Multi-Objective Evolutionary Algorithms

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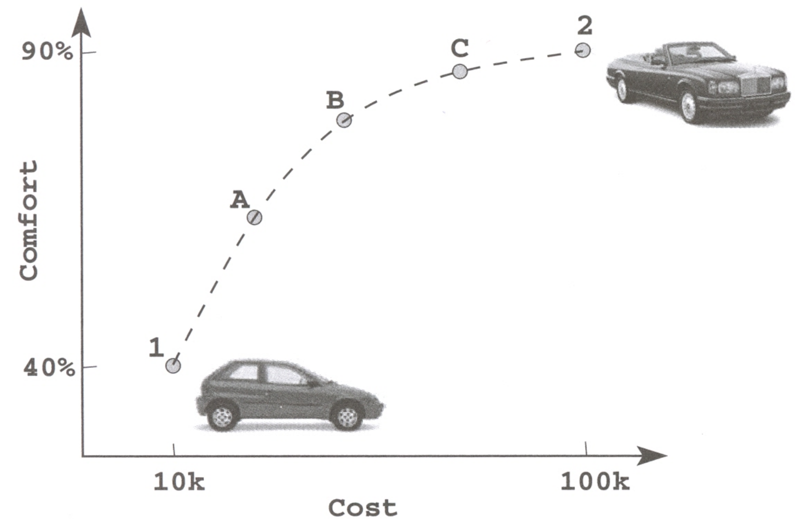
Multi-Objective Optimization

Many real-world problems involve multiple objectives

- **Conflicting objectives**
  - A solution that is extreme with respect to one objective requires a compromise in other objectives.
  - A sacrifice in one objective is related to the gain in other objective(s).

  Illustrative example: Buying a car
  - two extreme hypothetical cars 1 and 2,
  - cars with a trade-off between cost and comfort – A, B, and C.



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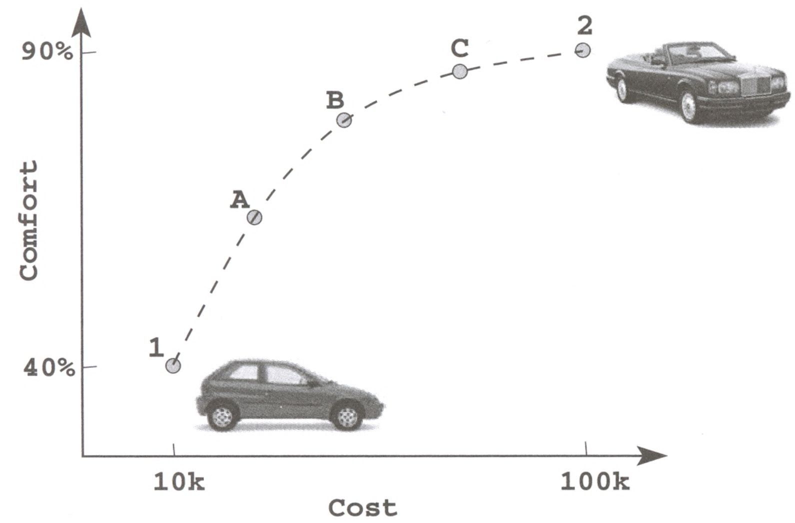

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- **Which solution** out of all of the trade-off solutions **is the best** with respect to all objectives?

  Without any further information those trade-offs are indistinguishable.

  $\Longrightarrow$ **a number of optimal solutions is sought in multiobjective optimization!**

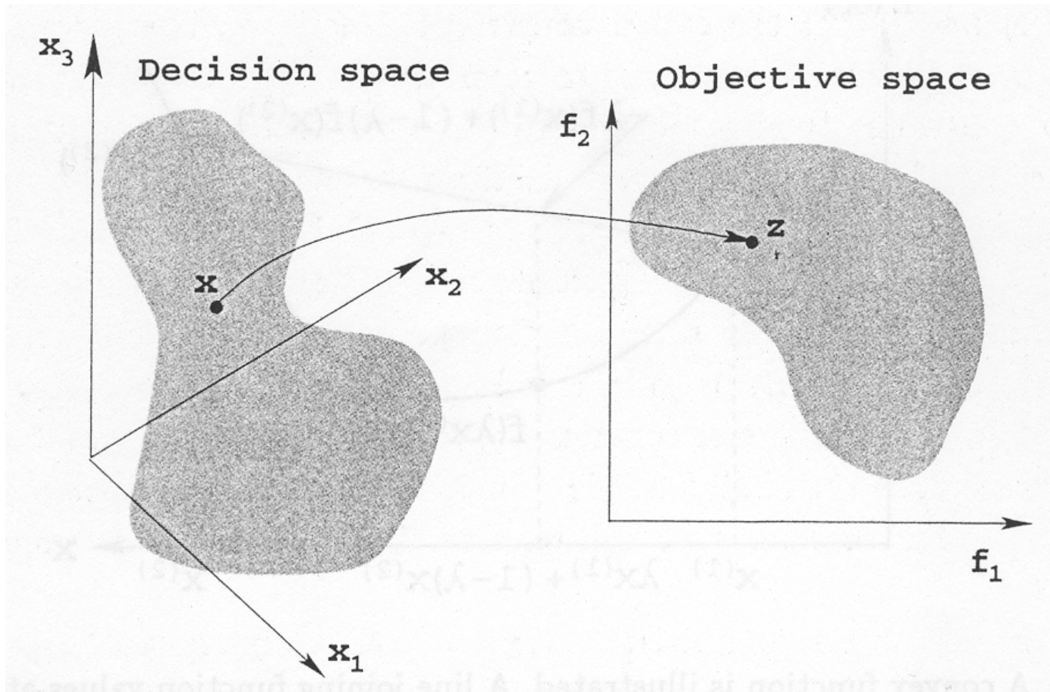
Multi-Objective Optimization: Definition

General form of multi-objective optimization problem

$$\begin{aligned}
\text{Minimize/maximize} \quad & f_m(x), && m = 1, 2, ..., M; \\
\text{subject to} \quad & g_j(x) \geq 0, && j = 1, 2, ..., J; \\
& h_k(x) = 0, && k = 1, 2, ..., K; \\
& x_i^{(L)} \leq x_i \leq x_i^{(U)}, && i = 1, 2, ..., n.
\end{aligned}$$

- x is a vector of n decision variables: $x = (x_1, x_2, ..., x_n)^T$;
- **Decision space** is constituted by variable bounds that restrict each variable x_i to take a value within a lower $x_i^{(L)}$ and an upper $x_i^{(U)}$ bound;
- Inequality and equality constraints
- A solution x that satisfies all constraints and variable bounds is a **feasible solution**, otherwise it si called an **infeasible solution**;
- **Feasible space** is a set of all feasible solutions;
- Objective functions $f(x) = (f_1(x), f_2(x), ..., f_M(x))^T$ constitute a multi-dimensional **objective space**.

Decision and Objective Space



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- For each solution x in the decision space, there exists a point in the objective space

$$f(x) = z = (z_1, z_2, ..., z_M)^T$$

Motivation Example: Cantilever Design Problem

Task is to design a beam, defined by two decision variables

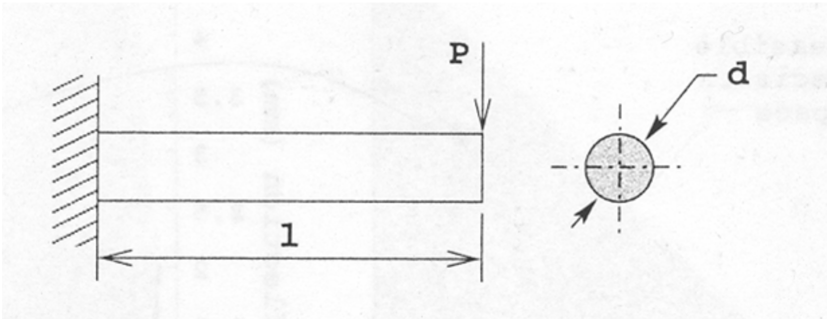
- diameter d,
- length l.

that can carry an end load P and is optimal with

respect to the following **objectives**

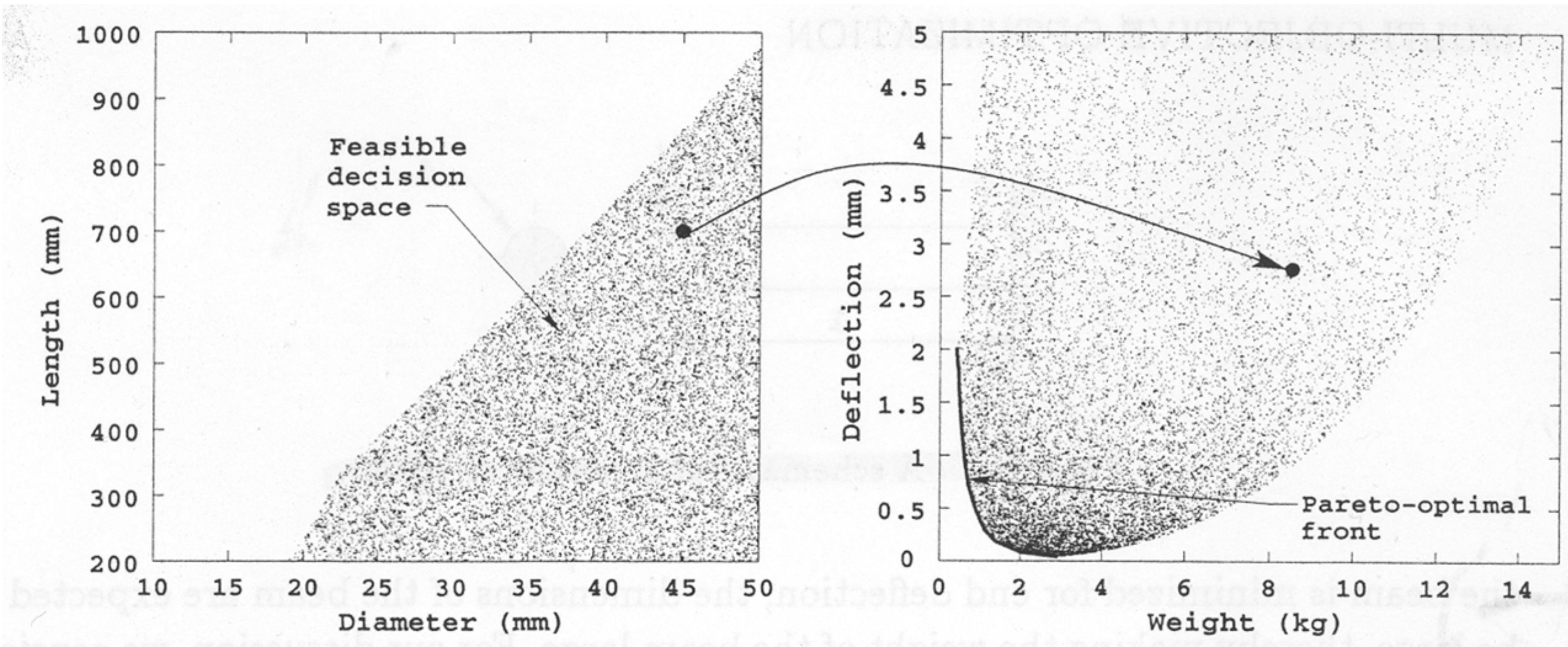
- f_1 – minimization of $weight$,
- f_2 – minimization of $deflection$.
  Obviously, conflicting objectives!

subject to the following **constraints**



- the developed maximum stress σ_{max} is less than the allowable strength S_y,
- the end deflection δ is smaller than a specified limit δ_{max}.

