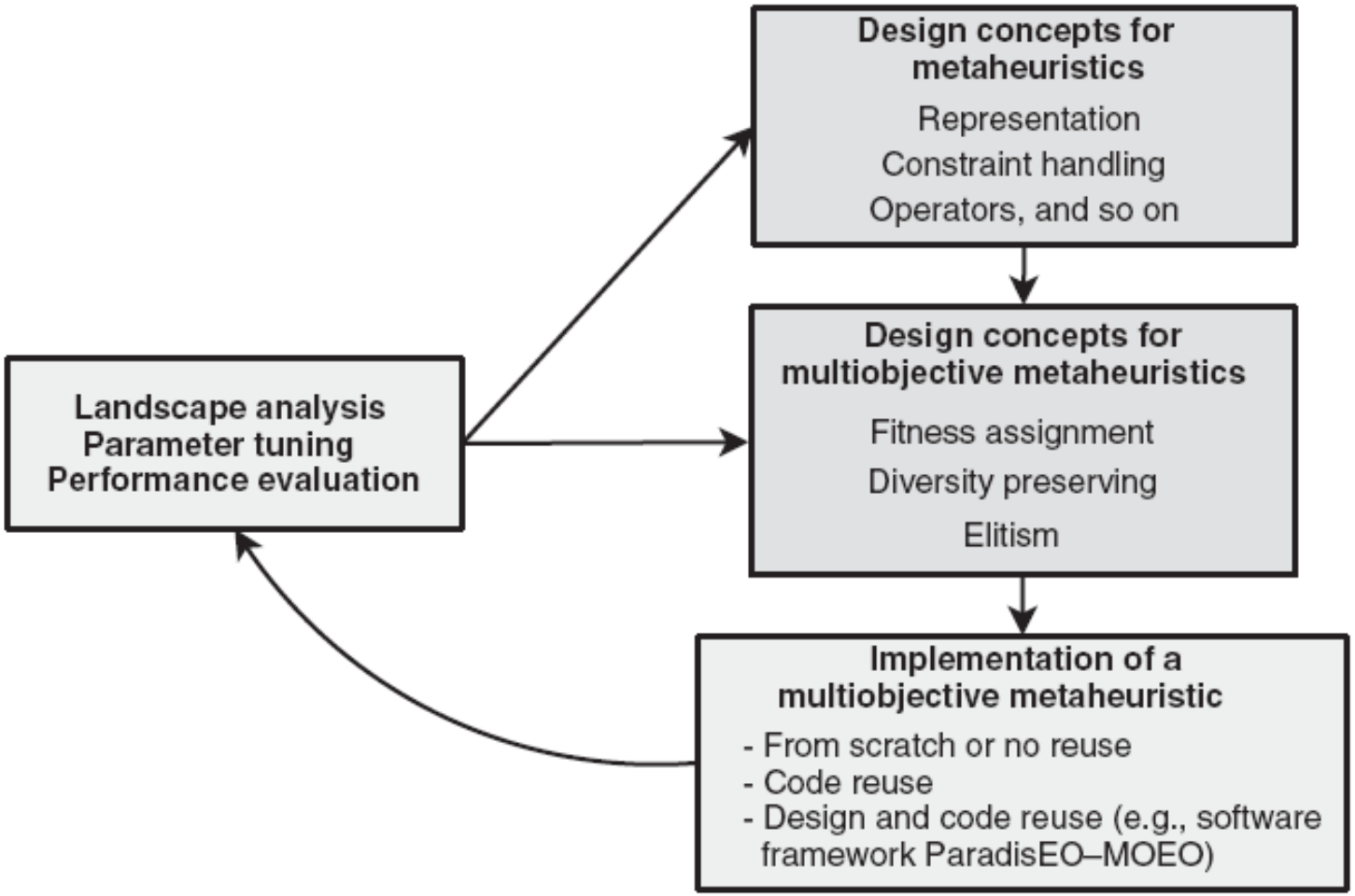
- Non-dominated solutions
- Unsupported solutions
- Convex hull
- Dominated solutions

Multi-objectivization

A way to improve solving single-objective optimization problems

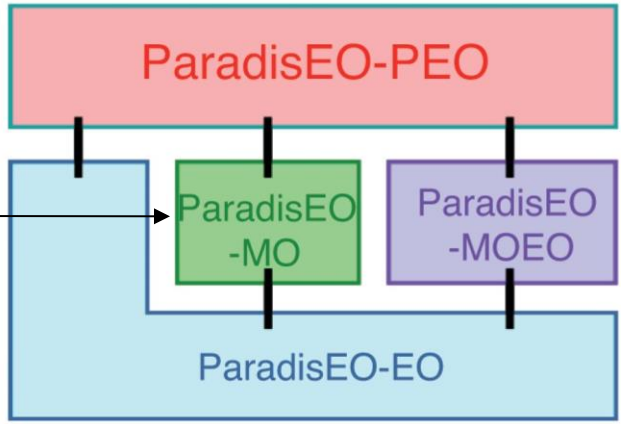
- Objective function decomposition
  - Several sub-objectives (separate conflicting goals)
  - Reduce the number of local optima
- Helper objectives
  - Adding new objectives correlated with the main objective
  - Break plateaus of the landscape → smooth landscape

Development process of a multi-objective metaheuristic



Framework for multi-objective metaheuristics: ParadisEO

parallel and distributed metaheuristics



single solution-based Metaheuristics (LS, SA, TS, TA, VNS, ILS)

multiobjective metaheuristics

population-based metaheuristics (GA, GP, ES, EDA, PSO, …)

http://paradiseo.gforge.inria.fr

ParadisEO

- Design and code reuse
  - Conceptual separation between the solution methods and the problem to be solved
- Flexibility and adaptability
  - Adding or updating other optimization methods, search mechanisms, operators, representation…
- Utility
  - Broad range of methods, components, parallel and distributed models, hybridization mechanisms…
- Transparent and easy access to performance and robustness
  - Parallel and hybrid implementation transparent to the hardware platform
- Portability
  - Operating systems: Windows, Linux, MacOS
  - Material architectures: sequential, parallel, distributed
- Usability and efficiency

Software Frameworks/Librairies for multi-objective metaheuristics

Framework/ Library	Meta	Type	Metrics	Hybrid	Parallel	Language
ParadisEO	S-meta P-meta	White	Many	Yes	Yes	C++
TEA	EA	White	No	No	Yes	C++
PISA	EA	Black	Many	No	No	Any
O. BEAGLE	EA	White	No	Yes	Yes	C++
MOMHLib++	EA,LS,SA	White	Many	Yes	No	C++
MOEA–Matlab	EA	Black	No	No	Yes	Matlab
MALLBA	S-meta P-meta	White	No	Yes	Yes	C++

S-meta: S-metaheuristics; P-meta: P-metaheuristics; White: white box software; Black: black box software; LS: local search; SA: simulated annealing; EA: evolutionary algorithms.

