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

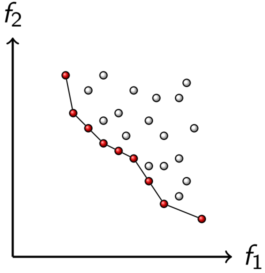
Pareto Dominance

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 individual
- 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

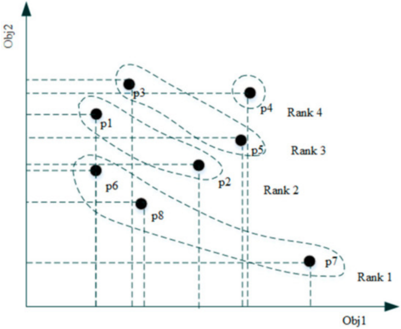


Figure 1: Image taken from SETNDS: A SET-Based Non-Dominated Sorting Algorithm for Multi-Objective Optimization Problems

Crowind distance

- Used for solutions on the *same* rank
- 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

The NSGA-II Algorithm

- 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 $\bigcup_{k \leq i} F_i$
- 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, $\lambda_1, \lambda_2, \ldots, \lambda_N$
- Each vector represents a different trade-off preference (e.g. $\lambda_1 = 0.1 \cdot f_1 + 0.9 \cdot f_2, \lambda_2 = 0.2 \cdot f_1 + 0.8 \cdot f_2, \ldots, \lambda_N = 0.9 \cdot f_1 + 0.1 \cdot f_2$)
- 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.

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.

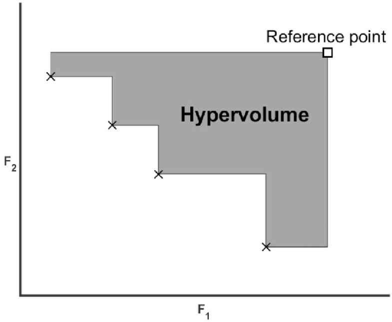
Spacing Measures the standard deviation of the distances between consecutive solutions. A low value means solutions are evenly spaced.

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 (≥ 30)
- Use non-parametric tests to compare the chosen metric (e.g., HV)
  - Wilcoxon Rank-Sum Test or
  - Mann-Whitney U Test