

# Multi Objective Optimization

Rui Mendes

# Rationale behind Multi-Objective Optimization

- Real world problems may have several objectives
- These are often contradictory:
  - ▶ Accuracy in a machine learning task versus the complexity of the model
  - ▶ Time needed to perform a given task versus its cost
  - ▶ Performance versus fuel consumption and emission of pollutants
- In non-trivial problems, it is not possible to satisfy all objectives at the same time

# Multi-Objective Optimization

$$\begin{array}{ll} \text{Minimize/Maximize} & f_m(x) \quad m \in \{1, \dots, M\} \\ \text{Subject to} & g_j(x) \geq 0 \quad j \in \{1, \dots, J\} \\ & h_k(x) = 0 \quad k \in \{1, \dots, K\} \\ & x_i^L \leq x_i \leq x_i^U \quad i \in \{1, \dots, N\} \end{array}$$

# Approaches for MOPs

- Penalty weights
- Objective sorting
- Pareto approaches

## Penalty weight approaches

- Fitness function combines all objectives
- Objectives are multiplied by weights
- Decision maker (DM) must estimate the correct weights for each objective
- If DM wants several trade-offs, she must run the optimization algorithm several times with different weights
- Best way of assigning weights for each objective is not trivial

## Objective sorting

- Objectives must be ranked in order of importance
- Solutions are sorted according to the objectives
- The lexicographic order is used
- It is also difficult to find several trade-offs

## Pareto approach

- Provides many solutions at the same time
- Solutions can have high quality in one of the objectives while having lower quality in others
- Allows the DM to select any trade-off solution
- Population holds solutions according to Pareto dominance

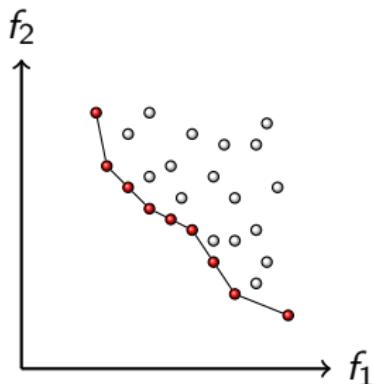
# Pareto Dominance

Assuming minimization of all objectives

strictly dominates	$x \prec\prec y$	$\iff f_m(x) < f_m(y) \forall m$
dominates	$x \prec y$	$\iff f_m(x) \leq f_m(y) \forall m \wedge \exists i : f_i(x) < f_i(y)$
weakly dominates	$x \preceq y$	$\iff f_m(x) \leq f_m(y) \forall m$
incomparable	$x \parallel y$	$\iff \neg(x \preceq y) \wedge \neg(y \preceq x)$
indifferent	$x \sim y$	$\iff f_m(x) = f_m(y) \forall m$

# Pareto Store and Pareto Front

- A Pareto store holds non-dominated solutions
- Figure shows a Pareto set in a two objective minimization problem
- The red points belong to the Pareto front



# Pareto Front and Archive

Pareto Set Set of non-dominated solutions in **decision space**

Pareto Front Set of non-dominated solutions in **objective space**

Pareto Archive Stores all non-domination solutions found so far

# Managing a Pareto Archive

## Adding to the archive

- Add new solutions to the archive if
- They are not dominated by any solution in it

## Cleaning archive

- When adding a new solution
- Remove all solutions dominated by it

## Pruning

- If the archive exceeds its max size
- Remove solutions from the most **crowded** regions

# Characteristics of Good algorithms

**Closeness** Solutions should be as **close** as possible to the true Pareto front. This gives a high quality information to the decision maker.

**Even distribution** Solutions should be equidistant. This gives the decision maker a wider range of trade-offs from which perform the final choice.

**High spread** Distance between extremes in objective space should be as high as possible. This ensures a good coverage of the Pareto Front.

