Two Novel Approaches for Many-Objective Optimization

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***Abstract*— In this paper, two novel evolutionary approaches for many-objective optimization are proposed. These algorithms integrate a fine-grained ranking of solutions to favor convergence, with explicit methodologies for diversity promotion in order to guide the search towards a representative approximation of the Pareto-optimal surface. In order to validate the proposed algorithms, we performed a comparative study where four state-of-the-art representative approaches were considered. In such a study, four well-known scalable test problems were adopted as well as six different problem sizes, ranging from 5 to 50 objectives. Our results indicate that our two proposed algorithms consistently provide good convergence as the number of objectives increases, outperforming the other approaches with respect to which they were compared.**

I. Introduction

Evolutionary algorithms (EAs) draw inspiration from the process of natural evolution in order to evolve a population of potential solutions for a given optimization problem through a series of probabilistic processes. EAs are suitable approaches to solve *multiobjective optimization problems* (MOPs), since they are able to explore simultaneously different regions of the search space and produce several elements of the Pareto optimal set within a single execution.

However, despite the considerable volume of research in this regard, several studies have shown that even the most popular multiobjective EAs (MOEAs) scale poorly with respect to the number of objectives [1], [2], [3]. The main reason is that *Pareto dominance* (PD) [4] (which has been the most commonly adopted relation to discriminate among solutions in the multiobjective context) loses its effectiveness when the number of objectives increases. As a consequence, it is not possible to impose preferences among individuals for selection purposes and the search process weakens since it is performed practically at random. MOPs having more than three objectives are referred to as *many-objective optimization problems* in the specialized literature [5].

PD's drawbacks have motivated researchers to explore the use of alternative ranking methods[1] in order to improve selection when dealing with many-objective problems [6], [7], [8], [9], [10], [11], [12], [13], [14]. In our previous work [6], [7], [8], we performed a series of comparative experiments in order to investigate the behavior provided by several of such approaches, regarding their scalability with respect to the number of objectives. In such a study, we analyzed the degree of discrimination induced by the studied approaches as well as their ability to guide the search process when they were incorporated into a generic MOEA.

One of our main findings was that, by using an effective ranking scheme, it is possible for a MOEA to converge in many-objective scenarios. Our experiments empirically showed that, in order to be effective, the ranking method must provide a fine-grained discrimination by considering how significantly better is a solution from the others with respect to each objective. Discarding this information can lead to wrong discrimination decisions and, can thus, negatively affect the search capabilities of a MOEA.

Nevertheless, it was also observed that a high selection pressure tends to sacrifice diversity and usually leads to converge towards a small region of the trade-off surface. The population tends to become homogenized from the early stages of the search process. Thus, the exploratory capabilities of a MOEA clearly deteriorate; practically, under these conditions the generation of new individuals relies solely on mutations. Also, the selection process, which is responsible for guiding the search, is biased because of the selective advantages of duplicate individuals [15]. Moreover, convergence towards a diversified set of Pareto-optimal solutions is an important requirement for MOEAs in order to provide the decision maker with a representative approximation of the Pareto front. However, the satisfaction of these requirements for a MOEA is, by itself, a multiobjective problem; the best diversity is commonly associated with a poor proximity [16].

Generally, diversity is promoted as a secondary criterion to discriminate among solutions which share the same rank. However, when using a fine-grained ranking procedure, each solution usually has a different rank and, therefore, such type of approach clearly has no effect; so, it is necessary to develop a more appropriate methodology in order to address this kind of scenarios.

In this paper, we propose two novel MOEAs whose peculiarity is the integration of a strict ranking procedure to favor convergence with an explicit mechanism for diversity promotion. The basic premise of our approaches is that convergence is to be maintained as the priority. In fact, we would prefer a poorly spread set of Pareto-optimal solutions rather than a well-spread set of solutions which are far from the Pareto-optimal surface [13]. Therefore, diversity preservation should be done in a way that does not affect convergence. In order to validate the two proposed MOEAs, we performed a comparative study where four approaches representative of

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[1]In this study, we will use indistinctly the terms fitness and rank to refer to the value which expresses the quality of solutions and which allows to compare them with respect to each other. Thus, it is equivalent to talk about ranking or fitness assignment approaches.

the state-of-the-art in the area were considered.

The remainder of this paper is structured as follows: Section II describes the baseline algorithm on which the proposed approaches were implemented. In Sections III and IV we present the details of the proposed MOEAs. Our experimental setup and the corresponding results are discussed in Section V. Finally, Section VI provides our conclusions as well as some possible directions for future research.