Multi-objective Metaheuristics

Multi-objective problem

Problem-dependent components

- Representation
- Evaluation
- Initialization
- Neighborhood
- Incremental evaluation
- Recombination
- Mutation

(shared by all metaheuristics)

Multiobjective-specific components

- Fitness assignment
- Diversity preservation
- Archiving

(shared by all multi-objective metaheuristics)

Implementation of an evolutionary algorithm

- Implement a representation
- Implement a population initialization strategy
- Implement a way of evaluating a solution
- Implement suitable variation operators

Problem-specific components

- Instantiate a fitness assignment strategy
- Instantiate a diversity preservation strategy
- Instantiate a selection strategy
- Instantiate a replacement strategy
- Instantiate an archive management strategy
- Instantiate a continuation strategy

Generic components

Multi-objective

Metaheuristic

Implementation

- Implement a representation
- Implement a population initialization strategy
- Implement a way of evaluating a solution
- Implement suitable variation operators
- Instantiate a fitness assignment strategy
- Instantiate a diversity preservation strategy
- Instantiate a selection strategy
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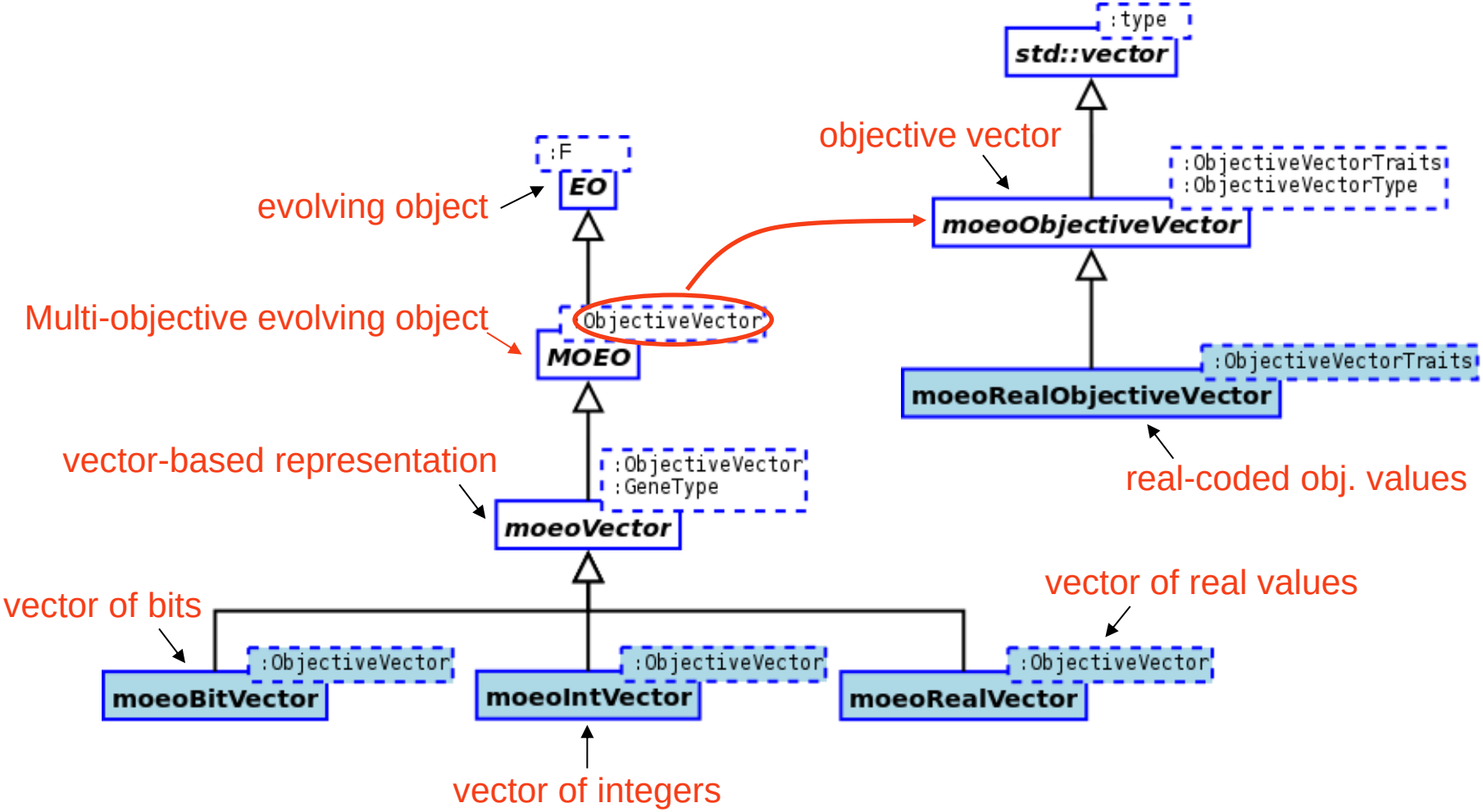
- Instantiate a continuation strategy

Representation



Implementation

- Implement a representation
- Implement a population initialization strategy → eolnit
- Implement a way of evaluating a solution
- Implement suitable variation operators
- Instantiate a fitness assignment strategy
- Instantiate a diversity preservation strategy
- Instantiate a selection strategy
- Instantiate a replacement strategy
- Instantiate an archive management strategy
- Instantiate a continuation strategy

Implementation

- Implement a representation
- Implement a population initialization strategy
- Implement a way of evaluating a solution → eoEvalFunc
- Implement suitable variation operators
- Instantiate a fitness assignment strategy
- Instantiate a diversity preservation strategy
- Instantiate a selection strategy
- Instantiate a replacement strategy
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Implementation

- Implement a representation
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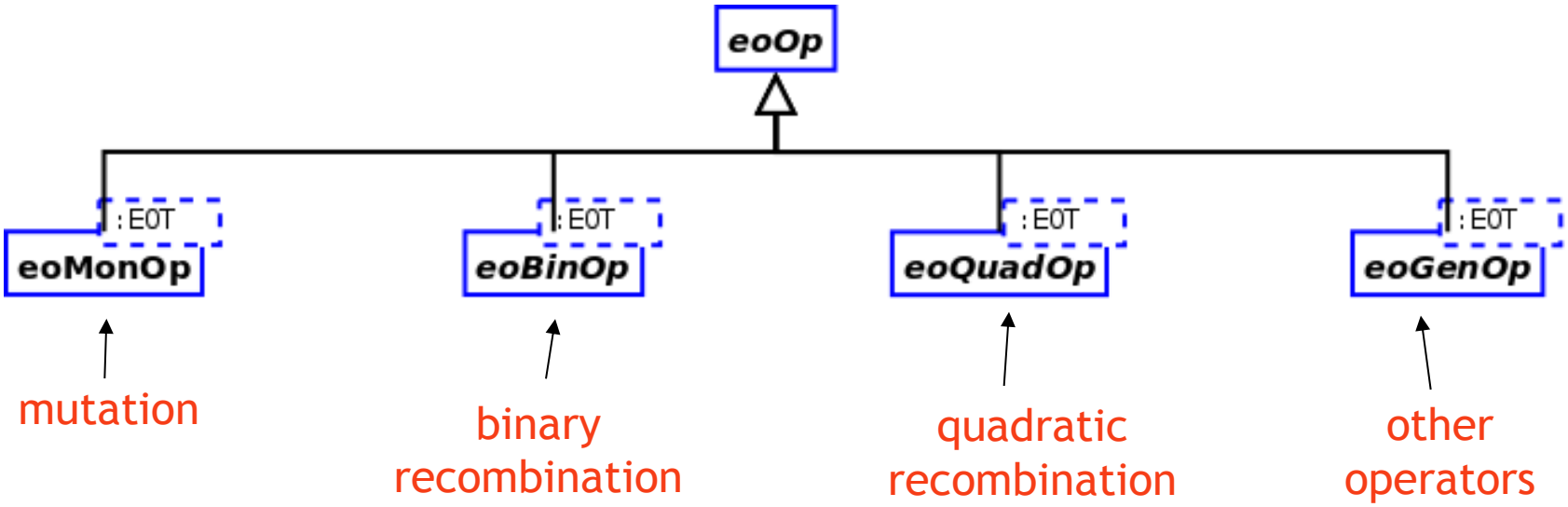
Variation operators



