Last class

- Fitness level
  - Original fitness level
  - Refined fitness level
- Drift analysis
  - Additive drift
  - Multiplicative drift
  - Negative drift
- Switch analysis
- Results of running time analysis

南京大学 人工智能学院
SCHOOL OF ARTIFICIAL INTELLIGENCE, NANJING UNIVERSITY

Heuristic Search and Evolutionary Algorithms

Lecture 11: Evolutionary Algorithms for Multi-objective Optimization

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Multi-objective optimization

Multi-objective optimization: optimize multiple objectives (which are usually conflicting) simultaneously

$$max_{x \in \mathcal{X}} \left(f_1(x), f_2(x), \ldots, f_m(x)\right)$$

feasible solution space, consisting of all solutions satisfying the constraints

- x weakly dominates y, denoted as $x \succcurlyeq y$, if

$$\forall i \in \{1,2,\ldots,m\}: \ f_i(x) \geq f_i(y)$$

- x dominates y, denoted as $x \succ y$, if

$$\forall i \in \{1,2,\ldots,m\}: \ f_i(x) \geq f_i(y) \text{ and } \exists i \in \{1,2,\ldots,m\}: \ f_i(x) > f_i(y)$$

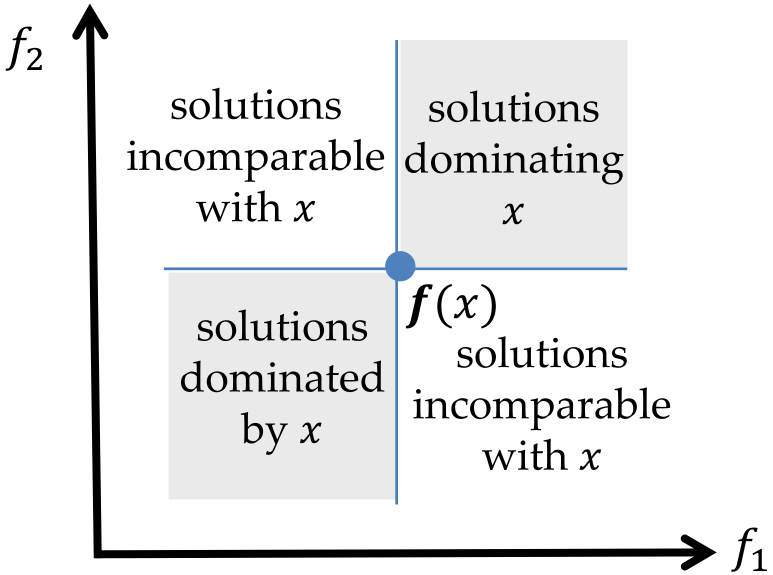
- x is incomparable with y, if neither $x \succcurlyeq y$ nor $y \succcurlyeq x$

Multi-objective optimization

Multi-objective optimization: optimize multiple objectives (which are usually conflicting) simultaneously

$$max_{x \in \mathcal{X}} \ \left(f_1(x), f_2(x), \ldots, f_m(x)\right)$$

Bi-objective maximization



Multi-objective optimization

Multi-objective optimization: optimize multiple objectives (which are usually conflicting) simultaneously

$$max_{x \in \mathcal{X}} \ \left(f_1(x), f_2(x), \ldots, f_m(x)\right)$$

A solution is Pareto optimal if no other solution dominates it

The collection of objective vectors of all Pareto optimal solutions is called the Pareto front

The goal of multi-objective optimization is to find a set of solutions whose objective vectors cover the Pareto front

Multi-objective optimization

Multi-objective optimization: optimize multiple objectives (which are usually conflicting) simultaneously

$$max_{x \in \mathcal{X}} \ \left(f_1(x), f_2(x), \ldots, f_m(x)\right)$$

However, the size of Pareto front can be exponentially large

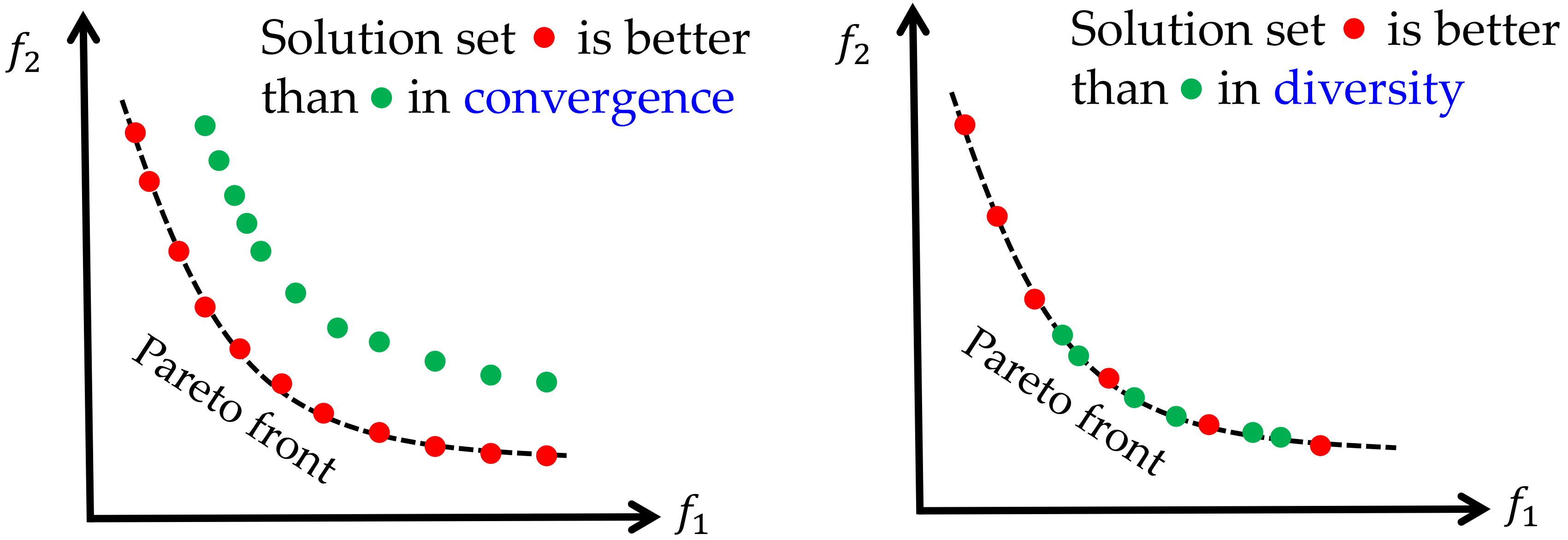
In practice, we want to find a set of solutions that is good in terms of:

- Convergence (to the Pareto front)
- Diversity (along the Pareto front)

Multi-objective optimization

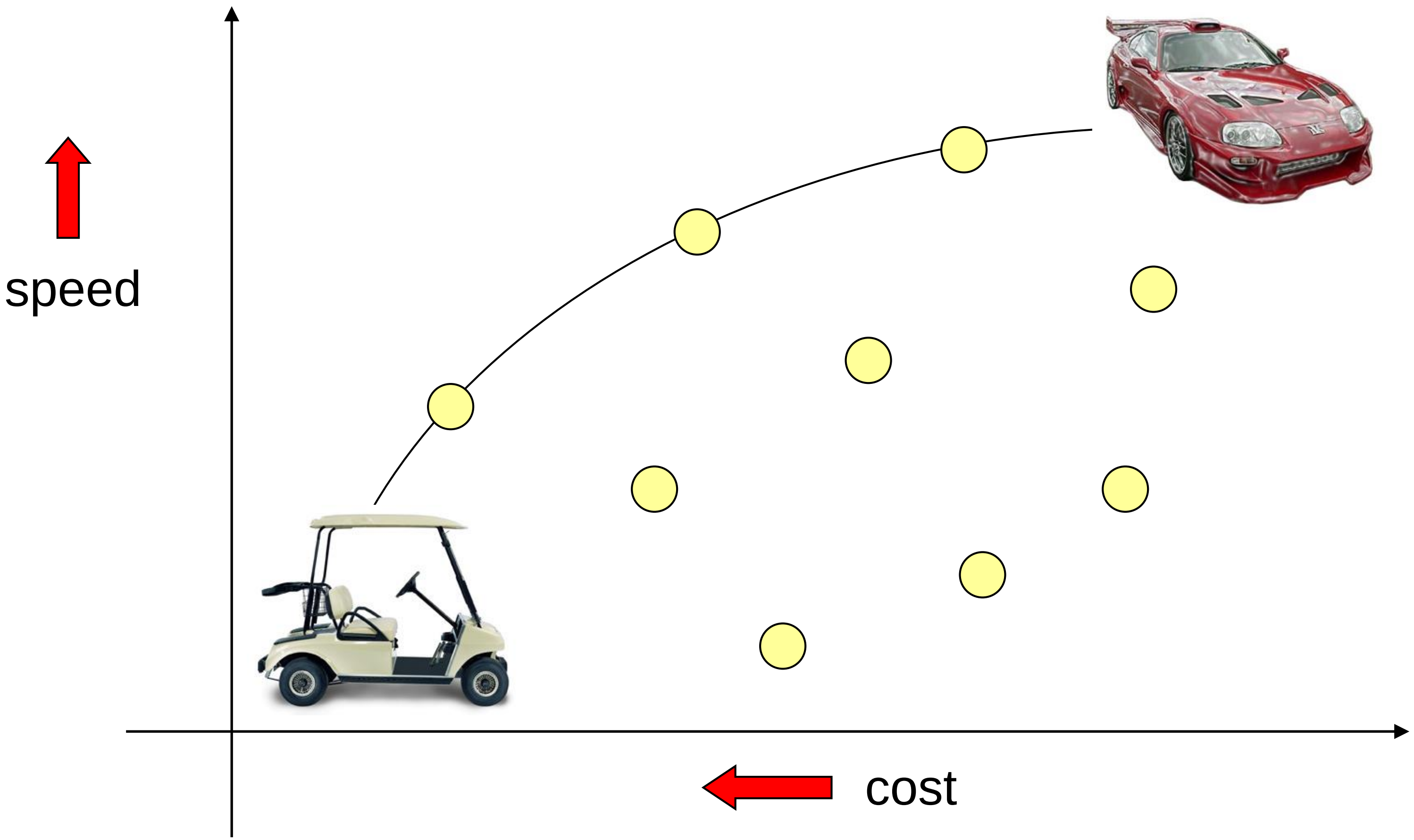
Multi-objective optimization: optimize multiple objectives (which are usually conflicting) simultaneously