## Ways of achieving these characteristics

- Elitism** Ensure that solutions closest to the true Pareto front are never eliminated  
The number of non-dominated solutions should increase in the population
- Crowding** Measure that penalizes solutions that are close to each other

## Evaluation

- Based on dominance
- Uses a *Pareto-rank*: number of individuals in the population that are dominated by this individuals
- Ordering often uses a secondary fitness to have a total order
- Evaluation is performed in *objective space*

# Non-dominated Sorting Genetic Algorithm (NSGA-II)

**Fast Non-Dominated Sorting** An efficient ( $O(MN^2)$ ) method for ranking the population based on dominance.

**Crowding Distance** A mechanism to maintain diversity along the Pareto Front without extra parameters.

**Elitism** Guarantees that the best solutions found are never lost.

## Fast sorting

- Find all non-dominated solutions (Rank 1)
- Temporarily remove them from the population
- All currently non-dominated solutions are assigned to the next rank (Rank 2)
- The procedure is iterated

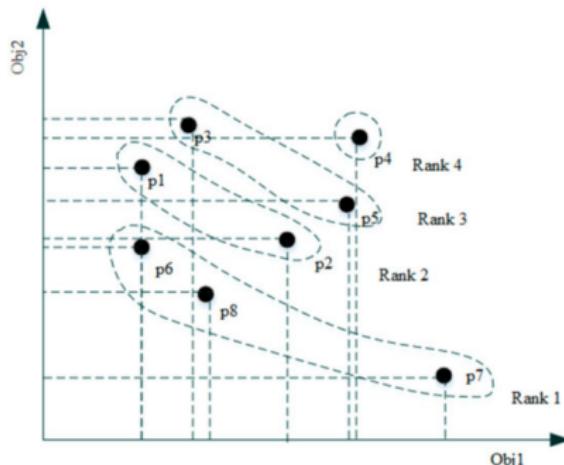


Figure 1: Image taken from SETNDS: A SET-Based Non-Dominated Sorting Algorithm for Multi-Objective Optimization Problems

## Crowding distance

- Used for solutions on the *same* front
- Perimeter of the *cuboid* formed by its nearest neighbors on either side
- Sum the distance from current solution to the nearest neighbors (e.g.,  $|f_1(i + 1) - f_1(i - 1)|$ ) on each objective
- Prefer solutions with the largest crowding distance

## NSGA-II

- Pareto store holds several layered fronts
- First layer  $F_1$  only holds non-dominated individuals
- Individuals belonging to front  $F_{i+1}$ :
  - ▶ can only be dominated by individuals in front  $F_i$  or lower
  - ▶ are non-dominated by all individuals not belonging to  $\bigcup_{k \leq i} F_k$
- Fitness rank of individuals in front  $F_i$  is  $i$
- *Crowding distance*, how close a solution is to its neighbors, in objective space, is calculated for each individual
- Individuals are ordered first by the *fitness rank* and then by the *crowding distance*
- Parents are selected by binary tournament selection based on their *rank* and *crowding distance*
- They create offspring using crossover and mutation
- Uses a  $(\mu + \lambda)$ -ES selection scheme

## Strength Pareto Evolutionary Algorithm 2 (SPEA2)

**Fixed-Size External Archive** Keeps all non-dominated solutions found so far, up to a limit.

**Strength Fitness** Fitness calculation is based on how many solutions a candidate dominates and how many dominate it.

**Density Estimation** Uses the  $k$ -th nearest neighbor distance to ensure diversity during archive maintenance.

# Strength Fitness

SPEA2 assigns fitness based on two properties derived from dominance:

## ① Strength Value $S(i)$

The **Strength** of a solution  $i$  is the number of solutions it **dominates** in the combined population (main population + archive). Solutions with higher strength are generally better candidates.

## ② Raw Fitness $R(i)$

The **Raw Fitness** is the sum of the strength values of all solutions that **dominate**  $i$ . If a solution  $i$  is non-dominated,  $R(i)$  will be 0. The goal is to **minimize** Raw Fitness.