Cantilever Design Problem: Decision and Objective Space



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Non-Conflicting Objectives

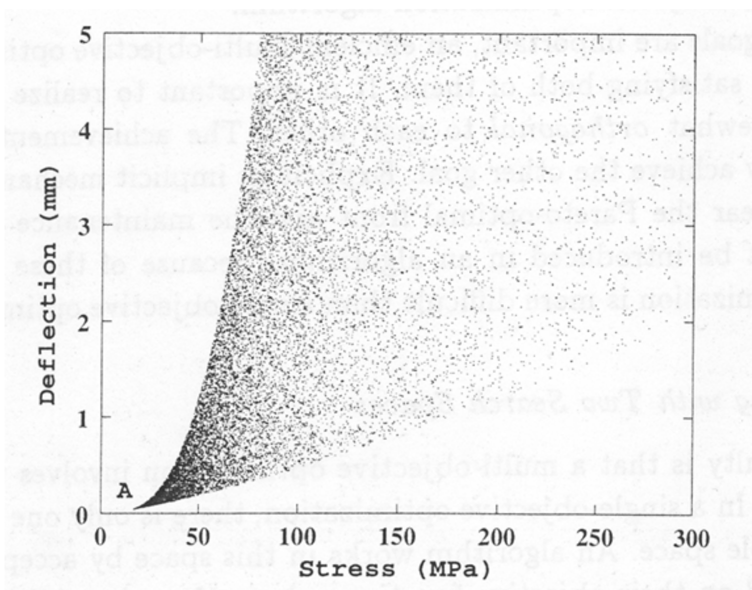
There exist multiple optimal solutions to the problem only if the objectives are conflicting to each other.

- If this does not hold then the cardinality of the Pareto-optimal set is one.

  This means that the optimum solution corresponding to any objective is the same.

Example: Cantilever beam design problem

- f_1 – minimizing the end deflection δ,
- f_2 – minimizing the maximum developed stress in the beam σ_{max}.



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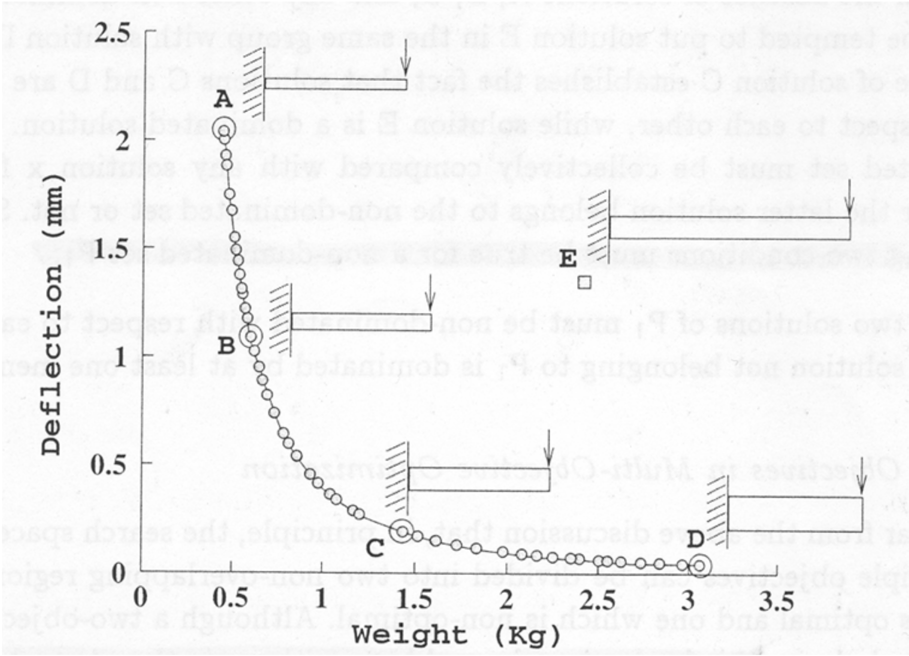
Dominance and Pareto-Optimal Solutions



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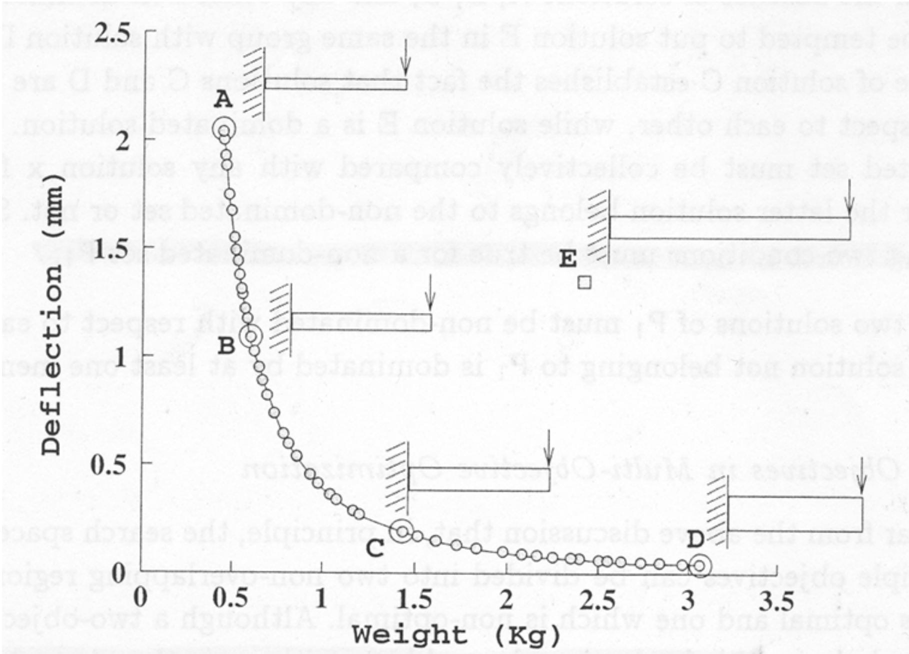
Dominance and Pareto-Optimal Solutions



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Domination: *A solution* $x^{(1)}$ *is said to dominate the other solution* $x^{(2)}$, $x^{(1)} \preceq x^{(2)}$, *if* $x^{(1)}$ *is no worse than* $x^{(2)}$ *in all objectives and* $x^{(1)}$ *is strictly better than* $x^{(2)}$ *in at least one objective.*

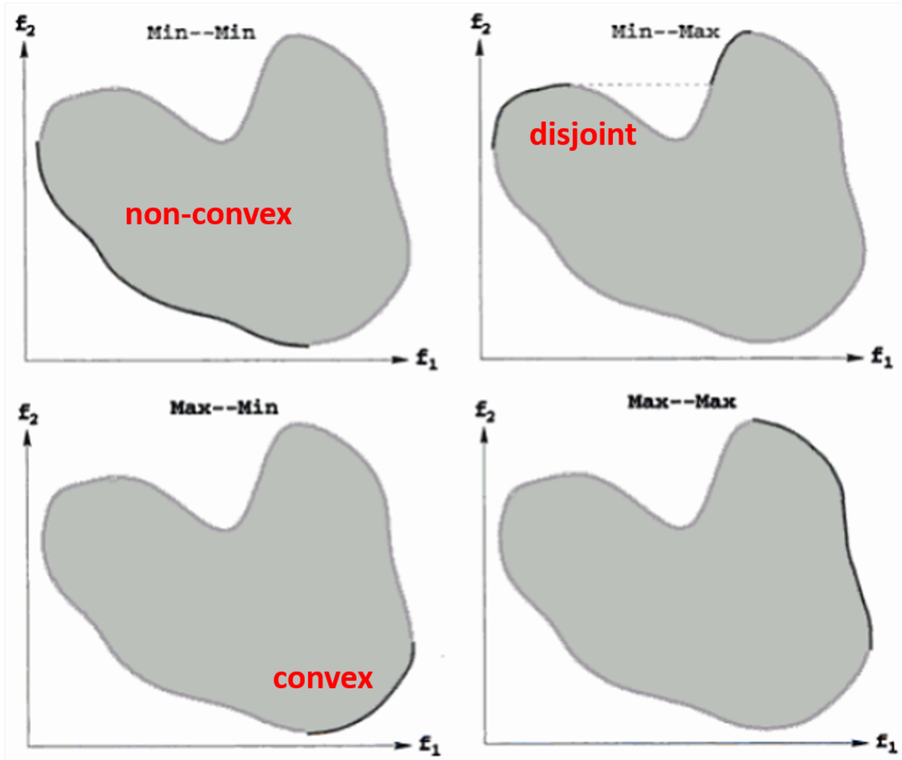
Solutions A, B, C, D are *non-dominated* solutions (Pareto-optimal solutions)

Solution E is *dominated* by C and B (E is non-optimal).

Properties of Dominance-Based Multi-Objective Optimization

Non-dominated set – Among a set of solutions P, the non-dominated set of solutions P' are those that are not dominated by any member of the set P.

The non-dominated set of the entire feasible search space is the **globally Pareto-optimal set**.