$$max_{x \in \mathcal{X}} \ \left(f_1(x), f_2(x), \ldots, f_m(x)\right)$$

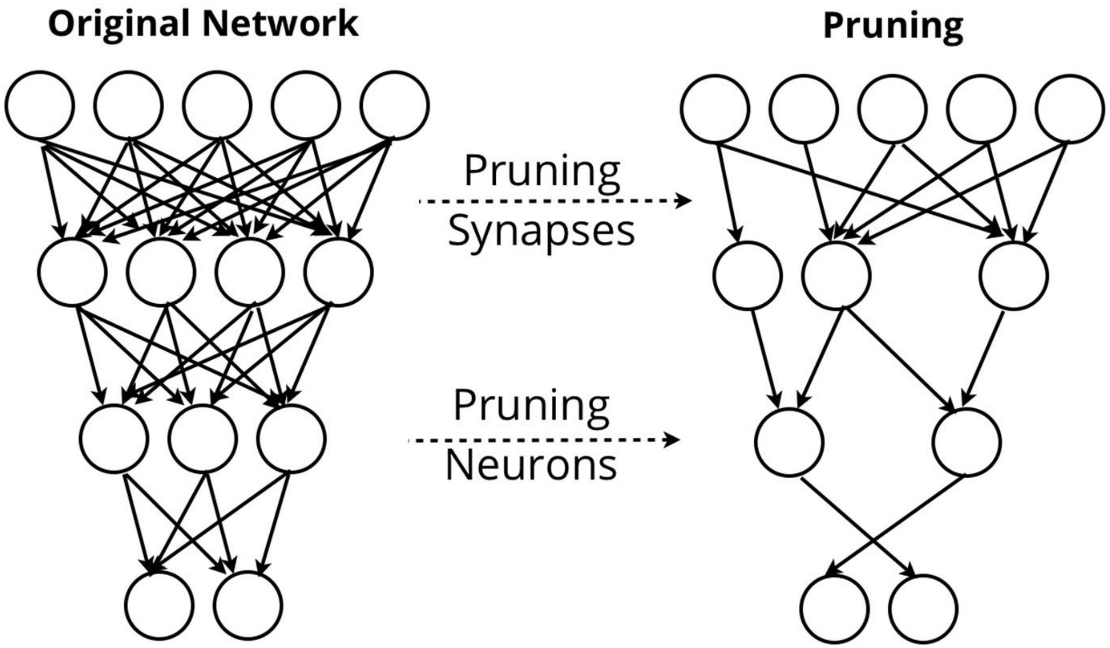


Bi-objective minimization

Example of multi-objective optimization

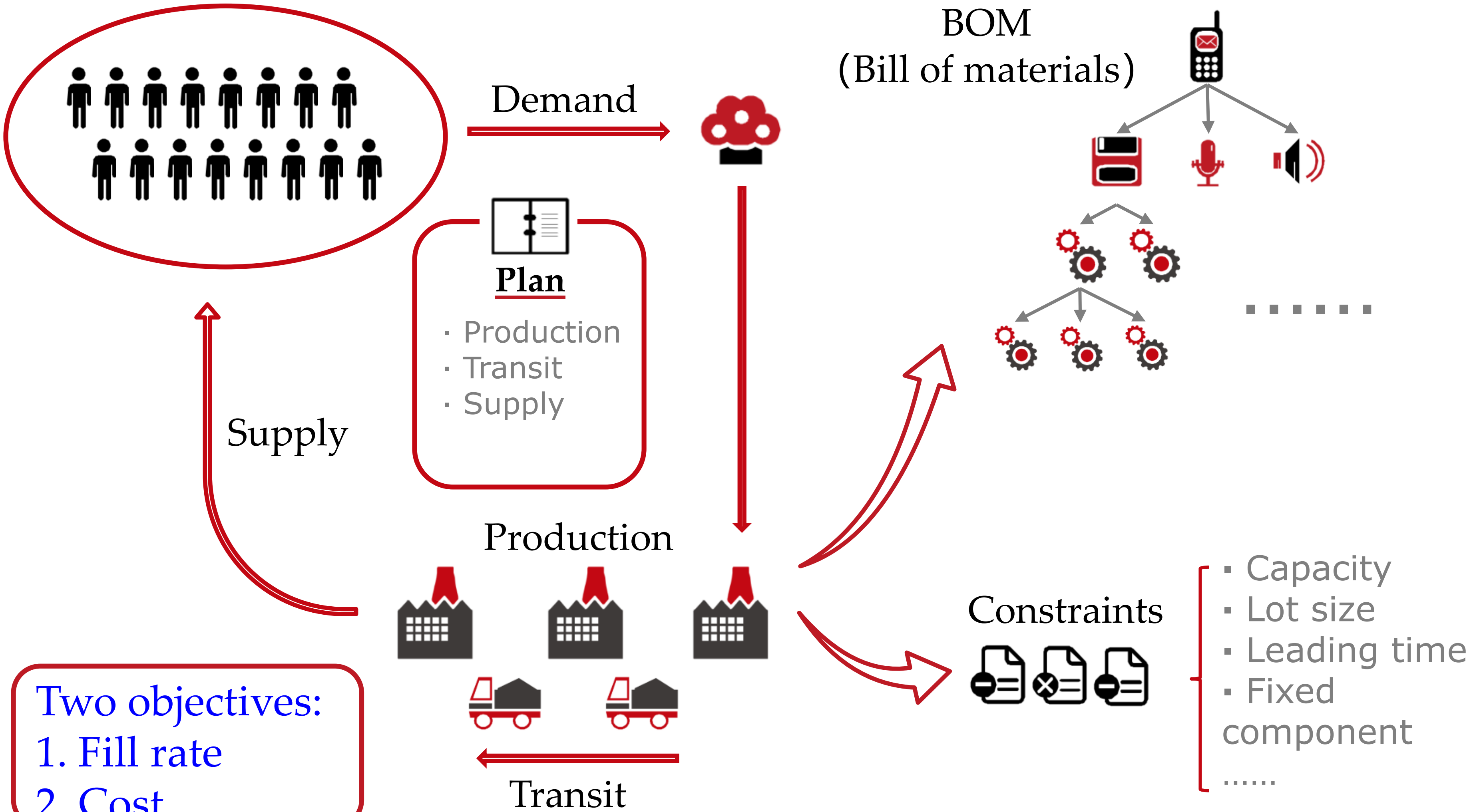


Example of multi-objective optimization



- Accuracy: the higher the better
- Complexity: the smaller the better

Example of multi-objective optimization



Two objectives:
1. Fill rate
2. Cost

Multi-objective evolutionary algorithms

- EAs for multi-objective optimization are usually called Multi-Objective Evolutionary Algorithms (MOEAs)
- Almost all types of EAs have their multi-objective version
- Become a prosperous sub-area of EAs since 1985

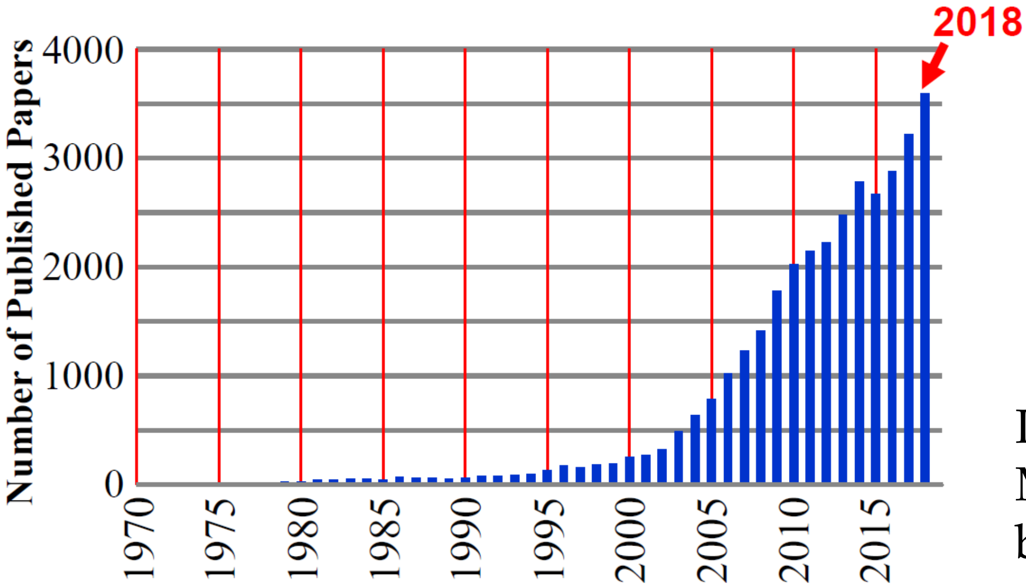


Image source: “Evolutionary Many-objective Optimization” by H. Ishibuchi

Variants of MOEA

- Pareto dominance based: NSGA-II, SPEA-II, …

K. Deb, A. Pratap, S. Agarwal and T. Meyarivan. A fast and elitist multiobjective genetic algorithm: NSGA-II. *IEEE Transactions on Evolutionary Computation*, 2002. (Google scholar引用：37988)

- Performance indicator based: SMS-EMOA, HyPE, ….

N. Beume, B. Naujoks and M. Emmerich. SMS-EMOA: Multiobjective selection based on dominated hypervolume. *European Journal of Operational Research*, 2007. (Google scholar引用：1625)

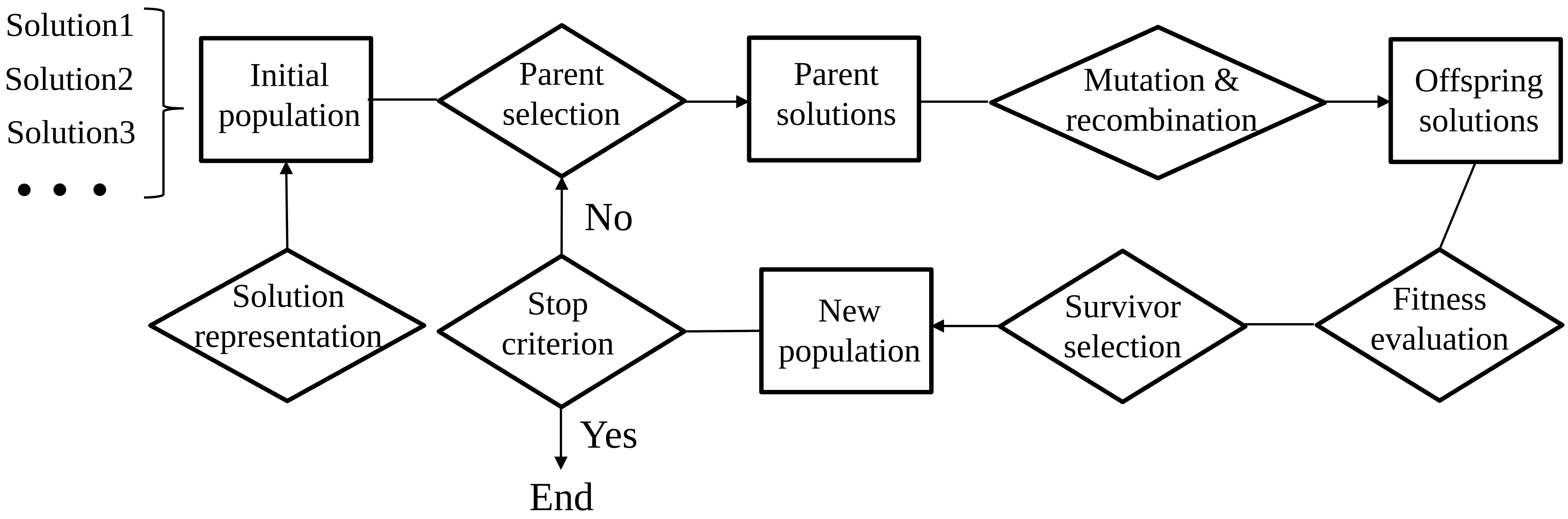
- Decomposition based: MOEA/D, ….

Q. Zhang and H. Li. MOEA/D: A multiobjective evolutionary algorithm based on decomposition. *IEEE Transactions on Evolutionary Computation*, 2007. (Google scholar引用：5940)

NSGA-II

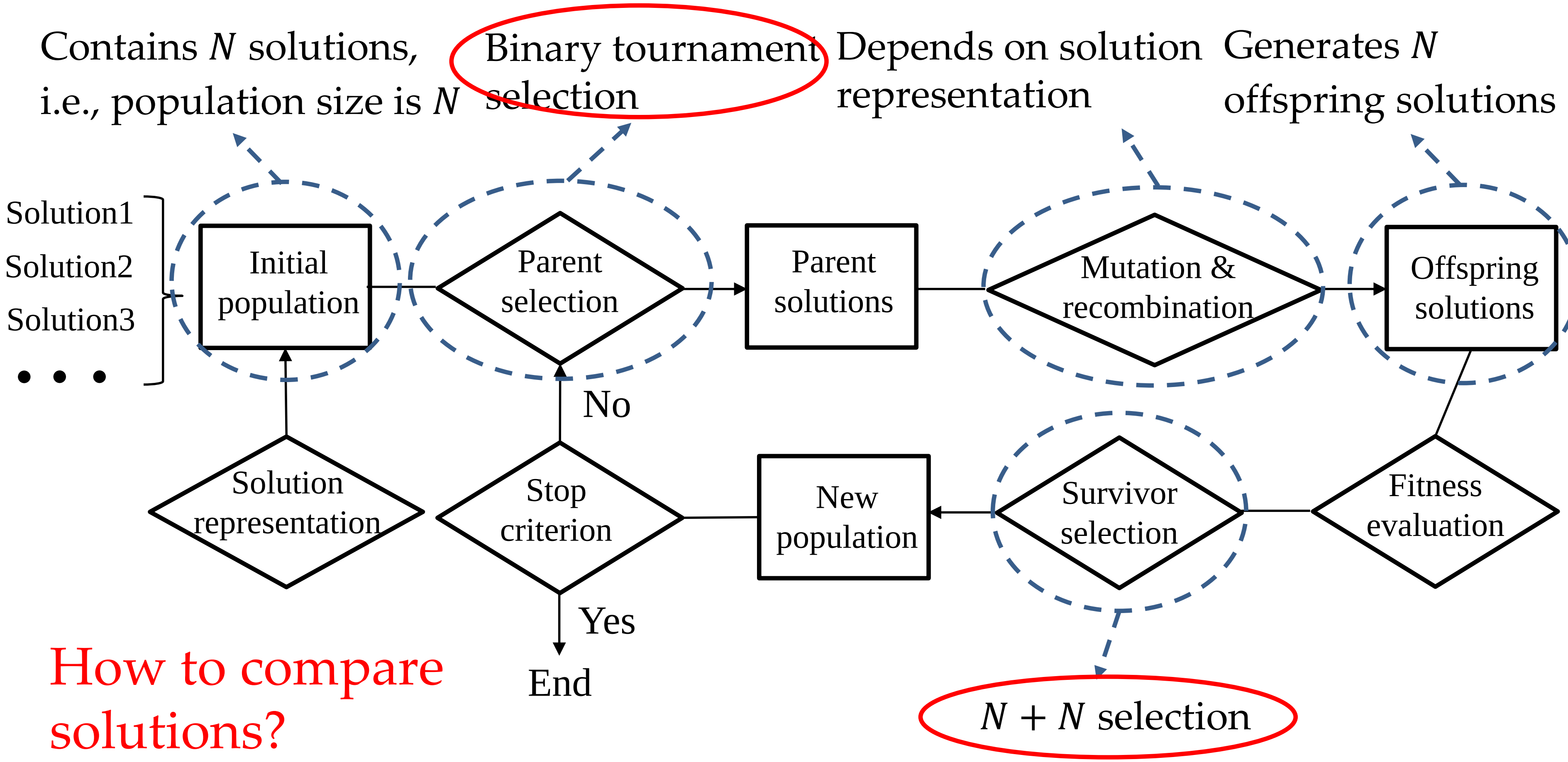
- NSGA-II: probably the most influential work on MOEAs
- Majority of papers on MOEAs emerge after this seminal work, and adopt similar framework as NSGA-II

Framework of NSGA-II



NSGA-II

Framework of NSGA-II



How to compare solutions?

NSGA-II

Non-dominated sorting

Input: $P = \{x_1, x_2, \dots, x_\mu\}$;

Initialize $k = 1$, $Q = \emptyset$

While $P \neq \emptyset$ Do

  for each $x_i \in P$

    if x_i is not dominated by any x_j in P

      rank$k(x_i) = k$;

      $Q = Q \cup \{x_i\}$

    end if

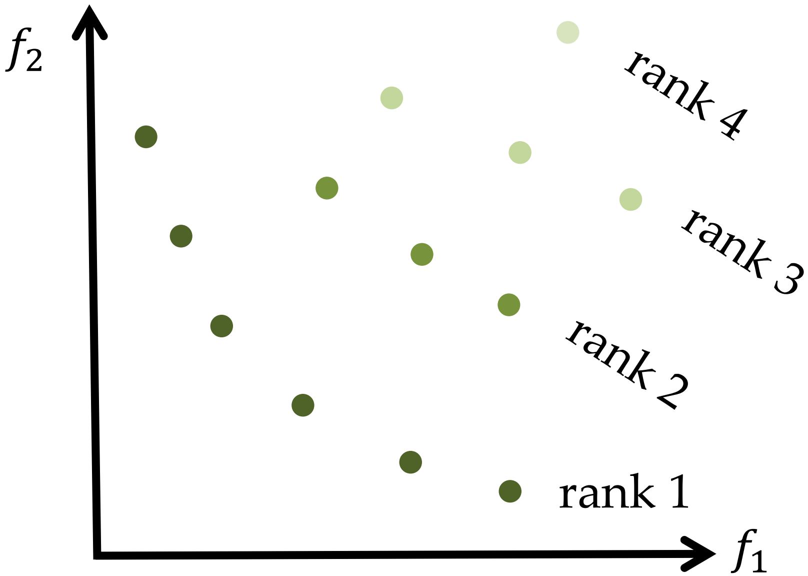
  end for

  $P = P/Q$;

  $k = k + 1$

End While

many redundant comparisons



Bi-objective minimization

NSGA-II

Fast non-dominated sorting

for each $x \in P$

$S_x = \emptyset$; $n_x = 0$;

for each $y \in P$

if $x \succ y$ then

$S_x = S_x \cup \{y\}$

else if $x \prec y$ then

$n_x = n_x + 1$

end if

end for

if $n_x = 0$ then

rank(x)=1; $F_1 = F_1 \cup \{x\}$

end if

end for

the set of solutions dominated by x

the number of solutions dominating x

if x dominates y, add y to S_x

if y dominates x, increase n_x

x is ranked by 1

$i = 1$;

while $F_i \neq \emptyset$

$Q = \emptyset$;

for each $x \in F_i$

for each $y \in S_x$

$n_y = n_y - 1$

if $n_y = 0$ then

rank(y)= $i + 1$;

$Q = Q \cup \{y\}$

end if

end for

end for

$i = i + 1$; $F_i = Q$

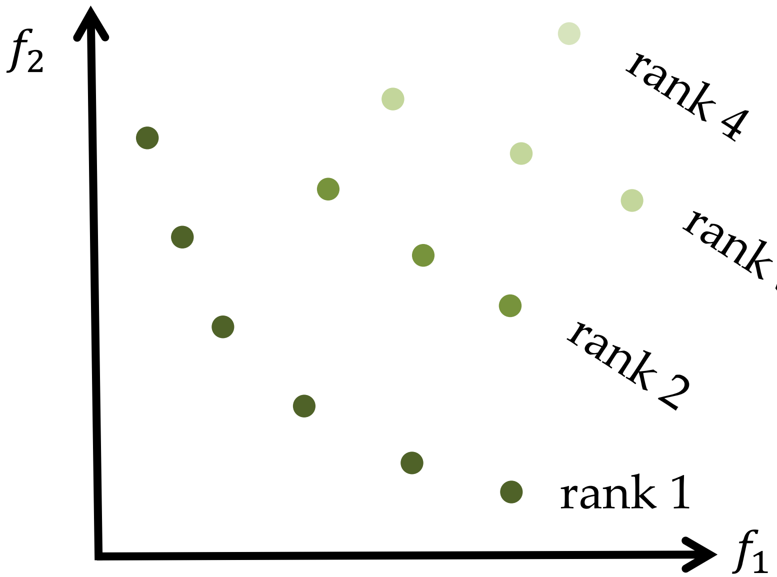
end while

store the solutions with the next rank

As x is excluded now, decrease n_y

y has the next rank

NSGA-II



Bi-objective minimization

For the solutions with the same rank, which one is better?