II. Baseline Algorithm

The two proposed approaches were implemented over a basic MOEA whose workflow is shown in Figure 1.

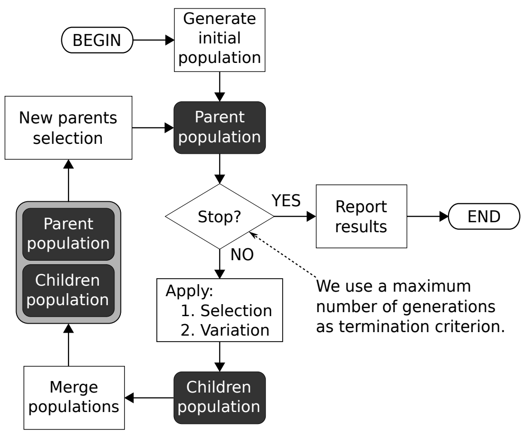


Fig. 1. Workflow of the baseline algorithm.

Initially, a parent population of N individuals is randomly generated. Then, this population is ranked and selection is performed in order to choose individuals for reproduction (*selection-for-variation*). A children population of N new individuals is generated by applying variation operators over the selected individuals. Finally, parent and children populations are combined and N individuals are selected to survive in order to form the new parent population (*selection-for-survival*). This process is repeated until a given number of generations is reached.

The implemented operators are: *binary tournament selection* based on the rank of solutions. *Simulated binary crossover* ($\eta_c = 15$) with probability of 1. *Polynomial mutation* ($\eta_m = 20$) with probability of $1/n$, where n is the number of decision variables.

III. Our First Proposal: The Clustering-based Elitist Genetic Algorithm

Our first proposed approach is called the *Clustering-based Elitist Genetic Algorithm* (**CEGA**) and it consists of a MOEA which incorporates clustering for diversity preservation and adopts a fine-grained ranking scheme to promote convergence. **CEGA** was implemented based on the algorithm described in Section II. Figure 2 shows the workflow of the resulting approach.

In Figure 2 the key elements of **CEGA** are highlighted with dotted boxes. On the one hand, it has a procedure which

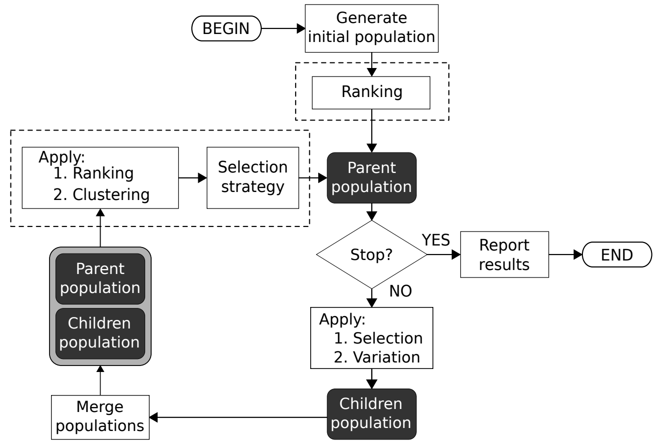


Fig. 2. **CEGA**'s workflow.

assigns to each individual a rank to compete at the selection-for-variation stage. On the other hand, it has a clustering-based strategy which guides the selection-for-survival process. These elements are to be separately described below.

A. Ranking scheme

CEGA incorporates the *Global Detriment* (GD) method, previously proposed in [8], as its discrimination strategy. According to GD, the fitness of a solution is obtained by accumulating the difference by which it is inferior to every other solution, with respect to each objective. Formally, the fitness of a solution $\mathbf{X}_i$ is calculated as follows:[2]

$$gd(\mathbf{X}_i) = \sum_{\mathbf{X}_j \neq \mathbf{X}_i} \sum_{m=1}^{M} \max(f_m(\mathbf{X}_i) - f_m(\mathbf{X}_j), 0) \qquad (1)$$

where M is the number of objectives and f_m is the m-th objective function. A solution $\mathbf{X}_i$ is said to be better than another solution $\mathbf{X}_j$ if it holds that $gd(\mathbf{X}_i) < gd(\mathbf{X}_j)$.

B. Clustering procedure

We implemented a hierarchical agglomerative clustering procedure.[3] Initially, each individual represents a different cluster and, iteratively, the two most similar clusters are combined until completing a fixed number of groups (see Figure 3).