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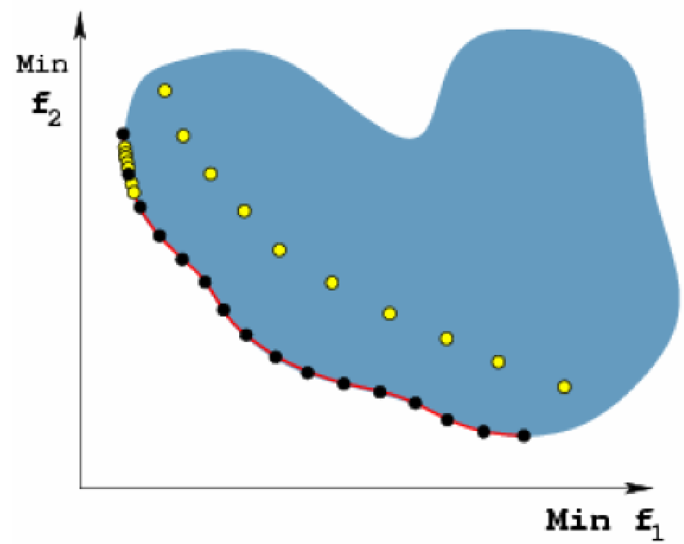
Goals of Dominance-Based Multi-Objective Optimization

Every finite set of solutions P can be divided into two non-overlapping sets

- non-dominated set P_1 – contains all solutions that do not dominate each other, and
- dominated set P_2 – at least one solution in P_1 dominates any solution in P_2.

In the absence of other factors (e.g. preference for certain objectives, or for a particular region of the tradeoff surface) there are **two goals of the multi-objective optimization**

- **Quality** – To find a set of solutions as close as possible to the Pareto-optimal front.
- **Spread** – To find a set of non-dominated solutions as diverse as possible.

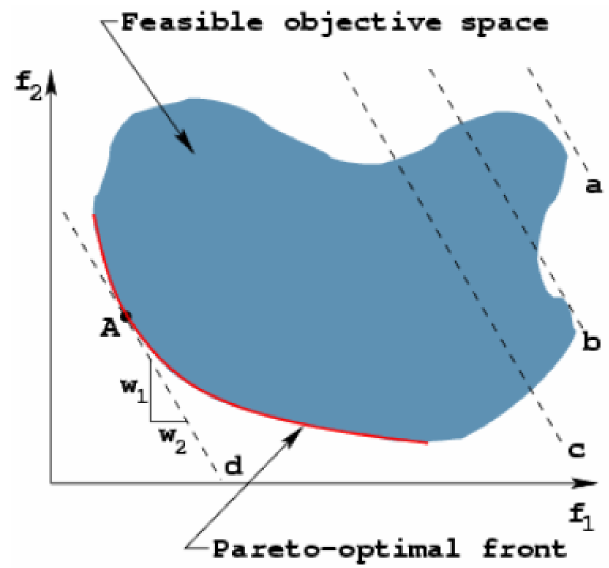


Classical Approaches: Weighted Sum Method

- Construct a weighted sum of objectives and optimize

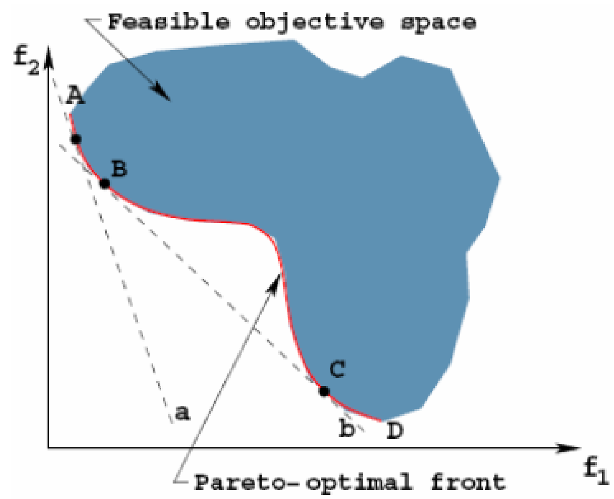
$$F(x) = \sum_{i=1}^{m} w_i \cdot f_i(x)$$

- User supplies weight vector w.
- Selection of weights w defines the slope of the line, which in turn determines the particular solution(s) on the boundary of the feasible space.



Difficulties with Weighted Sum Method

- Need to know weight vector w
- Non-uniformity in Pareto-optimal solutions
- Inability to find some Pareto-optimal solutions (in non-convex region)
- However, a solution of this approach is always Pareto-optimal



Classical Approaches: ε-Constraint Method

Method: Minimize a primary objective while expressing all the other objectives in the form of inequality constraints

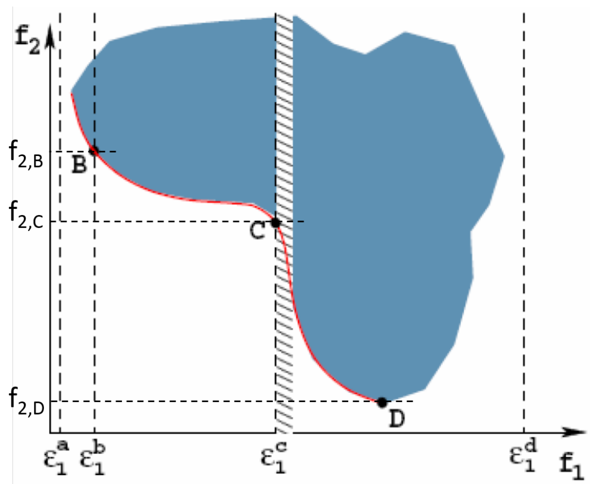
$$\text{Minimize } f_p(x)$$

$$\text{subject to } f_i(x) \leq \varepsilon_i; \qquad i = 1, \ldots, m; \qquad i \neq p$$

Remarks:

- Need to know relevant ε vectors to ensure a feasible solution
- Non-uniformity in Pareto-optimal solutions
- However, any Pareto-optimal solution can be found with this method

Ex.: Minimize $f_2(x)$
subject to $f_1(x) \leq \varepsilon_i$



Difficulties with Most Classical Approaches

- Need to run a single-objective optimizer many times
- Expect a lot of problem knowledge
- Even then, good distribution of solutions is not guaranteed
- Multi-objective optimization as an application of single-objective optimization

Why and How Use EAs for Multi-Objective Optimizations?

Why?

- **Population approach** suits well to find multiple solutions.
- **Niche-preservation methods** can be exploited to find diverse solutions.
- **Implicit parallelism** helps provide a parallel search.
  Multiple applications of classical methods do not constitute a parallel search.

How?

- Modify the **fitness computation**
- Emphasize non-dominated solutions for **convergence**
- Emphasize less-crowded solutions for **diversity**

Multi-Objective Evolutionary Algorithms

- **Pareto Archived Evolution Strategy** (PAES)

  Knowles, J.D., Corne, D.W. (2000) Approximating the nondominated front using the Pareto archived evolution strategy. Evolutionary Computation, 8(2), pp. 149-172

- **Multiple Objective Genetic Algorithm** (MOGA)

  Carlos M. Fonseca, Peter J. Fleming: Genetic Algorithms for Multiobjective Optimization: Formulation, Discussion and Generalization, In Genetic Algorithms: Proceedings of the Fifth International Conference, 1993

- **Niched-Pareto Genetic Algorithm** (NPGA)

  Jeffrey Horn, Nicholas Nafpliotis, David E. Goldberg: A Niched Pareto Genetic Algorithm for Multiobjective Optimization, Proceedings of the First IEEE Conference on Evolutionary Computation, IEEE World Congress on Computational Intelligence, 1994

- **SPEA2**

  Zitzler, E., Laumanns, M., Thiele, L.: SPEA2: Improving the Strength Pareto Evolutionary Algorithm For Multiobjective Optimization, In: Evolutionary Methods for Design, Optimisation, and Control, Barcelona, Spain, pp. 19-26, 2002

- **NSGA**

  Srinivas, N., and Deb, K.: Multi-objective function optimization using non-dominated sorting genetic algorithms, Evolutionary Computation Journal 2(3), pp. 221-248, 1994

- **NSGA-II**

  Kalyanmoy Deb, Samir Agrawal, Amrit Pratap, and T Meyarivan: A Fast Elitist Non-Dominated Sorting Genetic Algorithm for Multi-Objective Optimization: NSGA-II, In Proceedings of the Parallel Problem Solving from Nature VI Conference, 2000

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Non-Dominated Sorting Genetic Algorithm (NSGA)

Common features with the standard GA

- variation operators – crossover and mutation,
- selection method – Stochastic Reminder Roulette-Wheel,
- standard generational evolutionary model.

What distinguishes NSGA from the SGA

- fitness assignment scheme which **prefers non-dominated solutions**, and
- fitness sharing strategy which **preserves diversity among solutions of each non-dominated front**.

Algorithm NSGA

1. Initialize population of solutions
2. Repeat
   - Calculate objective values and assign fitness values
   - Generate new population

   Until stopping condition is fulfilled

Fitness Sharing

Diversity preservation method originally proposed for solving multi-modal optimization problems so that GA is able to sample each optimum with the same number of solutions.

Idea – diversity in the population is preserved by degrading the fitness of similar solutions

Algorithm for calculating the shared fitness value of i-th individual in population of size N

1. calculate *sharing function* value with all solutions in the population according to

$$Sh(d_{ij}) = \begin{cases} 1 - (\frac{d_{ij}}{\sigma_{share}})^{\alpha}, & \text{if } d_{ij} \leq \sigma_{share} \\ 0, & \text{otherwise.} \end{cases}$$

2. calculate niche count nc_i as follows

$$nc_i = \sum_{j=1}^{N} Sh(d_{ij})$$

3. calculate *shared fitness* as

$$f_i' = f_i / nc_i$$

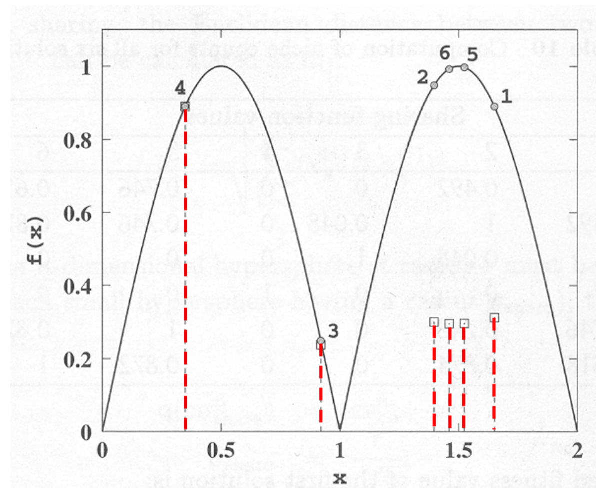
Remark: If $d = 0$ then $Sh(d) = 1$ meaning that two solutions are identical. If $d \geq \sigma_{share}$ then $Sh(d) = 0$ meaning that two solutions do not have any sharing effect on each other.

Fitness Sharing: Example

Bimodal function - six solutions and corresponding shared fitness functions

- $\sigma_{share} = 0.5$, $\alpha = 1$.

