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Optimizing Multi- and Many-Objective Problems on Varied Budgets: Hybridizing NSGA-III with Local Searches

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Abstract. This study addresses the challenges faced by Multi- and Many-Objective Evolutionary Algorithms in converging to the optimal Pareto Front under limited budgets. It proposes integrating these algorithms with deterministic single-objective local search techniques tailored for scalarized multi-objective optimization problems to accelerate convergence. Two integrations of NSGA-III with local search techniques based on SQP and BFGS algorithms are proposed and evaluated through numerical experiments on DTLZ1-4 problems across various budget scenarios. Performance profiles constructed using IGD+ and epsilon-indicator performance indicators demonstrate that the hybrid algorithms outperform NSGA-III. Statistical analysis confirms the superiority of the hybrid approaches, making them more efficient and reliable for the addressed problems.

Keywords. Many-Objective Problems, NSGA-III, Local Search.

1 Introduction

Evolutionary Algorithms (EAs) are widely used for solving both single- and multi-objective problems due to their adaptability and effectiveness across various domains. Inspired by natural selection, EAs iteratively evolve candidate solutions, incorporating genetic mechanisms to converge towards optimal or near-optimal solutions, addressing complex challenges where traditional methods may fall short. In a nutshell, the underlying mechanism of an EA consists of, for each iteration t, (i) creating a population called parents $P(t)$, in the search space of a problem; (ii) creating another population $\tilde{P}(t)$, called offspring, using genetics operators; (iii) combining the two sets of points into a single set, $R(t)$; (iv) and choosing, among its members, the best suited to compose the next population $P(t+1)$. The process is repeated until a convergence criteria is met.

In the construction of $\tilde{P}(t)$, points are influenced either by the parent distribution, as seen in algorithms like Genetic Algorithm and Differential Evolution, or by an independent distribution, as seen in basic Evolution Strategies. In single-objective optimization, as the population converges towards the optimal region, newly generated offspring tend to be located nearby, facilitating local

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exploration and refinement of solutions. However, in multi-objective optimization, where there is no singular optimum and multiple optimal solutions exist, algorithms must avoid concentrating the population in specific regions of the search space to ensure approximation of the optimal point set, which may lead to less effective local exploration and slower improvement over iterations.

Integrating local search mechanisms within the evolutionary cycle of Multi-Objective Evolutionary Algorithms (MOEAs) is one viable approach to promoting finer convergence toward the true Pareto front. Works incorporating local search techniques in MOEAs can be found in the literature, and this approach has been proven effective, as evidenced in several recent studies. For instance, [9] proposed a Pareto front model-based local search method to accelerate the exploration and exploitation of the Pareto front. The technique uses sparse points to guide the local search to promising sparse areas. Experimental results demonstrated the algorithm's efficiency and superiority. In another example, [1] proposes an iterative updating approach based on the Broyden method using improvement directions provided by Chebyshev scalarizing functions. The technique demonstrates better conditioning, especially near the Pareto set. Another notable contribution is presented in [14], which proposes an effective method of computing multi-objective descent directions seeking a compromise between feasibility and the decrement in the objective function values. The benefits of the novel approach are supported by numerical results.

In this paper, the well-known NSGA-III [4] is coupled with a deterministic local search procedure. The proposed hybrid approach involves the execution of the NSGA-III until meeting a termination condition. Upon establishing this condition, a local search method is applied to a subset of solutions situated on the Pareto front. The local search procedure transforms the multi-objective problem into a single-objective one using the Achievement Scalarizing Function (ASF). For each solution, the ASF is solved via two methods: using a Sequential Quadratic Programming algorithm [3] and a BFGS-like algorithm [6]. The new locally found solutions are integrated into the prior population, and the NSGA-III is re-executed until a new stagnation point is reached. This iterative process continues until a pre-defined maximum budget is attained.

The remainder of the paper is organized as follows. Section 2 defines the optimization problems and the NSGA-III, the reference-based evolutionary algorithm employed in this paper. Section 3 explores the proposed local search technique. Section 4 shows the computational experiments and an analysis of the results. Finally, Section 5 presents the conclusions and future work.

2 Multi- and Many-Objective Optimization Problems

Real-world problems frequently demand simultaneous optimization of multiple conflicting objective functions. Mathematically, these problems are typically formulated as equation (1):

$$\begin{aligned} & \mathbf{x}^* = \text{argmin}_{\mathbf{x}} \mathbf{f}(\mathbf{x}), \\ \text{subject to:} & \begin{cases} g_i(\mathbf{x}) \leq 0, & i = 1, 2, \ldots, r, \\ h_j(\mathbf{x}) = 0, & j = 1, 2, \ldots, p, \end{cases} \end{aligned} \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{f}(.) : \mathbb{R}^n \to \mathbb{R}^M$ with $M \geq 2$, $\mathbf{g}(.) : \mathbb{R}^n \to \mathbb{R}^r$, and $\mathbf{h}(.) : \mathbb{R}^n \to \mathbb{R}^p$. g_i and h_j represent inequality and equality constraints, respectively. $\mathbf{x} \in \mathbb{R}^n$ are named decision variable vectors, constituting the parameter space and the objective functions, denoted by $\mathbf{f}(\mathbf{x}) \in \mathbb{R}^M$, reside in the objective space. When $M = 2, 3$, these problems are called multi-objective optimization problems (MOPs). When $M \geq 4$, they are called many-objective optimization problems (MaOPs).

