Search-Based Software Engineering

Multi-Objective Optimization



Intelligent Software Systems

Bauhaus-Universität Weimar



Black Box Optimization Competition

BBComp

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* Please write an email to blackboxcompetition@gmail.com to register an account. Check the section How to Participate.

https://bbcomp.ini.rub.de/

For the Impatient

What is BBComp?

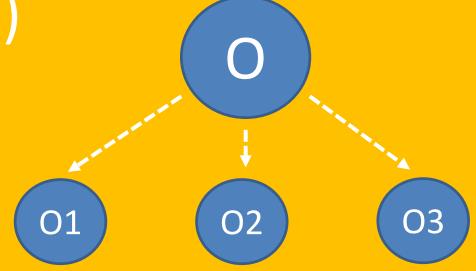
BBComp — the black box optimization competition — is the first competition in continuous black-box optimization where test problems are truly black boxes for participants. It is also the first web/online optimization competition in the direct search domain.

Quick links: [Downloads] [Rules] [FAQ] [Documentation] [Results]

Recap

- Exploit more to improve genetic and evolution algorithms
 - Ellitism
 - Hybrid approaches (ES+HC)
 - Memetic algorithms
- Differential Evolution:
 - Survival selection (do selection of the bred children)
 - Adaptive mutation based on variance in the population
- Particle swarm optimization:
 - Particles store position, velocity, and best positions
 - Particles move based on the velocity and neighbors' best solutions

Multi-Objective Optimization (MOO)



Introduction to MOO

- A practical problem: Optimize not for a single, but for multiple objectives
 - "I want a cheap, luxurious, fuel-efficient, fast, good-looking family car."
 - "I want a software system that is fast, reliable, energyefficient, secure, easy-to-use, bug free, and with low resource consumption."
 - "I want a set of test cases that cover all paths in my software, are fast to execute, reveal all bugs very quickly, and are easy to understand and maintain."



Find the best trade-off among multiple, possibly opposing objectives

MOO Formalization

Minimize
$$O(\vec{x}) = [O_1(\vec{x}), O_2(\vec{x}), ..., O_k(\vec{x})]$$

Subject to $G(\vec{x}) = [g_1(\vec{x}), g_2(\vec{x}), ..., g_m(\vec{x})] \geq 0$
 $H(\vec{x}) = [h_1(\vec{x}), h_2(\vec{x}), ..., h_r(\vec{x})] = 0$
 $x_i^L \leq x_i \leq x_i^U, i = 1, ..., n$

Where

 $\vec{x} = \langle x_1, x_2, ..., x_n \rangle^T$ is a vector of decision variables; k is the number of objectives O_i ; m inequality and r equality constraints x_i^L and x_i^U are respectively the lower and upper bound for each decision variable x_i

Defining the Objective

 Objective might be a vector F of k system responses or characteristics, we are trying to maximize or minimize

$$O = \begin{bmatrix} O_1 \\ O_2 \\ O_3 \\ O_i \\ \dots \\ O_k \end{bmatrix} = \begin{bmatrix} cost \ in \in \\ -range \ in \ km \\ weight \ in \ kg \\ -response \ time \ in \ s \\ \dots \\ -ROI \ in \ \% \end{bmatrix}$$
How to compute O ?

Simple solution: Weighted sum

Naïve: Weighted Sum

Idea: Define a linear function to combine all objectives

$$-0 = \omega_1 * O_1 + \omega_2 * O_2 + ... + \omega_k * O_k$$

- Example: F = 2 * performance + 5 * security + 0.5 * reliability + 1.3 * energy consumption

Problems:

- How to define the weights or how to express how much an objective is more worth than another one?
- What if the objectives are non-linear (i.e., the performance difference between 2-3s is of lower interest than the performance difference between 8-9s)?
- How to encode different value ranges of the objectives?
- Can we move toward the actual trade-off area of interest?