NSGA-II

Crowding distance assignment

Input: $Q = \{x_1, x_2, \dots, x_l\}$ with the same rank;

for each j, set $Q[j]_{distance} = 0$

the j-th solution in Q

for each objective f_i

$Q = sort(Q, f_i)$; in ascending order

$Q[1]_{distance} = \infty$;

$Q[l]_{distance} = \infty$;

boundary solutions

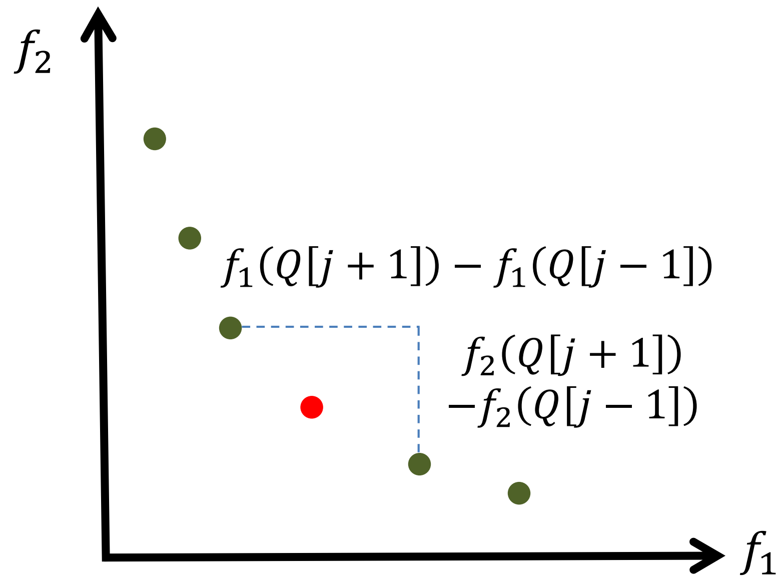
for $j = 2$ to $l - 1$

$$Q[j]_{distance} = Q[j]_{distance} + \frac{f_i(Q[j+1]) - f_i(Q[j-1])}{f_i.max - f_i.min};$$

normalization

end for

end for



Crowding distance: the larger the better

Prefer diversity

NSGA-II

Crowded comparison employed by NSGA-II

Given a set P of solutions, for any two solutions x, y in P, x is better than y, if

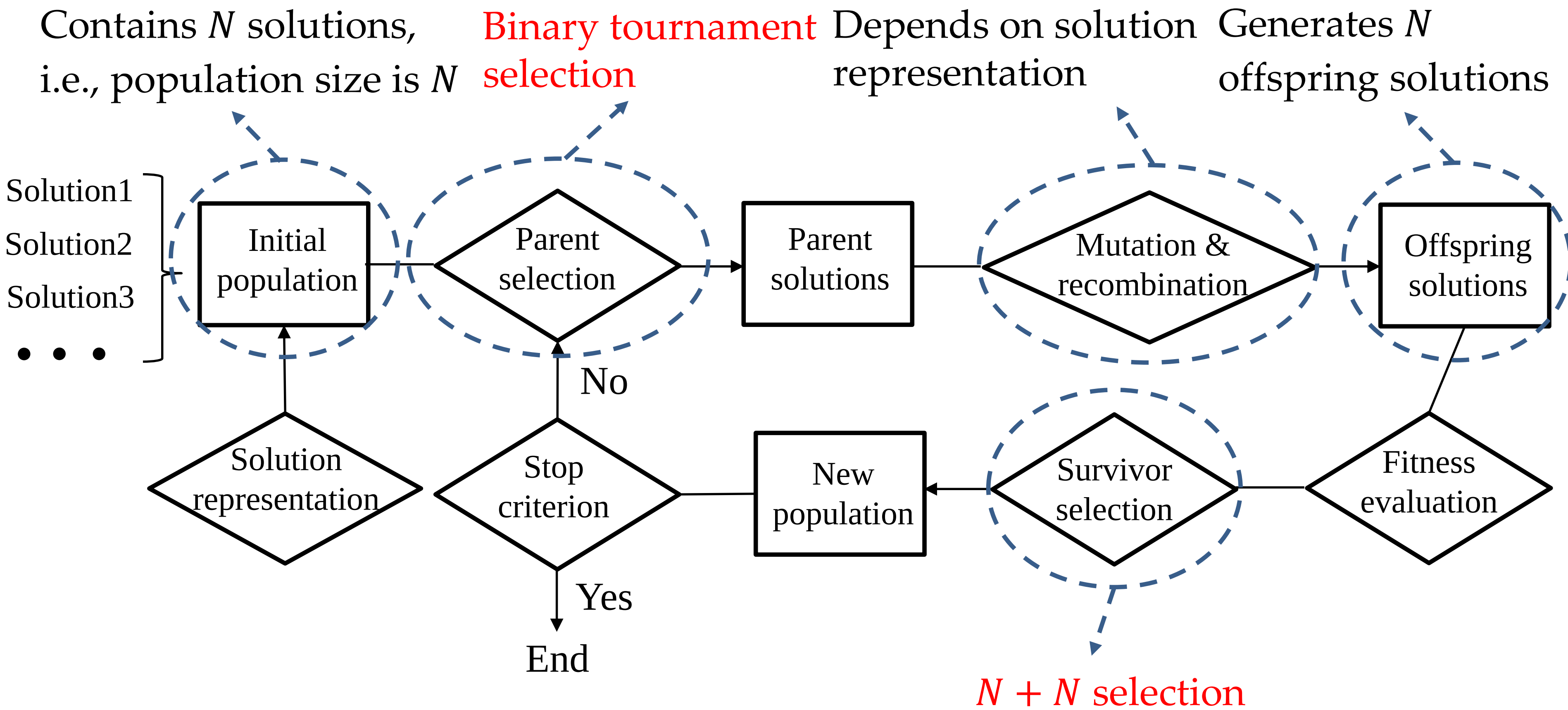
- rank(x) < rank(y)
- or rank(x) = rank(y) but distance(x) > distance(y)

Convergence

Diversity

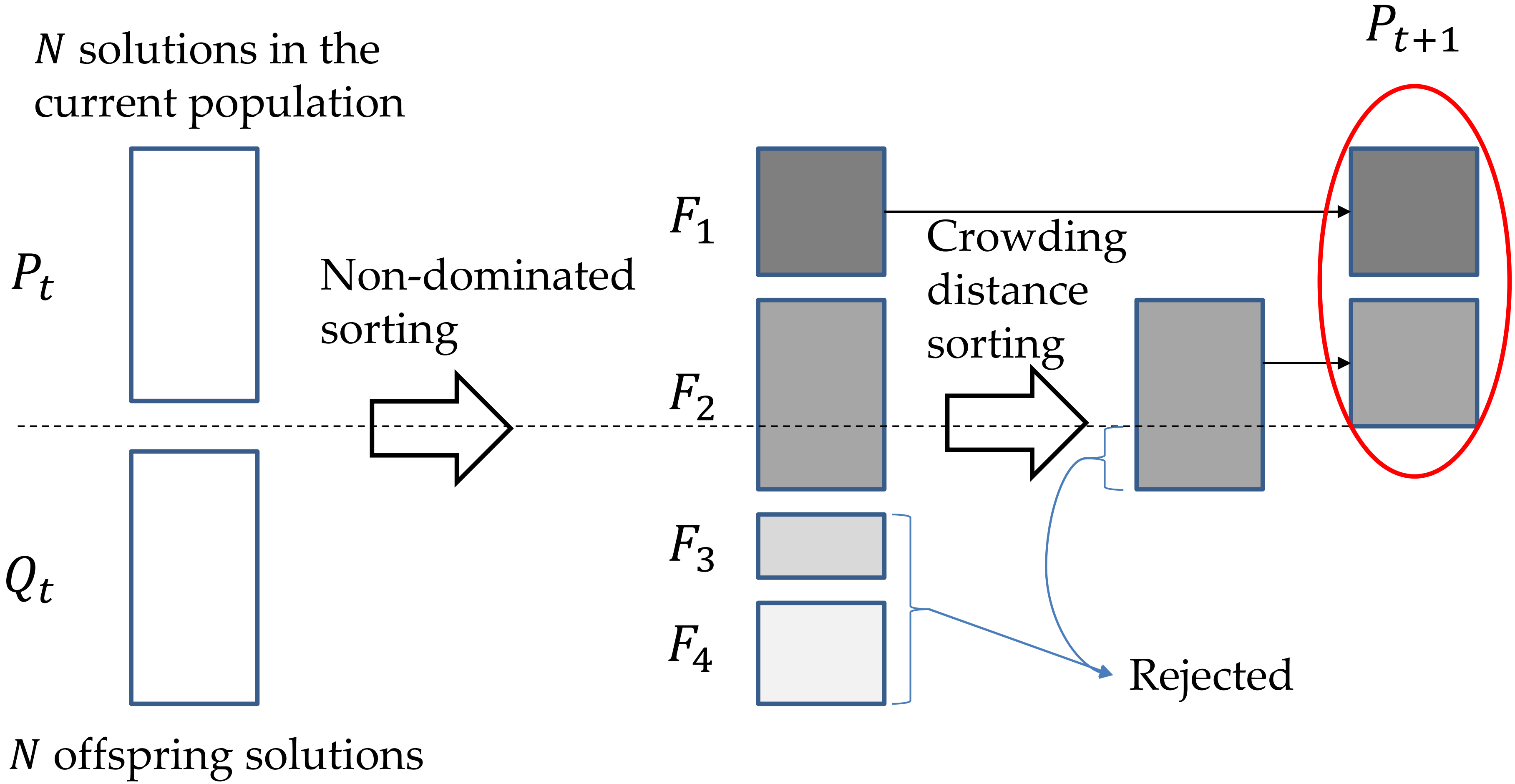
NSGA-II

Framework of NSGA-II



NSGA-II

$N + N$ survivor selection



NSGA-II: application illustration

NSGA-II: population size 40, SBX crossover with $\eta = 20$, crossover probability 0.9, polynomial mutation with $\eta = 20$, mutation probability $1/n$

DTLZ1:

$$
\begin{aligned}
&\text{Minimize } f_1(\mathbf{x}) = \tfrac{1}{2} x_1 x_2 \cdots x_{M-1}(1 + g(\mathbf{x}_M)),\\
&\text{Minimize } f_2(\mathbf{x}) = \tfrac{1}{2} x_1 x_2 \cdots (1 - x_{M-1})(1 + g(\mathbf{x}_M)),\\
&\qquad \vdots \quad \vdots\\
&\text{Minimize } f_{M-1}(\mathbf{x}) = \tfrac{1}{2} x_1 (1 - x_2)(1 + g(\mathbf{x}_M)),\\
&\text{Minimize } f_M(\mathbf{x}) = \tfrac{1}{2} (1 - x_1)(1 + g(\mathbf{x}_M)),\\
&\text{subject to } 0 \le x_i \le 1, \quad \text{for } i = 1, 2, \ldots, n.
\end{aligned}
$$

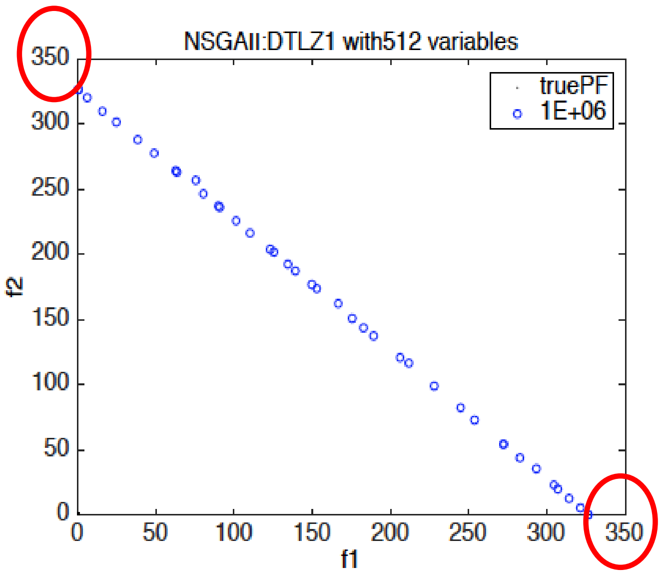
the vector containing the last $n - M + 1$ variables

$$
g(\mathbf{x}_M) = 100 \left[|\mathbf{x}_M| + \sum_{x_i \in \mathbf{x}_M} (x_i - 0.5)^2 - \cos(20\pi(x_i - 0.5)) \right]
$$