➔ variation operators must be embedded to an eoTransform object

Implementation

- Implement a representation
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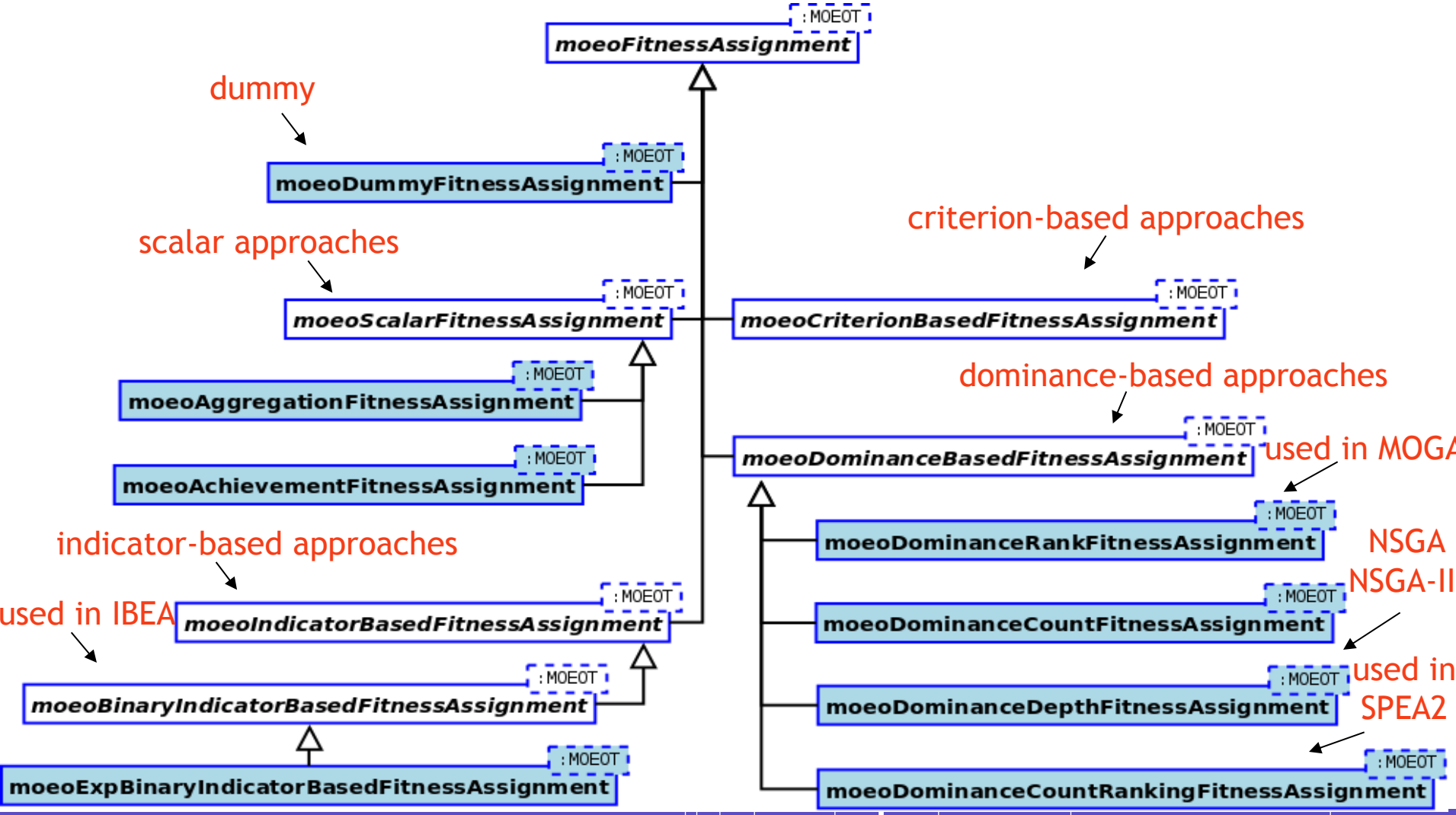
Fitness Assignment



Implementation

- Implement a representation
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- Implement suitable variation operators
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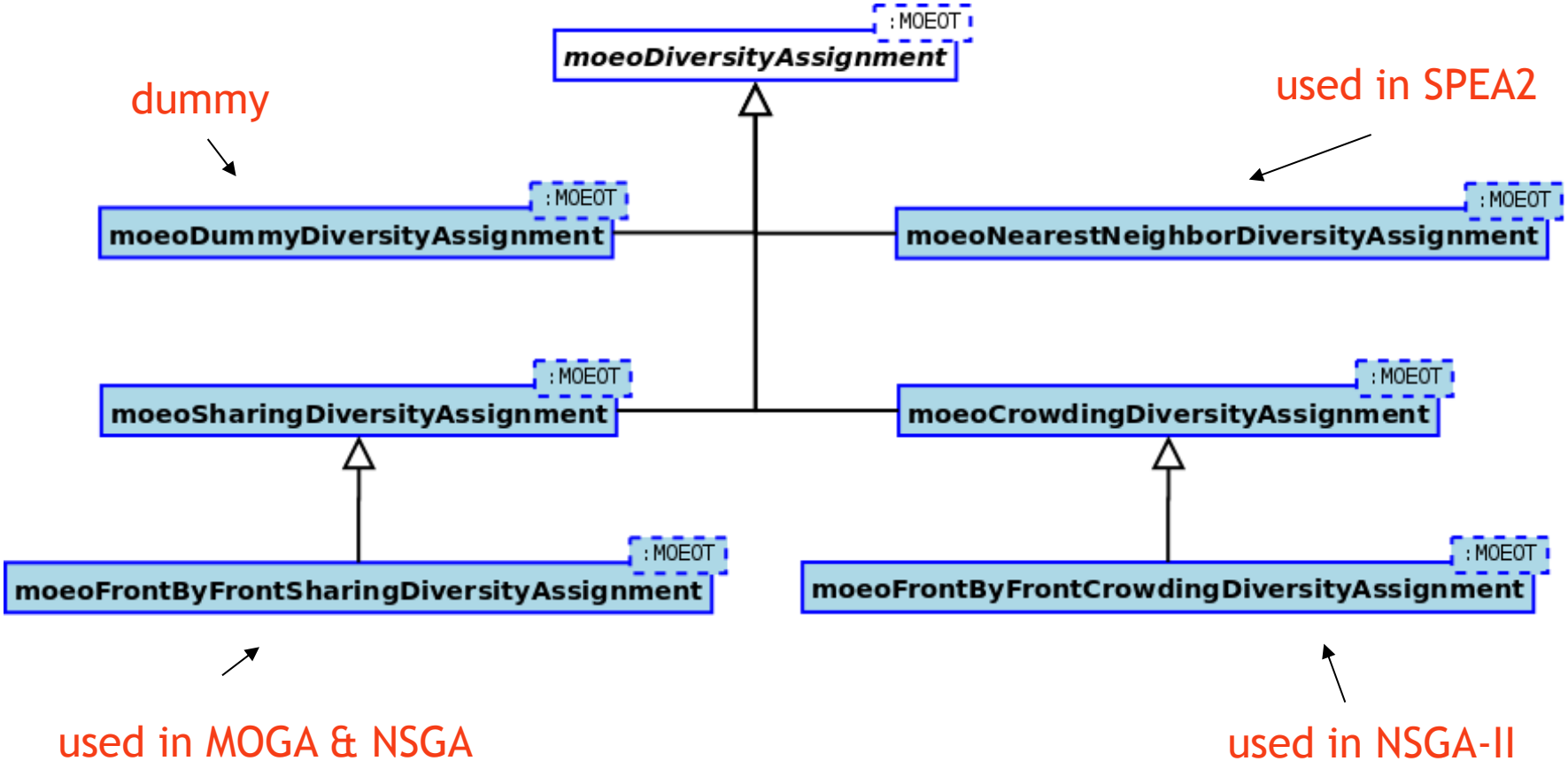
Diversity Assignment