Naïve: Preference Ranking

- Idea: Rank the objectives according to their importance
 - Individual x is better than y if it is superior in a higher ranked objective; if similar, go to the next objective and repeat
 - When comparing two individuals, go through the objectives from most to least important until we find one is clearly superior to the other one

```
Best ← individual picked at random from population with replacement O \leftarrow \{O_1, O_2, ..., O_k\} objectives t \leftarrow tournament size, t \geq 1 for i from 1 to t do

Next ← individual picked at random from population with replacement for j from 1 to k do

if ObjectiveValue(O_j, Next) > ObjectiveValue(O_j, Best) then Best ← Next; break

else if ObjectiveValue(O_j, Next) < ObjectiveValue(O_j, Best) then break

return Best
```

Adaptations to Preference Ranking

- (1) Pick objective at random each time to use for fitness
- (2) Use voting: An individual is preferred if it is better in *more* objectives than another one

```
Best \leftarrow individual picked at random from population with replacement
O \leftarrow \{O_1, O_2, \dots, O_k\} objectives
t \leftarrow \text{tournament size}, t \geq 1
for i from 1 to t do
  Next \leftarrow individual picked at random from population with replacement
  c \leftarrow 0
  for each objective O_i \in O do
    if ObjectiveValue(O_i, Next) > ObjectiveValue(O_i, Best) then
       c \leftarrow c + 1
    else if ObjectiveValue(O_i, Next) < ObjectiveValue(O_i, Best) then
       c \leftarrow c - 1
  if c > 0 then
    Best \leftarrow Next
return Best
```

Adaptations to Preference Ranking

- (3) Entrance-Based Tournament Selection
 - Tournament based on one objective
 - The individuals applicable for a tournament selection are selected using tournament selection of a second objective, and recursively further till all objectives have been covered

Entrance-Based Tournament Selection

```
Different weights are possible
0 \leftarrow \{0_1, 0_2, ..., 0_k\} objectives
T \leftarrow \{T_1, T_2, ..., T_k\} tournament sizes for the individual objectives in O, all \geq 1
return ObjectiveTournament(O,T)
                                              Recursive function with changing sets of objectives
                                              and tournament sizes
procedure ObjectiveTournament(O,T)
  Best \leftarrow individual picked at random from population with replacement
                                    Recursion abort
  n \leftarrow ||0||
  if O - \{O_n\} is empty then
    Best \leftarrow individual picked at random from population with replacement
                                                                 Recursion step
  else
    se 
Best \leftarrow ObjectiveTournament(O - \{O_n\}, T - \{T_n\})
  for i from 1 to T_n do
                                     This is the remaining object, so pick any individual for Next
    if O - \{O_n\} is empty then
      Next \leftarrow individual picked at random from population with replacement
                                      Get next individual by recursion as we got Best individual
    else
      Next \leftarrow ObjectiveTournament(O - \{O_n\}, T - \{T_n\})
    if ObjectiveValue(O_n, Next) > ObjectiveValue(O_n, Best) then
      Best \leftarrow Next
return Best
```

Open Problems

- Opposing objectives cancel each other out
 - We get solutions that are neither good in any objective
- We do not know what are the best options available
 - Trade-off must be represented by the set of final solutions/individuals
 - I want to be able to chose among them
- Still, I want only the best individuals that are superior to all other solutions in a certain objective
 - Called dominance relation
 - Set of individuals are the Pareto front of the solution space

Vilfredo Pareto



- Italian engineer, sociologist, economist, philosopher, and political scientist (1848-1923)
- First to analyze economic problems with mathematical tools
- Famous for two things:
 - 80/20 rule: For many events, roughly 80% of the effects come from 20% of the causes
 - True for many domains (engineering, economics, sales, politics, etc.)
 - Microsoft reported that by fixing the top 20% of most-reported bugs, 80% of the related errors and crashed would be eliminated
 - 80% of traffic in load testing occurs in 20% of the time
 - 20% of the code has 80% of the errors
 - 80% of use cases are easy to implement and 20% are way harder
 - Pareto front (see next)