The NSGA-III, one of the state-of-the-art algorithms for handling both MOPs and MaOPs, focuses on maintaining a diverse set of well-distributed solutions along the Pareto front, allowing an exploration of the trade-off solutions. It uses a reference point-based approach to non-dominated sorting to effectively handle a large number of objectives by guiding the evolution towards diverse regions of the Pareto front. Here, we use a PlatEMO implementation of NSGA-III [13].

3 The Proposed Local Search

Hybrid approaches aim to leverage the strengths of both multi-objective evolutionary algorithms (MOEAs) for global exploration and single-point methods for local search to enhance solution refinement. Two methods for triggering local searches are described in the literature: the serial approach, where the MOEA executes until a stopping condition is met before local search, and the concurrent approach, where local search is integrated into each iteration. The choice between these methods depends on the decision-maker's preferences.

In the present work, we adopt the serial approach to refine solutions while maintaining diversity similar to the MOEA. Additionally, we introduce a straightforward online stopping criterion that detects MOEA stagnation, prompting interruption and triggering the local search.

Suppose an MOEA has been executed for some time and stopped due to a given stopping criterion. Assuming that the current population ($P(t_{end})$) is in a neighborhood of the efficient set, exhibiting a reasonable distribution in the solution space, a possible way to perform a local search is to employ a single-point method on certain individuals, employing any scalarizing technique [10] (e.g., weighting method, ϵ-constraint, weighted metrics, etc). In this work, we opt to optimize an **achievement scalarizing function** (ASF), proposed in [15].

For each point selected for the local search and using a reference point given by $\bar{z} = \mathbf{f}(\mathbf{x})$, we use the ASF proposed in [12] to transformer the original problem into the following scalarized form as equation (2):

$$\begin{array}{c}\text{minimize} \\ \text{subject to } x\in\mathcal{X}\end{array} \max_{i=1}^{k} \frac{f_i(x) - \overline{z}_i}{z_i^{\max} - z_i^{\min}} + \rho \sum_{i=1}^{k} \frac{f_i(x) - \overline{z}_i}{z_i^{\max} - z_i^{\min}}, \tag{2}$$

where $z_i^{\max}$ and $z_i^{\min}$ are the currently available worst and best function values.

Once the scalarization method is defined, integrating it into the local search procedure becomes straightforward. Given $P(t_{end})$ containing individuals from the final MOEA iteration, the approach involves solving the single-objective problem described in (2) for each selected $\mathbf{x} \in P(t_{end})$ using $\mathbf{x}$ as the starting point and $\mathbf{f}(\mathbf{x})$ as a reference point.

For solving (2), two mathematical programming techniques are employed as local solvers: a Sequential Quadratic Programming (SQP) approach and a stochastic BFGS-like approach. The SQP method computes derivatives using the finite derivative method, while the **fastBFGS** solver, an accelerated stochastic quasi-Newton method, specializes in matrix inversion to ensure positive definite solutions. This approach, detailed in [6], offers efficient solutions and serves as an estimator for the inverse Hessian matrix, contributing to effective local optimization.

The minimization of the ASF ensures the attainment of a Pareto-optimal point, even if the initial point is distant from the global optima, provided a global optimizer is utilized. Determining when to stop the MOEA and initiate the local search procedure poses a crucial question. Performance indicators, such as the Moment of Inertia-based measure and a new indicator based on the ASF, serve to monitor population evolution and detect stagnation. The Moment of Inertia [11] quantifies population diversity in the variable space while the ASF-based indicator measures convergence by evaluating the improvement achievable for each reference point.

By aggregating these indicators over a time window and testing for horizontal regression lines, stagnation can be identified. To detect stagnation, we adopt an approach akin to that proposed by [7]. We fit a regression line $y = \beta_0 + \beta_1 t$ to t_w observations of the indicator, where y represents the performance indicator and t is the iteration number. By estimating the parameters β_0 and β_1 using a least squares approach, we examine whether the fitted line is nearly horizontal, indicating a slope close to zero. This is assessed through a hypothesis test on β_1, with a predetermined significance level $\alpha = 0.05$ and a given p-value P. If $P \geq \alpha$, we infer a zero slope. To enhance robustness, we utilize two indicators and stop only if both pass the stagnation test simultaneously. In our study, we employ a time window of $t_w = 15$ for these tests.