Sol. i	String	Decoded value	$x^{(i)}$	f_i	nc_i	f'_i
1	110100	52	1.651	0.890	2.856	0.312
2	101100	44	1.397	0.948	3.160	0.300
3	011101	29	0.921	0.246	1.048	0.235
4	001011	11	0.349	0.890	1.000	0.890
5	110000	48	1.524	0.997	3.364	0.296
6	101110	46	1.460	0.992	3.364	0.295



Let's take the first solution

- $d_{11} = 0.0$, $d_{12} = 0.254$, $d_{13} = 0.731$, $d_{14} = 1.302$, $d_{15} = 0.127$, $d_{16} = 0.191$
- $Sh(d_{11}) = 1$, $Sh(d_{12}) = 0.492$, $Sh(d_{13}) = 0$, $Sh(d_{14}) = 0$, $Sh(d_{15}) = 0.746$, $Sh(d_{16}) = 0.618$.
- $nc_1 = 1 + 0.492 + 0 + 0 + 0.746 + 0.618 = 2.856$
- $f'(1) = f(1)/nc_1 = 0.890/2.856 = 0.312$

NSGA: Fitness Assignment

Input: Set P of solutions with assigned objective values.

Output: Set of solutions with assigned fitness values (the bigger the better).

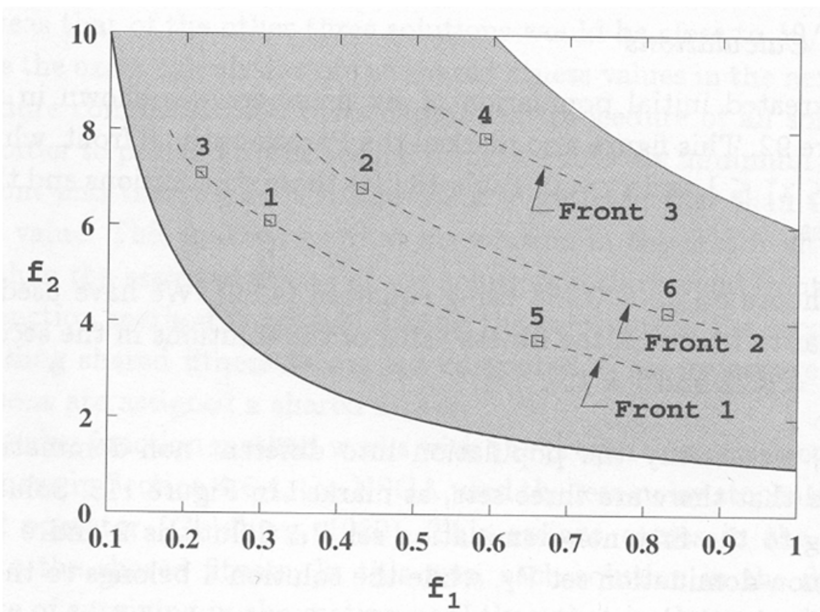
1. Choose sharing parameter σ_{share}, small positive number ϵ,
   initialize $F_{max} = PopSize$ and front counter $front = 1$
2. Find set $P' \subset P$ of non-dominated solutions
3. For each $q \in P'$
   - assign fitness $f(q) = f_{max}$,
   - calculate sharing function with all solutions in P' niche count nc_q among solutions of P' only,
     the normalized Euclidean distance d_{ij} is calculated
   - calculate shared fitness $f'(q) = f(q)/nc_q$.
4. $f_{max} = min(f'(q) : q \in P') - \epsilon$
   $P = P \setminus P'$
   $front = front + 1$
5. If not all solutions are assessed go to step 2, otherwise stop.

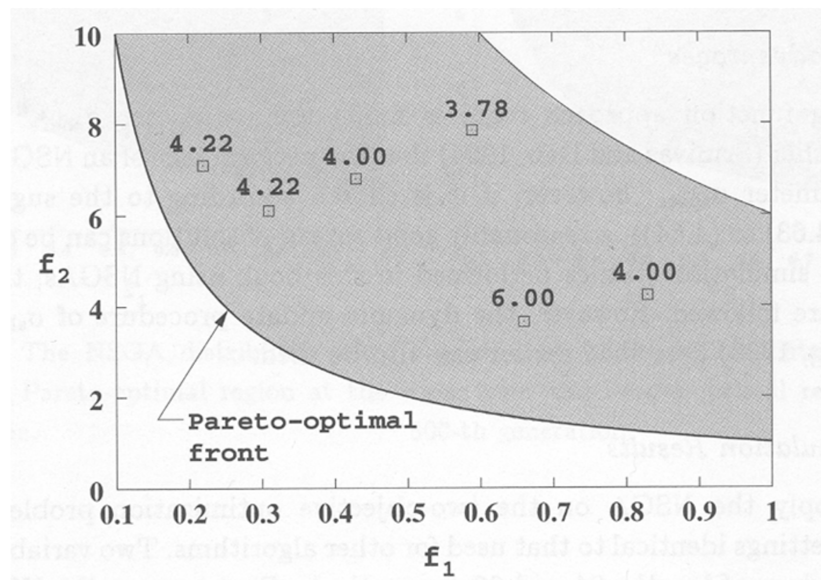
$$d_{ij} = \sqrt{\sum_{k=1}^{M} \left(\frac{f_k^{(i)} - f_k^{(j)}}{f_k^{max} - f_k^{min}}\right)^2}$$

NSGA: Fitness Assignment cont.

Example:

- First, 6 solutions are classified into different non-dominated fronts.
- Then, the fitness values are calculated according to the fitness sharing method.
  - The sharing function method is used front-wise.
  - Within a front, less dense solutions have better fitness values.





NSGA: Conclusions

Computational complexity

- Governed by the non-dominated sorting procedure and the sharing function implementation.
  - **non-dominated sorting** – complexity of $O(MN^3)$.
  - **sharing function** – requires every solution in a front to be compared with every other solution in the same front, total of $\sum_{j=1}^{\rho} |P_j|^2$, where ρ is a number of fronts.
    Each distance computation requires evaluation of n differences between parameter values.
    In the worst case, when $\rho = 1$, the overall complexity is of $O(nN^2)$.

Advantages

- Assignment of fitness according to non-dominated sets – makes the algorithm converge towards the Pareto-optimal region.
- Sharing allows phenotypically diverse solutions to emerge.

Disdvantages

- non-elitist
- sensitive to the sharing method parameter σ_{share}.
  requires some guidelines for setting the σ
  $\sigma_{share} = \frac{0.5}{\sqrt[n]{q}}$, for example based on the expected number of optima q

NSGA-II

Fast non-dominated sorting approach

- Computational complexity of $O(MN^2)$.

Diversity preservation

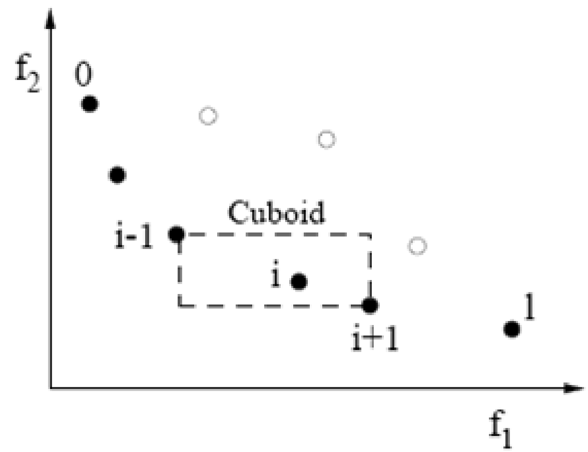
- the sharing function method is replaced with a **crowded comparison approach**,
- parameterless approach.

Elitist evolutionary model

- Only the best solutions survive to subsequent generations.

NSGA-II: Diversity preservation

Density estimation – crowding distance estimates how much unique the solution is.



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Crowded comparison operator

Every solution in the population has two attributes

1. non-domination rank (i^{rank}), and
2. crowding distance ($i^{distance}$).

A partial order $\prec_n$ is defined as:

$$i \prec_n j \text{ if}(i^{rank} < j^{rank}) \text{ or } ((i^{rank} = j^{rank}) and (i^{distance} > j^{distance}))$$

NSGA-II: Evolutionary Model

1. Current population P_t is sorted based on the non-domination

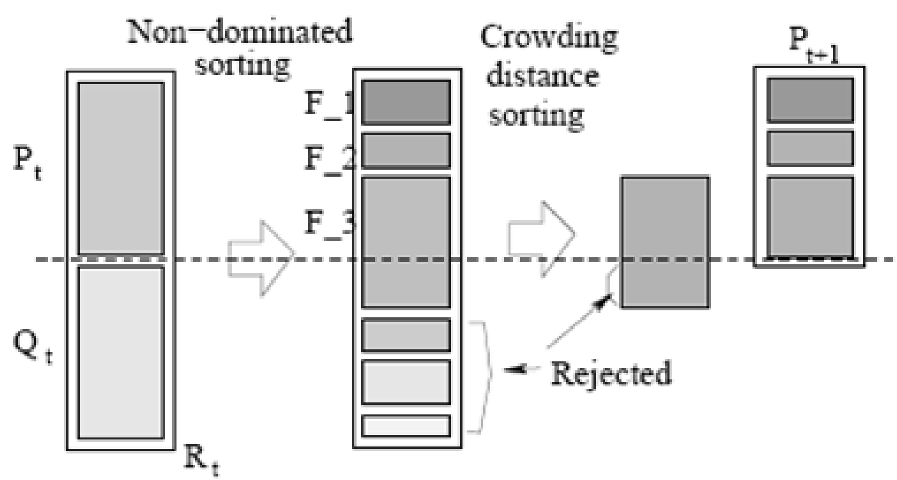
   Each solution is assigned a fitness equal to its non-domination level (1 is the best).

2. The usual binary tournament selection, recombination, and mutation are used to create a child population Q_t of size N.

3. Combined population $R_t = P_t \cup Q_t$ is formed.

   Elitism is ensured.

