INSTITUT NATIONAL
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EN INFORMATIQUE
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Metaheuristics for Multi-objective Optimization

May 2007

E.-G. Talbi and the ParadisEO team

http://paradiseo.gforge.inria.fr
paradiseo-help@lists.gforge.inria.fr

Outline

- Multi-objective optimization: definitions, problems, etc
- A taxonomy of the resolution methods
- Landscapes and performance analysis
- Conclusion

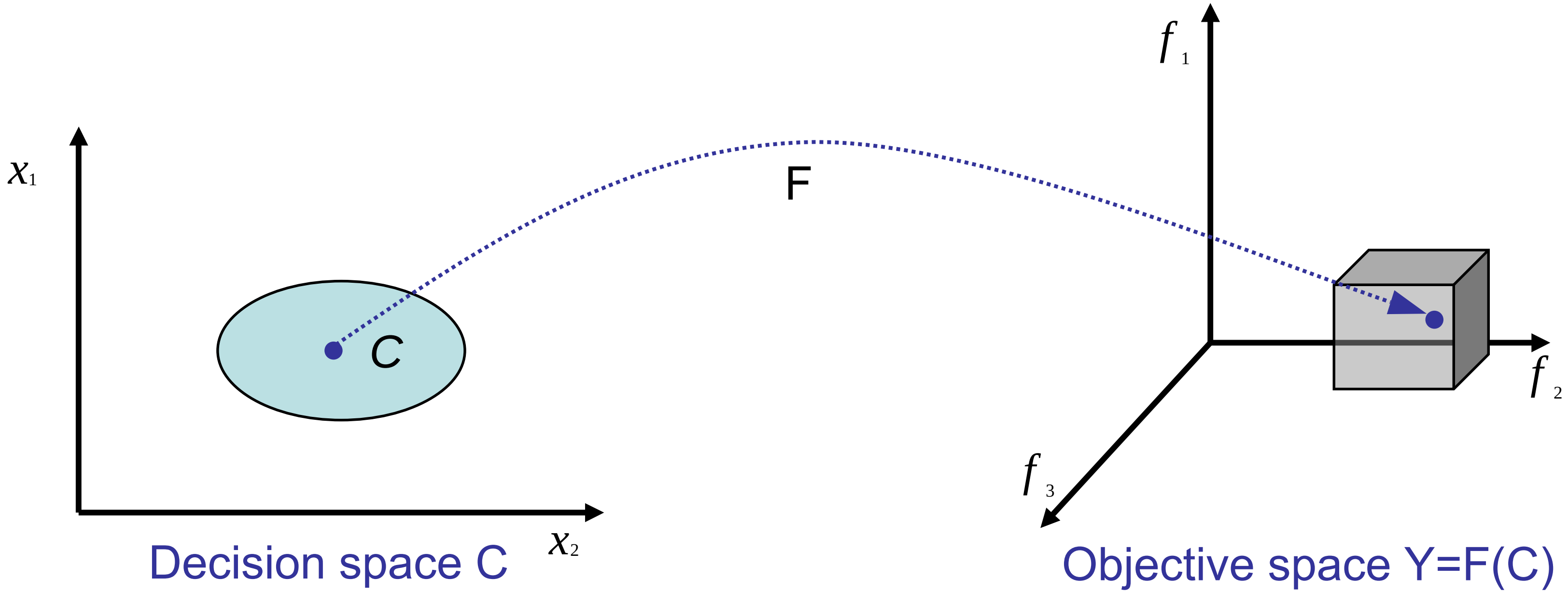
Multi-objective Optimization

- Many areas of industry are concerned
  - Telecommunication
  - Transport
  - Aeronautics
  - …
- Roots in the 19th century in economy from Edgeworth and Pareto
  - Management
  - Engineering
  - …
- Linear/Non linear Multi-objective Optimization [Steuer 86, White 90]
- Multi-objective Combinatorial Optimization

Multi-objective Optimization

$$(\text{MOP}) \begin{cases} \min F(x) = (f_1(x), f_2(x), \ldots, f_n(x)) & n \geq 2 \\ \text{s.t. } x \in C \end{cases}$$

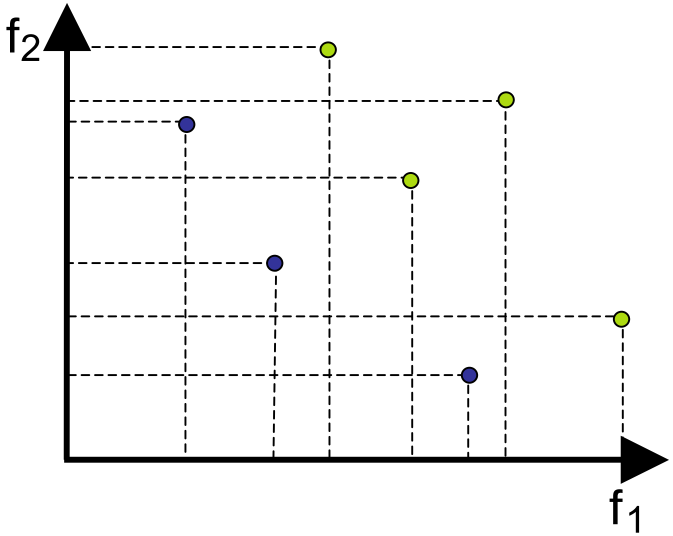
Decision variables $x = (x_1, x_2, \ldots, x_k)$



Definitions

Dominance: A solution x_1 dominates a solution x_2 if and only if:
$\forall i \in [1,\ldots,n],\ f_i(x_1) \leq f_i(x_2)$ and $\exists i \in [1,\ldots,n],\ f_i(x_1) < f_i(x_2)$

Non-dominated solution: A solution x is non-dominated if a solution which dominates x does not exist

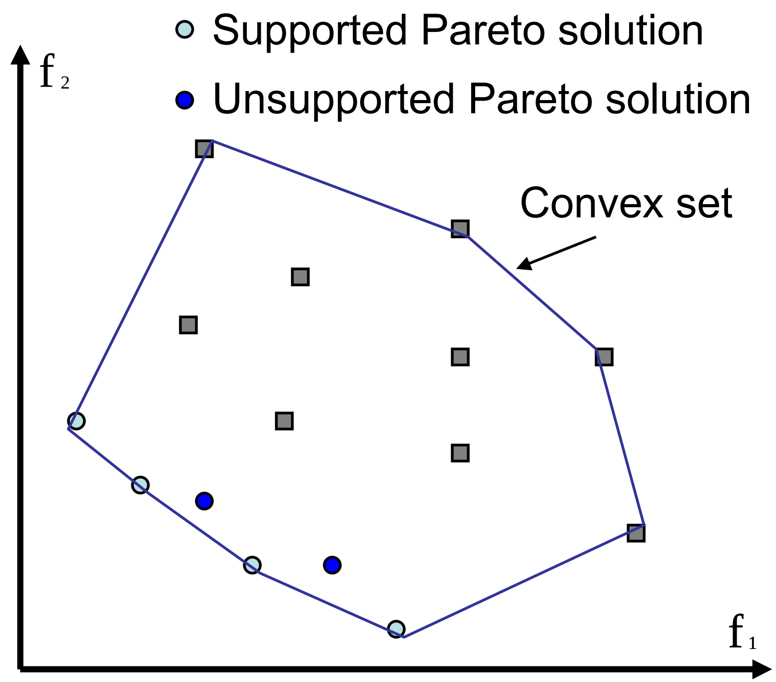


- Non-dominated solution (eligible, efficient, non inferior, Pareto optimal)
- Dominated feasible solution

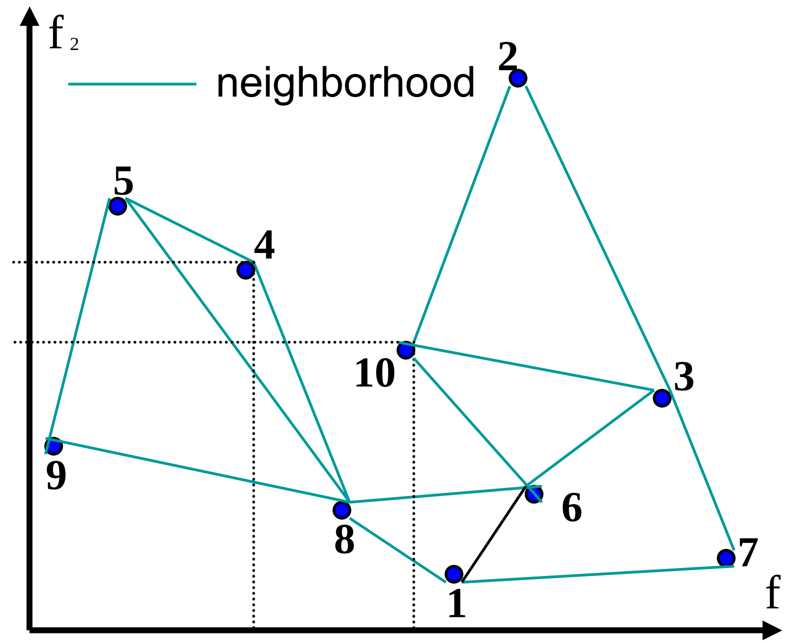
Goal: To find a well-converged and well-diversified Pareto set

Definitions

- Supported / Unsupported solutions
- Optimal vector y*
  Reference vector z*



- Locally Pareto optimal
- Neighborhood N: Local search
  - 1,8,9 : Pareto optimal
  - 4,10 : Locally Pareto optimal



Main Issues

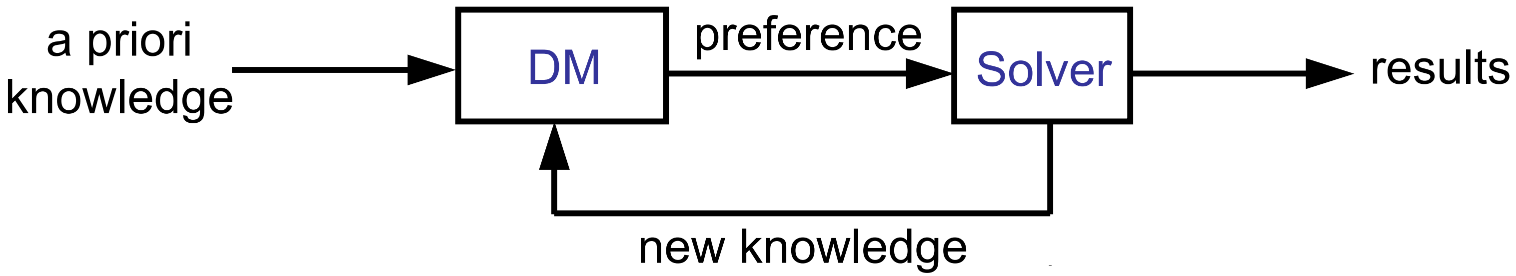
• What is optimality? Partial order, dynamic environment, the last choice belongs to the decision maker