# Density Estimation

- Unlike NSGA-II's Crowding Distance, SPEA2 uses a refined density metric based on distance.
  - ▶ The  **$k$ -th Nearest Neighbor** method finds the distance to the  $k$ -th closest solution in the objective space.
  - ▶ This distance is then used to calculate the **Density Value**  $D(i)$ .
  - ▶ The **Overall Fitness** is  $F(i) = R(i) + D(i)$ , where  $R(i)$  is the Raw Fitness.
- Solutions in less dense regions will have a smaller Density Value, making their overall fitness better (since  $F(i)$  is minimized).
- This metric is primarily used during the **archive truncation** step to remove clustered solutions.

# Robust Archive Truncation

- Calculate the  **$k$ -th nearest neighbor distance** for all solutions in the archive.
- Identify the two closest solutions (smallest distance).
- Remove the solution that is **least spread out** (i.e., the one with the smallest  $k$ -th nearest neighbor distance).
- Repeat this removal process until the archive returns to its fixed size.

# Multi-Objective Evolutionary Algorithm based on Decomposition (MOEA/D)

- It transforms the complex multi-objective problem into many simpler, single-objective *subproblems*
- It solves them **simultaneously** and **cooperatively**

## Weight Vectors

- The problem is broken down using a set of weight vectors (e.g.,  $\lambda_1, \lambda_2, \dots, \lambda_N$ )
- Each vector represents a different trade-off preference (e.g.  $0.1 \cdot f_1 + 0.9 \cdot f_2, 0.2 \cdot f_1 + 0.8 \cdot f_2, \dots, 0.9 \cdot f_1 + 0.1 \cdot f_2$ )
- These vectors are typically spread uniformly to guide the search for an evenly distributed Pareto Front
- Each vector  $\lambda_i$  is used to create one single-objective subproblem  $g_i$

## Creating subproblems

### Tchebycheff

- The most common method
- Finds the solution with the smallest 'weighted distance' to an ideal reference point
- Handles non-convex fronts well.

### Weighted Sum

- A simple sum of objectives, each multiplied by its weight
- Struggles with non-convex (concave) Pareto fronts.

### PBI

- Penalty-based Boundary Intersection
- Another popular method that measures both convergence and diversity effectively

# Neighborhood

- Each subproblem  $i$  has a *neighborhood*,  $B(i)$
- This is the set of the  $T$  closest subproblems (based on the distance between their weight vectors)
- Subproblems in a neighborhood have similar trade-offs
- Mating and replacement occurs within this neighborhood, allowing solutions to share information locally
- This is more efficient

## Algorithm

- Generate  $N$  weight vectors, create  $N$  subproblems, and initialize a population (one solution per subproblem)
- For each subproblem  $i$ , select parent solutions only from its neighborhood  $B(i)$
- Create a new offspring solution  $y'$  using genetic operators
- Check  $y'$  against all solutions in  $B(i)$ . If  $y'$  is better for any neighbor  $j$ , replace its solution  $x_j$

## Neighborhood Update

- A new solution  $y'$  is generated by parents from subproblem  $i$ 's neighborhood
- This solution  $y'$  is then used to update the solutions of neighboring subproblems ( $j, k$ , etc.)
- This allows good solutions to *move* between subproblems, driving the entire population towards the Pareto Front

# Advantages of MOEA/D

- Efficiency** Lower computational complexity per generation than many Pareto-based methods (like NSGA-II).
- Diversity** The use of evenly spread weight vectors naturally encourages a diverse set of solutions along the Pareto Front.
- Scalability** The framework can be adapted to handle many-objective problems (MaOPs) relatively well.
- Simplicity** The core concept is elegant and can be combined with many different decomposition methods and operators.

# Many-Objective Problems

- Curse of dimensionality
- Pareto Dominance Fails: Almost all solutions become non-dominated.
- Crowding Distance Fails: Density is impossible to calculate in high dimensions.

# NSGA-III

- Crowding distance from NSGA-II becomes ineffective
- It leads to poor selection pressure and loss of diversity
- NSGA-III replaces it with *Reference Points*

## Reference Points

- A set of structured reference points is generated on a normalized hyper-plane (e.g., using the *Das-Dennis* method)
- These points act as *guides* or *attractors* to maintain diversity across the entire objective space
- The algorithm's goal is to find at least one good solution close to each of these reference points

## Normalization

- Before selection, the algorithm normalizes the objective values for all solutions in the splitting front ( $F_1$ ).
- It finds the ideal point (minimums) and extreme points (maximums) to create a normalized hyperplane.
- This ensures distances are measured on a fair, uniform scale.