Implementation

- Implement a representation
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- Instantiate a selection strategy
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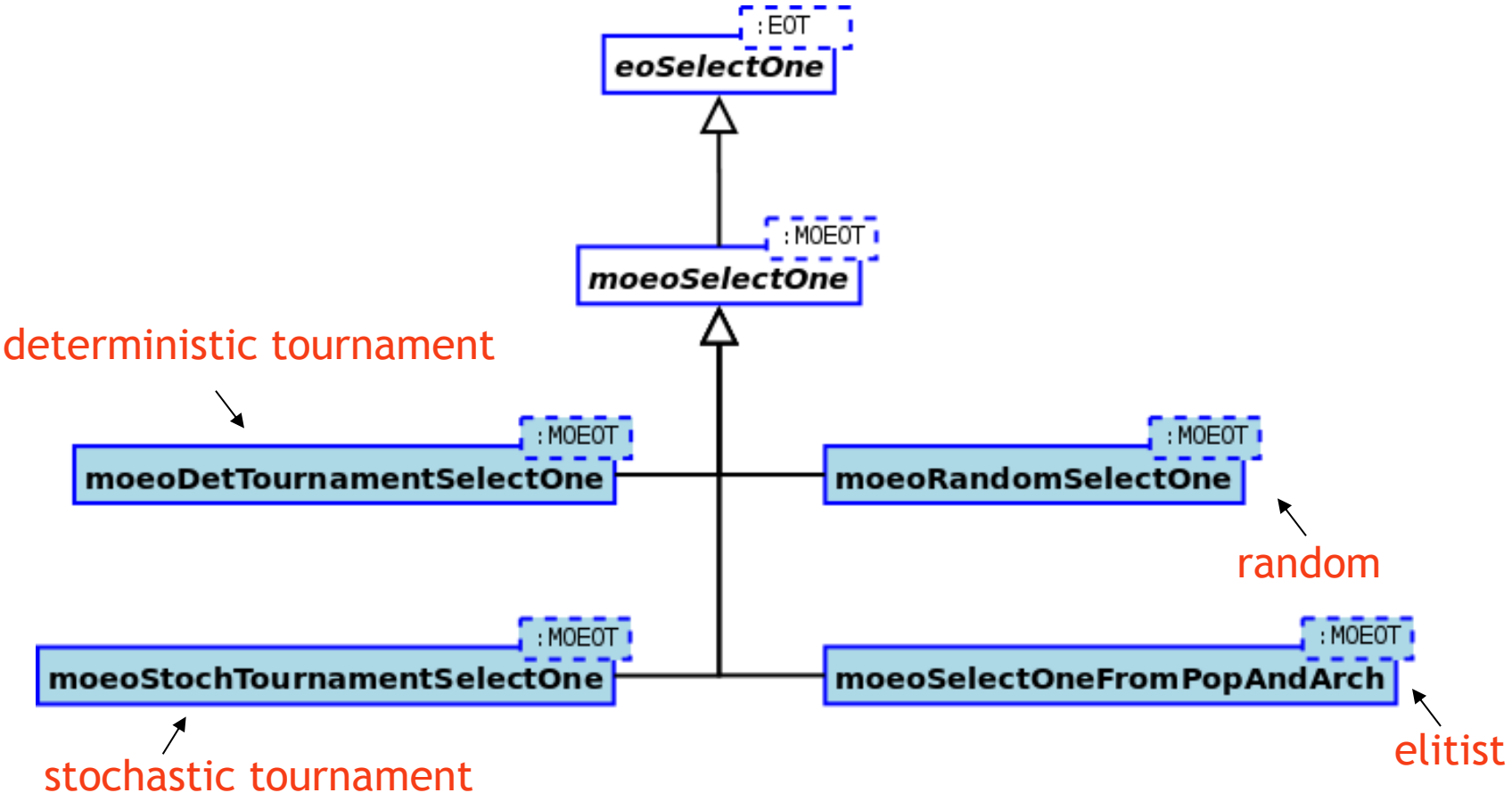
- Instantiate a continuation strategy

Selection


:EOT
eoSelectOne
:MOEOT
moeoSelectOne
deterministic tournament
:MOEOT
moeoDetTournamentSelectOne
:MOEOT
moeoRandomSelectOne
random
:MOEOT
moeoStochTournamentSelectOne
:MOEOT
moeoSelectOneFromPopAndArch
stochastic tournament
elitist

Implementation

- Implement a representation
- Implement a population initialization strategy
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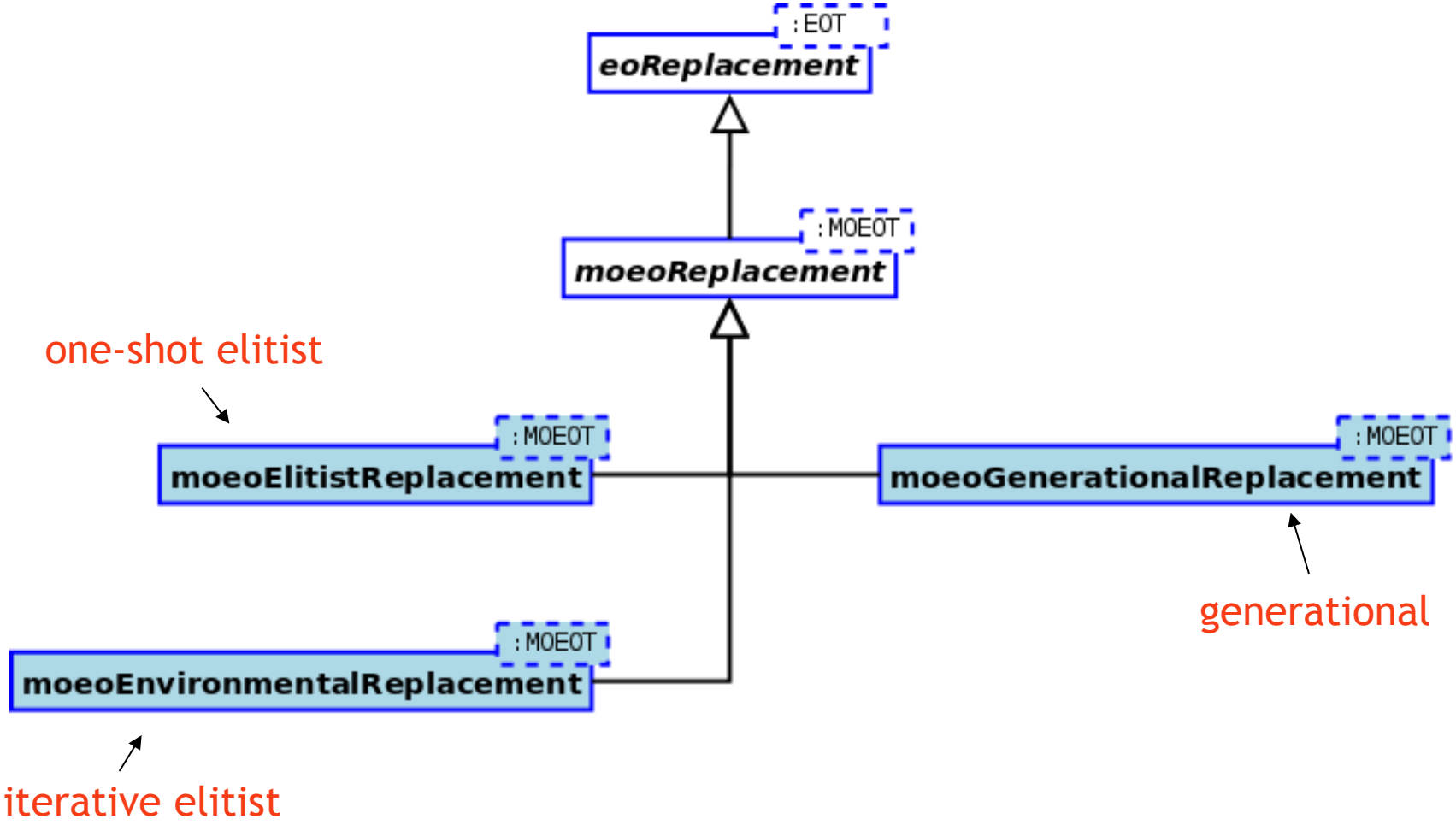
- Instantiate an archive management strategy
- Instantiate a continuation strategy