The clustering algorithm will be applied in decision variable space. We adopted the average linkage criterion to determine the closeness between a pair of clusters: the distance between two clusters c_1 and c_2 is the average of the Euclidean distances between each pair of solutions $\mathbf{X}_i$ and $\mathbf{X}_j$ such that $\mathbf{X}_i \in c_1$ and $\mathbf{X}_j \in c_2$. Clustering will be applied to the $2N$ individuals in the combined population (see Figure 2). The purpose of clustering the solutions is to guide the selection to a well-distributed set of individuals in order to promote diversity and to enhance the exploratory

[2]In this study, we assume that all objectives are equally important and, without loss of generality, we will refer only to minimization problems.

[3]There exist some other computationally less expensive clustering algorithms which might be explored with different results.

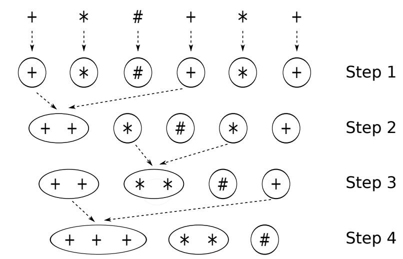


Fig. 3. Hierarchical agglomerative clustering.

capabilities of the algorithm. Since N individuals are to be selected, the number of required clusters lies in the range $[2, N]$. All our experiments involve a population size of $N = 100$ and, for reasons discussed in Section III-D, we will use a total of $C = N/2 = 50$ clusters.

C. Selection strategy

In order to reduce the combined parents and children population to N individuals, the survivor selection strategy to be followed is described below:

1) Compute the rank of individuals using the GD method described in Section III-A.
2) Generate C clusters as described in Section III-B.
3) Select a representative solution from each cluster using our *Distance To The Best Known Solution* method [6], [8]. This method uses a reference point which is to be referred to as GBEST and is composed by the best known value for each objective. The best solution will be the one with the minimum Euclidean distance from the GBEST point. However, as shown in Figure 4, this method will be applied locally to discriminate among solutions within the same cluster.

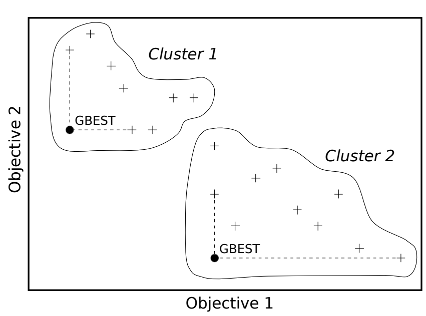


Fig. 4. Selection of the representative individual from each cluster.

4) In step 3, C individuals are selected. If $C < N$, then we select the remaining $N - C$ individuals according to their global rank obtained with GD in step 1.

$\mathbf{CEGA}$ preserves genetic variation in the population at the expense of the conservation of (probably) low-quality individuals through the search process. Specially in many-objective optimization, it is common the case in which these bad solutions are Pareto-nondominated with respect to other high-quality individuals in the population (the so-called *dominance resistant solutions* [17]). Thus, we implemented a filter which removes these *outliers* from the output of the algorithm (final population). We consider that a solution $\mathbf{X}_i$ is an outlier if the Euclidean distance of its objective values from the origin is $1.5 \times IQR$ (*inter-quartile range*) beyond the third quartile.

D. CEGA's parameters setting

In order to develop the $\mathbf{CEGA}$ algorithm, we implemented 14 different algorithmic designs. Also, we tested three different measures of the similarity between clusters: average, single and complete linkage. The number of clusters that $\mathbf{CEGA}$ requires lies in the range $[2, N]$. Considering a population size of $N = 100$, the values we tested for this parameter were $C = \{25, 50, 75\}$. Finally, we considered three different ranking approaches which, according to our previous work [6], [7], [8], provide good convergence. The combination of these parameters settings leads to a total of 378 $\mathbf{CEGA}$ configurations which were empirically evaluated: we performed a comparative study where six scalable test problems (from DTLZ1 to DTLZ6 [18]) and instances with $M = \{5, 10, 15, 20, 30, 50\}$ objectives were considered. Due to obvious space limitations, the details of such experiments are not provided here. However, the above description for $\mathbf{CEGA}$ corresponds to the (statistically) best-performing configuration according to the obtained results.

The number of clusters, C, determines the trade-off between the convergence and diversity provided by $\mathbf{CEGA}$. That is, the higher the value for C, the better the diversity at the expense of convergence. Even though we empirically determined that a value of $C = 50$ provides an acceptable performance in our experiments, the proper value for this parameter should be carefully investigated for the problem at hand.