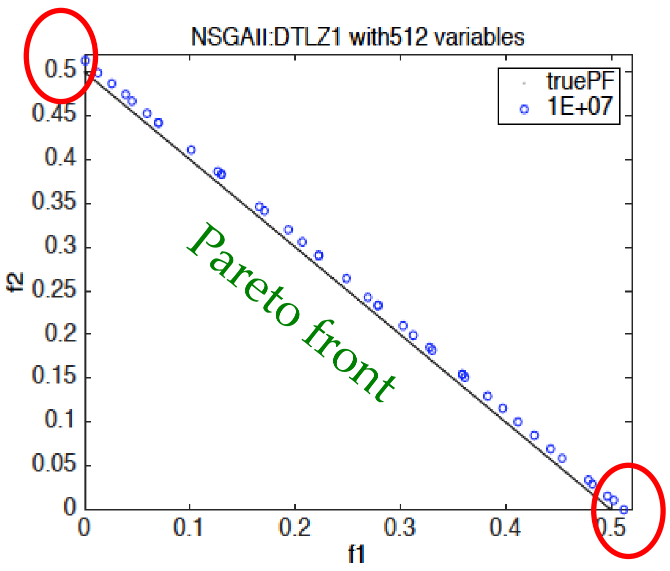
$n - M + 1$

NSGA-II: application illustration

For NSGA-II solving DTLZ1 with $M = 2$ and $n = 512$



The population
after 10^6 fitness evaluations



The population
after 10^7 fitness evaluations

NSGA-II: application illustration

NSGA-II: population size 40, SBX crossover with $\eta = 20$, crossover probability 0.9, polynomial mutation with $\eta = 20$, mutation probability $1/n$

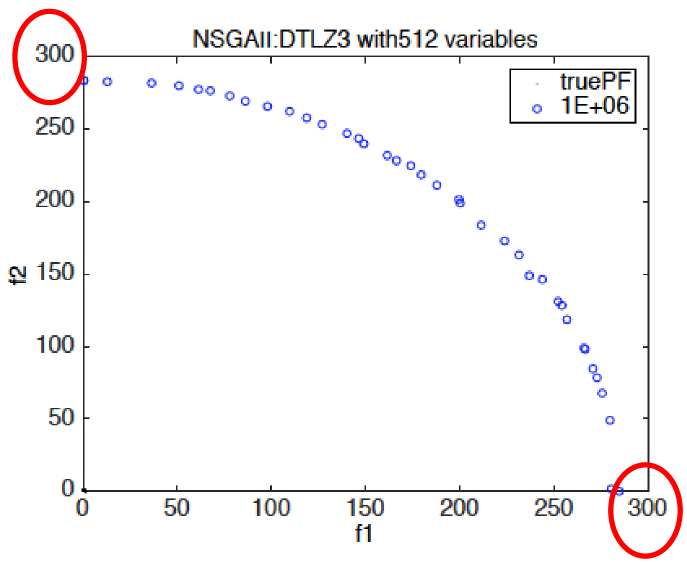
DTLZ3:

$$
\begin{aligned}
\text{Min. } & f_1(\mathbf{x}) = (1 + g(\mathbf{x}_M)) \cos(x_1\pi/2) \cdots \cos(x_{M-2}\pi/2) \cos(x_{M-1}\pi/2), \\
\text{Min. } & f_2(\mathbf{x}) = (1 + g(\mathbf{x}_M)) \cos(x_1\pi/2) \cdots \cos(x_{M-2}\pi/2) \sin(x_{M-1}\pi/2), \\
\text{Min. } & f_3(\mathbf{x}) = (1 + g(\mathbf{x}_M)) \cos(x_1\pi/2) \cdots \sin(x_{M-2}\pi/2), \\
\vdots \quad & \vdots \\
\text{Min. } & f_M(\mathbf{x}) = (1 + g(\mathbf{x}_M)) \sin(x_1\pi/2), \\
\text{with } & g(\mathbf{x}_M) = 100 \left[|\mathbf{x}_M| + \textstyle\sum_{x_i \in \mathbf{x}_M} (x_i - 0.5)^2 - \cos(20\pi(x_i - 0.5)) \right], \\
& 0 \le x_i \le 1, \quad \text{for } i = 1, 2, \ldots, n.
\end{aligned}
$$

the vector containing the last $n - M + 1$ variables

NSGA-II: application illustration

For NSGA-II solving DTLZ3 with $M = 2$ and $n = 512$



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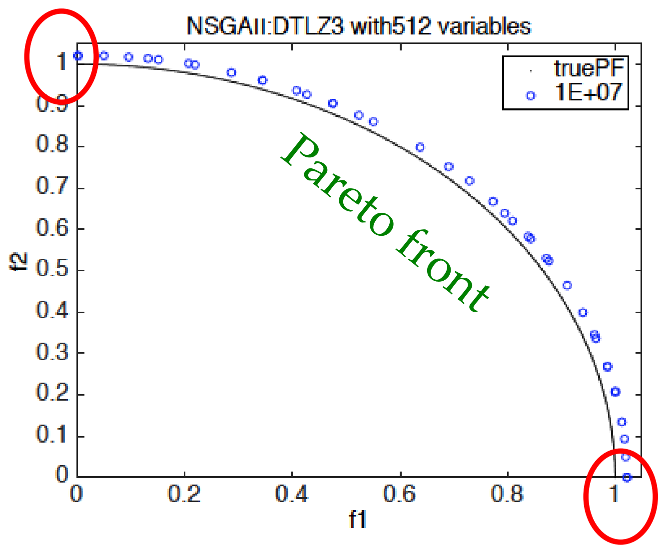


The population
after 10^7 fitness evaluations

NSGA-II: application illustration

NSGA-II: population size 40, SBX crossover with $\eta = 20$, crossover probability 0.9, polynomial mutation with $\eta = 20$, mutation probability $1/n$

WFG:

to be optimized

Given $\quad \mathbf{z} = \{z_1, \ldots, z_k, z_{k+1}, \ldots, z_n\}$

Minimise $\quad f_{m=1:M}(\mathbf{x}) = x_M + S_m h_m(x_1, \ldots, x_{M-1})$

where

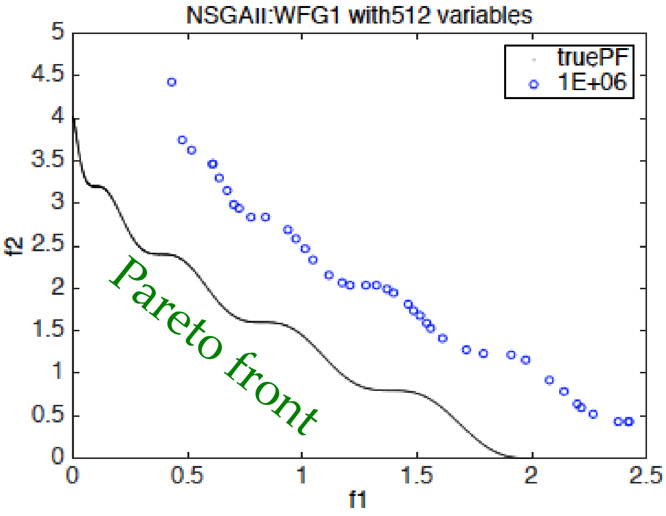
$$\mathbf{x} = \{x_1, \ldots, x_M\} = \{\max(t_M^p, A_1)(t_1^p - 0.5) + 0.5, \ldots, \max(t_M^p, A_{M-1})(t_{M-1}^p - 0.5) + 0.5, t_M^p\}$$

$$\mathbf{t}^p = \{t_1^p, \ldots, t_M^p\} \leftarrow\![\ \mathbf{t}^{p-1} \leftarrow\![\ \ldots \leftarrow\![\ \mathbf{t}^1 \leftarrow\![\ \mathbf{z}_{[0,1]}$$

$$\mathbf{z}_{[0,1]} = \{z_{1,[0,1]}, \ldots, z_{n,[0,1]}\} = \{z_1/z_{1,\max}, \ldots, z_n/z_{n,\max}\}$$

NSGA-II: application illustration

For NSGA-II solving WFG1 with $M = 2$ and $n = 512$



The population
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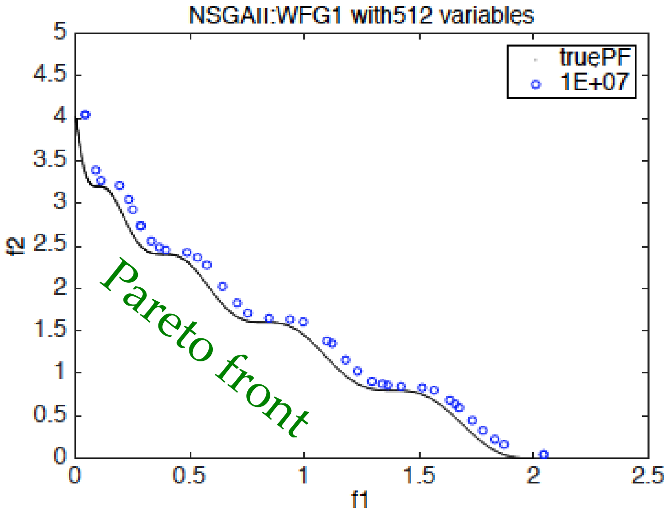


The population
after 10^7 fitness evaluations

SMS-EMOA

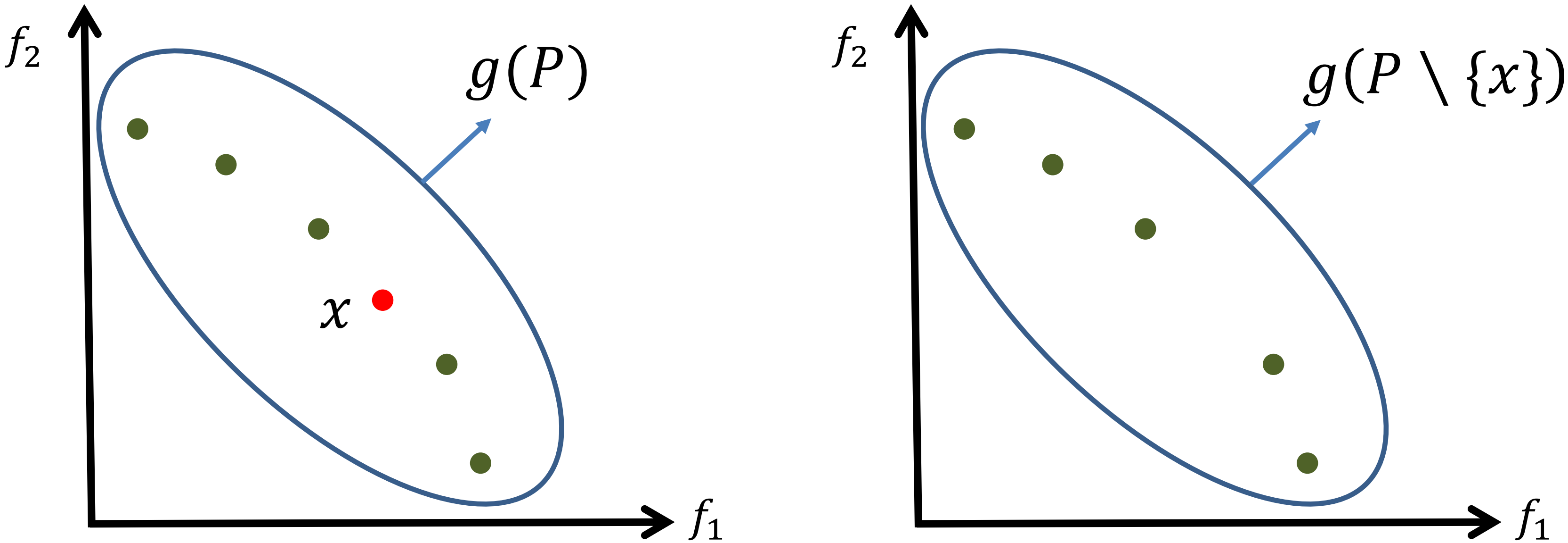
- Similar to NSGA-II, except the goodness measure for the solutions with the same rank

- Make use of quality indicators to measure the goodness

- Typically, the goodness of a solution is defined based on how much the quality indicator decreases if the solution is removed

SMS-EMOA

Quality indicator: $g(P)$, where P is a set of solutions



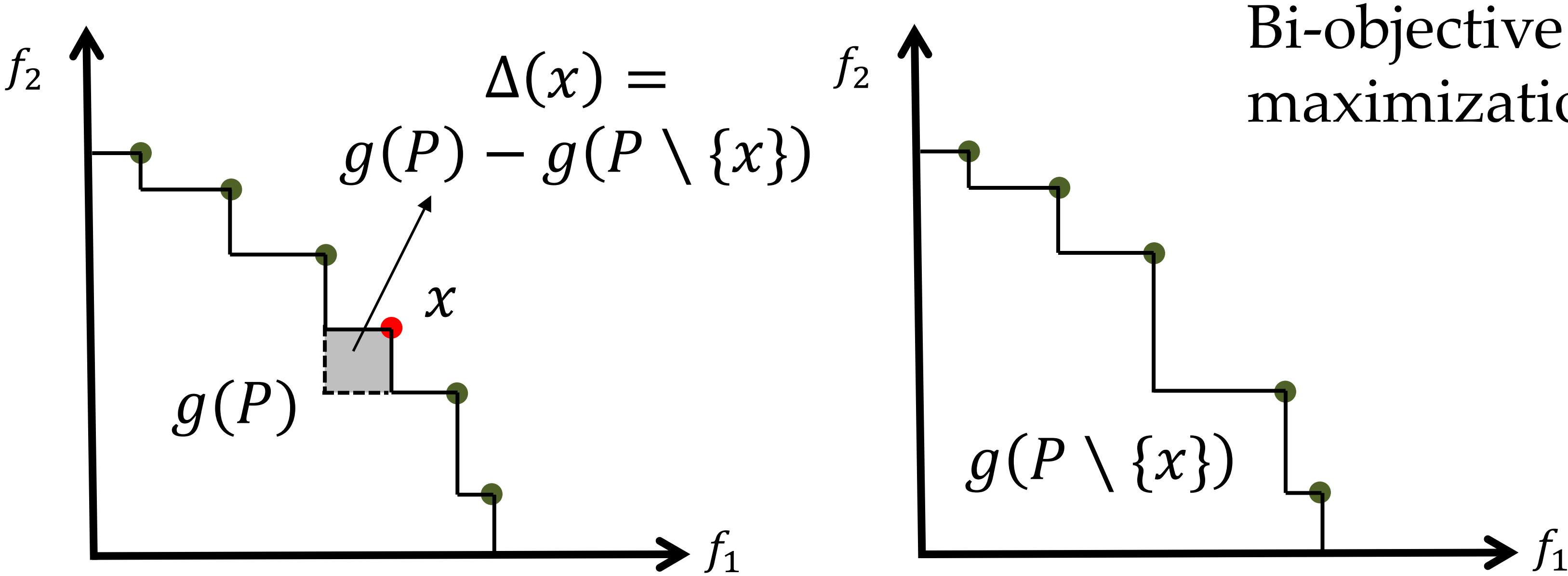
$$\Delta(x) = g(P) - g(P \setminus \{x\})$$