Pareto Front / Optimum

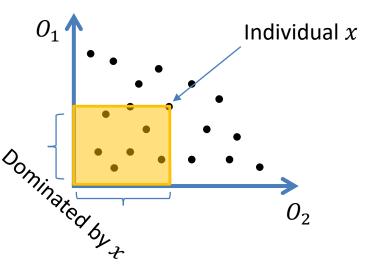
Pareto Optimum

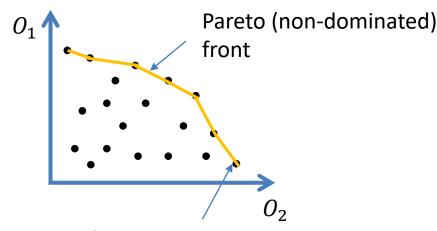
- "The optimum allocation of the resources of a society is not attained so long as it is possible to make at least one individual better off in his own estimation while keeping others as well off as before in their own estimation."
- Reference: Pareto, V., Manuale di Economia Politica, Societa Editrice Libraria, Milano, Italy, 1906.
- What does this mean?

Pareto Dominance

- Two candidate solutions x and y
- x is Pareto dominant to y if x is at least as good as y in all
 objectives and superior to y in at least one objective
 - Why select y in any case, when x is always as good as y or sometimes even better?

Objective space





Individuals/solutions that are non-dominated

Dominance Relation Properties I

Reflexive

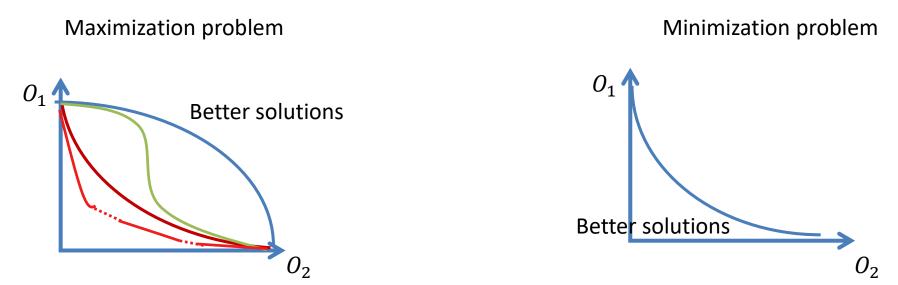
- Is **not reflexive**, because any solution x does not dominate itself by definition of dominance
- Symmetric
 - Is **not symmetric** because $x \le y$ does not imply $y \le x$. The opposite is true: if $x \le y$, then $y \not \le x$
- Antisymmetric
 - Since dominance relation is not symmetric and not reflexive, it cannot be antisymmetric as well
- Transitive
 - Is **transitive**, because $x \le y$ and $y \le z$, then $x \le z$

Dominance Relation Properties II

- Consider: x does not dominate y, does it mean that y dominates x?
 - No! Both can be non-dominating!
- Dominance relation qualifies as an ordering relation due to its transitivity property

Shapes of Fronts

- Convex: curved outwards towards better solutions
- Concave: curved inwards away from better solutions
- Nonconvex: contains subparts of both kinds
- Discontinuous: regions that are impossible to achieve



Open Questions

- Which solutions on the Pareto front to compute?
 - Better have diversity / spread to not have a small group of very similar solutions, but more of the whole front
- What about many objectives (>4)?
 - Open problem in research (not covered here)
 - Idea: Use hypervolume spanned by the multi-dimensional
 Pareto front as a metric for diversity
 - E.g. see: HypE: An Algorithm for Fast Hypervolume-Based
 Many-Objective Optimization, J. Bader and E. Zitzler. In
 Evolutionary Computation. 2011, Vol. 19, No. 1, Pages: 45-76

Dominance Practice

Which individuals are non-dominated?