IV. Our Second Proposal: Multi-Directional Fitness Assignment

Our second proposal is called *Multi-Directional Fitness Assignment* ($\mathbf{MDFA}$). As its name indicates, it is a fitness assignment method whose aim is to guide the search process, simultaneously, in multiple directions. $\mathbf{MDFA}$ uses a set of weighted vectors in order to set different search directions. A weighted vector is a set of coefficients which denote the relative importance of each objective. Thus, we assume that different weighted vectors will direct the search towards different regions of the objective space. Figure 5 shows the workflow of $\mathbf{MDFA}$, which is based on the generic algorithm described in Section II.

The ranking process is specifically our proposal in this case. This element has been highlighted with a dotted box in Figure 5 and it will be described below.

A. Fitness assignment

The fitness assignment process is done to guide both the selection-for-variation and the selection-for-survival stages. Considering a population P of size N, this method requires a set V with N different weighted vectors ($|V| = N$). Algorithm 1 describes the proposed fitness assignment procedure.

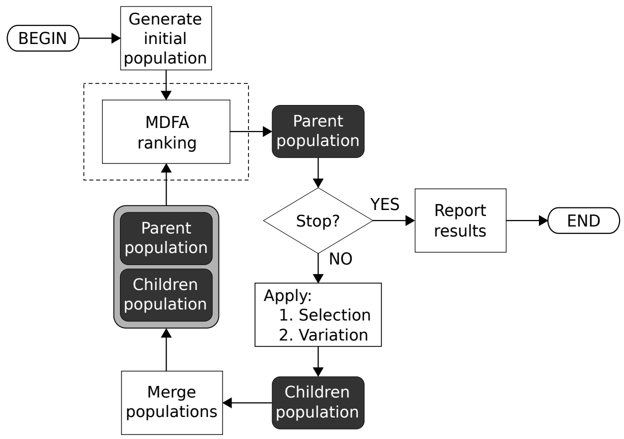


Fig. 5. **MDFA**'s workflow.

Algorithm 1 **MDFA**'s fitness assignment process.

DEFINE MDFA(P, V)
$fitness[\mathbf{X}_i] \leftarrow \infty \quad \forall \mathbf{X}_i \in P$
-[STAGE 1]-
for all $v \in V$ **do**
  Find $\mathbf{X}_i \in P \; : \; wsum(\mathbf{X}_i, v) < wsum(\mathbf{X}_j, v)$ $\forall \mathbf{X}_j \in P : \mathbf{X}_j \neq \mathbf{X}_i$
  if $wsum(\mathbf{X}_i, v) < fitness[\mathbf{X}_i]$ **then**
    $fitness[\mathbf{X}_i] \leftarrow wsum(\mathbf{X}_i, v)$
-[STAGE 2]-
$worst\_stage1 \leftarrow \max(fitness[\mathbf{X}_i])$ $\forall \mathbf{X}_i \in P : fitness[\mathbf{X}_i] \neq \infty$
for all $\mathbf{X}_i \in P : fitness[\mathbf{X}_i] = \infty$ **do**
  $fitness[\mathbf{X}_i] \leftarrow \max\limits_{v \in V}(wsum(\mathbf{X}_i, v)) + worst\_stage1$
END

Initially, all individuals in the population are evaluated for each $v \in V$ by using an aggregating approach. We adopted a simple but effective weighted sum technique. The weighted sum for a solution $\mathbf{X}_i$ with respect to a vector v is given by:

$$wsum(\mathbf{X}_i, v) = \sum_{m=1}^{M} v_m f_m(\mathbf{X}_i) \tag{2}$$

where v_m is the weighting coefficient which denotes the relative importance of the m-th objective. Then, the individual with the best performance for each $v \in V$ is identified and the obtained fitness value (with respect to v) is assigned to it. Since the same individual may be the best for several weighted vectors, its final fitness will be the best of all the fitness values obtained for those vectors. Individuals which were not ranked (since they are not the best for any weighted vector) use their worst performance for all vectors as their fitness value. This will allow to prefer solutions showing a better average performance for the given set of vectors. Additionally, the fitness of these individuals is penalized by adding the worst fitness assigned in the first stage. This will ensure these individuals to be less preferred than the first set of individuals.

B. **MDFA***'s parameters setting*

We implemented five different algorithmic designs during the development of **MDFA**. Also, we experimented with 3 sets of weighted vectors which were generated in different ways: 1) vectors generated with a tool developed by Hughes for his MSOPS algorithm [19] (available for academic use at `http://code.evanhughes.org/`), 2) vectors of randomly generated weights in the range $[0.5, 1]$ and 3) vectors of randomly generated weights in the range $[0.25, 1]$. The combination of such elements leads to a total of 15 algorithmic configurations. As in the case of **CEGA**, the 15 configurations for **MDFA** were statistically evaluated with respect to six test cases (from DTLZ1 to DTLZ6 [18]) and we used $M = \{5, 10, 15, 20, 30, 50\}$ objectives in each problem. Due to space limitations, the details are not provided here. However, the above description of **MDFA** corresponds to the strategy which performed the best.