• Number of Pareto solutions increases function of the dimension(s) of the tackled problems and the number of objectives

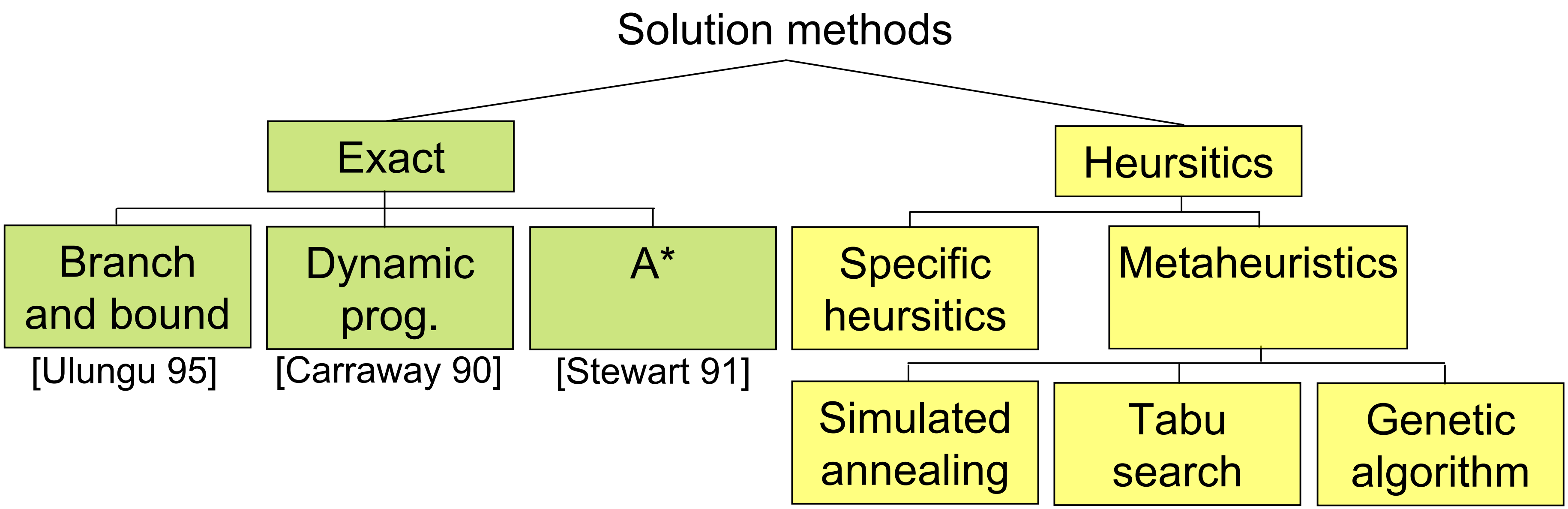
• For non-convex MOPs, Pareto solutions are located on the frontiers and in the convex hulls

Solver-Decision Maker Cooperation

- A priori
  - Preference → Search
  - A priori knowledge of the tackled problem
- A posteriori
  - Search → Preference
  - Cardinality of the reduced PO set
- Interactive
  - Search ↔ Preference
  - Decision helping is not addressed



Taxonomy of Optimization Methods



- Exact algorithms: bi-criterion problems of small size
- Metaheuristics:
  - Solution-based: simulated annealing, tabu search, ...
  - Population-based: genetic algos, scatter search, ants systems, ...

PO*: Approximation of PO

Academic MOPs

- Scheduling [Sayin et al. 99]
- Flow [Warburton 87], Spanning tree [Zhou et Gen 99]
- TSP [Serafini 92], Affectation [Teghem 95]
- Vehicle Routing [Park et Koelling 89], ...
- Bag packing [Teghem et al. 97]:

$$\begin{cases} Max\left(f_i(x)\right) = \sum_{j=1}^{m} c^i_j x_j \\ (i = 1,\dots, n), x \in C \\ C = x \Big/ \sum_{j=1}^{m} w_j x_j < W \\ x_j \in \{0,1\}, \forall j = 1,\dots, m \end{cases}$$

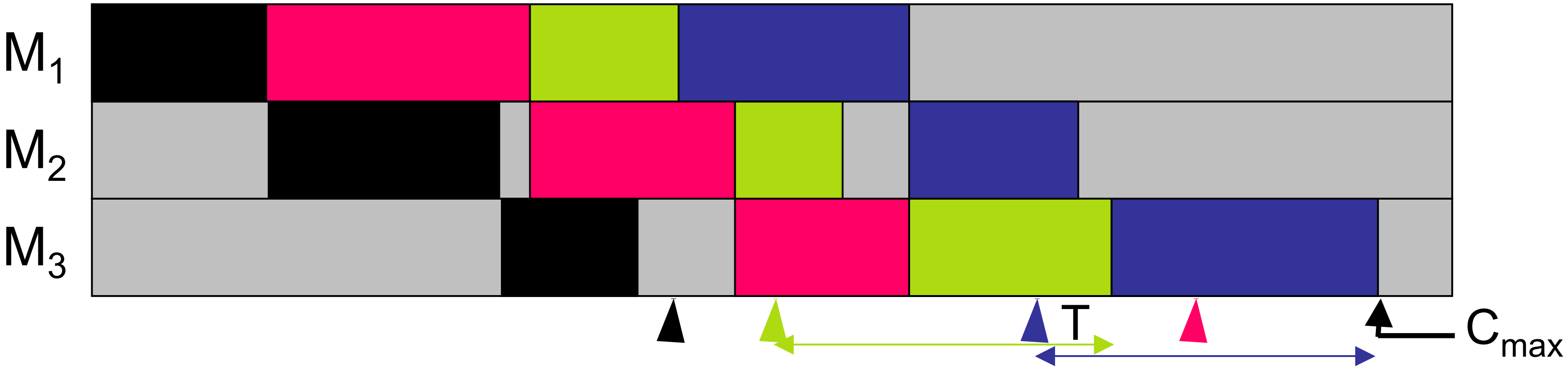
$$x_j = \begin{cases} 1 & \text{if } j \text{ is in the bag} \\ 0 & \text{else} \end{cases}$$

w_j : weight of j

c^i_j : usefulness of j / objective i

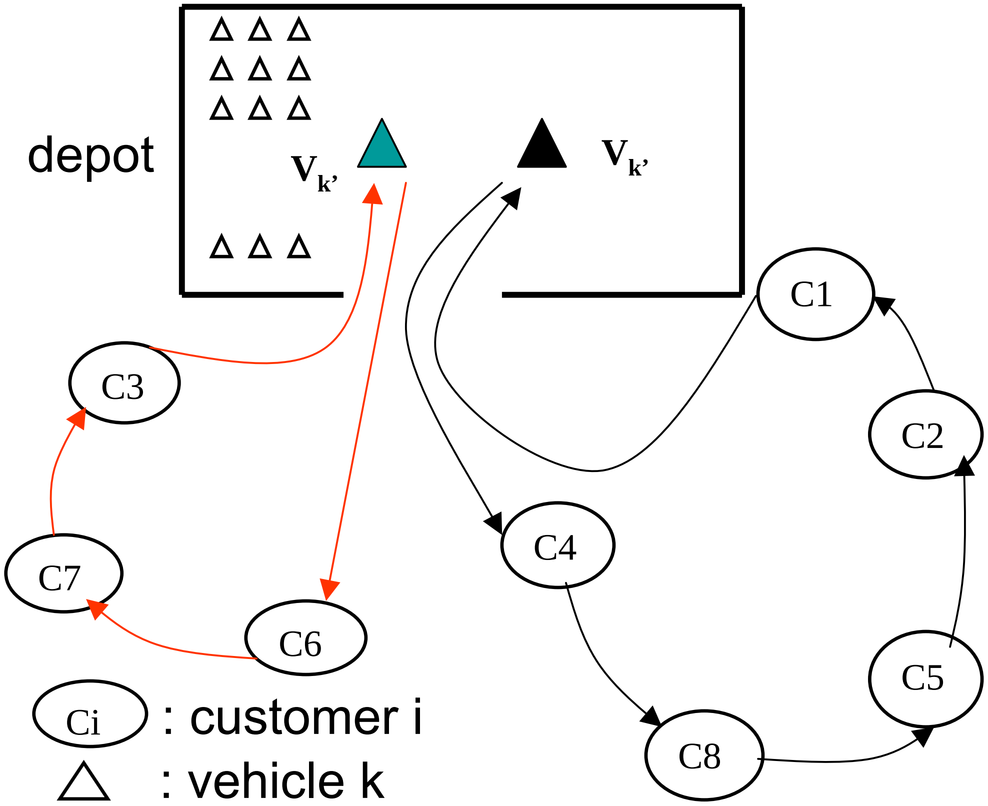
Bi-objective Flow-shop Scheduling Problem

- Scheduling problem F/perm, $d_i/(C_{max},T)$ [Graham 79]
- N jobs to schedule on M machines
- 2 objectives to minimize
  - Makespan (C_{max})
  - Total tardiness (T)



M. Basseur, F. Seynhaeve, E-G. Talbi: "**Design of multiobjective evolutionary algorithms: Application to the flow-shop scheduling problem**", *CEC'2002*, pp. 1151-1156, Hawaii, 2002

Bi-objective VRP



A multi-objective problem by nature

Bi-objective model:

- First criteria
  - Minimizing the tour length

$$\sum_{i,j=1}^{N} d_{ij} \sum_{k=1}^{M} x_{ijk}$$

- Second criteria
  - Minimizing the balance

$$\max_{k} \sum_{i,j=1}^{N} d_{ij}\, x_{ijk} - \min_{k'} \sum_{i,j=1}^{N} d_{ij}\, x_{ijk'}$$