Replacement



Implementation

- Implement a representation
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- Implement suitable variation operators
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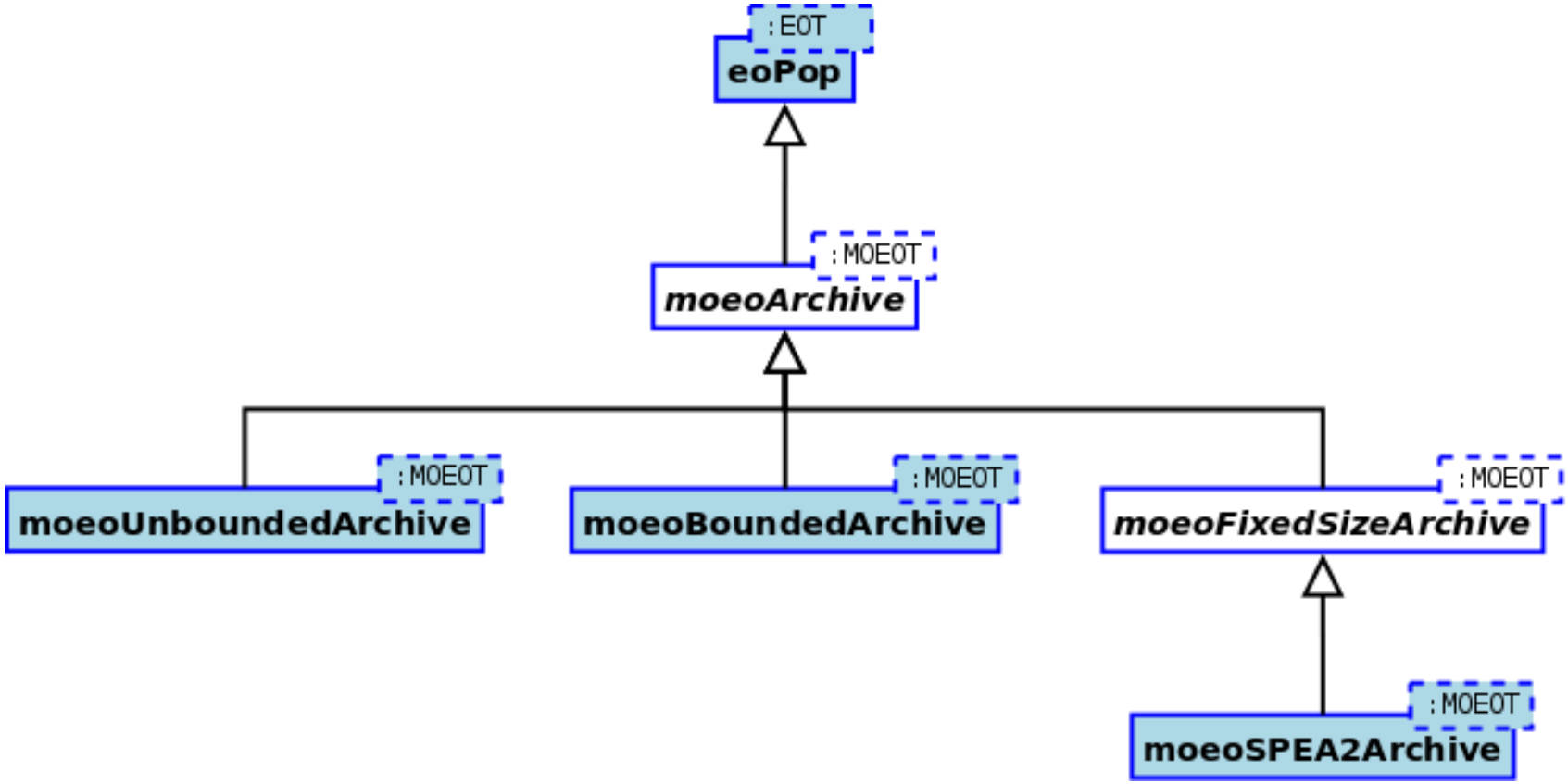
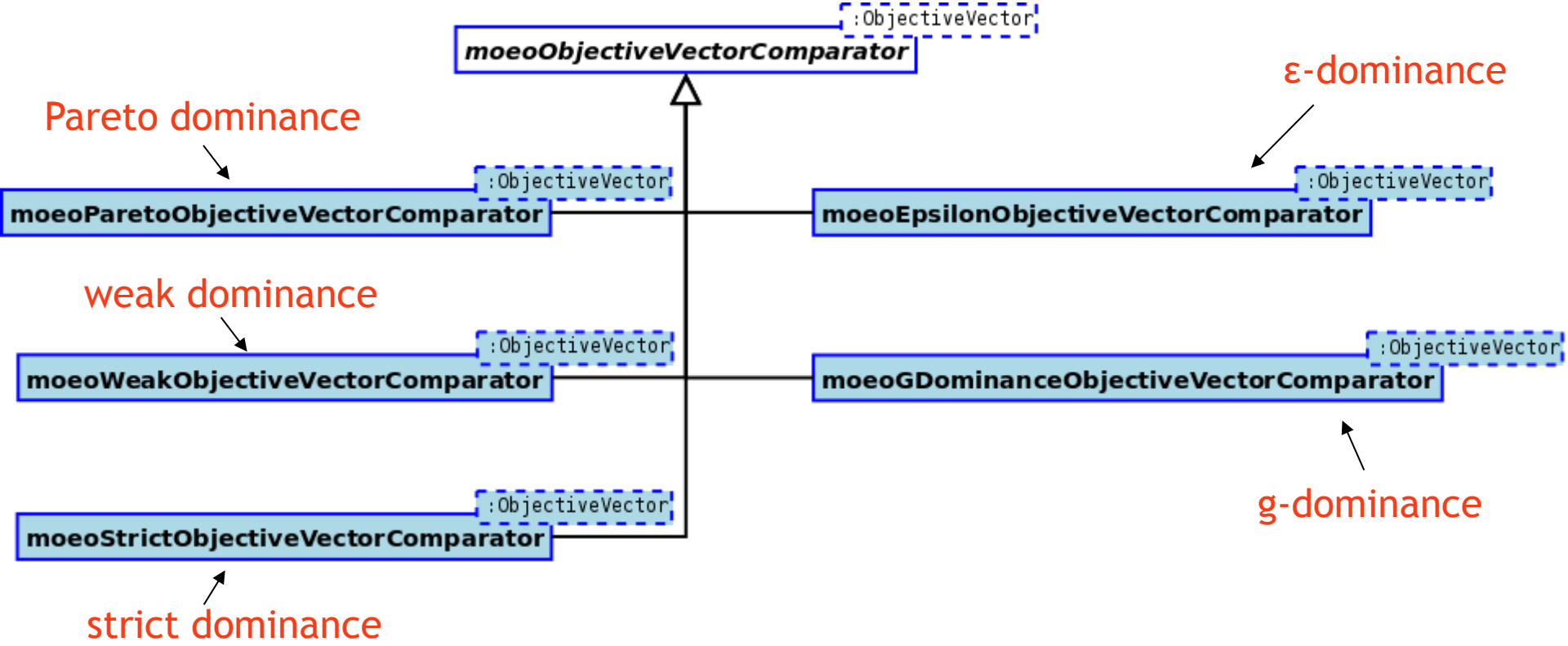
- Instantiate a diversity preservation strategy
- Instantiate a selection strategy
- Instantiate a replacement strategy
- Instantiate an archive management strategy
- Instantiate a continuation strategy