The features of the adopted weighted vectors directly affect the performance of **MDFA**. According to our observations, the weighted vectors must satisfy $v_m > 0$ for all $v_m \in v$, for each $v \in V$; that is, all objectives are to be considered in each weighted vector. In our experiments, the set of weighted vectors randomly generated in the range $[0.25, 1]$ provided the best performance.

V. Experimental Results

We performed an experimental study in order to investigate the behavior of the proposed approaches in terms of convergence and diversity, as well as their scalability with respect to the number of objective functions.

A. Experimental setup

Due to space limitations, only four test problems were adopted for this study: DTLZ{1,3,4,6} [18]. These problems can be scaled to any number of objectives and decision variables. The total number of variables in these problems is $n = M + k - 1$, where M denotes the number of objectives and k is a difficulty parameter which was set to $k = 5$ for DTLZ1 and $k = 10$ for the remaining problems. In this study, we considered problems instances with $M = \{5, 10, 15, 20, 30, 50\}$ objectives.

As a convergence measure, we computed the average distance from the Pareto-nondominated solutions in the approximation set obtained by the MOEA to the true Pareto front [20]. Since equations defining the true Pareto front are known for all the test problems adopted, this measure was analytically determined.

Additionally, we implemented the *Inverted Generational Distance* (IGD) performance measure which allows to evaluate both convergence and diversity. IGD is a variation of the *Generational Distance* indicator [21] and is defined by IGD $= \left(\sqrt{\sum_{i=1}^{|P^*|} d_i^2}\right) / |P^*|$, where P^* is a reference set of points in the true Pareto front and d_i is the Euclidean distance between the i-th solution in P^* and the nearest point in the approximation set obtained by the MOEA.

The two adopted performance measures are to be minimized. For all the approaches compared, we used a population size of $N = 100$ individuals, a maximum number of 300 generations and we performed 31 independent executions of each experiment.

B. State-of-the-art approaches

We considered four state-of-the-art MOEAs for comparing our results:

- *Nondominated Sorting Genetic Algorithm II* (**NSGA-II**) [22]. This is perhaps the most representative MOEA in the literature. **NSGA-II** implements the *Nondominated Sorting*, which is a ranking method based on Pareto dominance, and an explicit mechanism for diversity preservation, the *Crowding Distance*, which is used as a secondary criterion to discriminate among equally ranked solutions.
- *Diversity Management Operator* (**DMO**) [23]. **DMO** is a methodology to manage the use of diversity preservation operators when dealing with many-objective problems. According to the authors, diversity promotion can be harmful in many-objective scenarios, since it tends to prefer solutions with a poor convergence and, therefore, to guide the search away from the Pareto front. **DMO** is an adaptive strategy: diversity promotion is performed only when it is required.
- *Hypervolume Estimation Algorithm* (**HypE**) [24]. **HypE** is a many-objective optimizer which uses the hypervolume metric to guide the search. Since the calculation of this metric becomes computationally expensive with the increase in the number of objectives, **HypE** approximates it by using a Monte Carlo simulation.
- *Multiple Single Objective Pareto Sampling* (**MSOPS**) [19]. **MSOPS** was proposed as an alternative to deal with many-objective problems. As our **MDFA** algorithm, **MSOPS** uses a set of weighted vectors to guide the search in multiple directions simultaneously.

For a more detailed description of these approaches, the reader is referred to their original publications.

C. Convergence results

Figures 6 to 9 present the results obtained by the studied algorithms for problems DTLZ$\{1,3,4,6\}$, respectively, with respect to the convergence metric described in Section V-A.

From these figures it is clear that our algorithms **CEGA** and **MDFA** performed the best for this experiment. For all the instances of the adopted test problems, the two proposed MOEAs reached the lowest values for the convergence metric, significantly outperforming the 4 approaches taken from the literature. By specifically comparing our approaches with respect to each other, we can see that for problems DTLZ1 and DTLZ4 (Figures 6 and 8, respectively) **CEGA** achieved better results than those obtained by **MDFA**, and the superiority of **CEGA** becomes more evident as the number of objectives increases. On the other hand, for problems DTLZ3 and DTLZ6 (Figures 7 and 9, respectively) the differences between our two proposed algorithms are not significant enough as to argue superiority of any of them.