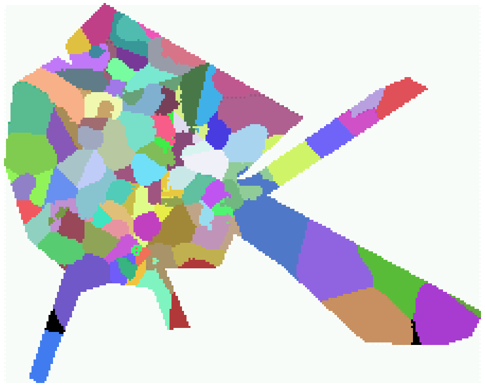
N. Jozefowiez, F. Semet, E.-G. Talbi: "**The bi-objective covering tour problem**", *Computers and Operations Research (COR)*, vol. 34, pp. 1929-1942, 2007

Industrial MOPs

- Telecommunications
    - Frequencies assignment [Dahl et al. 95], Wire antenna geometry design [Sandlin et al. 97]…
- Bioinformatics
- Aeronautics
    - Wings [Obayashi 98], Motors [Fujita 98]…
- Environment
    - Air quality [Loughlin 98], Water distribution…
- Transports
    - Motorway layout , Container Management [Tamaki 96]…
- Finances, Computer-integrated manufacturing, Robotics, Mechanics…

Cellular Network Design
[France Telecom]

- Network design (antennae on sites, configuration of antennae)
- Objectives
  - Minimizing the number of sites
  - Minimizing interferences
  - Minimizing traffic loss
  - Maximizing resource use
- Constraints
  - Covering
  - Handover

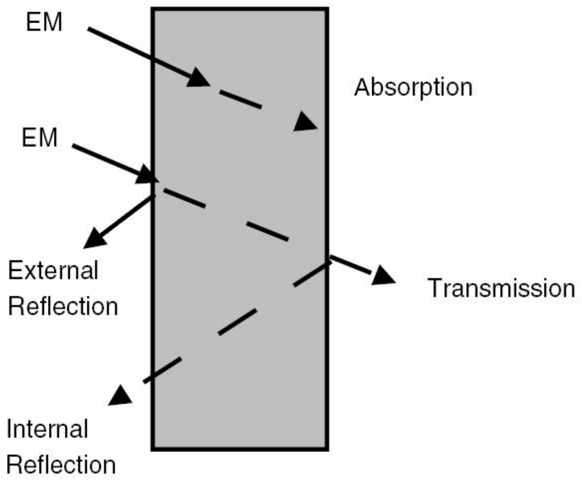


E.-G. Talbi, H. Meunier: "**Hierarchical parallel approach for GSM mobile network design**", *Journal of Parallel and Distributed Computing*, vol. 66(2), pp. 274-290, 2005

Design of Conducting Polymer Composites for Electromagnetic Shielding

4 objectives:

- Maximizing the electromagnetic shielding
- Min/Max the high reflecting coefficient
- Minimizing the mass percentage
- Minimizing the thickness



O. Schuetze, L. Jourdan, T. Legrand, E.-G. Talbi, J.-L. Wojkiewicz: "**A Multi-Objective Approach to the Design of Conducting Polymer Composites for Electromagnetic Shielding**", EMO'2007, LNCS vol. 4408, pp. 590-603, Matsushima, Japan, 2007

Knowledge Discovery in Biological Data

- Exponential growth of amount of available data
- Analyzing microarray is a major issue in genomics
- Often used techniques
  - Clustering and classification
- New high throughput technologies
  - Association rules

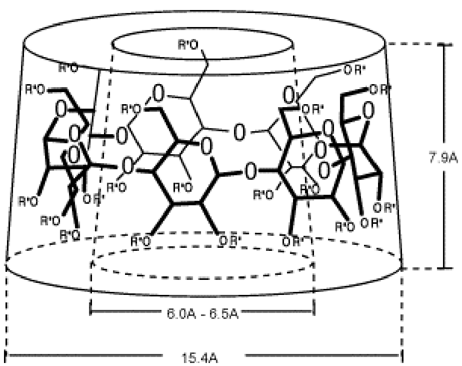
➔ Multi-objective rule-mining problem

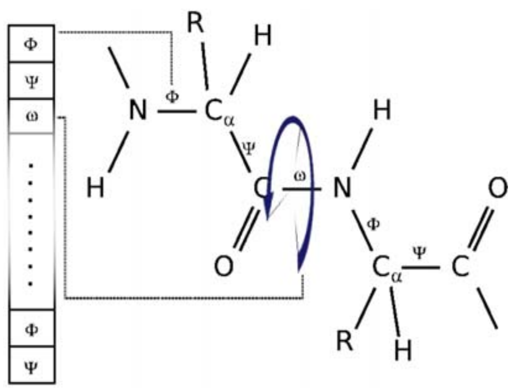
L. Jourdan, M. Khabzaoui, C. Dhaenens, E.-G. Talbi: "**A hybrid metaheuristics for knowledge discovery in microarray experiments**", *Handbook of Bioinspired Algorithms and Applications*, Chapter 28, pp. 489-505, CRC Press, USA, 2005

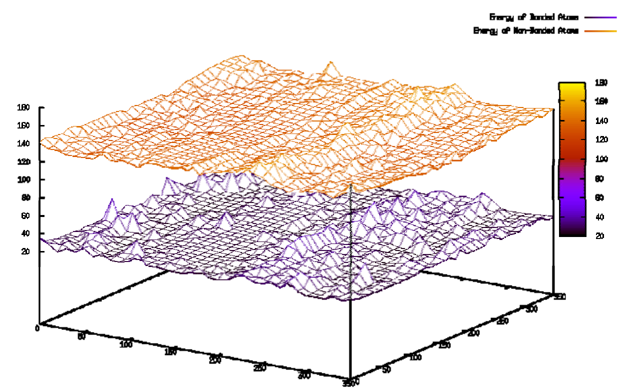
Bicriterion Molecular Structure Prediction

- A molecule with 40 residues and 10 conformations per residue
  - 1040 conformations are obtained (in average)
  - 1018 years are required (with 1014 conformations per second)

➔ Island-deployed Lamarckian genetic algorithm







A.-A. Tantar, N. Melab, E.-G. Talbi, B. Toursel: "**Solving the Protein Folding Problem with a Bicriterion Genetic Algorithm on the Grid**", *BioGrid'06*, Singapore, 2006

A Taxonomy of the Resolution Methods

Methods classification

- Scalar approaches
  - Aggregation method
  - ε-constraint method
  - Goal programming method

- Non-Pareto approaches
  - Each objective is treated separately

- Pareto approaches
  - The concept of Pareto dominance is used

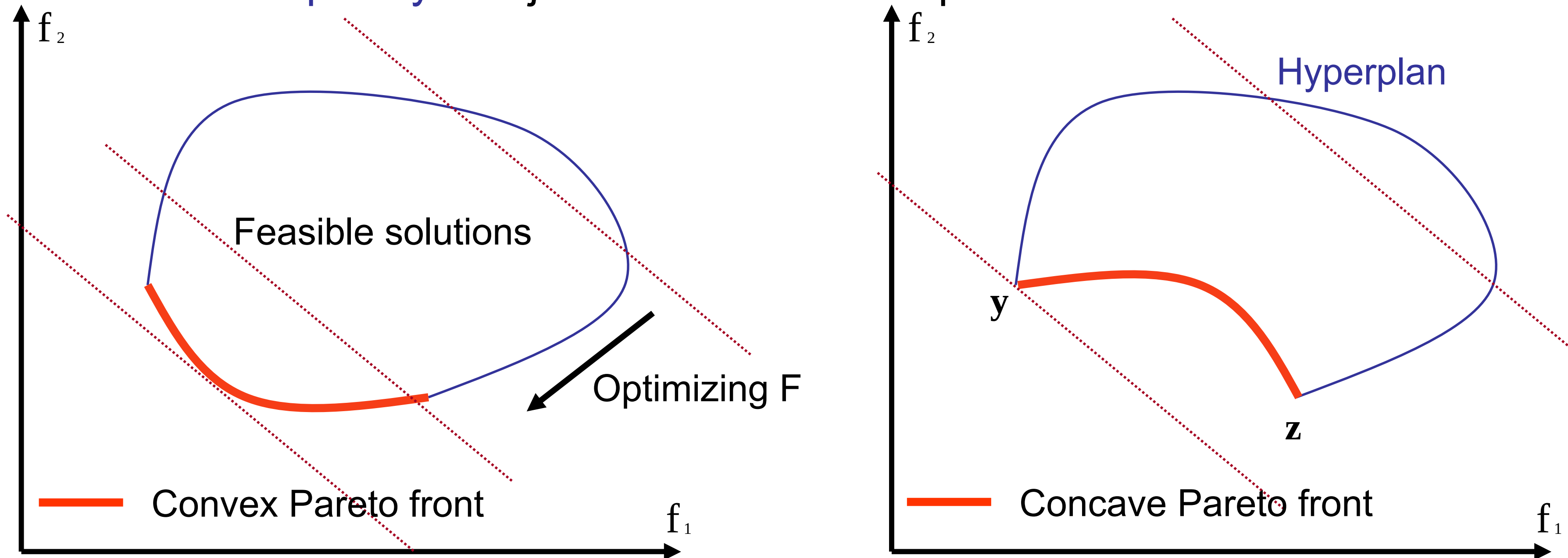
Aggregation Approach

[Gass & Saaty 55]

$$(MOP_w) \begin{cases} \min F(x) = \sum w_i f_i(x) \\ \text{s.t. } x \in C \\ \text{where } w_i \geq 0 \text{ for all } i=1,\dots,n \text{ and } \sum w_i = 1 \end{cases}$$

linear aggregation

Complexity: subjacent combinatorial problem



Aggregation Metaheuristics

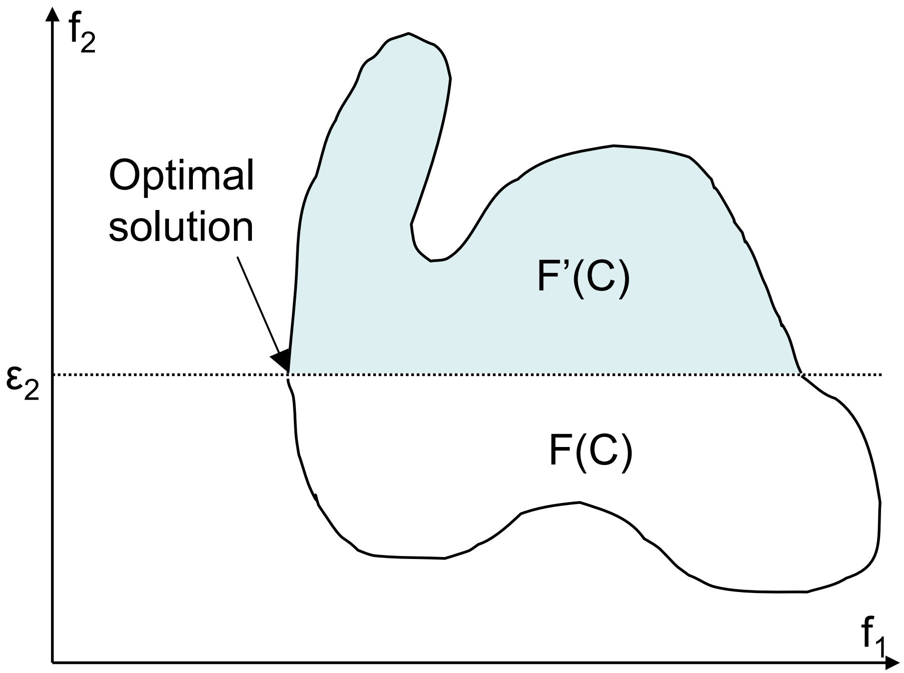
- Genetic algorithms [Hajela et Lin 92]
  - Individual representation: solution + λ
  - Goal: generating various Pareto solutions
- Simulated annealing [Serafini 92]
  - Acceptance probability
- Tabu search [Dahl et al. 95]
  - Weight = priority of the objective
- Hybrid metaheuristics [Talbi 98]
  - 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)