4 Numerical Experiments

After combining the NSGA-III and the proposed local search described in Section 3, two hybrid approaches are proposed: (i) NSGA-III solving the ASF via SQP (H-NSGA-III-SQP) and (ii) NSGA-III solving the ASF via the stochastic BFGS-like method (H-NSGA-III-fBFGS). The hybrid approaches have been compared to the classical NSGA-III in the DTLZ 1-4 problems with 3, 5, 8, 10, and 15 objectives.

Twenty-one independent runs for all algorithms have been performed. The population size (PopSize) for NSGA-III, for each number of objectives (M), and the maximum number of generations (MaxGen) for NSGA-III in each DTLZ problem have been chosen as defined in [4] and are shown in Table 1. Three different budgets, the maximum number of objective function evaluations, have been analyzed: $b1 = \dfrac{\text{PopSize} \times \text{MaxGen}}{3}$; $b2 = \dfrac{\text{PopSize} \times \text{MaxGen}}{M}$; $b3 = \text{PopSize} \times 150$. These budgets have been defined to assess the algorithms' performance in scenarios with diverse budgets, involving variations in both problems and dimensions, as recommended in [4]. Additionally, evaluations have been conducted in scenarios with fixed-size budgets.

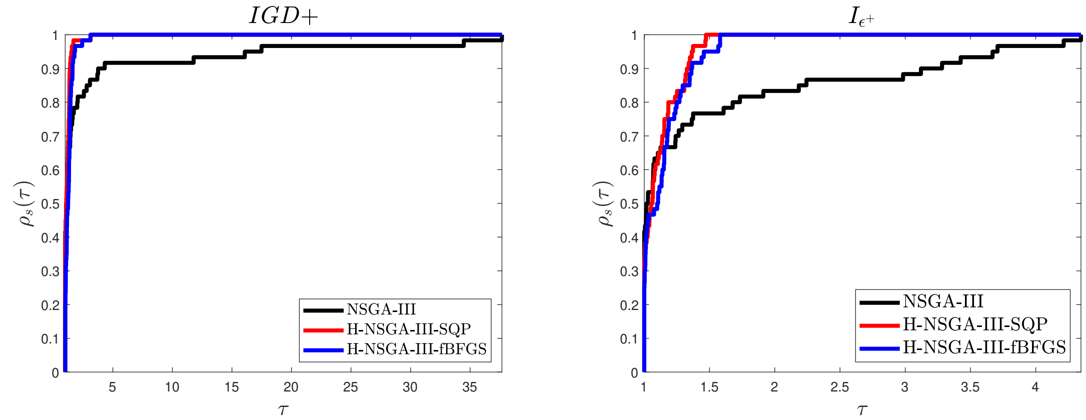
In both hybrid approaches, following the stagnation of NSGA-III, the local search is applied to 1/4 of the current population. The individuals selected for local search are chosen from the fronts based on their non-dominated rank and crowding distance. Individuals with higher non-dominated ranks and higher crowding distances (excluding the ones having an infinite crowding distance) are preferred. Both solvers, SQP and fBFGS, terminate when one of the following stopping criteria is met: reaching a maximum of 20 iterations or when the maximum difference in any decision variable between two successive iterations is less than or equal to 10^{-6}.

Table 1: Population sizes and Maximum number of generation (MaxGen) used in NSGA-III for each problem and each number of objectives.

# of objectives (M)	3	5	8	10	15
Pop. Size	92	212	156	276	136
MaxGen(DTLZ1)	400	600	750	1000	1500
MaxGen(DTLZ2)	250	350	500	750	1000
MaxGen(DTLZ3)	1000	1000	1000	1500	2000
MaxGen(DTLZ4)	600	1000	1250	2000	3000

The performance of each hybrid algorithm has been tested against the classical version of NSGA-III in each problem, considering specific budgets for each assessment. The other NSGA-III parameters used in this paper are the values set as default in PlatEMO [13]. The additive epsilon indicator (I_{ϵ^+}) [16] and IGD+ [8], are utilized to assess the convergence and distribution of non-dominated fronts generated by the algorithms. For each problem, the non-dominated solutions obtained from the union of results by all considered algorithms serve as the reference set for calculating the performance indicators. The non-parametric Wilcoxon Rank Sum statistical test, using $\alpha = 0.05$, is used to verify whether there is a statistically significant difference in performance between the results, i.e., whether two samples are likely to come from the same population. A post hoc test is applied to determine the directionality of the difference.