- Idea: Pairwise comparison
 - If one individual is always equal and at least one time better, it dominates the other one

Pareto Domination Algorithm

 Idea: Implement tournament selection operator based on Pareto domination

```
A \leftarrow \text{individual } A
B \leftarrow \text{individual } B
O \leftarrow \{O_1, O_2, ..., O_k\} objectives
a \leftarrow false
for each objective O_i \in O do
   if ObjectiveValue(O_i, A) > ObjectiveValue(O_i, B) then
   a \leftarrow true
   else if ObjectiveValue(O_i, A) < ObjectiveValue(O_i, B) then
   return false
return a
```

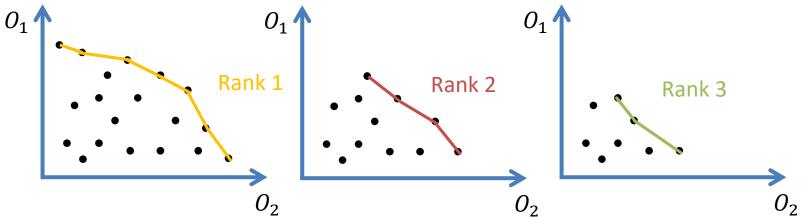
Pareto Domination Binary Tournament Selection

```
P \leftarrow \text{population}
P_A \leftarrow \text{individual picked at random from } P \text{ with replacement}
P_B \leftarrow \text{individual picked at random from } P \text{ with replacement}
if P_A \text{ Pareto Dominates } P_B \text{ then}
return P_A
else if P_B \text{ Pareto Dominates } P_A \text{ then}
return P_B
else
return either P_A \text{ or } P_B \text{ chosen at random}
```

- Improvement: if two individuals do not Pareto dominate each other, we might be interested in the individual that is least dominated by other individuals in the population
- Idea: Use a metric specifying the closeness of a solution to the Pareto front

Pareto Front Rank

- Rank defines distance to the Pareto front
 - Individuals in the front have rank 1
- Idea: Remove all rank 1 individuals from the set
 - Now, new individuals form a new Pareto front (rank 2 front)
 - Recursively, remove elements from the population of the current front and build the next front, such that all individuals belong to a certain rank



Computing the Pareto Front

```
G \leftarrow \{G_1, G_2, \dots, G_m\} Group of individuals for computing the front
0 \leftarrow \{0_1, 0_2, \dots, 0_k\} objectives
F \leftarrow \{\}
                                   —— Pareto front
for each individual G_i \in G do
  F \leftarrow F \cup \{G_i\}
                               \leftarrow Assume G_i is in the Pareto front
  for each individual F_i \in F do
    if F_i Pareto Dominates G_i given O then
                                                                    Check wether G_i can stay in the
       F \leftarrow F - \{G_i\}
                                                                   front or G_i dominates another
       break
     else if G_i Pareto Dominates F_i given O then
                                                                    individual in the front that has to
       F \leftarrow F - \{F_i\}
                                                                    be removed
return F
```

From Pareto Front To Ranks

- Compute the Pareto front as shown before
- Remove the individuals of the front
- Compute the Pareto front again for the reduced subset
- Repeat until there are no individuals in the population
- Why is this useful?
 - Lower ranked individuals are better (closer to the Pareto front)

$$-Fitness(i) = \frac{1}{1 + ParetoFrontRank(i)}$$

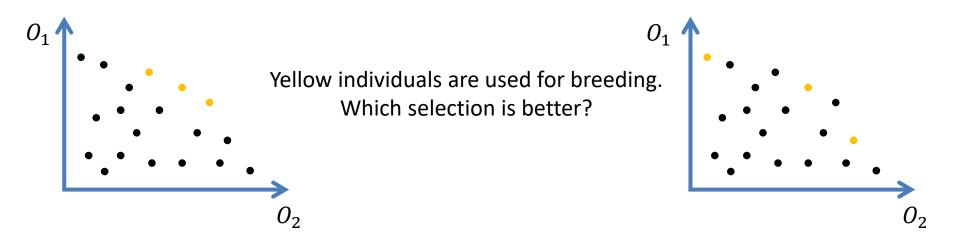
Store each group of individuals separately and store rank in each individual
 Non-Dominated Sorting