ε-constraint Approach

[Haimes et al. 71]

$$
(MOP_k(\varepsilon)) \begin{cases} \min f_k(x) \\ \text{s.t. } x \in C, \\ f_j(x) \leq \varepsilon_j \text{ for all } j=1,\ldots,n,\ j \neq k \end{cases} \qquad \varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)
$$

- Variations of ε
- F(C) = objective space of the initial problem
- F'(C) = objective space of the modified problem



ε-constraint Metaheuristics

- Genetic algorithms
  - Individual = ε [Loughlin 98]

$$\varepsilon_i = \varepsilon_{\min} + \frac{(i-1).(\varepsilon_{\max} - \varepsilon_{\min})}{(k-1)}$$

k = size of the population

- Tabu search [Hertz et al. 94]
  - Set of sub-problems
  - Priority order
  - Threshold (f') = Optimum (f*)
  - + Allowed deterioration

$$(MOP_q) \begin{cases} f_q^* = \min f_q(x) \\ \text{s.t. } x \in C \\ f_r(x) \leq f'_r,\ r=1, \ldots, q-1 \end{cases}$$

- Hybrid metaheuristics [Quagliarella et al. 97]
  - Genetic algorithm + Local search

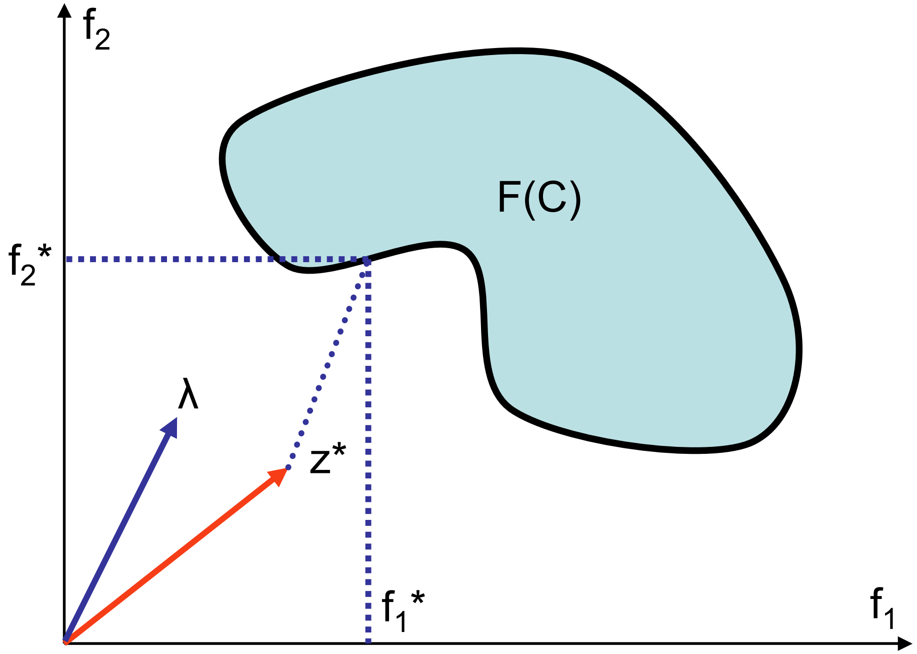
Goal Programming Approach

$$(MOP_{\lambda,z^*}) \begin{cases} \min \left(\sum \lambda_i \, |f_i(x) - z_i^*|^p\right)^{1/p} \\ \text{s.t. } x \in C \end{cases}$$

z^*: ideal or reference vector

- Tchebycheff metric
- L_p metric

- p=2 → Euclidian metric
- p=∞ → Min-Max



Goal Programming Metaheuristics

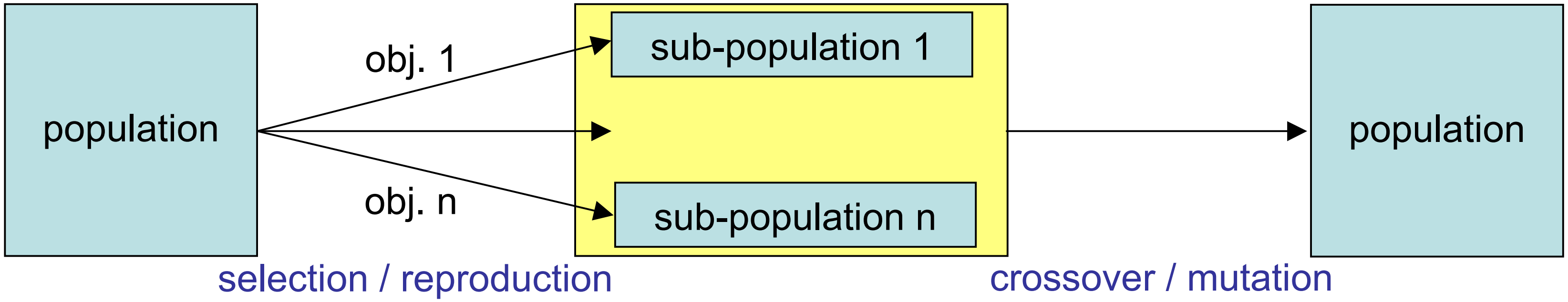
- Genetic algorithms
  - Min-max function + parallel GA with various weights [Coello Coello 98]
  - Fuzzy rules during the evaluation of F [Reardon 98]
- Simulated annealing [Serafini 92]
  - Acceptance probability
  - Iteration = λi = λi + [-0.05, +0.05]
- Tabu search [Gandibleux 96]
  - Best neighbor = best non-tabu compromise
  - Compromise = L_p norm of Tchebycheff to the ideal vector
  - Saving the M best individuals

Scalar Approaches: Critical Analysis

- Research space ≠ initial problem
  - The problem loses its eventual properties
- An execution produces one solution only
- A priori knowledge (to determine parameters)
- Sensitive to the landscape of the Pareto front
  - Convexity, discontinuity…
- Sensitive to various parameters
  - Weights, constraints, goals…
- Noisy objectives or uncertain data
- Cost associated to the algorithms (multiple executions)

Non-Pareto Approaches

- Parallel selection (VEGA) [Schaffer 85]



- Lexicographic selection (priority order)
  - Genetic algorithms [Fourman 85]
  - Evolutionary strategies [Kursawe 91]
- Multi-sexual reproduction [Lis & Eiben 96]
  - One class per objective
  - Reproduction (crossover) over several individuals

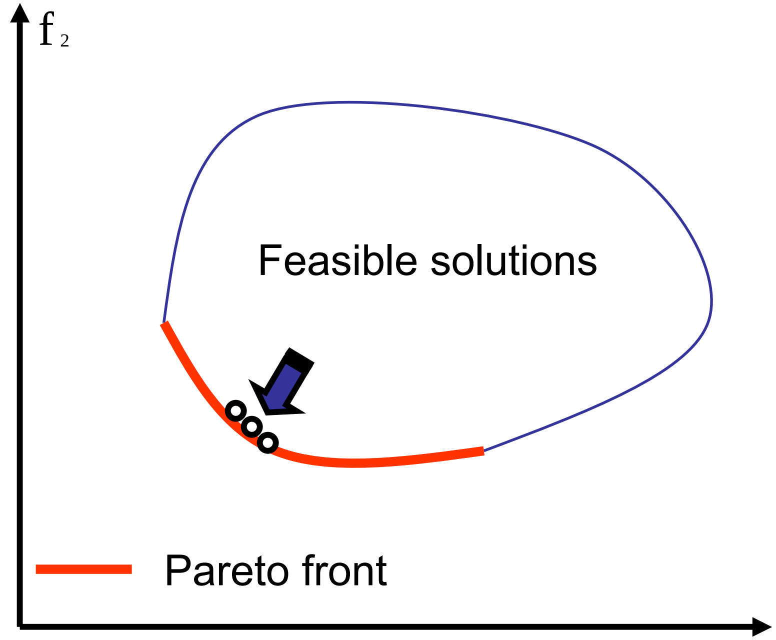
➔ Tends to ignore compromised solutions

Pareto Approaches

Goals

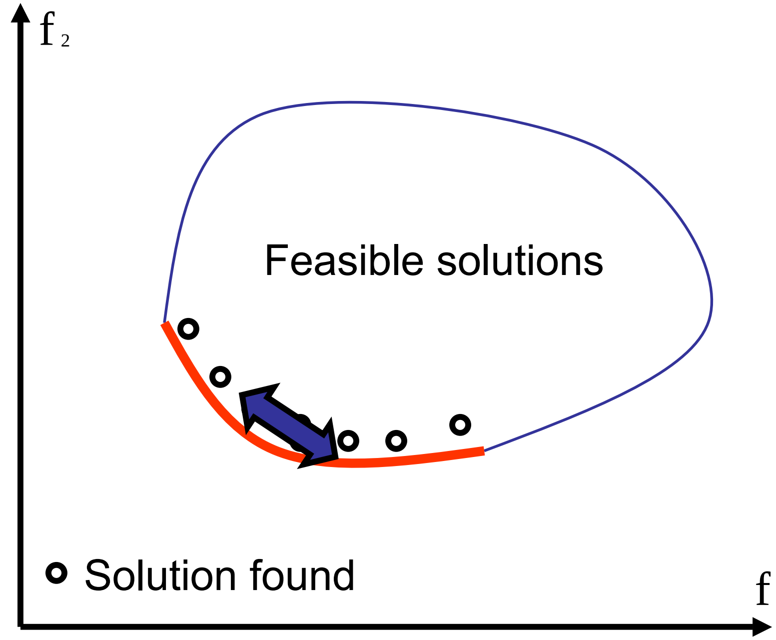
Convergence
(fitness)