DMO showed a better performance than **NSGA-II** in most instances of this experiment. These results confirm that, as stated by Adra and Fleming [23], diversity promotion mechanisms can be harmful when many objectives are to be optimized, supporting the need for a more appropriate management of these operators when are combined with a Pareto-based ranking procedure. However, the improvements of **DMO** are not so significant as to achieve good values for the convergence metric, since this method is based on Pareto dominance which, as discussed in Section I, loses its effectiveness to guide the search process as the number of objectives increases. Among the considered state-of-the-art MOEAs, the **MSOPS** algorithm performed the best in most cases, while the ranking among the three other approaches is not clear.

D. IGD metric results

This section provides the results obtained for the IGD metric described in Section V-A. Figures 10 to 13 show the results obtained by the studied MOEAs at solving problems DTLZ$\{1,3,4,6\}$, respectively.

From these figures, we can clearly see that **CEGA** and **MDFA** achieved the best results for the IGD metric in most configurations of this experiment.

In the case of the problem DTLZ1 (Figure 10), the results of **MSOPS** are very close to those attained by our approaches in all instances. However, the size of its corresponding boxes and outliers indicate a more inconsistent behavior. Regarding problems DTLZ3 and DTLZ6 (Figures 11 and 13, respectively), the superiority of our proposed approaches is more clear.

On the other hand, some important conclusions can be drawn from the results for problem DTLZ4 (Figure 12). As we can see, for all the instances of this problem, some state-of-the-art approaches performed equal or better than ours. For the smallest instance ($M = 5$) our algorithms performed the worst, while **MSOPS** achieved the best results. However, these differences were reduced for larger instances, where **HypE**, **MSOPS** as well as our proposed approaches **CEGA** and **MDFA** behaved similarly, competing in performance at the top of the ranking. Contrasting these results with those for the convergence metric in Section V-C, it is possible to observe that both **CEGA** and **MDFA** are inferior in their ability to maintain a diversified set of solutions. Although state-of-the-art approaches did not show the best convergence, they are superior enough at maintaining diversity as to achieve competitive results with respect to the IGD metric. It is important to mention that similar results were obtained for problems DTLZ2 and DTLZ5, which were not reported here due to space constraints.

When comparing the performance of our approaches, it is not possible to distinguish significant improvements to claim the superiority of one approach with respect to the other. However, **CEGA** achieved slightly better results

Fig. 6. Convergence metric. DTLZ1 problem.

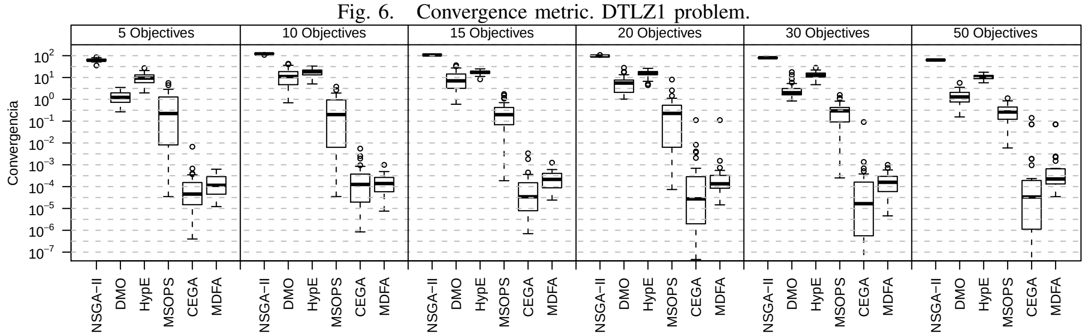


Fig. 7. Convergence metric. DTLZ3 problem.

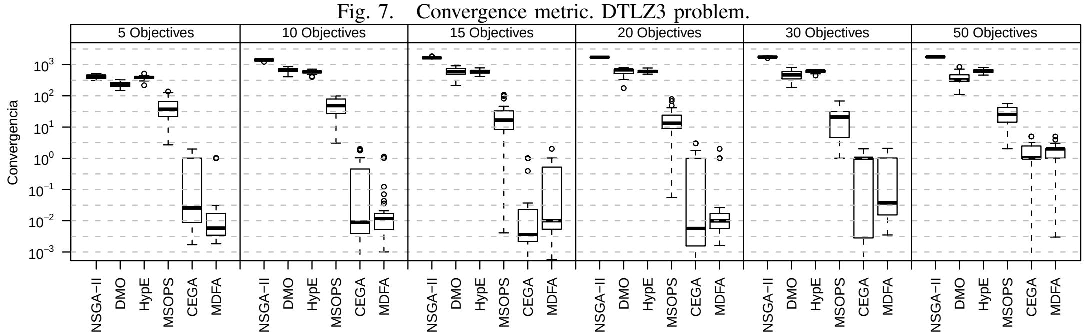


Fig. 8. Convergence metric. DTLZ4 problem.