## Association

- Each normalized solution ( $s$ ) in the splitting front is “associated” with the closest reference point.
- “Closest” is measured by the perpendicular distance from the solution to the vector (line) defined by the reference point.

## Niching and Selection

- Count: The algorithm counts how many solutions are associated with each reference point (the “niche count”).
- Select: To fill the remaining K spots in the new population, the algorithm iteratively selects solutions.
- Priority: It picks from reference points with the lowest niche count (least crowded niches).
- Diversity: This process explicitly maintains diversity by ensuring all reference points (all regions of the front) are represented.

## Advantages of NSGA-III

- Solves MaOPs: Specifically designed for problems with 4 or more objectives.
- Maintains Diversity: Reference points effectively preserve diversity across the entire Pareto front.
- Strong Selection: The niche-ing mechanism maintains selection pressure even when most solutions are non-dominated.
- Flexible: A well-established and powerful tool for complex engineering and design problems.

# Comparing Algorithms

**Convergence** how close is the generated front from the true pareto front?

**Diversity** how well are the solutions spread across the front?

**Combined** metrics that combine both convergence and diversity

## Generational Distance (GD)

- Evaluate the quality of a set of solutions
- Compares how well they converge to the true Pareto front
- Measures the average distance between each solution in the set and its closest solution in the true Pareto front

## Computing the GD

**Calculate the distance** For each point in the obtained solution set, calculate the Euclidean distance to every point in the reference Pareto set.

**Find the minimum** For each point from the obtained set, identify the minimum distance to any point in the reference set.

**Average the minimums** Average these minimum distances across all points in the obtained set. This provides the final GD value.

**Interpretation** A lower GD value means the obtained solution set is closer to the true Pareto front, indicating better performance.

## Variants and related metrics

**Inverted Generational Distance (IGD)** A variant that uses a reference set from the true Pareto front and can be used to evaluate both convergence and diversity.

**Generational Distance Plus ( $GD^+$ )** A variant that modifies the distance calculation to be more robust.

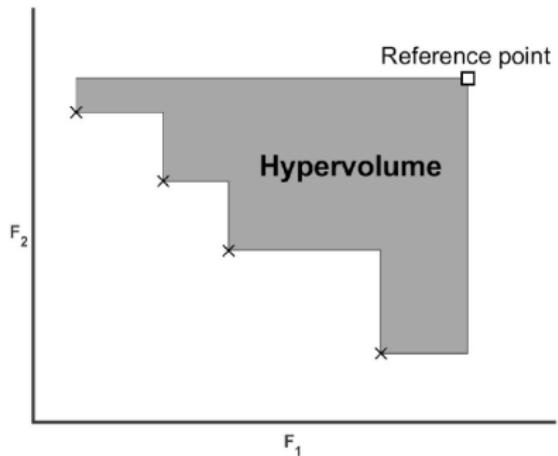
**Spacing** Measures the standard deviation of the distances between consecutive solutions. A low value means solutions are evenly spaced.

**Hypervolume (HV)** A different metric that measures the volume of the dominated space by the obtained solutions relative to a reference point, without needing a true Pareto set.

**Spread** Another common metric that measures the spread or diversity of the obtained solutions along the Pareto front

# Hypervolume (HV)

- Most popular and powerful metric
- Measures the volume of the objective space that is dominated by the found pareto front, relative to a reference point
- Combines both convergence and diversity.
- Does not require the true Pareto front.
- A larger HV is better.



# Comparing Algorithms

- Run each algorithm a large number of times ( $\geq 30$ )
- Use non-parametric tests to compare the chosen metric (e.g., HV)
  - ▶ Wilcoxon Rank-Sum Test or
  - ▶ Mann-Whitney U Test