- Ranking, elitism, …



Diversification
(diversity)

- Niching, sharing, …



Fitness assignment

Solution x → Evaluation of x in the objective space → Fitness (x) (scalar value)

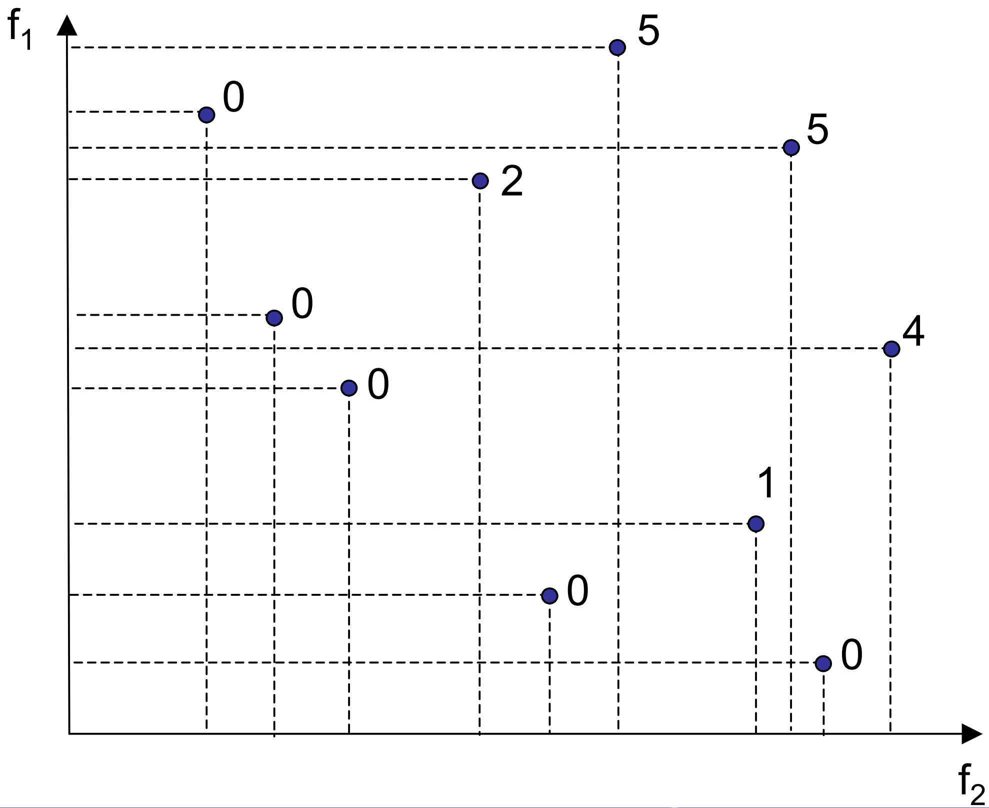
- Fitness (x) reflects the quality of x in term of convergence

- Pareto-based fitness assignment strategies
  - Dominance rank (*e.g.* used in MOGA)
  - Dominance depth (*e.g.* used in NSGA and NSGA-II)
  - Dominance count (*e.g.* combined with dominance rank in SPEA and SPEA2)
  - Indicator-based (e.g. used in IBEA)

Pareto Ranking

[Fonseca & Fleming 93]

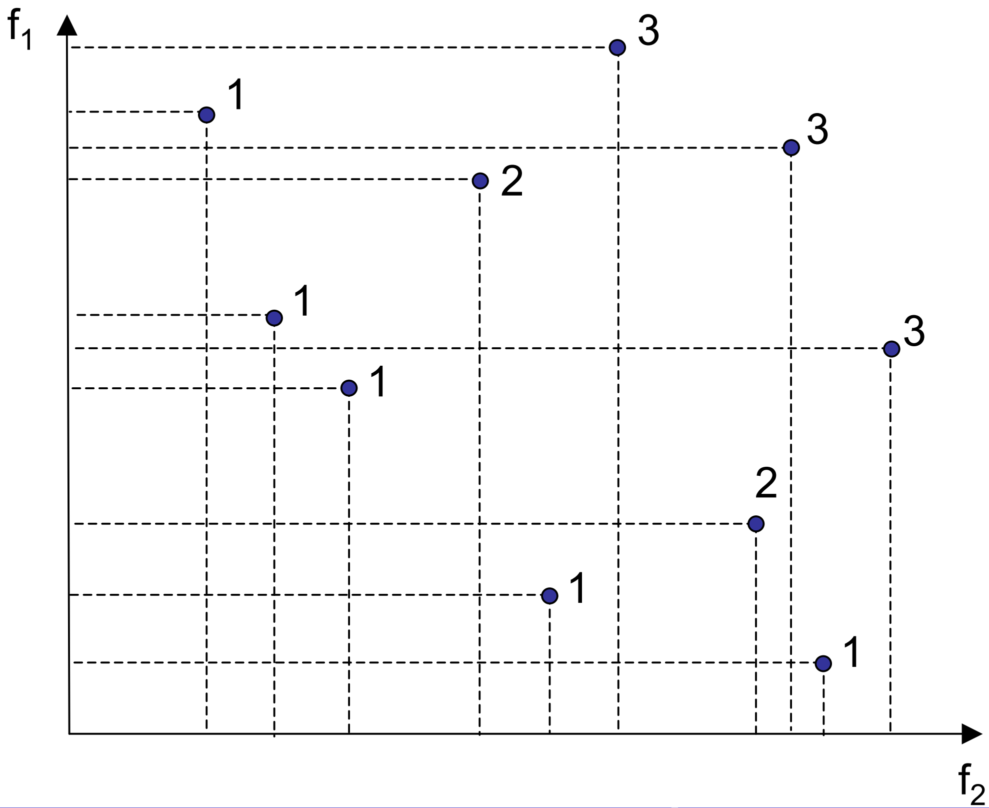
Fitness (x) = number of solutions by which the solution x is dominated



Fast Non-dominated Sorting

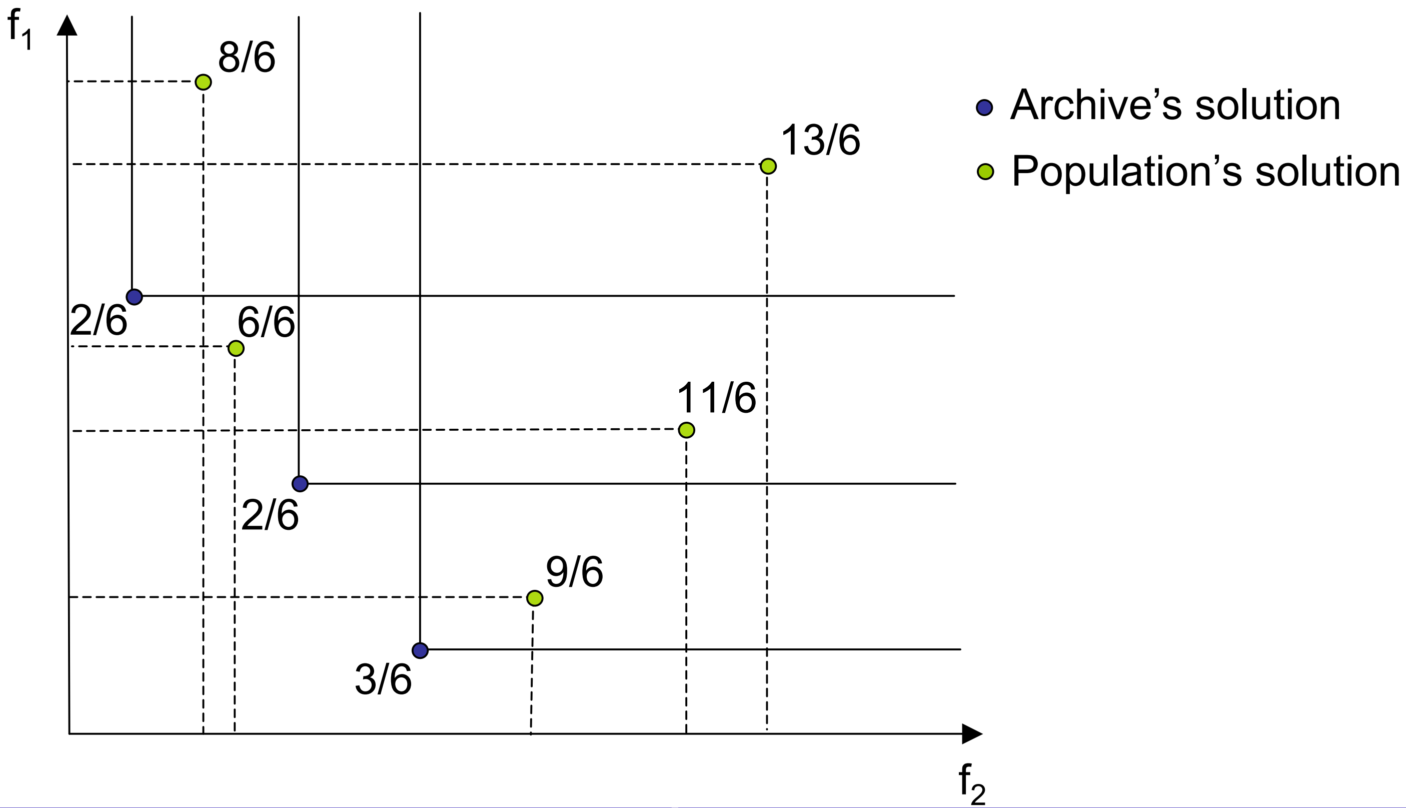
[Srinivas & Deb 94]

Solutions classified into several fronts



Strength Pareto Fitness Assignment
[Zitzler & Thiele 99]

Fitness (x) depends on the strength values of the archive's members that dominate x



