Multi Objective Optimization

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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

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

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

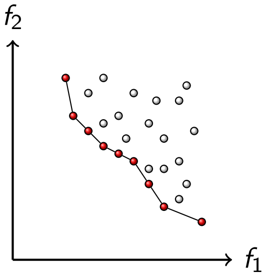
Pareto Dominance

Assuming minimization of all objectives

$$
\begin{array}{rcll}
\text{strictly dominates} & x \prec\prec y & \iff & f_m(x) < f_m(y)\ \forall m \\
\text{dominates} & x \prec y & \iff & f_m(x) \leq f_m(y)\ \forall m \wedge \exists i : f_i(x) < f_i(y) \\
\text{weakly dominates} & x \preceq y & \iff & f_m(x) \leq f_m(y)\ \forall m \\
\text{incomparable} & x \parallel y & \iff & \neg(x \preceq y) \wedge \neg(y \preceq x) \\
\text{indifferent} & x \sim y & \iff & f_m(x) = f_m(y)\ \forall m
\end{array}
$$

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

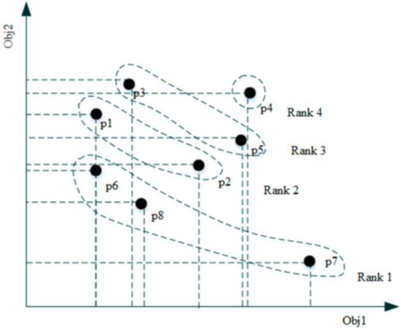


Figure 1: Image taken from SETNDS: A SET-Based Non-Dominated Sorting Algorithm for Multi-Objective Optimization Problems

Crowind 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 $\bigcup\limits_{k \leq i} F_i$
- 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., $\lambda_1, \lambda 2, \ldots, \lambda_N$)
- Each vector represents a different trade-off preference (e.g. $0.1 \cdot f_1 + 0.9 \cdot f_2, 0.2 \cdot f_1 + 0.8 \cdot f_2, \ldots, 0.9 \cdot f_1 + 0.1 \cdot f_2$)
- These vectors are typically spread uniformly to guide the search for an evenly distributed Pareto Front
- Each vector λ_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

- Crowiding 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 (`Fl`).
- 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 ($\mathbf{s}$) 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.