Quality indicator loss: the larger the better

SMS-EMOA

The quality indicator $g(P)$ should be coherent with "convergence" and "diversity"

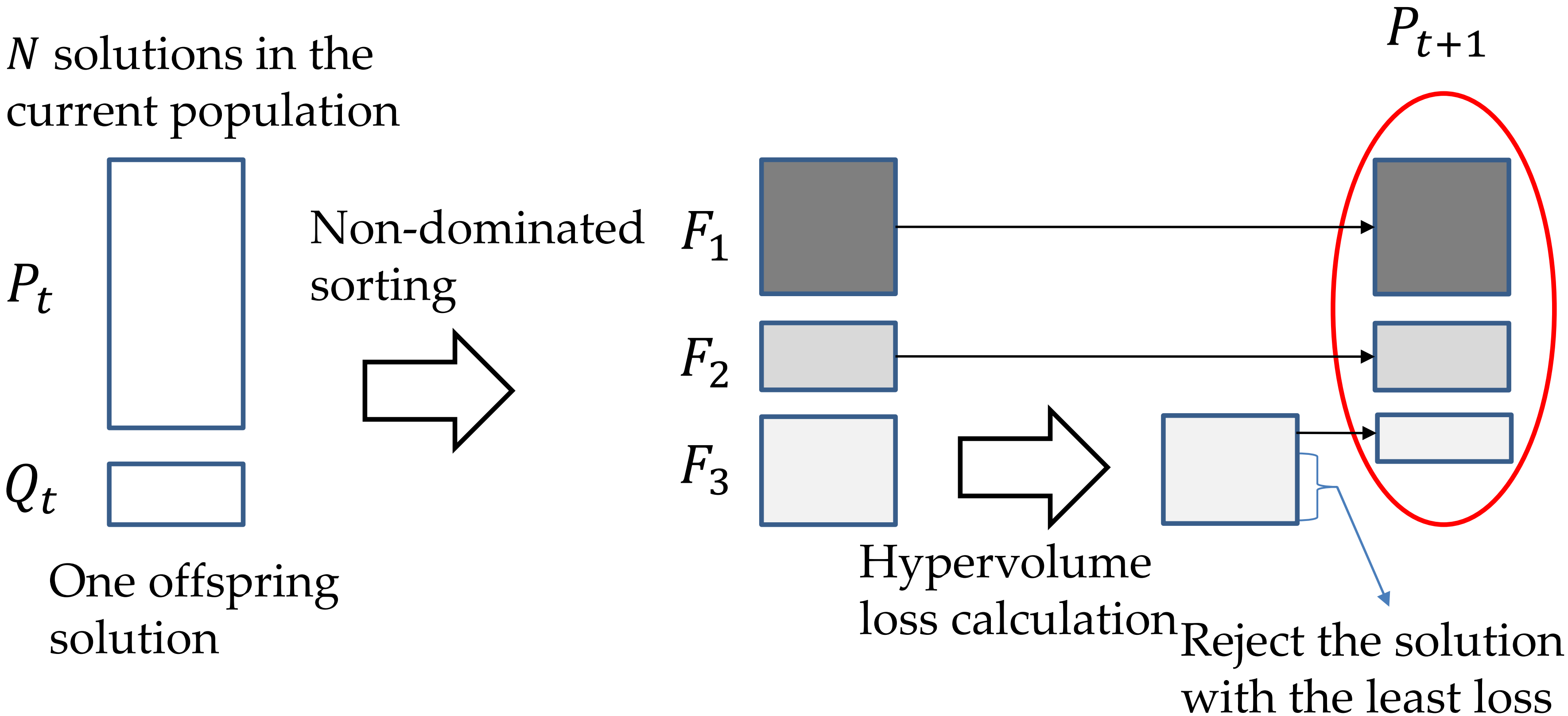
E.g., the hypervolume indicator



Bi-objective maximization

SMS-EMOA

- The basic SMS-EMOA generates only one offspring solution



SMS-EMOA: application illustration

SMS-EMOA: population size 40, SBX crossover with $\eta = 20$, crossover probability 0.9, polynomial mutation with $\eta = 20$, mutation probability $1/n$

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&\quad \vdots \quad \vdots\\
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DTLZ3:

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&\text{Min. } f_3(\mathbf{x}) = (1+g(\mathbf{x}_M))\cos(x_1\pi/2)\cdots\sin(x_{M-2}\pi/2),\\
&\vdots \qquad \vdots\\
&\text{Min. } f_M(\mathbf{x}) = (1+g(\mathbf{x}_M))\sin(x_1\pi/2),\\
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WFG:

$$
\begin{aligned}
&\text{Given} && \mathbf{z} = \{z_1, \ldots, z_k, z_{k+1}, \ldots, z_n\}\\
&\text{Minimise} && f_{m=1:M}(\mathbf{x}) = x_M + S_m h_m(x_1, \ldots, x_{M-1})\\
&\text{where} && \mathbf{x} = \{x_1, \ldots, x_M\} = \{\max(t^p_M, A_1)(t^p_1 - 0.5) + 0.5, \ldots,\\
& && \qquad \max(t^p_M, A_{M-1})(t^p_{M-1} - 0.5) + 0.5, t^p_M\}\\
& && \mathbf{t}^p = \{t^p_1, \ldots, t^p_M\} \leftarrow\![\ \mathbf{t}^{p-1} \leftarrow\![\ \ldots \leftarrow\![\ \mathbf{t}^1 \leftarrow\![\ \mathbf{z}_{[0,1]}\\
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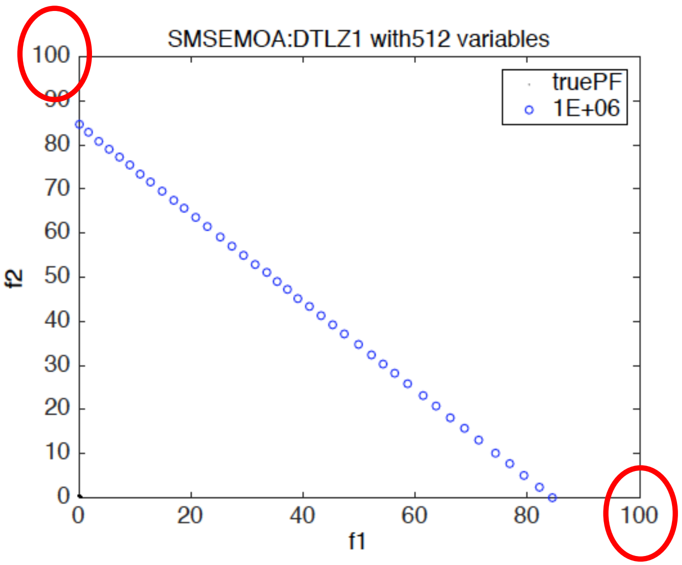
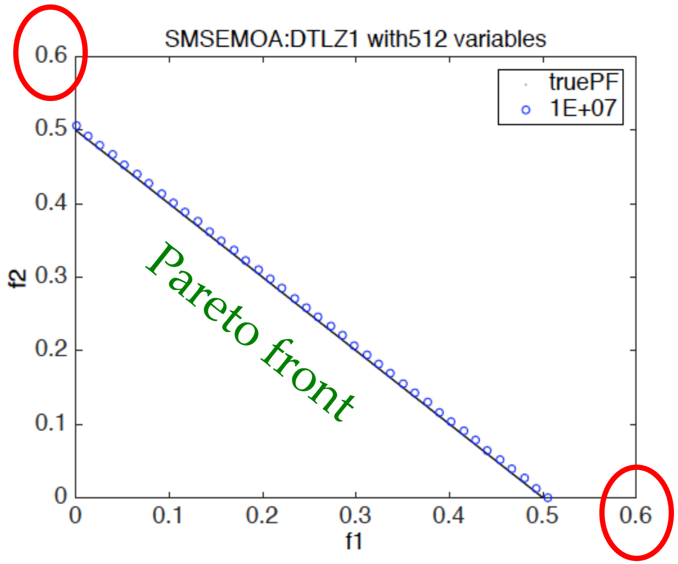
\end{aligned}
$$

SMS-EMOA: application illustration

For SMS-EMOA solving DTLZ1 with $M = 2$ and $n = 512$



The population
after 10^6 fitness evaluations

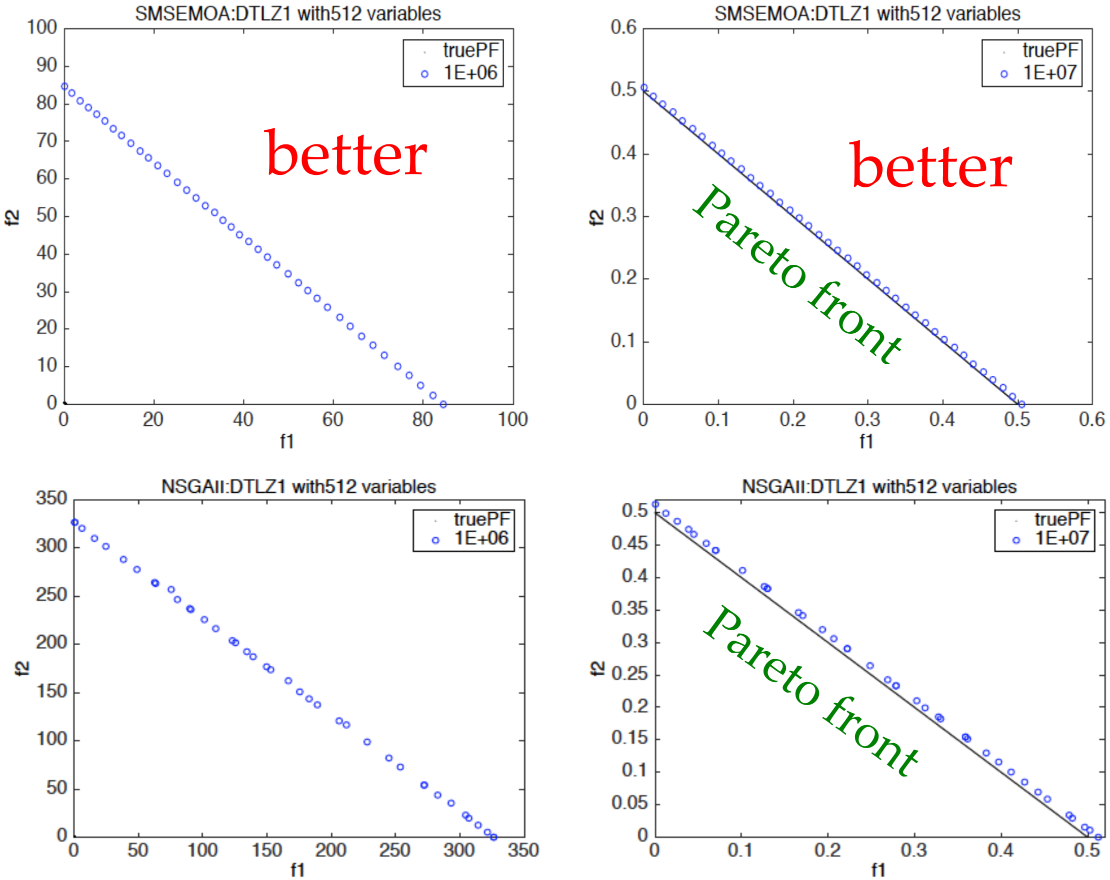


The population
after 10^7 fitness evaluations

SMS-EMOA vs. NSGA-II

SMS-EMOA

NSGA-II

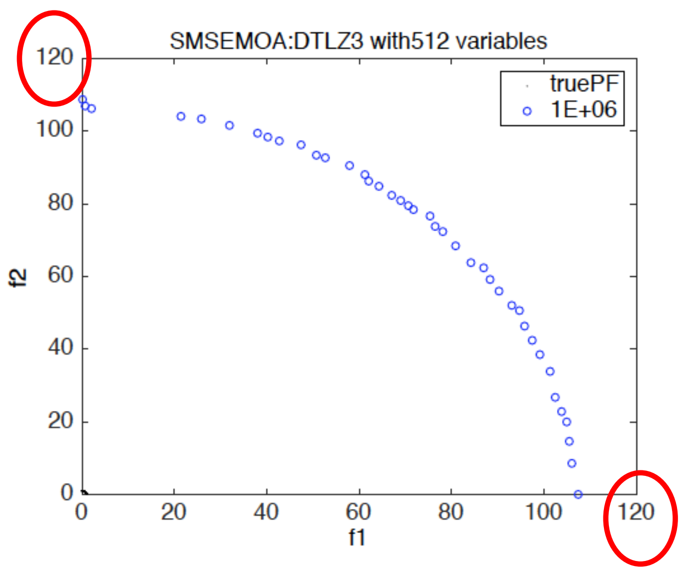


The population after 10^6 fitness evaluations

The population after 10^7 fitness evaluations

SMS-EMOA: application illustration

For SMS-EMOA solving DTLZ3 with $M = 2$ and $n = 512$



The population
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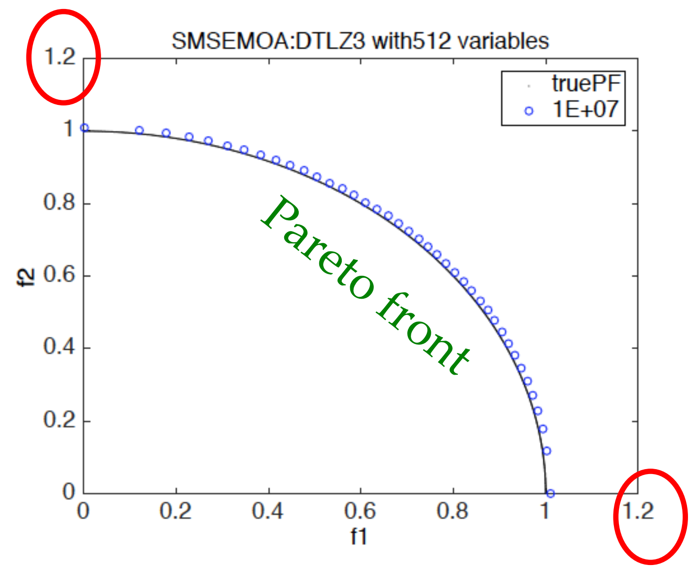