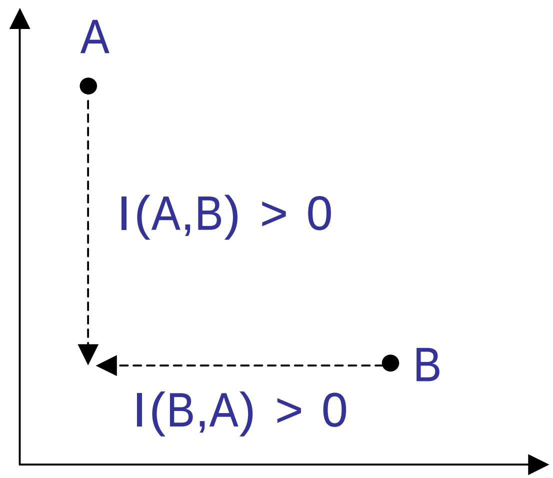
Indicator-Based Fitness Assignment

[Zitzler & Künzli 04]

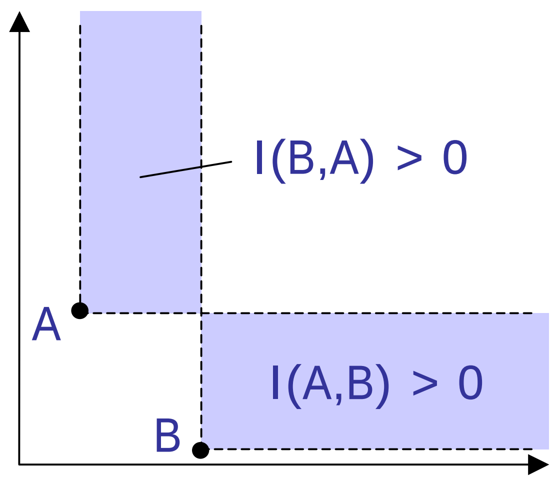
Solutions compared on the basis of a binary quality indicator I

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

Examples of binary quality indicators:



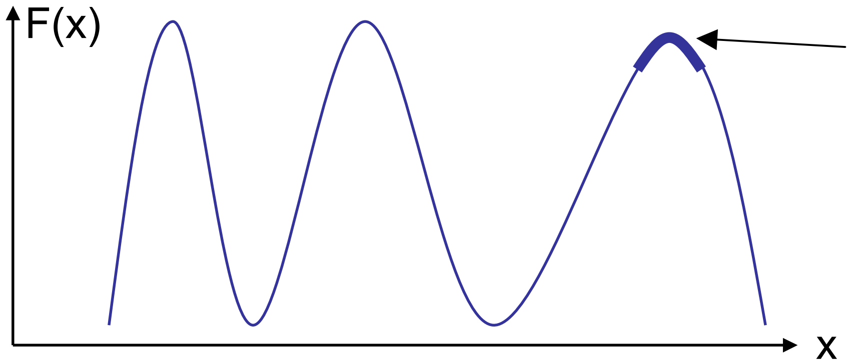
Additive epsilon indicator ($I_{\epsilon+}$)



Hypervolume indicator (I_{HD})

Diversity

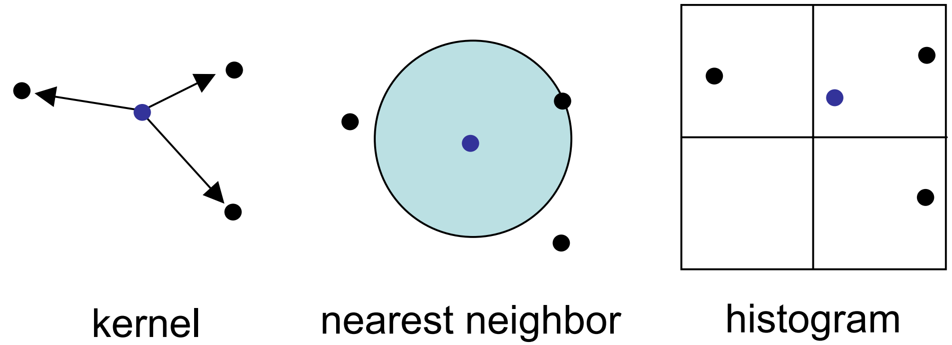
Multi-modal optimization: locating every optima of the problem



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

Diversity

- 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 k^{th} nearest neighbour
- Histograms
  - Space divided onto neighbourhoods by an hypergrid



➔ decision / objective space

Sharing

➔ Reduce the cost of an individual / number of similar individuals

$$f(x) = f(x) / \sum sh(\, dist(x,y)\,)$$

$$sh(\, dist(x,y)\,) = \begin{cases} 1 - (\, dist(x,y) / \sigma_{sh}\,)^{\alpha} & \text{if } dist(x,y) < \sigma_{sh} \\ 0 & \text{else} \end{cases}$$

- Objective space and/or decision space?
- Distance used (dist)?
- Niches size (σ_{sh})?

Pareto-based Metaheuristics

- Mainly evolutionary algorithms
  - MOGA [Fonseca & Fleming 1993]
  - NSGA-II [Deb et al. 2000]
  - SPEA2 [Zitzler et al. 2001]
  - IBEA [Zitzler & Künzli 2004]

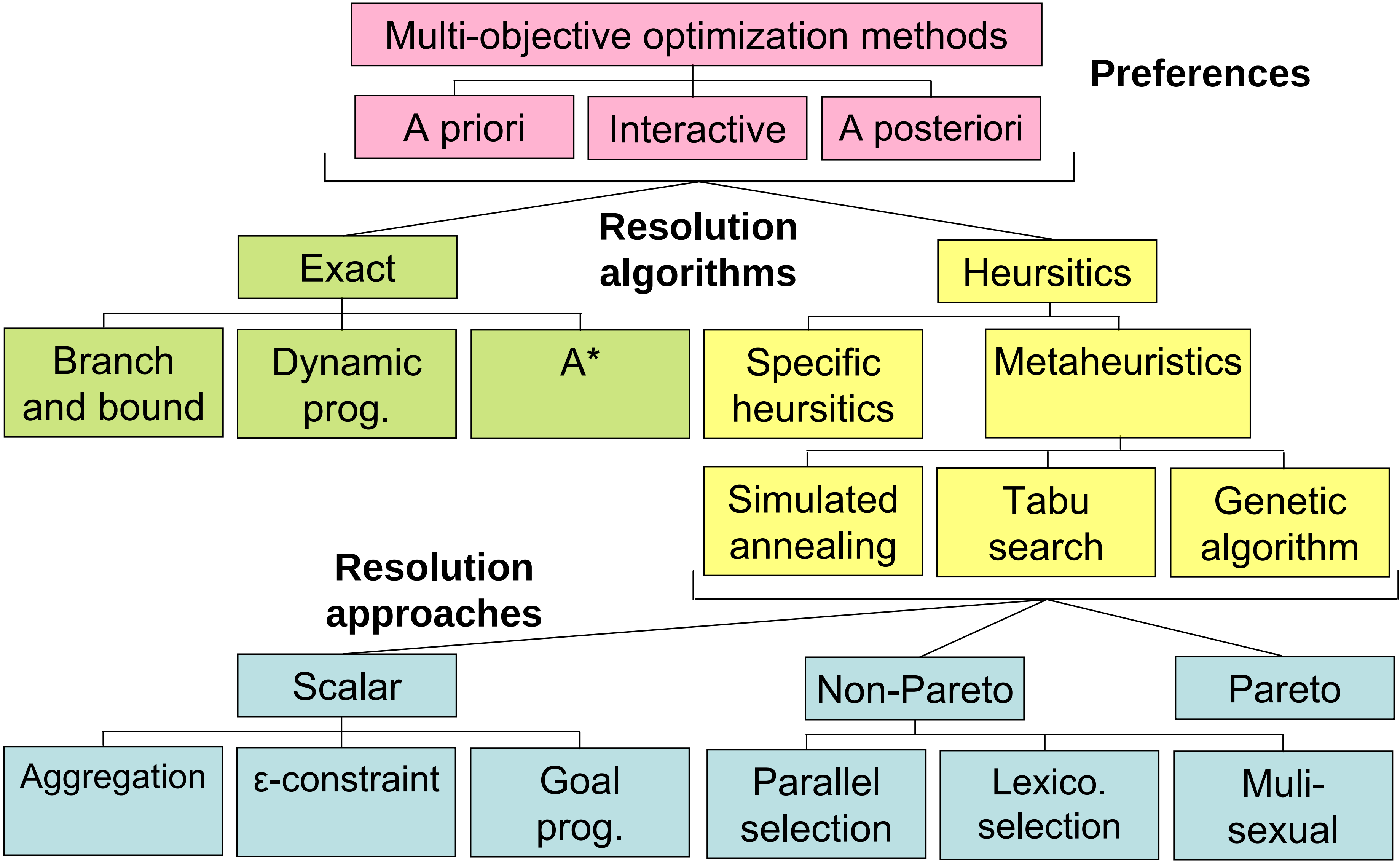
- Genetic programming
  - MOGP [Rodriguez-Vasquez et al. 97]

- Ant colony

Pareto-based Metaheuristics

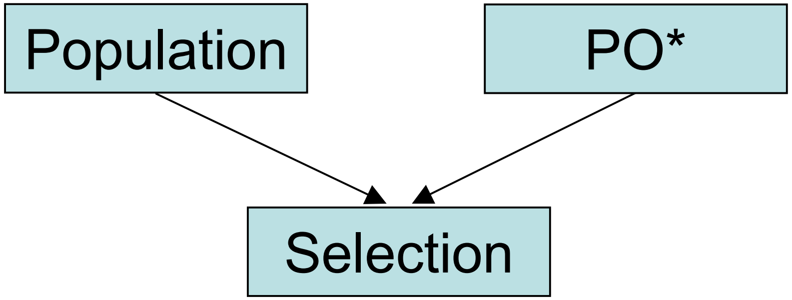
- Scatter search
  - SSPMO [Molina et al. 05]
  - MOSS [Beausoleil 06]
- Local search
  - PLS [Basseur et al. 03]
- Tabu search
  - MOTS [Hansen et al. 97]
  - TAPaS [Jozefowiez et al. 03]
- Simulated annealing

Classification



Advanced Techniques

- Elitism (archive PO*) [Zitzler & Thiele 98]



- Clustering of the PO* set [Roseman et Gero 85]
- Hybridization
  - Genetic Algorithm + Local Search (Tabu, Archive PO*)

E-G. Talbi, M. Rahoual, M-H. Mabed, C. Dhaenens: "**A Hybrid Evolutionary Approach for Multicriteria Optimization Problems: Application to the Flow Shop**", *EMO'01, LNCS 1993, Springer-Verlag*, pp.416-428, Zurich, Switzerland, 2001

Advanced Techniques

- Parallel models (genetic algorithms)
  - Quicker research
  - Results improved (cooperation)

N. Jozefowiez, F. Semet, E-G. Talbi: "**Parallel and hybrid models for multi-objective optimization: Application to the vehicle routing problem**", *PPSN VII, LNCS 2439, Springer-Verlag,* pp. 271-280, Granada, Spain, 2002

- Adaptive operators
  - Mutation, crossover, …

M. Basseur, F. Seynhaeve, E-G. Talbi: "**Adaptive mechanisms for multi-objective evolutionary algorithms**", *CESA'2003*, Lille, France, 2003

- Path relinking

M. Basseur, F. Seynhaeve, E-G. Talbi: "**Path Relinking in Pareto Multi-objective Genetic Algorithms**", *EMO'05, LNCS 3410, Springer-Verlag*, pp.120-134, Guanajuato, Mexico, 2005

Landscapes and Performance Analysis

PO known

[Teghem et al.]