Archive


:EOT
eoPop
:MOEOT
moeoArchive
:MOEOT
moeoUnboundedArchive
:MOEOT
moeoBoundedArchive
:MOEOT
moeoFixedSizeArchive
:MOEOT
moeoSPEA2Archive

Dominance Relation

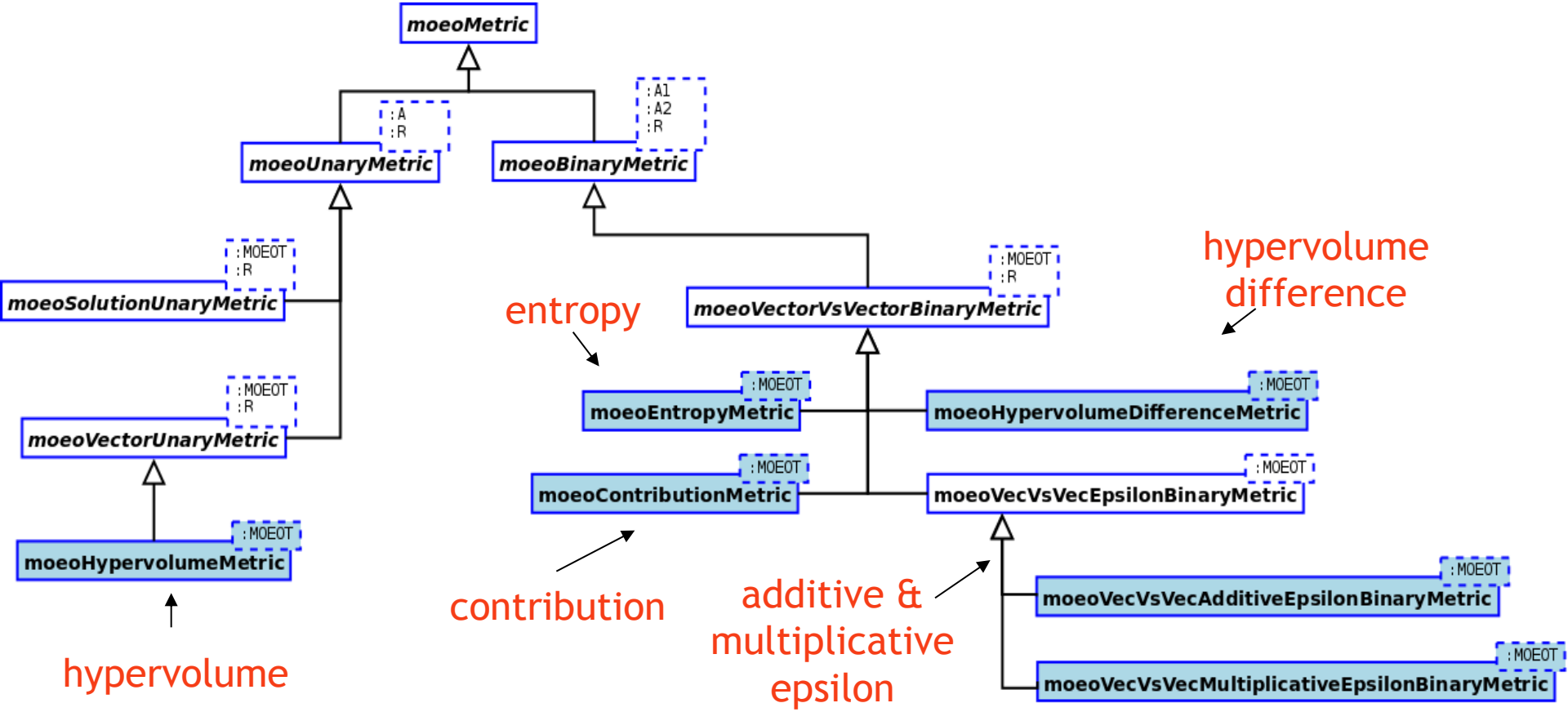


Implementation

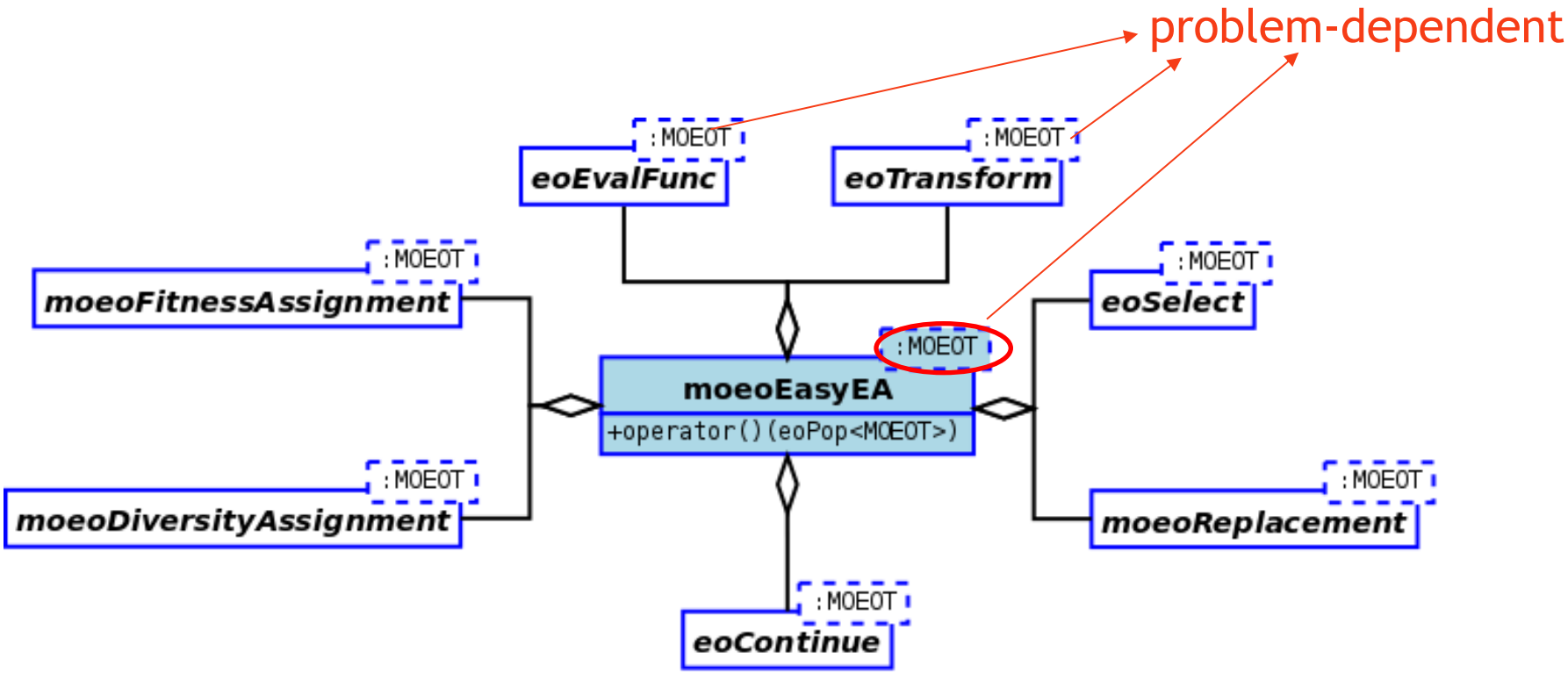
- Implement a representation
- Implement a population initialization strategy
- Implement a way of evaluating a solution
- Implement suitable variation operators
- Instantiate a fitness assignment strategy