Away from Naïve: Non-Dominated Sorting

Invented by N. Srinvas and K. Deb in 1994

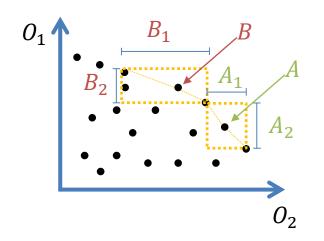
```
P \leftarrow \text{population}
0 \leftarrow \{0_1, 0_2, \dots, 0_k\} objectives
P' \leftarrow P Initially, all elements are considered to compute the current front
R \leftarrow \langle \rangle Empty vector of Pareto front ranks
i \leftarrow 1 Start with the first front
repeat
                                                                     Compute all individuals of the
  R_i \leftarrow \text{Pareto Non-Dominated Front of } P' \text{ using } O \longleftarrow
                                                                     current front that are still in P'
  for each individual r \in R_i do
    ParetoFrontRank(r) \leftarrow i Go through these individuals, store their rank, and
    P' \leftarrow P' - \{r\}
                                   remove them from the population
  i \leftarrow i + 1
until P' is empty
return R
```

Spread out the Population: Sparsity



- To better show the tradeoff and allow exploration, we want to have individuals with a certain distance to each other
- Idea: Use sparsity of a region as a measure of spread

Sparsity using Manhattan Distance



- To get the surrounding region of an individual:
 - Get the direct neighbors of the same Pareto front rank
 - Span the region
- Compute the Manhattan distance over every objective between an individual's left and right neighbors
 - Far end individuals get an infinite sparsity to be always selected
 - Example: $A_1 + A_2 < B_1 + B_2$ so that B is in a sparser region
- Requires the value range of every objective function

Multi-Objective Sparsity Assignment

```
F \leftarrow \langle F_1, F_2, \dots, F_m \rangle Pareto front rank of individuals
0 \leftarrow \{0_1, 0_2, \dots, 0_k\} objectives
Range(O_i) function providing the range (max - min) of possible values for given objective O_i
for each individual F_i \in F do
                            First, set sparsity to zero for all individuals
  Sparsity(F_i) \leftarrow 0
for each objective O_i \in O do
                                                                                    Sort individuals based on
  F' \leftarrow F sorted by objective value given objective O_i
                                                                                   current objective
   Sparsity(F'_1) \leftarrow \infty
  Sparsity(F'_1) \leftarrow \infty

Sparsity(F'_{||F||}) \leftarrow \infty Assign infinity to the ends
                                                                                                   Region of neighbors
  for j from 2 to ||F'|| - 1 do Sparsity based on previous objectives
Sparsity(F'_{j}) \leftarrow Sparsity(F'_{j}) + \frac{ObjectiveValue(O_{i}, F'_{j+1}) - ObjectiveValue(O_{i}, F'_{j-1})}{Prove (O_{i})}
                                                                              Range(O_i)
return F with assigned Sparsities by F'
                                                                                                Normalization
```

- How to compute sparsity for the whole population?
 - Break population into ranks and compute for each rank the sparsity

Tournament Selection with Sparsity and Non-Dominated Sorting

 Selected individuals are both close to the Pareto front and spread throughout the front

Non-Dominated Sorting Genetic Algorithm II (NSGA-II)