4. Population P_{t+1} is formed according to the following schema



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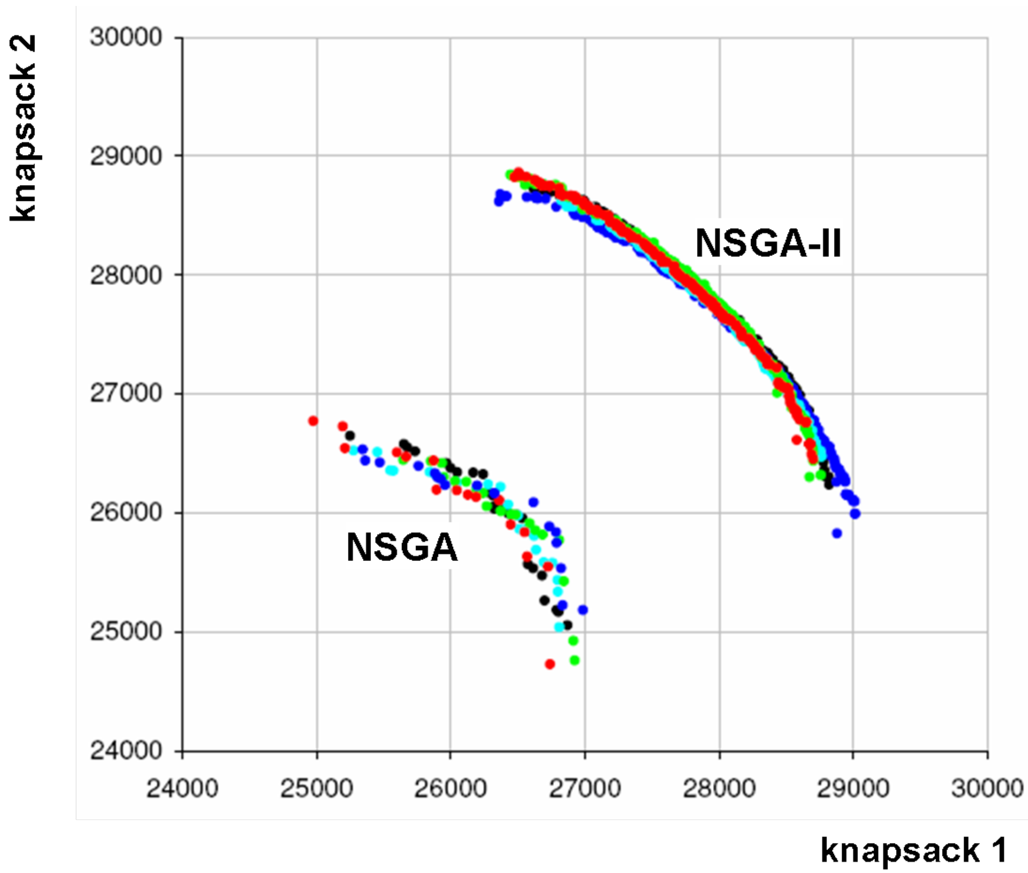
Simulation Results: NSGA vs. NSGA-II

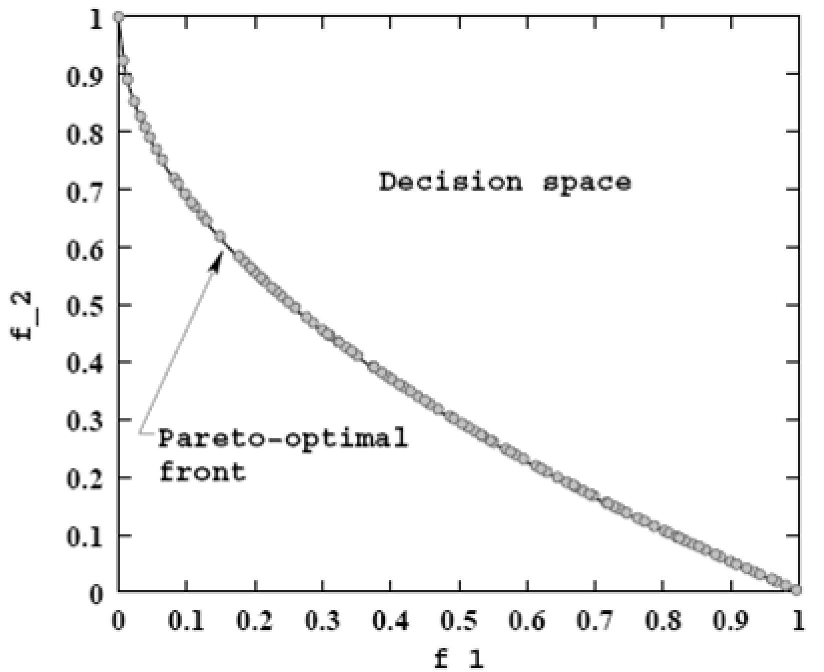
Comparison of NSGA nad NSGA-II on bi-objective 0/1 Knapsack Problem with 750 items.

NSGA-II outperforms NSGA with respect to both performance measures.

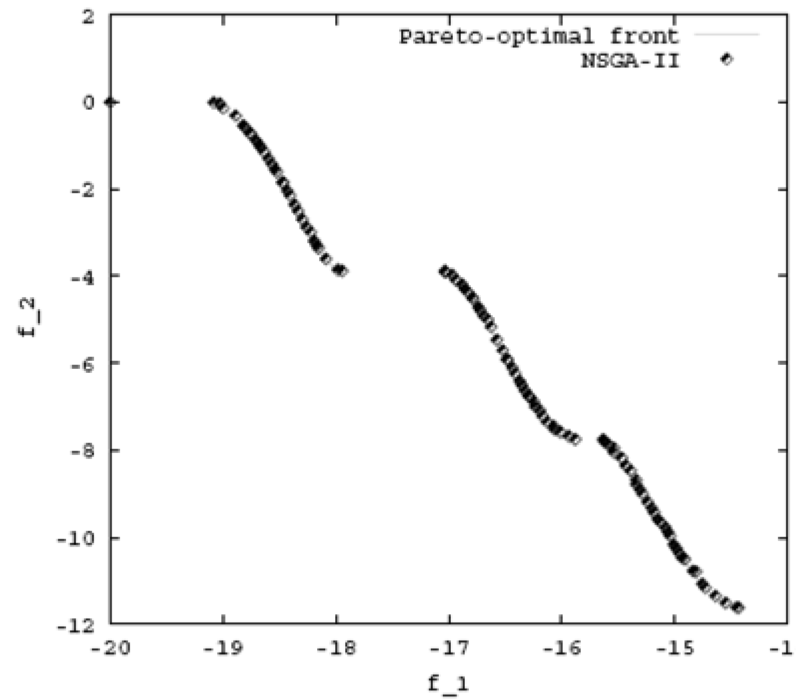


NSGA-II: Simulation Results on Different Types of Problems

Problem with continuous Pareto-optimal front



Problem with discontinuous Pareto-optimal front



NSGA-II: Constraint Handling Approach

Binary tournament selection with modified domination concept is used to choose the better solution out of the two solutions i and j, randomly picked up from the population.

In the presence of constraints each solution in the population can be either **feasible** or **infeasible**, so that there are the following three possible situations:

1. both solutions are feasible,
2. one is feasible and other is not,
3. both are infeasible.

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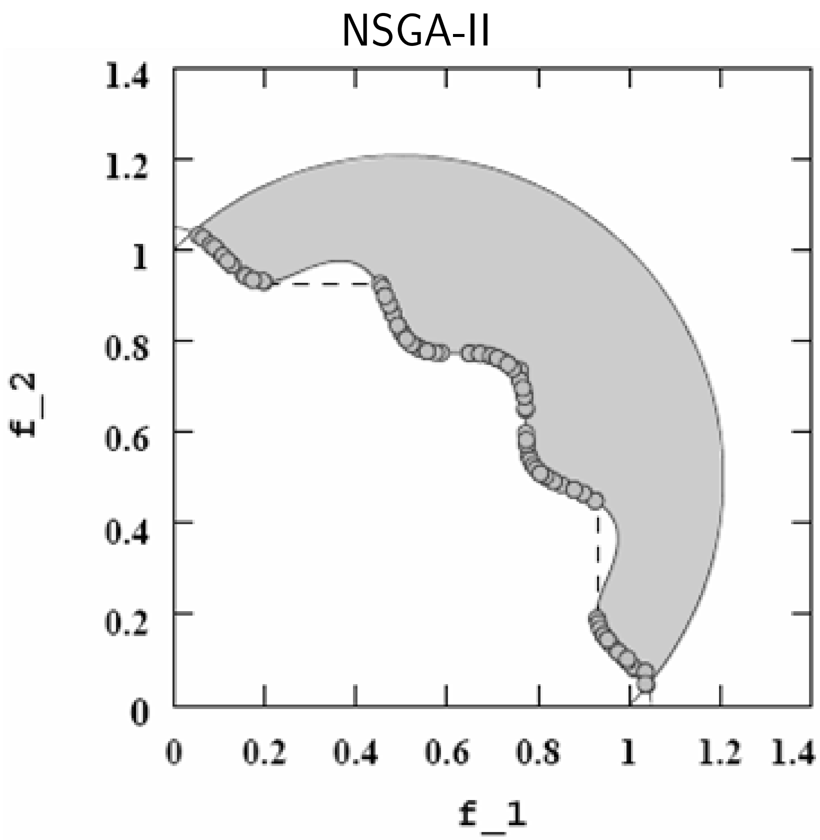
Constrained-domination: A solution i is said to constrained-dominate a solution j, if any of the following conditions is true

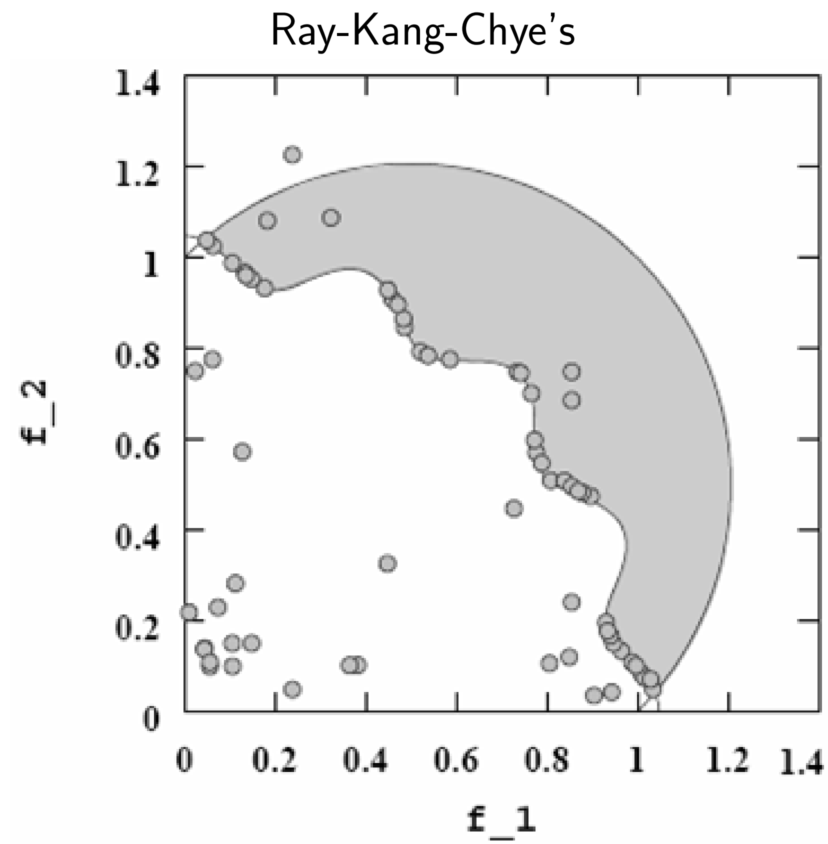
1. Solution i is feasible and solution j is not.
2. Solutions i and j are both infeasible, but solution i has a smaller overall constraint violation.
3. Solutions i and j are feasible, and solution i dominates solution j.