Observing the results for all problems DTLZ 1-4, in all dimensions and all budgets, it is possible to note that, in the majority of the tests, except for a few instances with 5 and 8 objectives, the hybrid approaches consistently demonstrated superior performance compared to their classical counterparts. The H-NSGA-III-SQP achieved a better mean in 62.5% of the MaOPs with dimensions 10 and 15 for the IGD+ indicator. Regarding the I_{ϵ^+} indicator, the best mean was confirmed



(a) NSGA-III = 0.9434, H-NSGA-III-SQP = 1, H-NSGA-III-fBFGS= 0.9971.

(b) NSGA-III = 0.8861, H-NSGA-III-SQP = 1, H-NSGA-III-fBFGS =0.9914.

Figure 1: The Performance Profiles relative to all problems and budgets and the areas under the curves (proportionally to the biggest). Fonte: dos autores

in 50% of the problems. In both indicators, H-NSGA-III-SQP performed significantly better in most problems where it obtained the best mean. In the same dimensions, the H-NSGA-III-fBFGS get a better mean for the IGD+ in 29.17% of the cases and 37.5% for the I_{ϵ^+}, holding statistically significant differences in the most problems where it obtained the best mean. Furthermore, H-NSGA-III-SQP outperformed H-NSGA-III-fBFGS in budgets $b1$ and $b2$, while the opposite was observed in budget $b3$.

Aiming to visualize and interpret the results of IGD+ and I_{ϵ^+}, Performance Profiles [5] have been employed. Performance profile provides a graphical representation of the distribution of performance measures over a given problem set considering the number of problems solved and the cost (calculated here as the performance measure) it took to solve it. Let P be a set of problems, S a set of algorithms, and $t_{p,s}$ any performance measure evaluated in problem p by algorithm s. Considering an algorithm s and each value of a positive factor τ, the Performance Profile represents the percentage of problems extracted from P on which the performance of s is within a factor of τ of the best performance of other algorithms. [2] highlighted that the area below $\rho_s(\tau)$ can be used as an overall performance measure (larger area corresponds to an increased algorithm efficiency).

The Performance Profiles, depicted in Figures 1a and 1b, assess the algorithms' performance across all problems when I_{ϵ^+} and IGD+ are considered, jointly with the areas under the curves for I_{ϵ^+} and IGD+, respectively. Figure 2 displays the Overall Performance Profile when both indicators are combined. Considering the areas under these curves, it can be observed that both the hybrid algorithms proposed here outperformed NSGA-III, highlighting H-NSGA-III-SQP, which achieved the best performance regarding both indicators and the Overall Performance Profile (Figure 2).

5 Conclusions

This study proposed a hybrid approach to tackle multi- and many-objective optimization problems by enhancing NSGA-III with deterministic mathematical programming local search techniques. The hybrid method employed NSGA-III until a predefined stopping criterion, measured by population quality stagnation using two distinct performance indicators. Local search was then applied to a subset of Pareto optimal solutions, transforming the multi-objective problem

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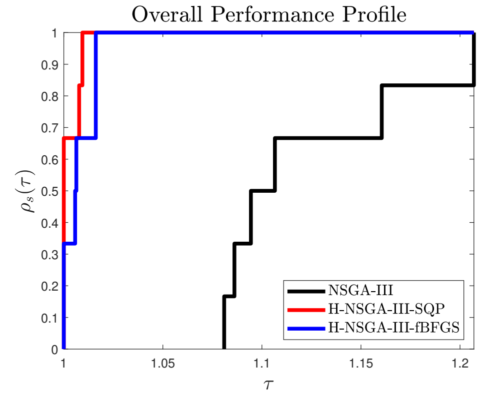

Figure 2: The Overall Performance Profiles relative to the inverted values of the areas under the Performance Profiles curves in Figures 1a and 1b. The areas under the curves (proportionally to the biggest) for NSGA-III, H-NSGA-III-SQP and H-NSGA-III-fBFGS are, respectively, 0.4134, 1, 0.9778. Fonte: dos autores

into a single-objective one using the Achievement Scalarizing Function (ASF). For each selected point, ASF was solved using Sequential Quadratic Programming and a stochastic BFGS-like algorithm. The discovered local solutions were integrated into the population, and NSGA-III was re-executed until a new stagnation point was reached, iteratively continuing until a maximum budget was reached. Comparative experiments with classical NSGA-III were conducted across various objective functions and budget scenarios. H-NSGA-III-SQP demonstrated superior performance, achieving the best results in terms of performance indicators and mean values across most problems, with statistically significant differences in several cases. H-NSGA-III-fBFGS also performed competitively, ranking second overall. Performance Profiles constructed based on these results consistently favored the hybrid algorithms over classical NSGA-III across all addressed problems. In future work, the hybrid approaches will be applied to address a broader range of MOPs and MaOPs in both constrained and unconstrained situations. The investigation will include new budget scenarios and MaOPs involving more than 15 objective functions.

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