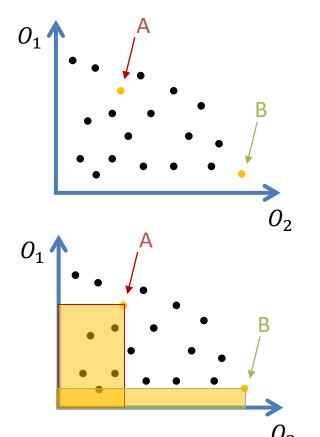
- Developed by K. Deb, A. Pratap, S. Agarwal, and T.
 Meyarivan in 2000: A fast elitist non-dominated sorting genetic algorithm for multi-objective optimization: NSGA-II
 - State of the art technique
- Idea: Keep all the best known individuals so far (similar to $(\mu+\lambda)$ or elitist)
 - -A is a store of the best n individuals discovered so far
 - Breed a new population P from A and let the individuals of both sets compete to stay in A
 - Highly exploitative?
 - Not really, since we use Sparsity to spread out in the optimization space

NSGA-II Algorithm

```
m \leftarrow desired population size
a \leftarrow desired archive size, usually a = m
P \leftarrow \{P_1, P_2, ..., P_m\} population with Pareto front ranks assigned to the individuals
A \leftarrow \{ \} archive
repeat
  AssessFitness(P) Calculate objective values to obtain Pareto front ranks
  P \leftarrow P \cup A
  BestFront \leftarrow Pareto front of P
  A \leftarrow \{ \}
  R \leftarrow \text{Compute front ranks of } P
  for each front rank R_i \in R do \blacksquare Go through the front ranks and fill the archive
    Compute sparsities of individuals in R_i
    if ||A|| + ||R_i|| \ge a then \leftarrow Last front rank, whose members can come into A
      A \leftarrow A \cup the sparsest a - |A| individuals in R_i, breaking ties arbitarily
      break Insert only as many as the archive can fill and break the for-loop
    else
      A \leftarrow A \cup R_i
  P \leftarrow Breed(A), using tournament selection with sparsity and non-dominated sorting
until BestFront is optimal or out of time
return BestFront
```

Pareto Strength

Alternative fact measure to compute the fitness and do parent selection



If you would have to chose between A and B, so far, we would select B, because it has a front rank 1 vs. A with a front rank 2. But is this a good choice?

What if we look at the number of individuals that an individual dominates?

A dominates 5 individuals
B dominates only 1 individual
-> so why don't pick A?

It does not necessarily correspond to closeness to the Pareto front and corner individuals are weak.

Wimpiness

- Use weakness instead:
 - Number of individuals that dominate the current individual
 - Pareto front individuals have weakness of 0
 - Individuals far away from the front have a high weakness
- Improve weakness using the strength of the individuals that dominate the current individual: Wimpiness
- Wimpiness(i) = $\sum_{g \in G \text{ that } Pareto \text{ Dominate } i} Strength(g)$

•
$$Fitness(i) = \frac{1}{1 + Wimpiness(i)}$$



Non-dominated individuals have a fitness of 1

Strength Pareto Evolutionary Algorithm2 (SPEA2)

- Developed by E. Zitzler, M. Laumanns, and L. Thiele in 2002: SPEA2: Improving the strength pareto evolutionary algorithm for multiobjective optimization
 - Similar to NSGA-II, SPEA2 maintains a store of the best known
 Pareto front individuals + other members found so far
 - Uses Pareto measure (using Wimpiness) and crowding measure (using distance to other individuals in the multi-objective space and no ranks) for its fitness assessment
- Similarity measure computes a distance to other individuals in the population (i.e., to the kth closest individual)
 - Simple solution: Compute distance from everyone to everyone and for each individual sort them to its own distance and take the kth closest individual ($O(n^2 lgn)$), for n individuals