- Absolute efficiency
  - 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

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

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

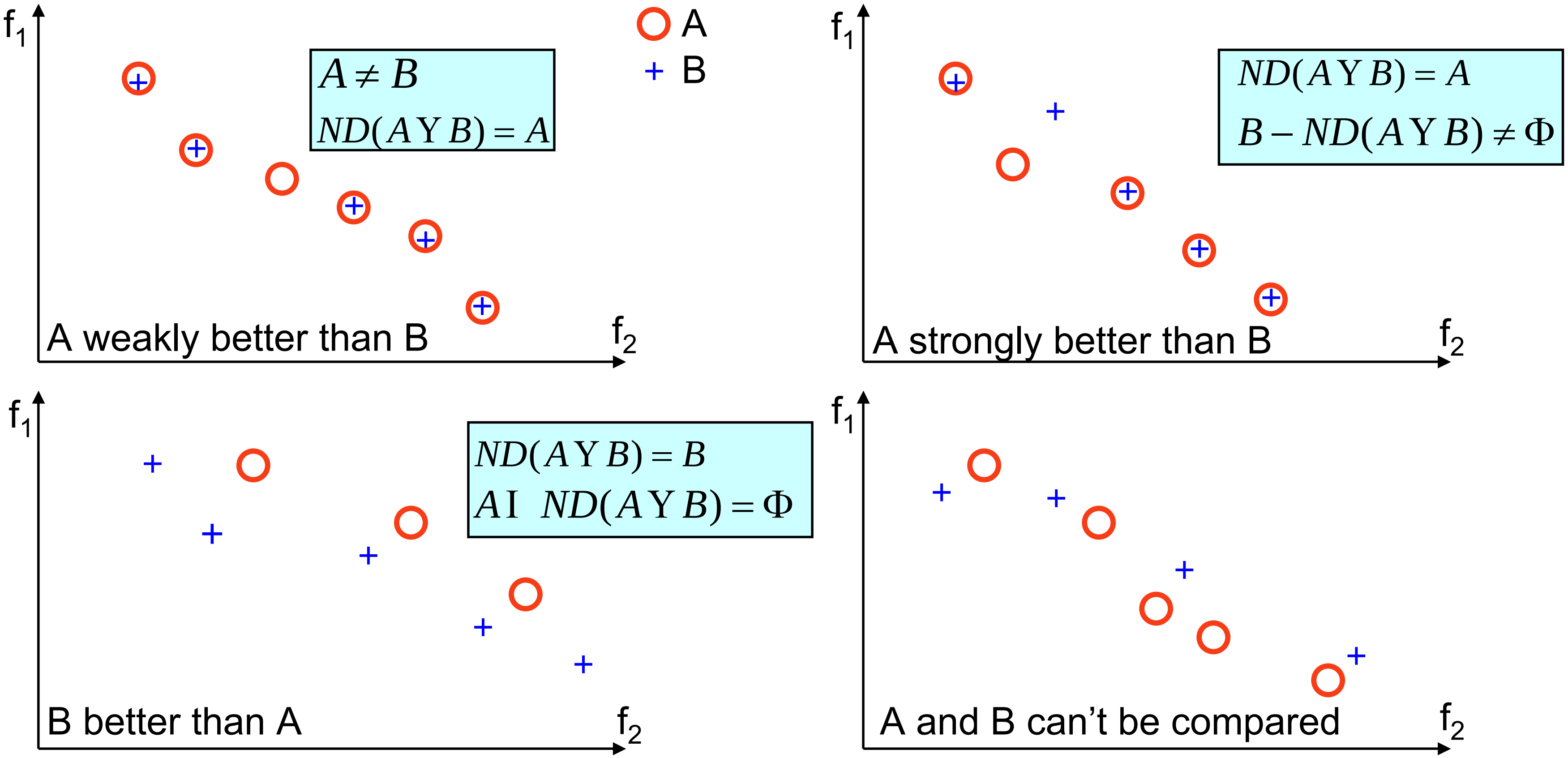
$$d(x,y) = \sum_{i=1}^{n} \lambda_i \left| f_i(x) - f_j(y) \right|$$

- Uniformity

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

PO unknown

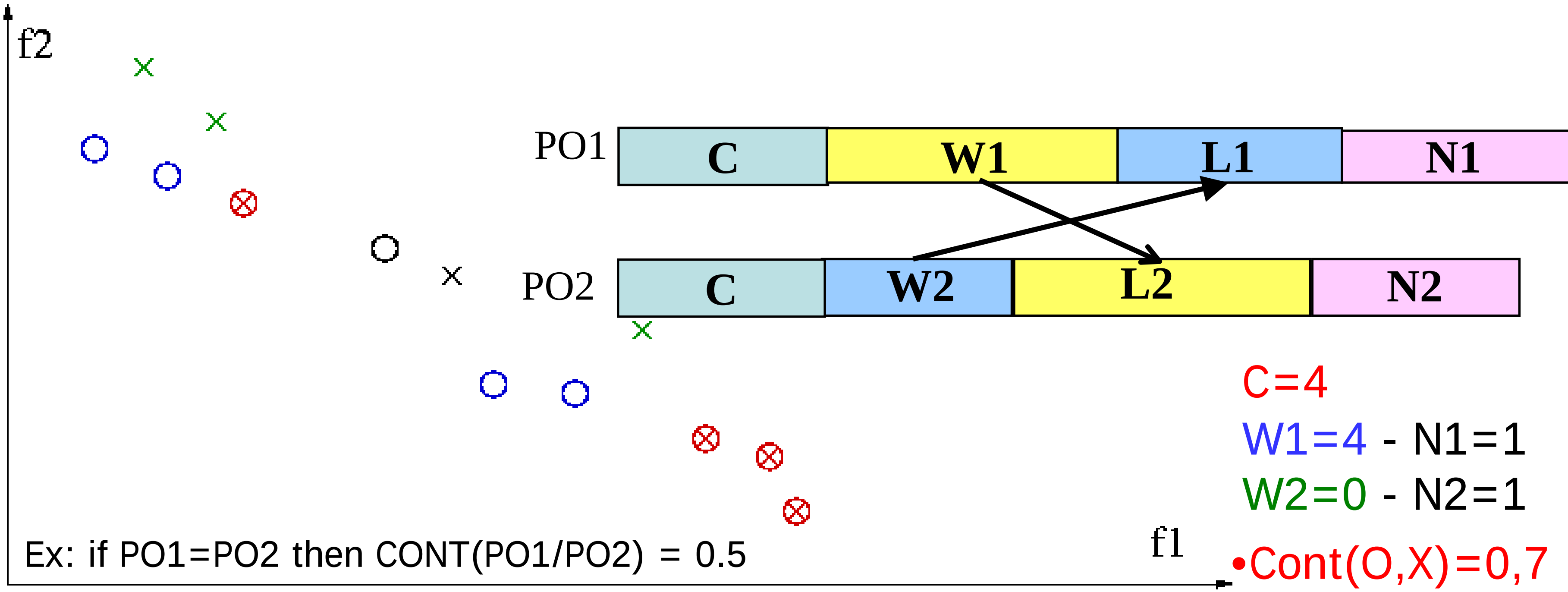
- Relative efficiency: number of solutions from A dominated by B