- Instantiate a diversity preservation strategy
- Instantiate a selection strategy
- Instantiate a replacement strategy
- Instantiate an archive management strategy
- Instantiate a continuation strategy → eoContinue

Performance Metrics

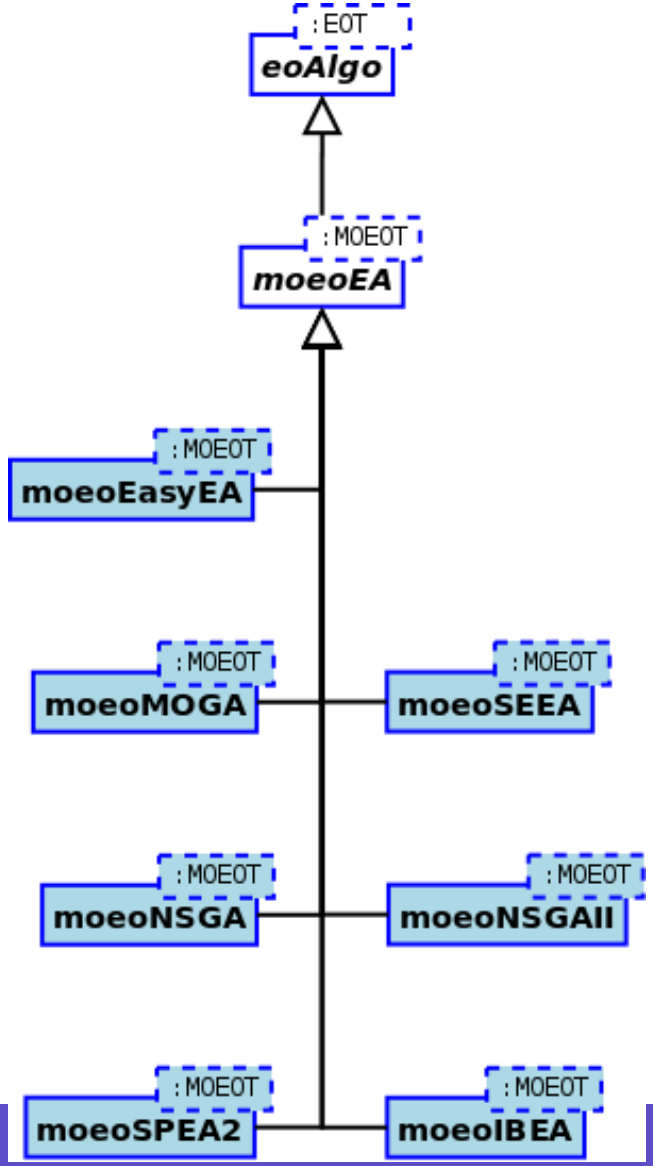
➔ Online computation



General-Purpose EMO Algorithm



State-of-the-art EMO Algorithms

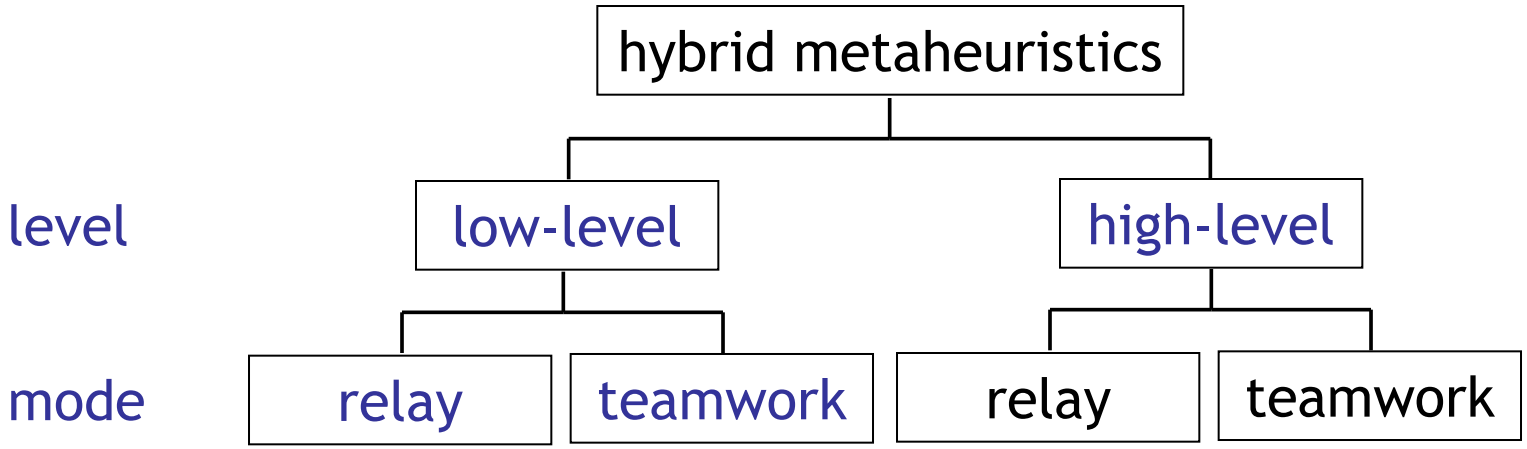


- To instantiate a state-of-the-art multi-objective metaheuristic for a novel continuous MOP