The population
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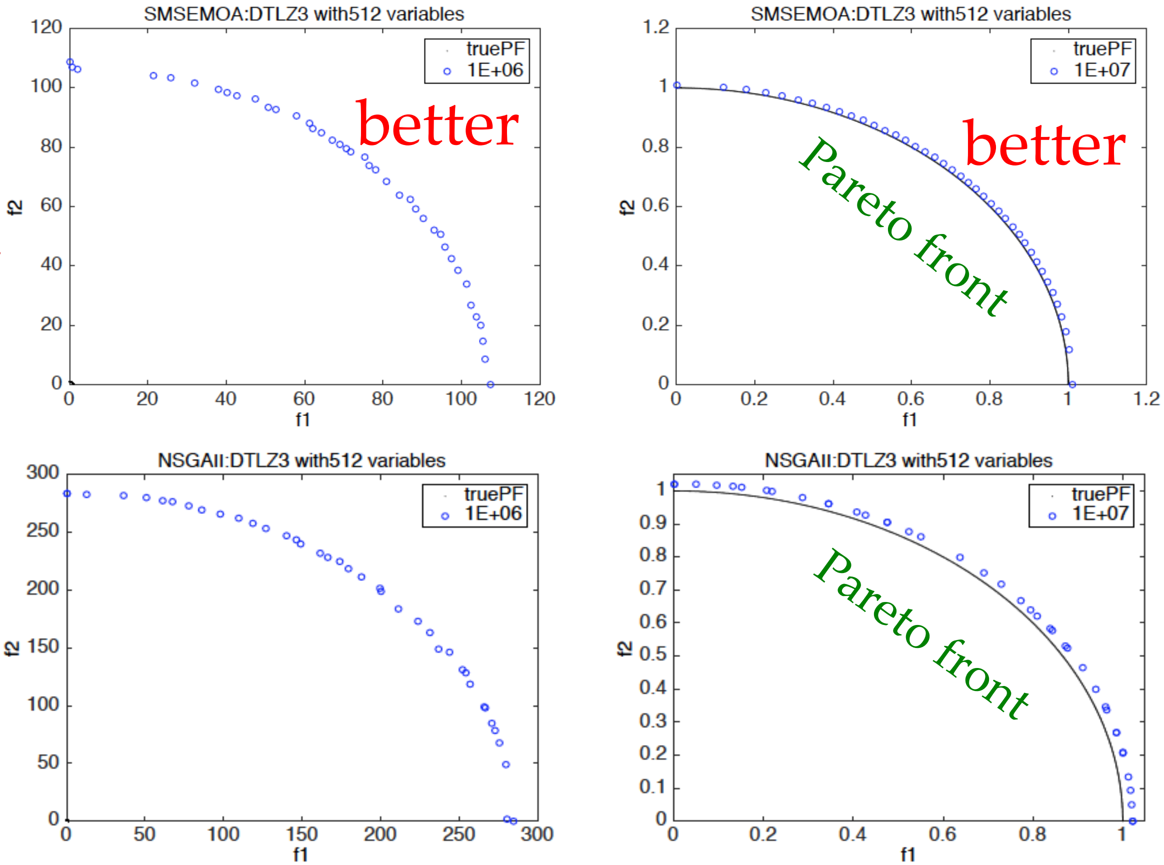
SMS-EMOA vs. NSGA-II

SMS-EMOA

NSGA-II

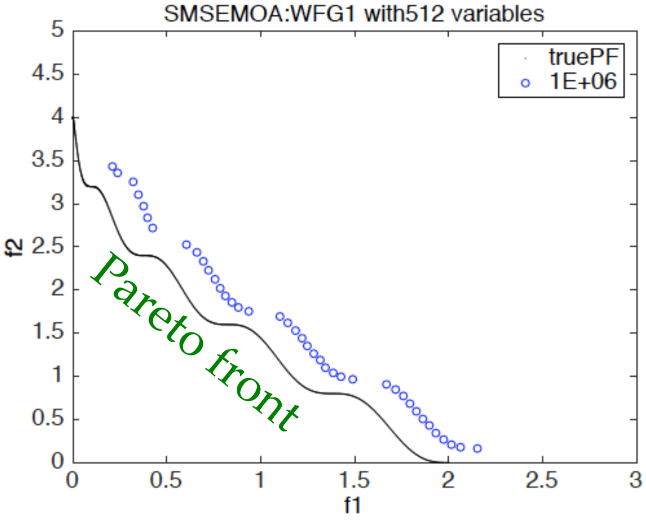


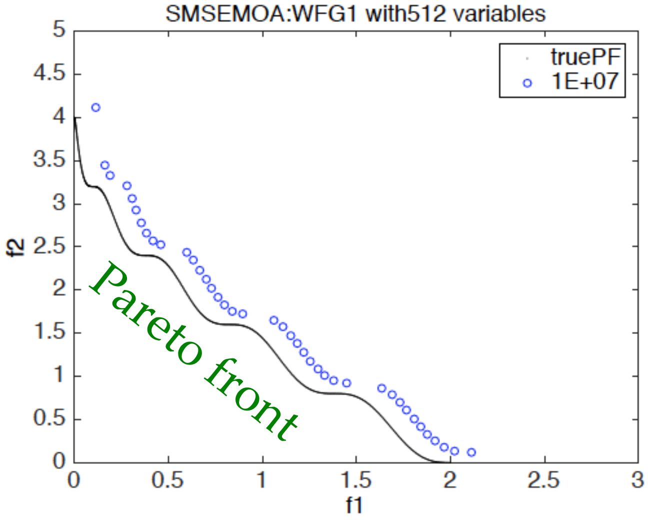
The population after 10^6 fitness evaluations

The population after 10^7 fitness evaluations

SMS-EMOA: application illustration

For SMS-EMOA solving WFG1 with $M = 2$ and $n = 512$





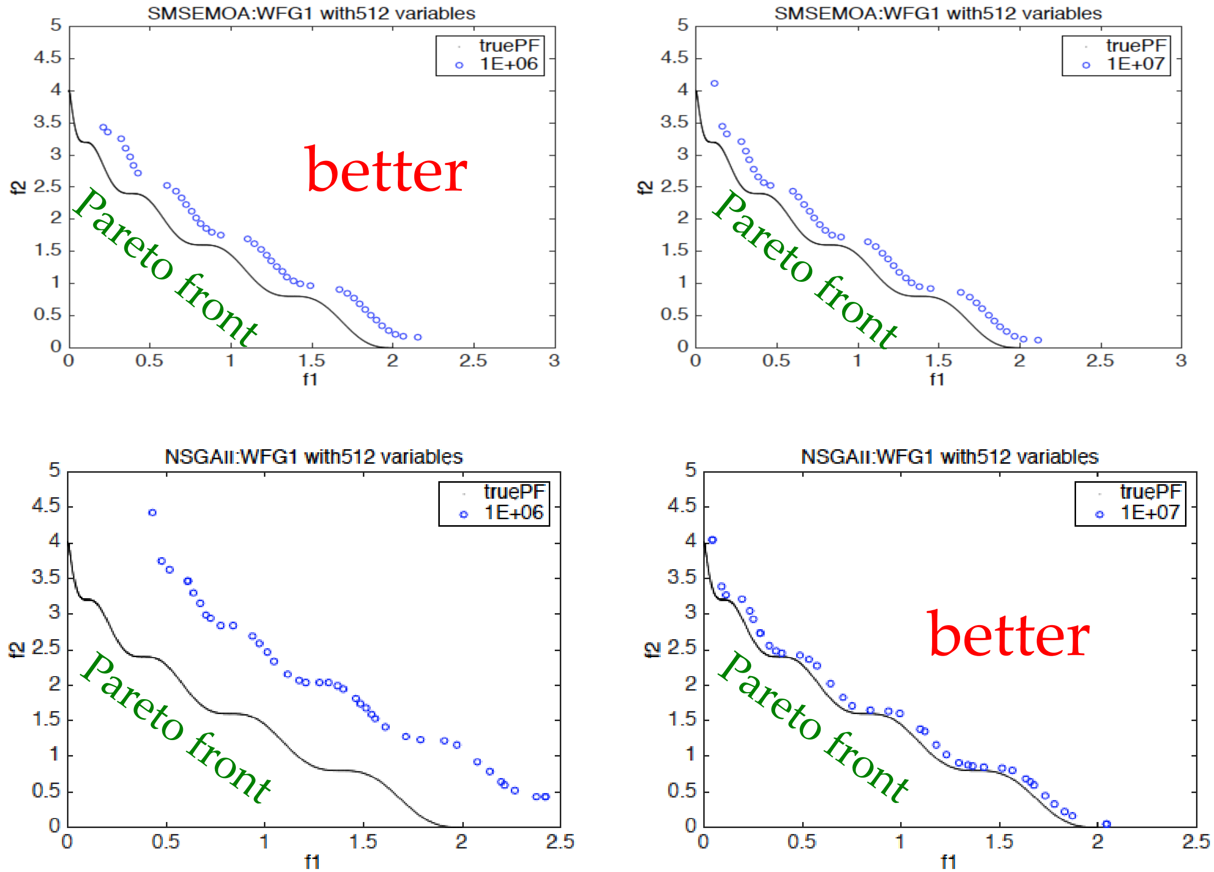
The population after 10^6 fitness evaluations

The population after 10^7 fitness evaluations

SMS-EMOA vs. NSGA-II

SMS-EMOA

NSGA-II

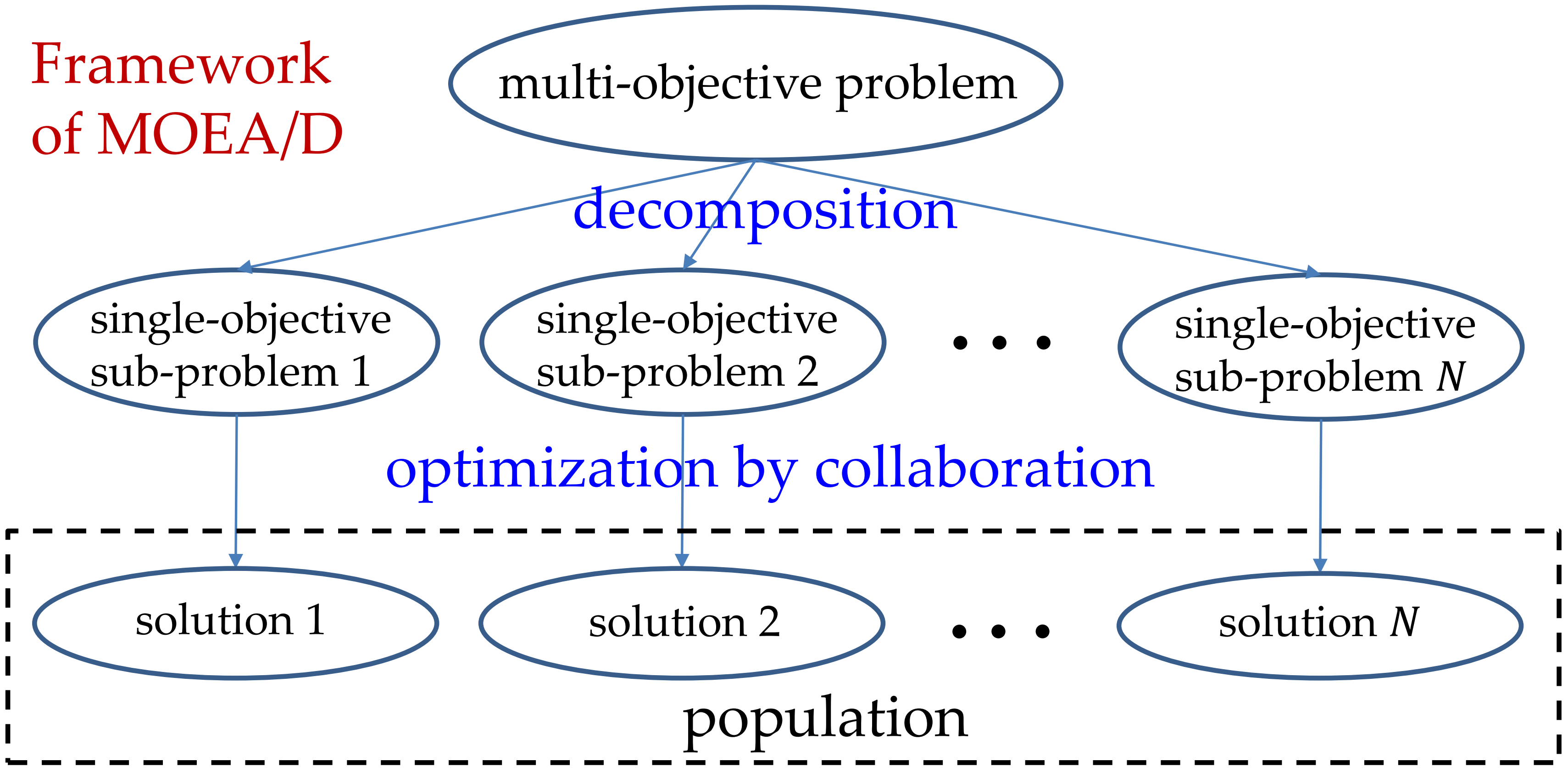


The population after 10^6 fitness evaluations

The population after 10^7 fitness evaluations

MOEA/D

- MOEA based on Decomposition (MOEA/D): old things become new again



MOEA/D - decomposition

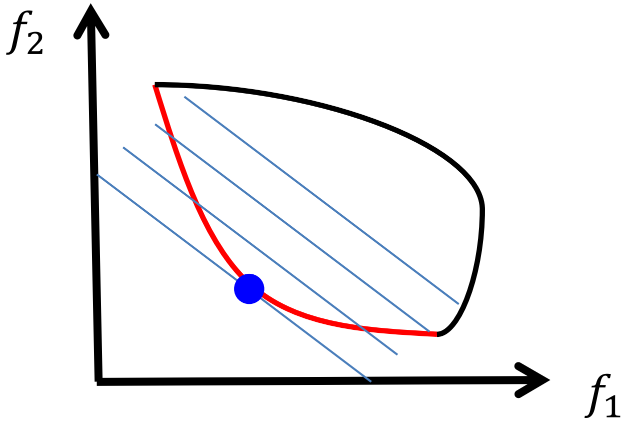
- Weighted sum approach

$$min_{x \in \mathcal{X}} \ \left(f_1(x), f_2(x)\right)$$

⇩

$$min_{x \in \mathcal{X}} \ g^{ws}(x \mid \boldsymbol{\lambda}) = \lambda_1 f_1(x) + \lambda_2 f_2(x)$$

where $\lambda_1 + \lambda_2 = 1, \lambda_1, \lambda_2 \geq 0$



An optimal solution for $g^{ws}(x \mid \boldsymbol{\lambda})$ must be Pareto optimal