PO unknown

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

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



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

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

C=4

W1=4 - N1=1

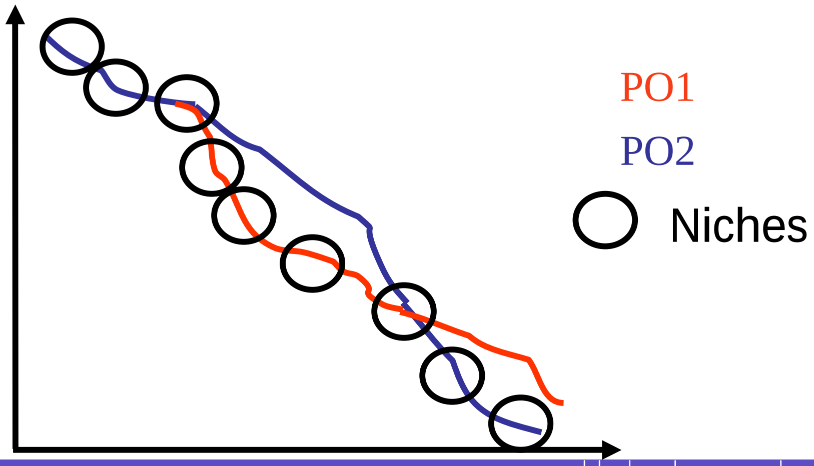
W2=0 - N2=1

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

PO unknown

- 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*

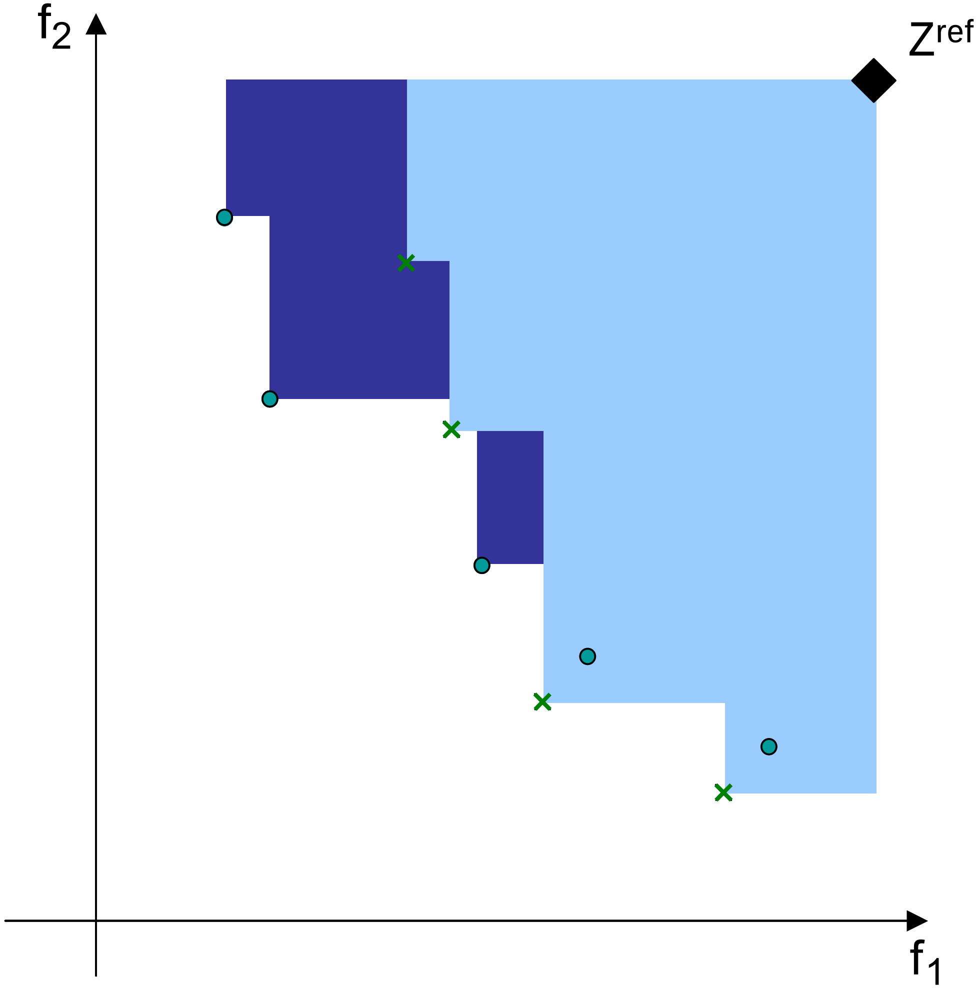
$$E(PO_1,PO_2)=\frac{-1}{\ln(\gamma)}\sum_{i=1}^{|PO^*|}\left(\frac{1}{Ni}\frac{n_i}{\|PO_1\|}\ln\frac{n_i}{\|PO_1\|}\right)$$



PO unknown

• S-metric / Hypervolume
[Zitzler 99]

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



Landscapes

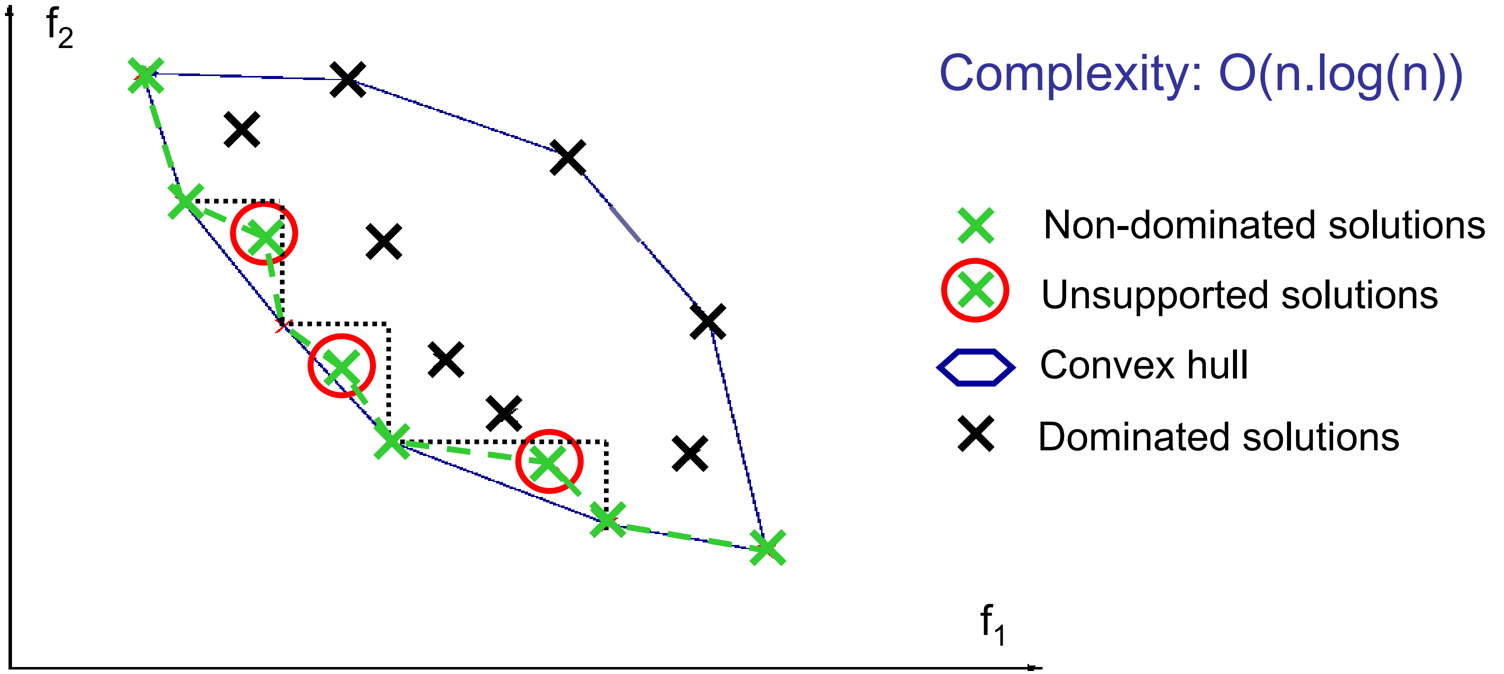
How to describe a Pareto front?

- Convexity of PO (supported or not)
- Multi-modality
- Deception (deceptive attractors)
- Isolated optimum (Flat space)
- Discontinuity
- Uniform distribution

Landscapes

Aggregation: supported solutions only

Convexity: Proportion of Pareto solutions belonging to the convex hull



Complexity: O(n.log(n))

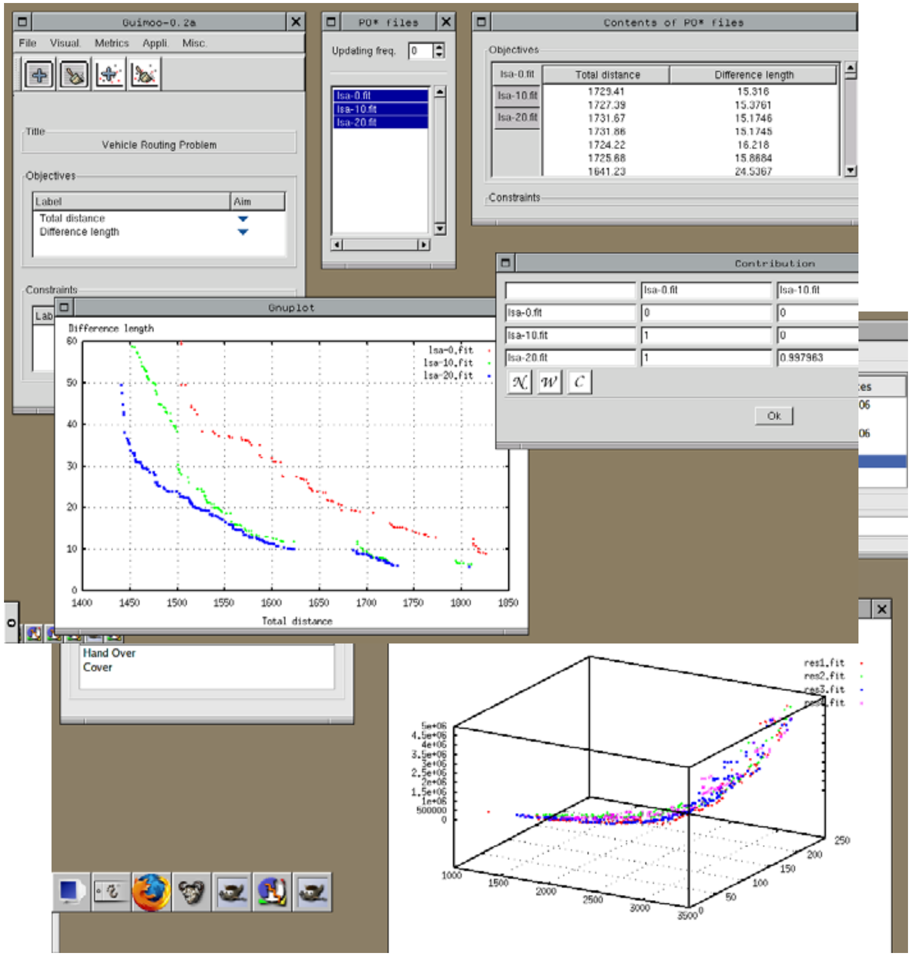
GUIMOO

a Graphical User Interface for Multi-objective Optimization

http://guimoo.gforge.inria.fr

GUIMOO

- Graphical tool dedicated to the analysis of multi-objective optimization results
- Free software (open source)
- Platform-independent
- Different input/output formats
- Easily customized for specific applications
    - Telecom, genomics, engineering design, …
- On-line user manual



GUIMOO

- On-line and off-line visualization (2D or 3D) of Pareto fronts
  - (dis)continuity, (dis)convexity, multi-modality, …
  - Distribution of the solutions among the objective space
- Metrics for quantitative and qualitative performance evaluation
  - Contribution
  - Entropy
  - Generational distance
  - Spacing
  - Coverage of two sets, coverage difference
  - S-metric, D-metric
  - R-metrics

Conclusion

Conclusion

- Important research area orientation for scientists and engineers (real problems, open questions)
- Population-based metaheuristics naturally efficient
- Hybrid approaches
- Performance analysis
- Interactive approach
- ParadisEO-MOEO: a framework for multi-objective optimization
  - http://paradiseo.gforge.inria.fr
- GUIMMO: a graphical user interface for multi-objective optimization
  - http://guimoo.gforge.inria.fr

Conclusion

- Academic problems (benchmarks : www.lifl.fr/OPAC/)
  - TSP / VRP
  - Scheduling problems
- Real-world applications
  - Bioinformatics
    - Protein docking
    - Protein folding
    - Knowledge discovery in biological data
  - Telecom
    - Cellular networks design
  - Polymer composites in the microwave band