➔ The evaluation is the only component to be implemented

Conclusion

- Unified view of hybrid multi-objective metaheuristics

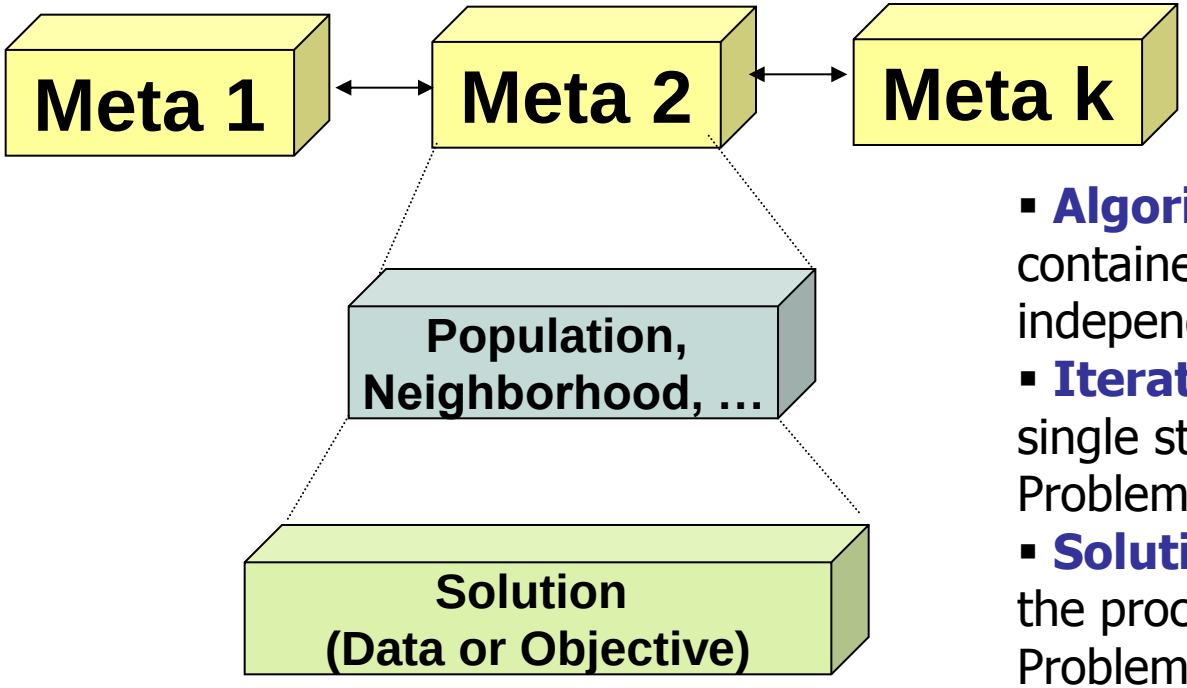


- **Low-level :** Functional composition of a single method.
- **High-level :** Different methods are self-contained.

- **Relay :** Pipeline fashion.
- **Teamwork :** Parallel cooperating agents.

Conclusion

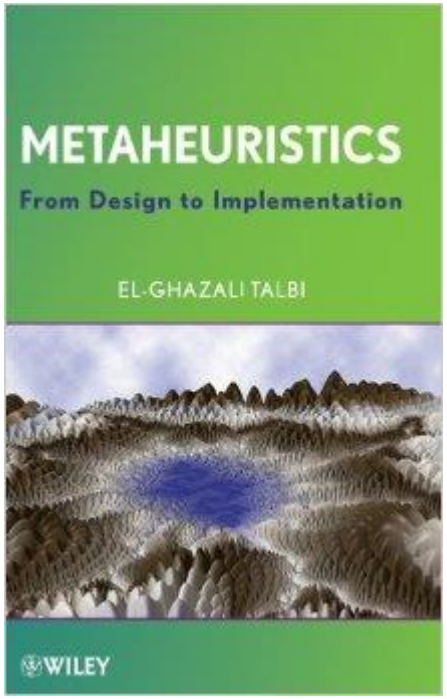
- Unified view of parallel multi-objective metaheuristics



- **Algorithm-Level**: Cooperative self-contained metaheuristics: Problem independent
- **Iteration-Level**: Parallelization of a single step of the metaheuristic: Problem independent
- **Solution-Level**: Parallelization of the processing of a single solution: Problem dependent

Exercises: what has to be done (design & implementation ?

- From the mono-objective resolution to the multi-objective resolution
- From the application of NSGA-II to IBEA evolutionary algorithms
- From the application of NSGA-II evolutionary algorithm to particle swarm optimization MOPSO and multi-objective scatter search
- Design of interactive multi-objective metaheuristics
- Handling many-objective MOPs
- Design of multi-objective metaheuristics for MOP with uncertainties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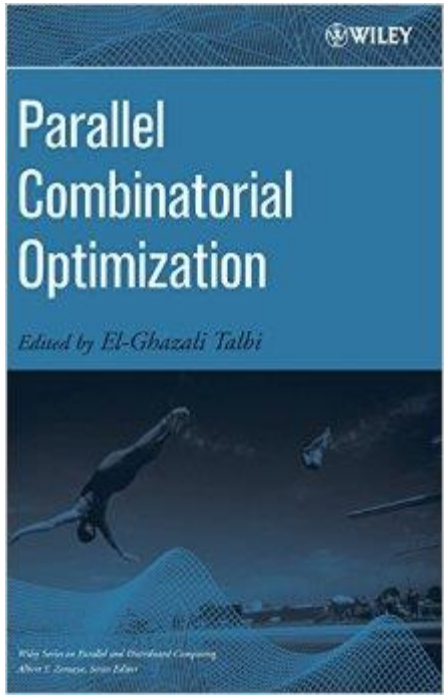
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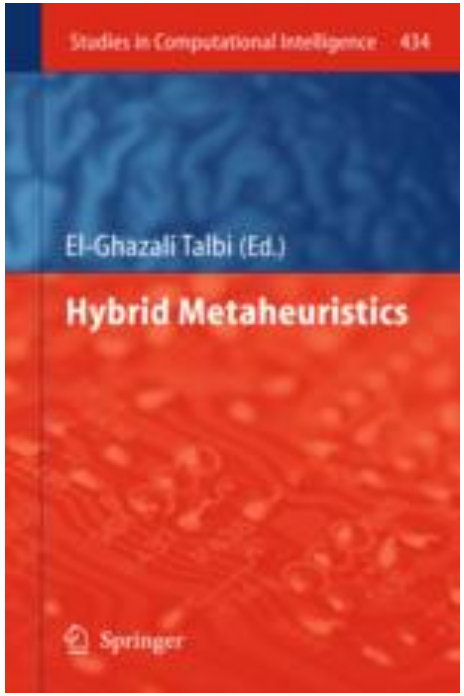
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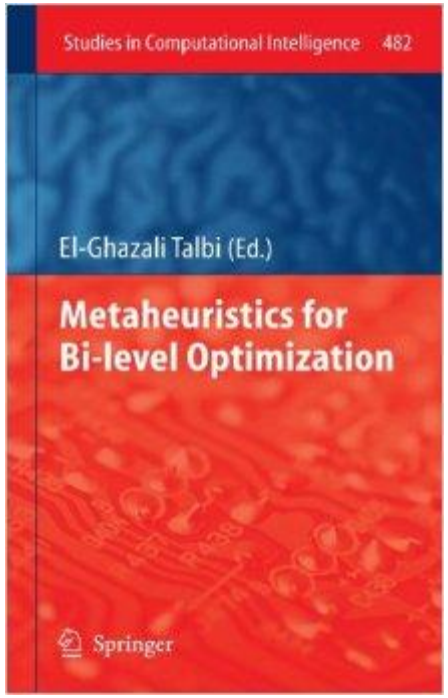
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