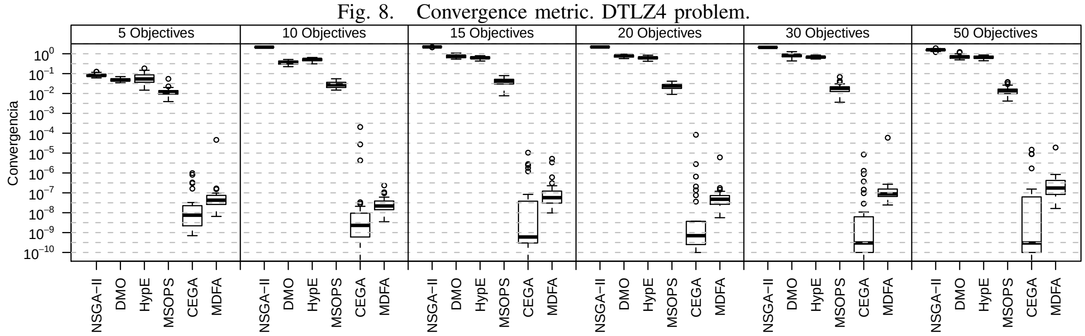
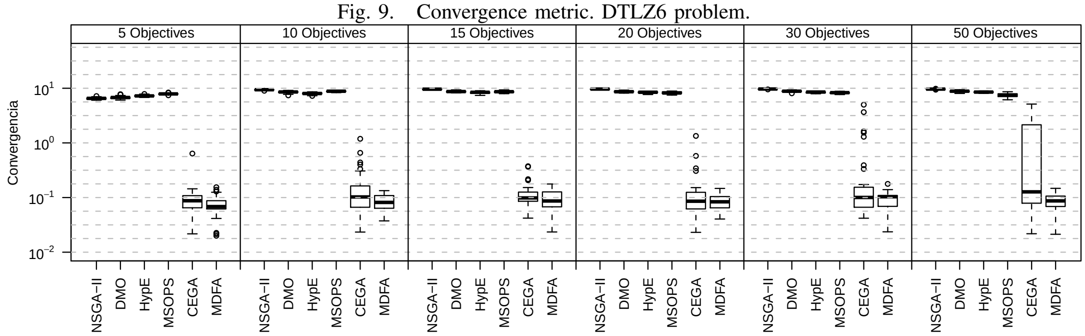


Fig. 9. Convergence metric. DTLZ6 problem.



than **MDFA** in most cases. Regarding state-of-the-art approaches, **MSOPS** showed the best performance in this experiment, particularly as the number of objectives was increased.

VI. Conclusions and Future Work

In this paper, we proposed **CEGA** and **MDFA**, two new MOEAs to deal with many-objective optimization problems. The peculiarity of the proposed MOEAs is the integration of a fine-grained ranking procedure with an explicit mechanism for diversity preservation. Thus, these approaches provide a strong selection pressure to enhance convergence while guiding the search towards a well-spread set of solutions.

In order to validate our two proposed MOEAs, we performed a comparative study in which four state-of-the-art approaches were considered. The results of this study indicated that **CEGA** and **MDFA** provide a good performance

Fig. 10. IGD metric. DTLZ1 problem.

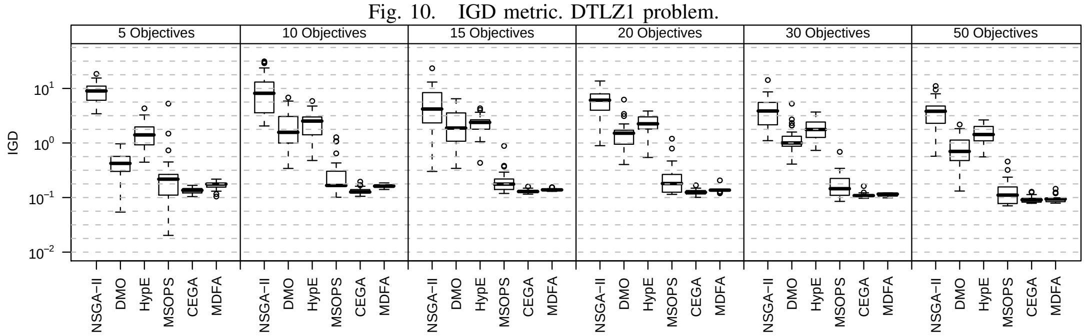


Fig. 11. IGD metric. DTLZ3 problem.