NSGA-II: Simulation Results cont.

Comparison of NSGA-II and Ray-Kang-Chye's Constraint handling approach

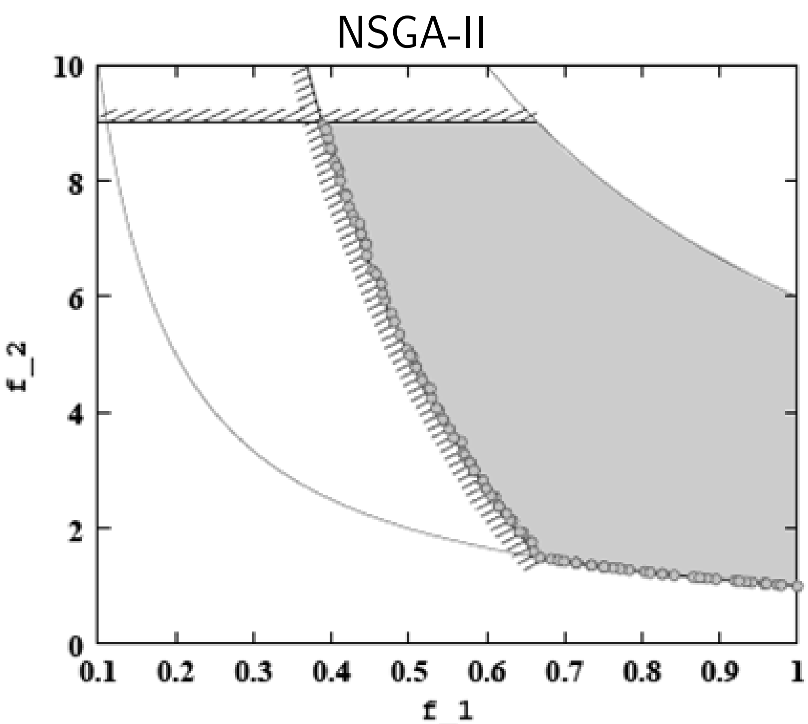
- Ray, T., Tai, K. and Seow, K.C. [2001] "Multiobjective Design Optimization by an Evolutionary Algorithm", Engineering Optimization, Vol.33, No.4, pp.399-424

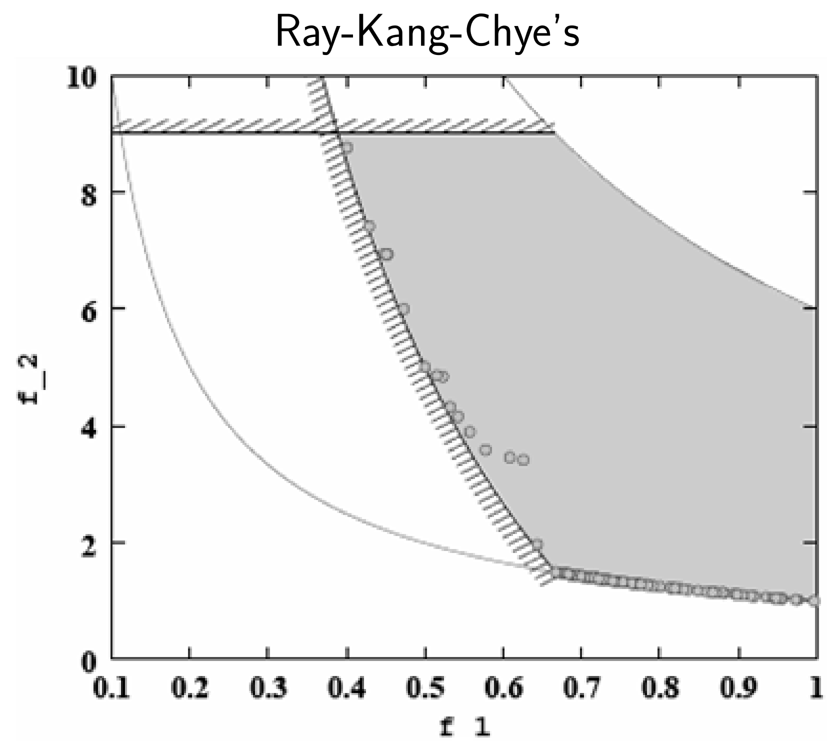




NSGA-II: Simulation Results cont.

Comparison of NSGA-II and Ray-Kang-Chye's Constraint handling approach





NSGA-II: Bi-objective Symbolic Regression

Optimization objectives:

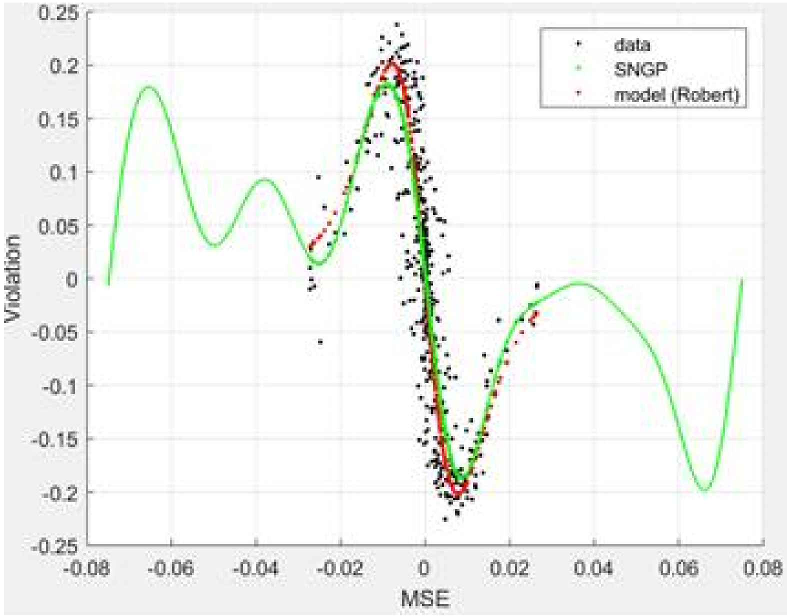
- Minimize MSE on the training data set
- Minimize deviation of the symbolic models from the desired properties

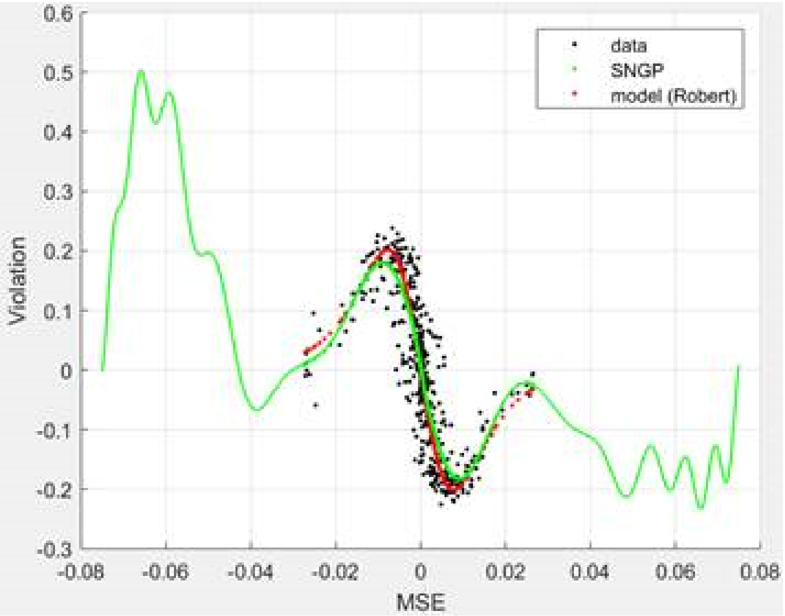
Desired properties:

- Monotonically increasing in the intervals $y = \langle -0.075, -0.01 \rangle$ and $y = \langle 0.01, 0.075 \rangle$
- Monotonically decreasing in the interval $y = \langle -0.07, 0.07 \rangle$
- $F(y) \geq$, for $y \in \langle -0.075, 0.0 \rangle$
- $F(y) \leq$, for $y \in \langle 0.0, 0.075 \rangle$
- $|F(0.0)| < 0.005$
- $|F(-0.075) - 0.001| < 0.0005$
- $|F(0.075) + 0.001| < 0.0005$

NSGA-II: Bi-objective Symbolic Regression

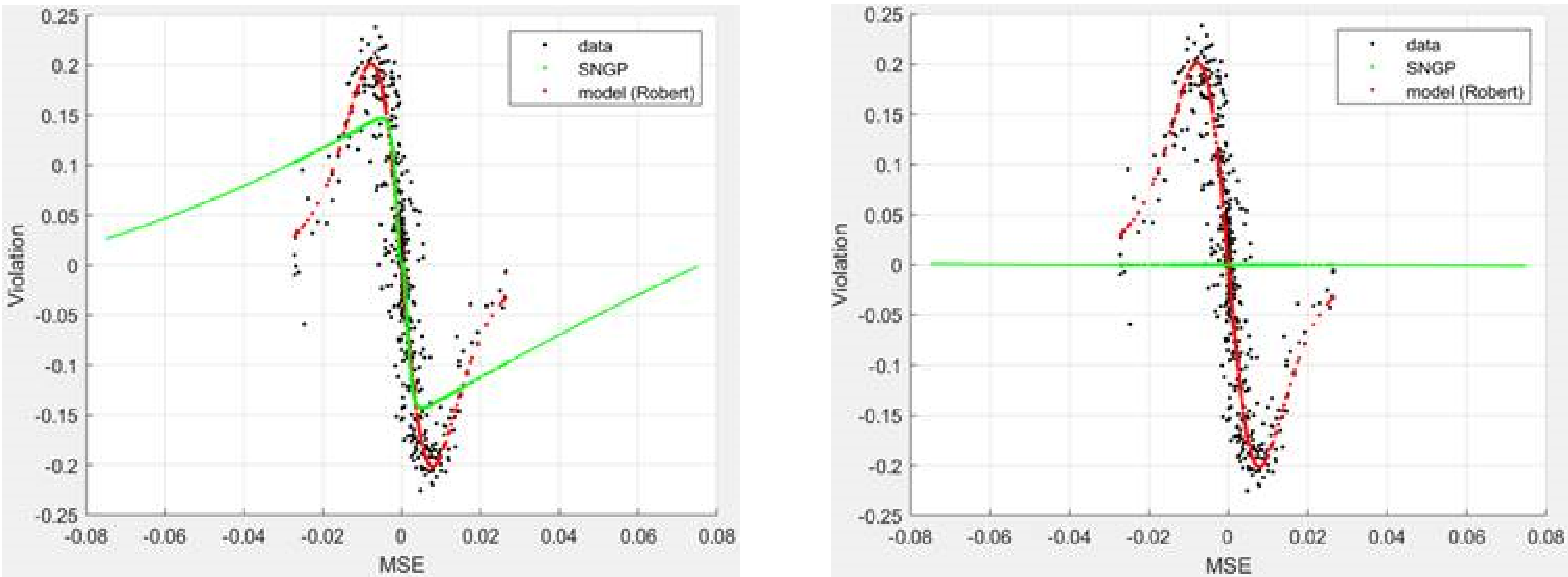
Well-fit models w.r.t. the MSE on training data only