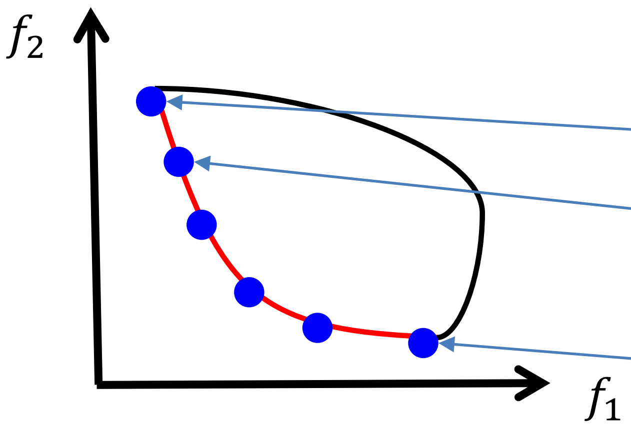
MOEA/D - decomposition

- Weighted sum approach

$$min_{x \in \mathcal{X}} \ \left(f_1(x), f_2(x)\right)$$

$$min_{x \in \mathcal{X}} \ g^{ws}(x \mid \boldsymbol{\lambda}) = \lambda_1 f_1(x) + \lambda_2 f_2(x)$$

where $\lambda_1 + \lambda_2 = 1, \lambda_1, \lambda_2 \geq 0$



N single-objective sub-problems

$g^{ws}(x \mid \boldsymbol{\lambda})$ with $\lambda_1 = 1, \lambda_2 = 0$

$g^{ws}(x \mid \boldsymbol{\lambda})$ with $\lambda_1 = \frac{N-2}{N-1}, \lambda_2 = \frac{1}{N-1}$

• • •

$g^{ws}(x \mid \boldsymbol{\lambda})$ with $\lambda_1 = 0, \lambda_2 = 1$

MOEA/D - decomposition

- Tchbycheff approach

$$min_{x \in \mathcal{X}} \left(f_1(x), f_2(x)\right)$$

$$\Downarrow$$

$$min_{x \in \mathcal{X}} \; g^t(x \mid \boldsymbol{\lambda}, \boldsymbol{z}^*) = \max\{\lambda_1 |f_1(x) - z_1^*|, \lambda_2 |f_2(x) - z_2^*|\}$$

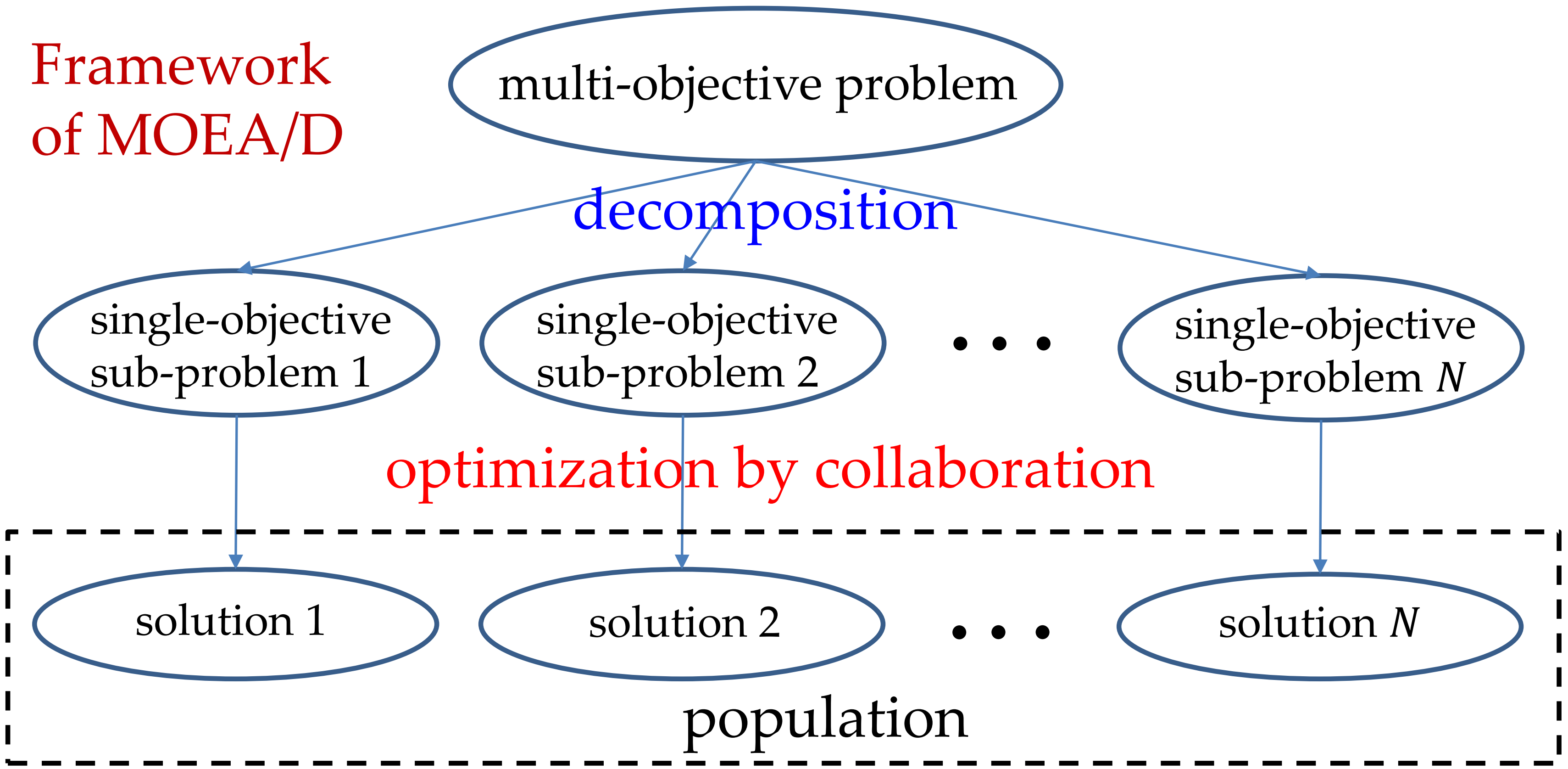
where $\lambda_1 + \lambda_2 = 1, \lambda_1, \lambda_2 \geq 0$

$\boldsymbol{z}^*$ is an Utopian point,
where $z_1^* < \min\{f_1(x)\}$ and $z_2^* < \min\{f_2(x)\}$

For any Pareto optimal solution x^*, there is a $\boldsymbol{\lambda}$ such that x^* is optimal to $g^t(x \mid \boldsymbol{\lambda}, \boldsymbol{z}^*)$

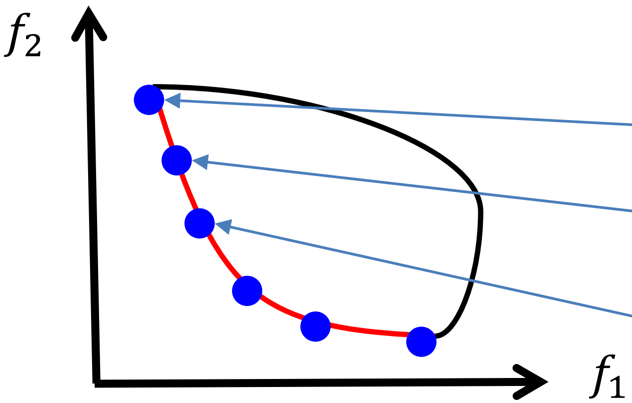
MOEA/D - optimization

Framework of MOEA/D



For each sub-problem, one needs to find neighboring sub-problems, e.g., sub-problems with close weight vectors

MOEA/D - optimization



N single-objective sub-problems

$g^{ws}(x \mid \boldsymbol{\lambda})$ with $\lambda_1 = 1, \lambda_2 = 0$

$g^{ws}(x \mid \boldsymbol{\lambda})$ with $\lambda_1 = \frac{N-2}{N-1}, \lambda_2 = \frac{1}{N-1}$

$g^{ws}(x \mid \boldsymbol{\lambda})$ with $\lambda_1 = \frac{N-3}{N-1}, \lambda_2 = \frac{2}{N-1}$

• • •

neighboring sub-problems

For optimizing each sub-problem in each iteration

1. Mating selection: obtain the current solutions of some neighbours
2. Reproduction: generate a new solution by applying reproduction operators on its own solution and borrowed solutions
3. Replacement:
   3.1 replace its old solution by the new one if the new one is better
   3.2 pass the new solution on to some of its neighbours, and update its neighbor's solutions when better

MOEA/D: application illustration

MOEA/D: Tchbycheff decomposition approach, population size 40, SBX crossover with $\eta = 20$, crossover probability 0.9, polynomial mutation with $\eta = 20$, mutation probability $1/n$

DTLZ1:

$$
\begin{aligned}
&\text{Minimize } f_1(\mathbf{x}) = \tfrac{1}{2} x_1 x_2 \cdots x_{M-1}(1 + g(\mathbf{x}_M)),\\
&\text{Minimize } f_2(\mathbf{x}) = \tfrac{1}{2} x_1 x_2 \cdots (1 - x_{M-1})(1 + g(\mathbf{x}_M)),\\
&\quad \vdots \quad \vdots\\
&\text{Minimize } f_{M-1}(\mathbf{x}) = \tfrac{1}{2} x_1 (1 - x_2)(1 + g(\mathbf{x}_M)),\\
&\text{Minimize } f_M(\mathbf{x}) = \tfrac{1}{2} (1 - x_1)(1 + g(\mathbf{x}_M)),\\
&\text{subject to } 0 \le x_i \le 1, \quad \text{for } i = 1, 2, \ldots, n.
\end{aligned}
$$

DTLZ3:

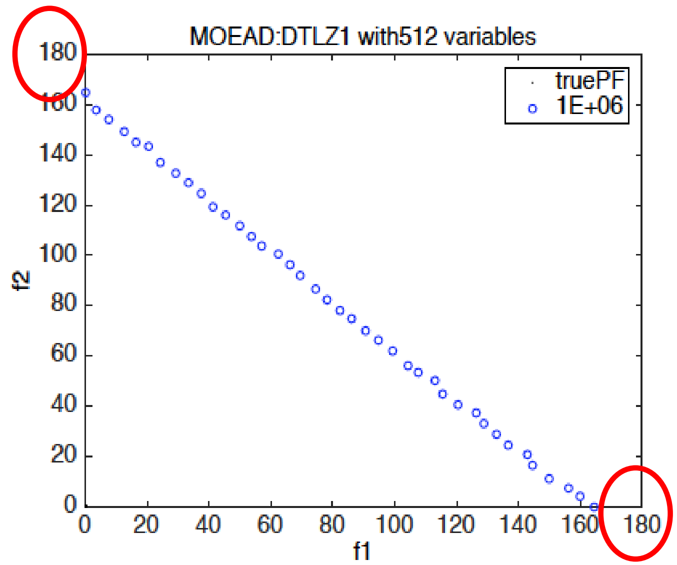
$$
\begin{aligned}
&\text{Min. } f_1(\mathbf{x}) = (1 + g(\mathbf{x}_M)) \cos(x_1 \pi/2) \cdots \cos(x_{M-2}\pi/2) \cos(x_{M-1}\pi/2),\\
&\text{Min. } f_2(\mathbf{x}) = (1 + g(\mathbf{x}_M)) \cos(x_1 \pi/2) \cdots \cos(x_{M-2}\pi/2) \sin(x_{M-1}\pi/2),\\
&\text{Min. } f_3(\mathbf{x}) = (1 + g(\mathbf{x}_M)) \cos(x_1 \pi/2) \cdots \sin(x_{M-2}\pi/2),\\
&\vdots \qquad \vdots\\
&\text{Min. } f_M(\mathbf{x}) = (1 + g(\mathbf{x}_M)) \sin(x_1 \pi/2),\\
&\text{with } g(\mathbf{x}_M) = 100 \left[|\mathbf{x}_M| + \textstyle\sum_{x_i \in \mathbf{x}_M} (x_i - 0.5)^2 - \cos(20\pi(x_i - 0.5)) \right],\\
&\qquad 0 \le x_i \le 1, \quad \text{for } i = 1, 2, \ldots, n.
\end{aligned}
$$

WFG:

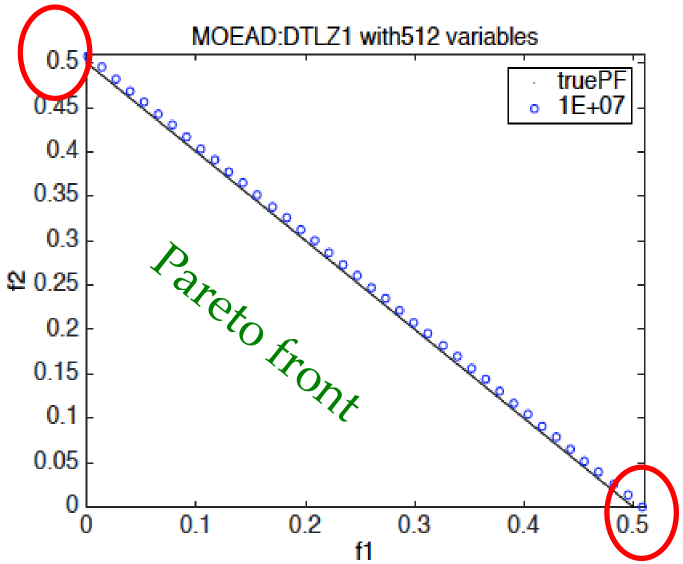
$$
\begin{aligned}
&\text{Given} && \mathbf{z} = \{z_1, \ldots, z_k, z_{k+1}, \ldots, z_n\}\\
&\text{Minimise} && f_{m=1:M}(\mathbf{x}) = x_M + S_m h_m(x_1, \ldots, x_{M-1})\\
&\text{where} && \mathbf{x} = \{x_1, \ldots, x_M\} = \{\max(t_M^p, A_1)(t_1^p - 0.5) + 0.5, \ldots,\\
& && \qquad \max(t_M^p, A_{M-1})(t_{M-1}^p - 0.5) + 0.5, t_M^p\}\\
& && \mathbf{t}^p = \{t_1^p, \ldots, t_M^p\} \leftarrow\![\ \mathbf{t}^{p-1} \leftarrow\![\ \ldots \leftarrow\![\ \mathbf{t}^1 \leftarrow\![\ \mathbf{z}_{[0,1]}\\
& && \mathbf{z}_{[0,1]} = \{z_{1,[0,1]}, \ldots, z_{n,[0,1]}\} = \{z_1/z_{1,\max}, \ldots, z_n/z_{n,\max}\}
\end{aligned}
$$