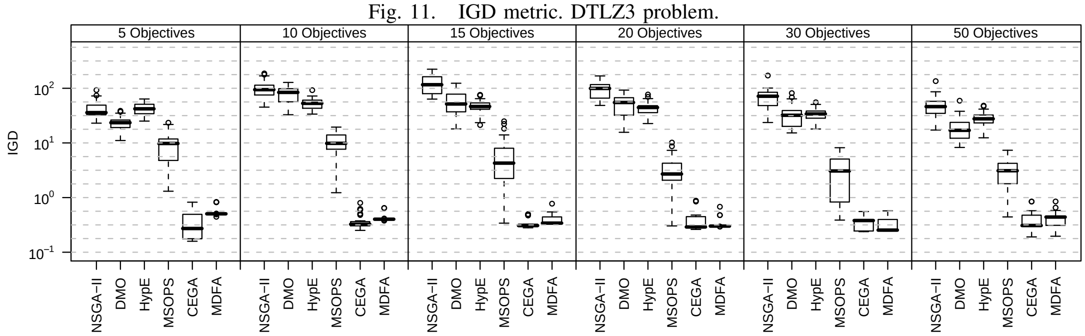


Fig. 12. IGD metric. DTLZ4 problem.

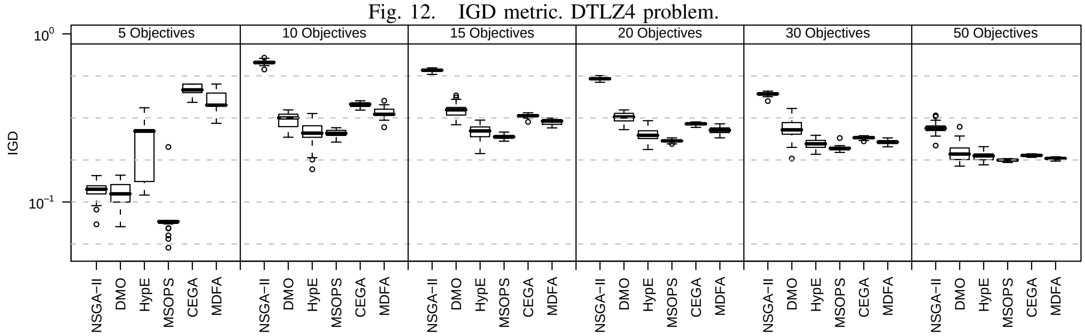
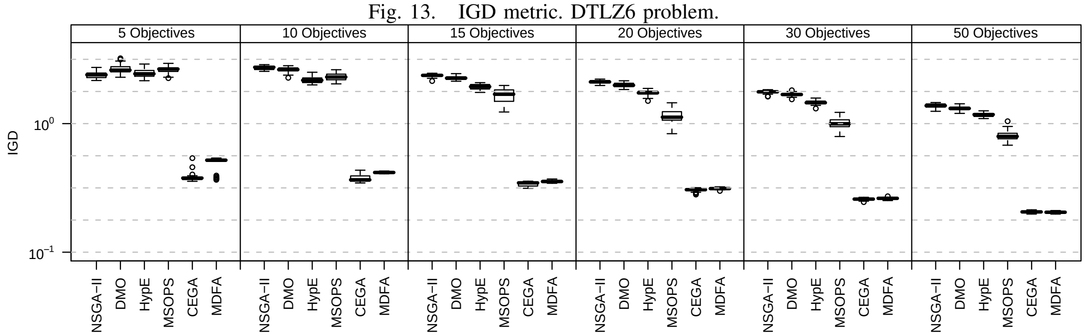


Fig. 13. IGD metric. DTLZ6 problem.



in terms of convergence, and that such behavior remains consistent as the number of objectives increases. The success of our proposed approaches is mainly due to the use of an appropriate discrimination scheme, since this was identified in our previous work to be a key aspect to perform an effective search through high-dimensional objective spaces.

Nevertheless, our results for the IGD metric indicate that our proposed approaches are less effective in terms of diversity preservation than the considered state-of-the-art algorithms. Thus, the development of algorithms being able to converge in high-dimensional objective spaces, while maintaining good diversity, remains as a research challenge.

Due to space limitations we have presented results for only four test cases, but similar results (not reported here) were obtained for two additional problems. However, it is necessary to extend these experiments to a larger set of test functions as well as to adopt real-world many-objective problems in order to generalize our results. Also, the consideration of a wider set of performance metrics is required in order to derive more general conclusions about the performance of the studied approaches.

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