Distance Computation

```
P \leftarrow \langle P_1, P_2, ..., P_m \rangle population
O \leftarrow \{O_1, O_2, \dots, O_n\} objectives
P_l \leftarrow \text{individual to compute } k \text{th klosest individuals}
k \leftarrow desired individual index (the kth individual from l)
global D \leftarrow m \ vectors, each of size m \leftarrow D_i holds a vector of distances of various
perform only once
                                     D_i has already
  for each individual P_i \in P do
                                     been sorted
    V \leftarrow \{ \}
    for each individual P_i \in P do
                                                                                             Computes the
      V \leftarrow V \cup \{\sqrt{\sum_{m=1}^{n} \left(ObjectiveValue(O_m, P_i) - ObjectiveValue(O_m, P_j)\right)^2}\}
                                                                                             distances among
                                                                                             all individuals
    D_i \leftarrow V
    S_i \leftarrow false
                             Sum the distances over all objectives
perform each time
  if S_l is false then
    Sort D_l, smallest first
    S_1 \leftarrow true
  W \leftarrow D_I
                          Since W_0 is the distance to ourself (i.e., 0), we return the
return W_{k+1}
                          distance of the k+1 closest neighbor
```

SPEA2: Putting Everything Together

- $G_i \leftarrow Wimpiness(i) + \frac{1}{2+d_i}$ where d_i is the distance of i to the kthe closest neighbor
 - Typically, set $k = \lceil \sqrt{||P||} \rceil$
 - A smaller G_i , is better, because a large distance makes G_i smaller and so we get more diversity and spread and smaller Wimpiness is better, too
- Each iteration of SPEA2 builds an archive/store of size n with the current Pareto front of the population
 - If not enough individuals for n, fill with other fit individuals
 - If too many individuals for n, remove the ones with the smallest distance kth closest distance (starting with k=1, continuing with k=2, etc.)

SPEA2: Archive Construction Algorithm

```
P \leftarrow \langle P_1, P_2, \dots, P_m \rangle population
0 \leftarrow \{0_1, 0_2, \dots, 0_n\} objectives
a \leftarrow desired archive size
A \leftarrow Pareto non-dominated front of P \leftarrow Initialize the archive with Pareto front individuals
Q \leftarrow P - A \leftarrow \Box Get the remaining individuals
if |A| < a then \longrightarrow If not enough individuals in the archive, add fittest
  Sort Q by fitnes individuals to the archive
  A \leftarrow A \cup \text{the } a - |A| fittest individuals in Q, breaking ties arbitarily
while |A| > a do \leftarrow If too many individuals in the archive, remove the k-closest ones
  Closest \leftarrow A_1
  c \leftarrow \text{index of } A_1 \text{ in } P
  for each individual A_i \in A except A_1 do
     l \leftarrow \text{index of } A_i \text{ in } P
    for k from 1 to m-1 do
       if DistanceOfKthNearest(k, P_l) < DistanceOfKthNearest(k, P_c) then
         Closest \leftarrow A_i
         c \leftarrow l; break
       else if DistanceOfKthNearest(k, P_l) > DistanceOfKthNearest(k, P_c) then
         break
  A \leftarrow A - \{Closest\}
return A
```

SPEA2: Algorithm

NSGA_II and SPEA2 are both version of $(\mu+\lambda)$ in multi-objective space, combined with a diversity mechanism and a technique for selecting individuals that are closer to the Pareto front

Take Home Message:

- Multiple objectives are more common in practice
- Not a single solution is the optimum, but a set of solutions
- Pareto front represents the individuals that are nondominated by others
 - Dominance relation: an element dominates another if it is better in at least one objective and not worse in all others
- Ranks of dominance/Pareto fronts can be recursively computed for all elements in the population and represent as a way to assess the fitness
- Another factor for fitness is the diversity of the individuals in the front, so we add a measure based on sparsity to favor individuals that are farther away from other

Take Home Message:

- Combining sparsity and Pareto front ranks plus a storage of the best found individuals so far is realized by NSGA-II
- An alternative approach is SPEA2
 - With a more complex diversity measure, using the distance to the kth nearest individual
 - With a different Pareto front distance measure, using the weakness of individuals (i.e., number of individuals that dominate it)

Next Lecture

- Combinatorial Optimization
 - Greedy randomized adaptive search
 - Ant colony optimization
 - Guided local search