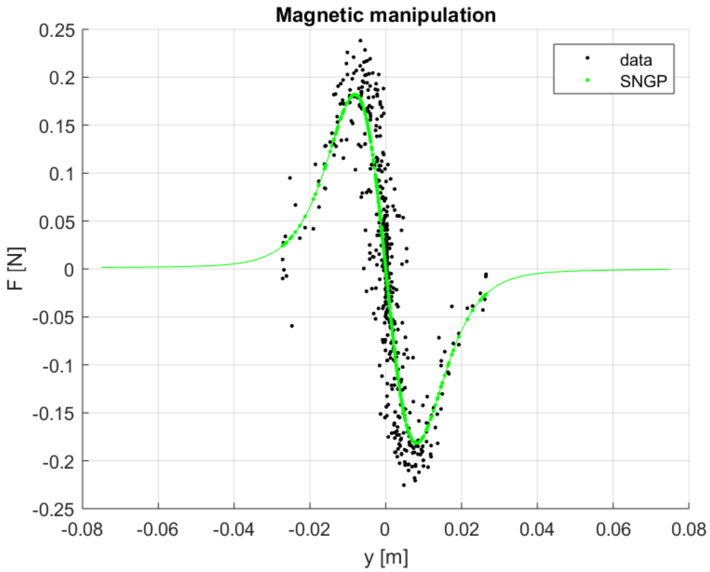
NSGA-II: Bi-objective Symbolic Regression

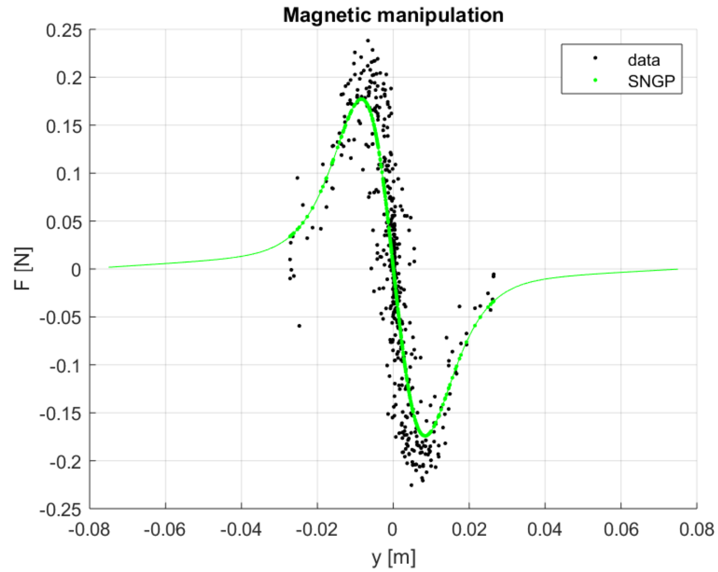
Well-fit models w.r.t. the constraint violations



NSGA-II: Bi-objective Symbolic Regression

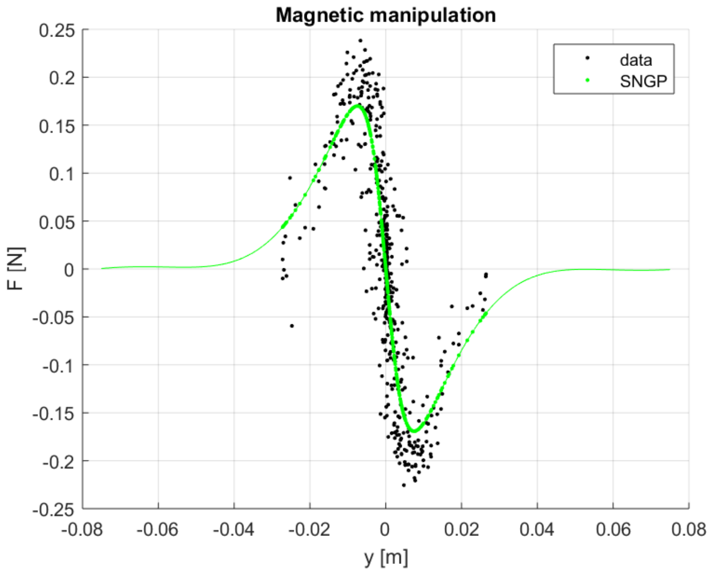
Models with small MSE on training data that fully comply with the constraints

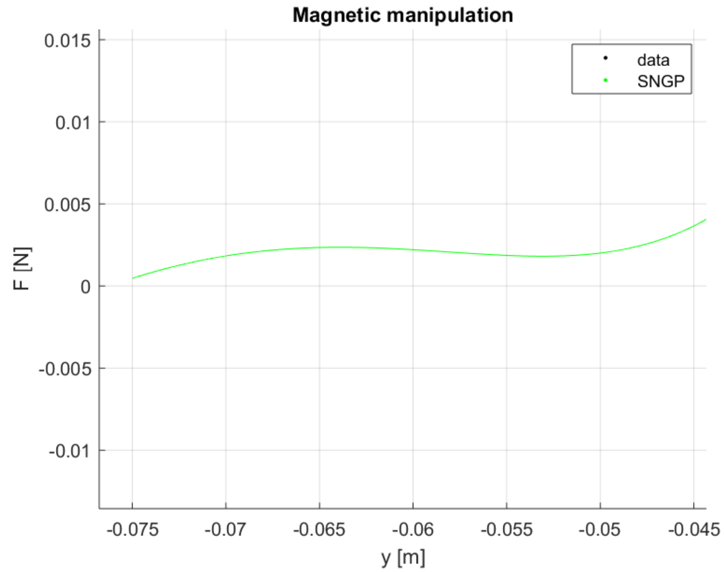




NSGA-II: Bi-objective Symbolic Regression

Models with small MSE on training data that almost fully comply with the constraints





Strength Pareto Evolutionary Algorithm 2 (SPEA2)

SPEA2 maintains two sets of solutions

- **regular population** of newly generated solutions, and
- **archive**, which contains a representation of the nondominated front among all solutions considered so far.

  The archive size is fixed, i.e., whenever the number of nondominated individuals is less than the predefined archive size, the archive is filled up by *good* dominated individuals.

  A **truncation method** is invoked when the nondominated front exceeds the archive limit.

  A member of the archive is only removed if

  1. a solution has been found that dominates it or
  2. the maximum archive size is exceeded and the portion of the front where the archive member is located is overcrowded.

  Using the archive makes it possible not to lose certain portions of the current nondominated front due to random effects.

  All individuals in the archive participate in selection.

SPEA2: Algorithm

Input: N is the population size, $\overline{N}$ is the archive size.

1. **Initialization**: Generate an initial population P_0 and create the empty archive $\overline{P}_0 = \emptyset$. Set $t = 0$.
2. **Fitness assignment**: Calculate fitness of individuals in P_t and $\overline{P}_t$.
3. **Environmental selection**: Copy all nondominated individuals in P_t and $\overline{P}_t$ to $\overline{P}_{t+1}$.
   If size of $\overline{P}_{t+1}$ exceeds $\overline{N}$ then reduce $\overline{P}_{t+1}$ using the truncation operator.
   If size of $\overline{P}_{t+1}$ is less than $\overline{N}$ then fill $\overline{P}_{t+1}$ with dominated solutions in P_t and $\overline{P}_t$.
4. **Termination**: If $t \geq T$ then return nondominated solutions in $\overline{P}_{t+1}$. Stop.
5. **Mating selection**: Perform binary tournament selection with replacement on $\overline{P}_{t+1}$ in order to fill the mating pool.
6. **Variation**: Apply recombination and mutation operators to the mating pool and fill P_{t+1} with the generated solutions,
   increment generation counter $t = t + 1$,
   go to Step 2.

SPEA2: Fitness Assignment

Fitness assignment (fitness is to minimized) – for each individual both dominating and dominated solutions are taken into account.

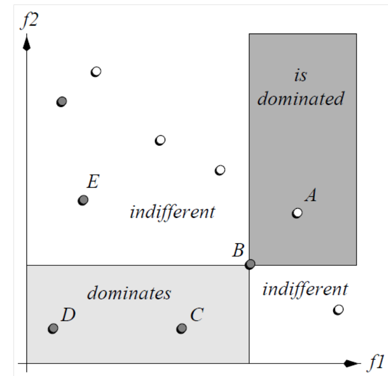
- Each individual i in the archive $\overline{P}_t$ and the population P_t is assigned a **strength value** $S(i)$, representing the number of solutions it dominates.
- The raw fitness $R(i)$ of an individual i is calculated as

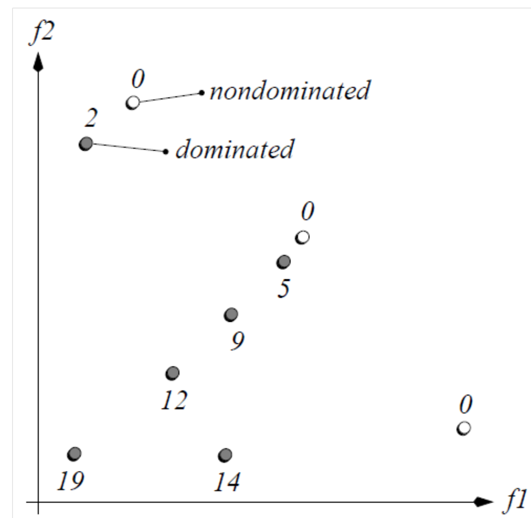
$$R(i) = \sum_{j \in P_t + \overline{P}_t, j \succ i} S(j)$$

  that is $R(i)$ is determined by the strengths of its dominators in both archive and population.