MOEA/D: application illustration

For MOEA/D solving DTLZ1 with $M = 2$ and $n = 512$



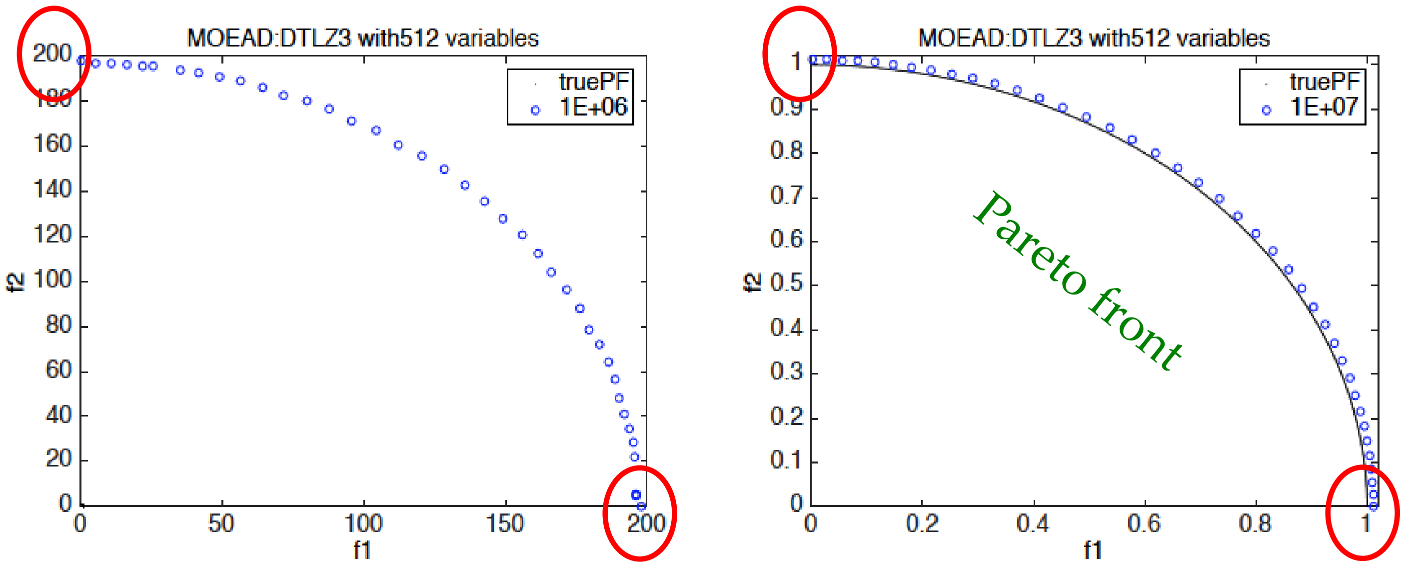
The population
after 10^6 fitness evaluations



The population
after 10^7 fitness evaluations

MOEA/D: application illustration

For MOEA/D solving DTLZ3 with $M = 2$ and $n = 512$

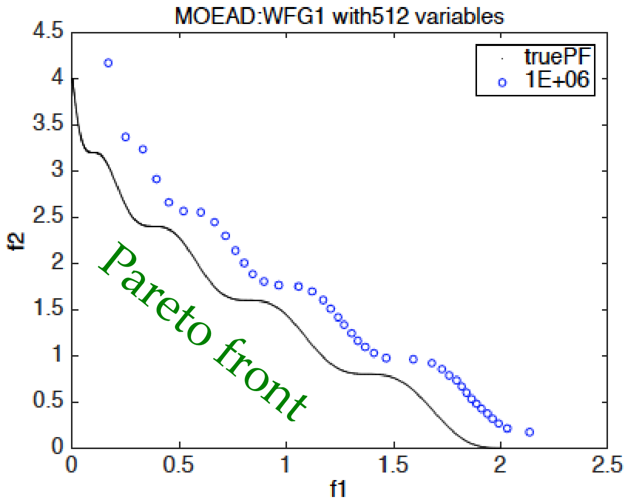


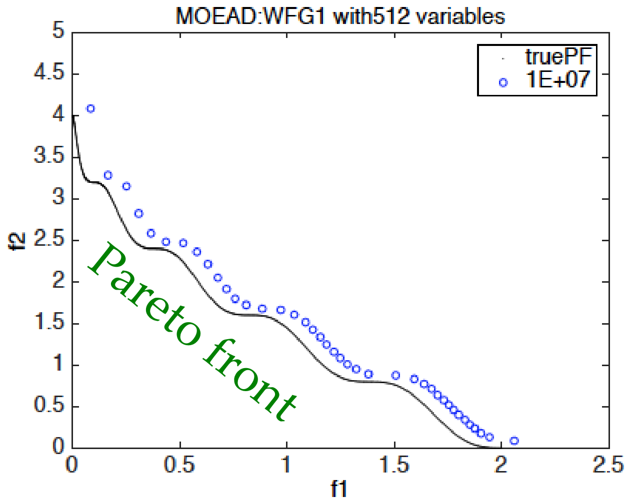
The population after 10^6 fitness evaluations

The population after 10^7 fitness evaluations

MOEA/D: application illustration

For MOEA/D solving WFG1 with $M = 2$ and $n = 512$



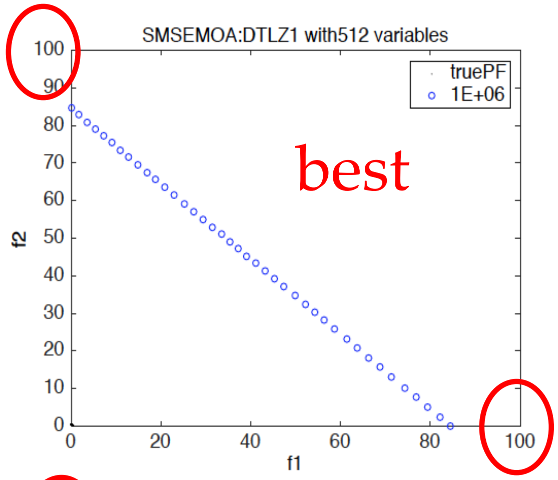


The population after 10^6 fitness evaluations

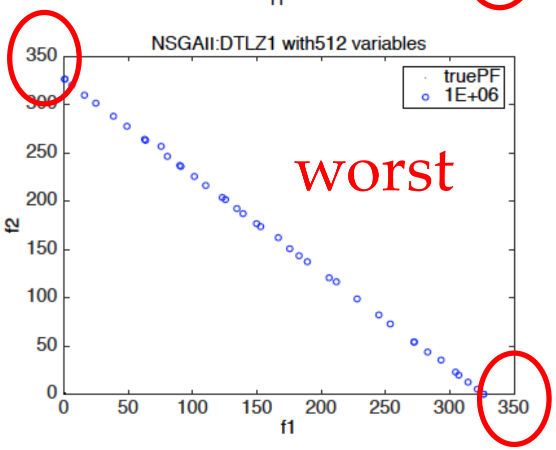
The population after 10^7 fitness evaluations

Comparison on DTLZ1

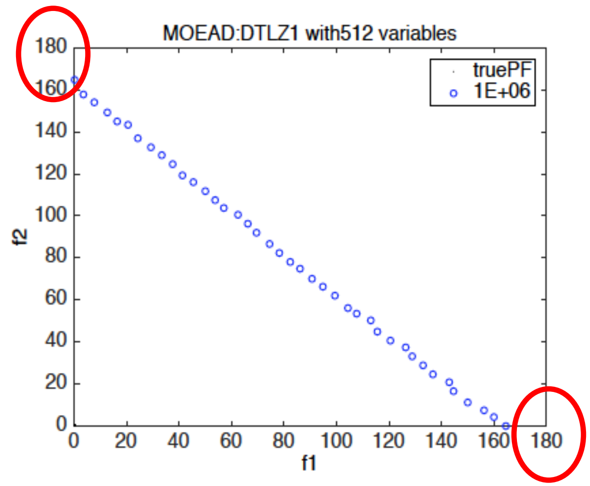
SMS-EMOA



NSGA-II



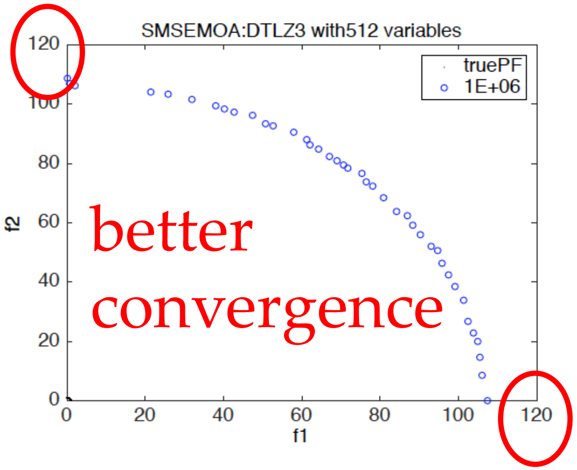
MOEA/D



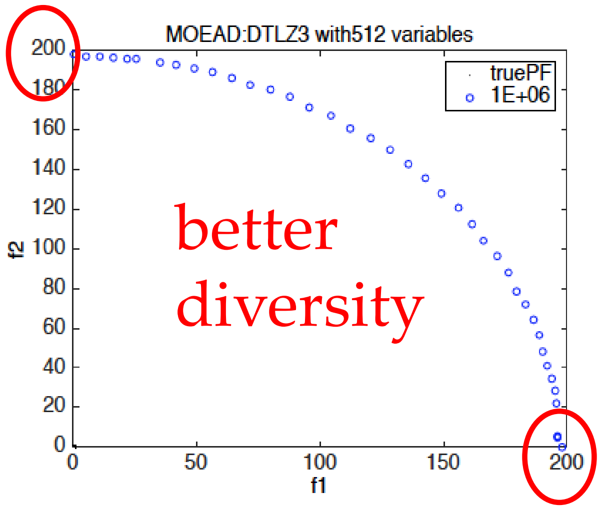
The population after 10^6 fitness evaluations

Comparison on DTLZ3

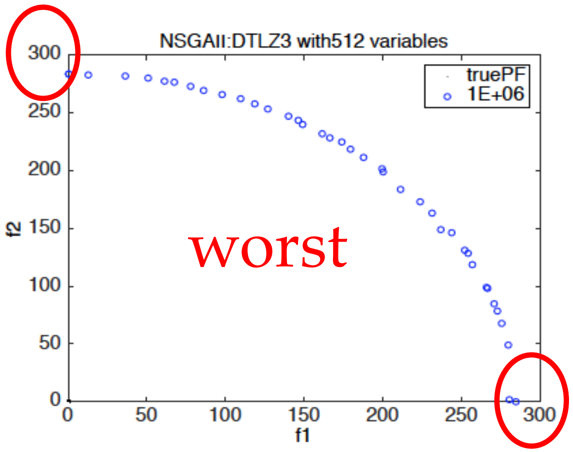
SMS-EMOA



MOEA/D



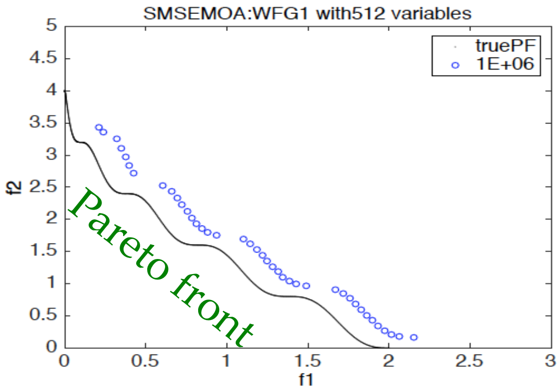
NSGA-II



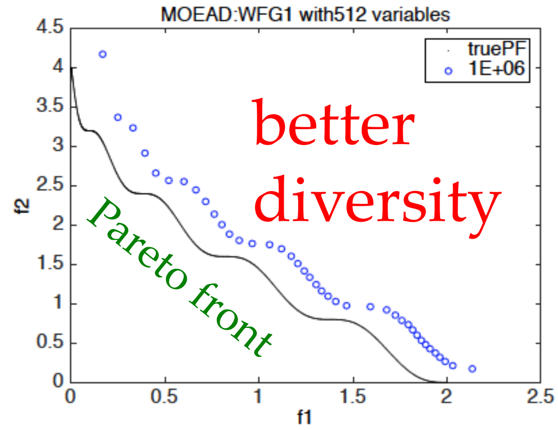
The population after 10^6 fitness evaluations

Comparison on WFG1

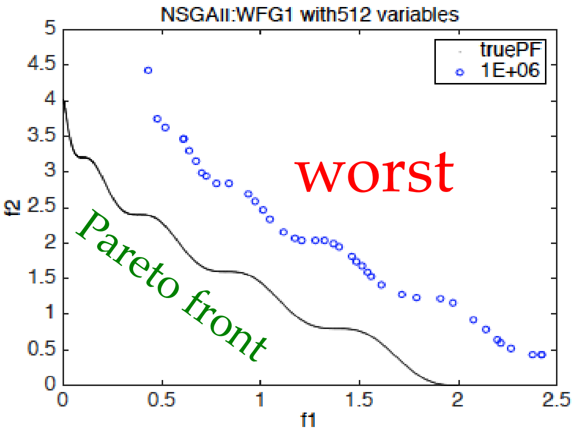
SMS-EMOA



MOEA/D



NSGA-II



The population after 10^6 fitness evaluations

Summary

- Multi-objective optimization
- NSGA-II
- SMS-EMOA
- MOEA/D

} Popular variants of MOEA

References

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