  $R(i) = 0$ corresponds to a nondominated solution.

  Since the **raw fitness assignment** is based on the concept of Pareto dominance, it **may fail when most individuals do not dominate each other**.





SPEA2: Density Estimation

Density information is incorporated to discriminate between individuals having identical raw fitness values.

The density at any point is estimated as a (decreasing) function of the distance to the k-th nearest data point – calculated as the inverse of the distance to the k-th nearest neighbor.

- k equal to the square root of the sample size is used: $k = \sqrt{N + \overline{N}}$.
- Density $D(i)$ is calculated as

$$D(i) = \frac{1}{\sigma_i^k + 2}$$

  where σ_i^k is the distance to the k-th nearest neighbor and it is made sure that $D(i) < 1$.

Final fitness is given as

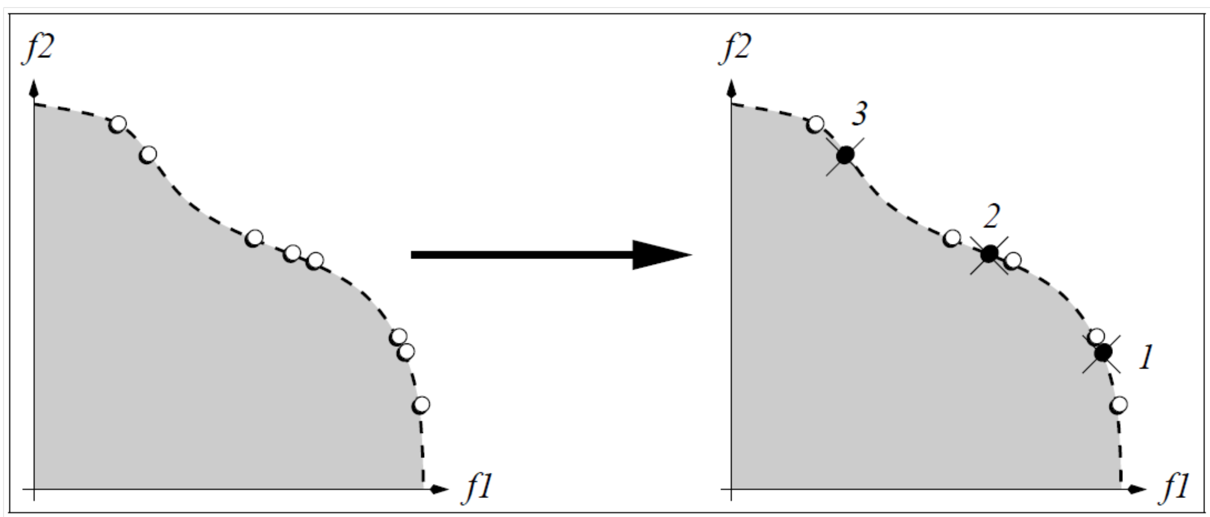
$$F(i) = R(i) + D(i)$$

SPEA2: Environmental Selection

If after copying all nondominated individuals from archive and population to the archive of the next generation

- the archive is too small (i.e. $|\overline{P}_{t+1} < \overline{N}|$), the best $\overline{N} - |\overline{P}_{t+1}|$ dominated solutions (w.r.t. fitness) in the previous archive and population are copied to the new archive;
- the archive is too large (i.e. $|\overline{P}_{t+1} > \overline{N}|$), individuals from $\overline{P}_{t+1}$ are iteratively removed until $|\overline{P}_{t+1}| = \overline{N}$.

  At each iteration, the individual which has the minimum distance to another individual is chosen (a tie is broken by considering the second smallest distances and so forth).



SPEA2: Conclusions

SPEA2

- uses the concept of **Pareto dominance** in order to assign scalar fitness values to individuals;
- uses a **fine-grained fitness** assignment strategy which **incorporates density information** in order to distinguish between solutions that are indifferent, i.e., do not dominate each other;
- uses environmental selection in order to keep the optimal diversity in the archive;
- seems to have advantages over NSGA-II in higher dimensional objective spaces.

MOEA Performance Measures

The result of a MOEA run is not a single scalar value, but a collection of vectors forming a non-dominated set.

- Comparing two MOEA algorithms requires comparing the non-dominated sets they produce. However, there is no straightforward way to compare different non-dominated sets.

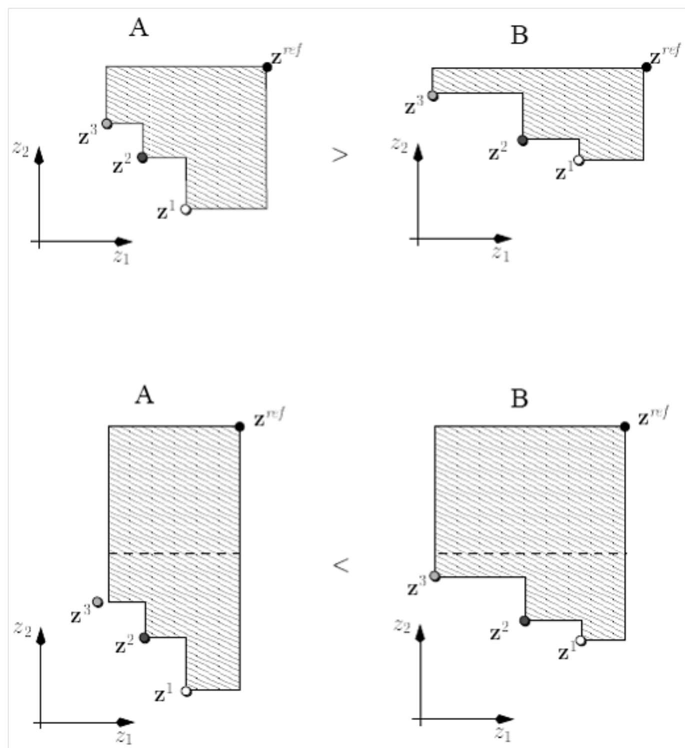
Three goals that can be identified and measured:

1. The distance of the resulting non dominated set to the Pareto-optimal front should be minimized.
2. A good (in most cases uniform) distribution of the solutions found is desirable.
3. The extent of the obtained non dominated front should be maximized, i.e., for each objective, a wide range of values should be present.

S Metric

Size of the space covered $S(X)$ – it calculates the *hypervolume* of the multi-dimensional region enclosed by a set A and a *reference point* Z^{ref}. The hypervolume expresses the size of the region that is dominated by A.

So, the bigger the value of this measure the better the quality of A is, and vice versa.



S Metric cnd.

Pros:

- Given two non-dominated sets, A and B, if each point in B is dominated by a point in A then A will always be evaluated as being better than B.
- Independent – the hypervolume calculated for the given set is not dependent on any other, or any reference set.
- Differentiates between different degrees of complete outperformance of two sets.
- Intuitive meaning/interpretation.

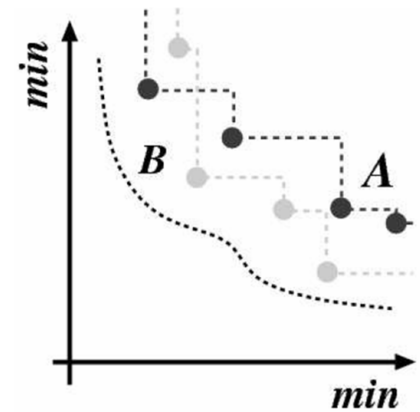
Cons:

- Requires defining some upper boundary of the region.
  This choice does affect the ordering of non-dominated sets.
- It has a large computational overhead, $O(n^{k+1})$, where n is the number of nondominated solutions and k is the number of objectives, rendering it unusable for many objectives or large sets.
- It multiplies apples by oranges, that is, different objectives together.

C Metric

Coverage of two sets $C(X, Y)$ – given two sets of non-dominated solutions X and Y found by the compared algorithms, the measure $C(X, Y)$ returns a ratio of a number of solutions of Y that are dominated by or equal to any solution of X to the whole set Y.

- It returns values from the interval [0, 1].
- The value $C(X, Y) = 1$ means that all solutions in Y are covered by solutions of the set X. And vice versa, the value $C(X, Y) = 0$ means that none of the solutions in Y are covered by the set X.
- Always both orderings have to be considered, since $C(X, Y)$ is not necessarily equal to $1 - C(Y, X)$.



$C(A, B) = 0.25$, $C(B, A) = 0.75$

Properties:

- It has low computational overhead.
- If two sets are of different cardinality and/or the distributions of the sets are non-uniform, then it gives unreliable results.

C Metric cnd.

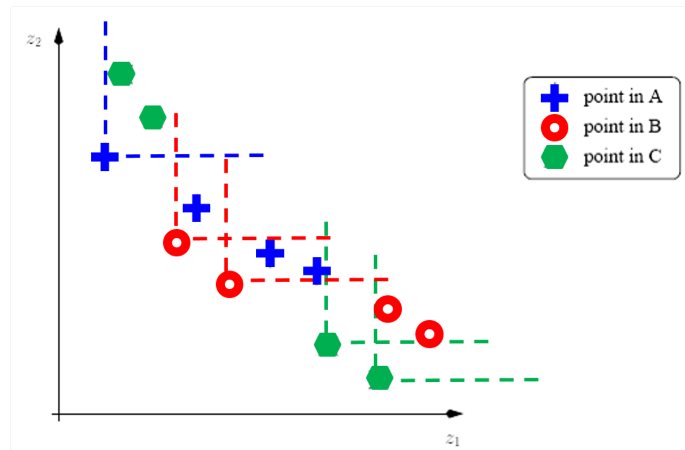
Properties:

- Any pair of C metric scores for a pair of sets A and B in which neither $C(A,B)=1$ nor $C(B,A)=1$, indicates that the two sets are incomparable according to the weak outperformance relation.
- It is cycleinducing – if three sets are compared using C, they may not be ordered.

Example:

- $C(A,B)=0$, $C(B,A)=3/4$
- $C(B,C)=0$, $C(C,B)=1/2$
- $C(A,C)=1/2$, $C(C,A)=0$

B considered better than A, A better than C, but C better than B.



©Knowles J. and Corne D.: On Metrics for Comparing Non-Dominated Sets.

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