Improving the Diversity Preservation of Multi-objective Approaches used for Single-objective Optimization

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—The maintenance of a proper diversity is an important issue for the correct behavior of Evolutionary Algorithms (EAs). The loss of diversity might lead to stagnation in suboptimal regions, producing the effect known as "premature convergence". Several methods to avoid premature convergence have been previously proposed. Among them, the use of Multi-objective Evolutionary Algorithms (MOEAs) is a promising approach. Several ways of using MOEAs for single-objective optimization problems have been devised. The use of an additional objective based on calculating the diversity that each individual introduces in the population has been successfully applied by several researchers. Several ways of measuring the diversity have also been tested. In this work, the main weaknesses of some of the previously presented approaches are analyzed. Considering such drawbacks, a new scheme whose aim is to maintain a better diversity than previous approaches is proposed. The proposed approach is empirically validated using a set of well-known single-objective benchmark problems. Our preliminary results indicate that the proposed approach provides several advantages in terms of premature convergence avoidance. An analysis of the convergence in the average-case is also carried out. Such an analysis reveals that the better ability of our proposed approach to deal with premature convergence produces a reduction in the convergence speed in the average-case for several of the benchmark problems adopted.

I. Introduction

Evolutionary Algorithms (EAs) are one of the most popular strategies for solving complex optimization problems. EAs have shown great promise for obtaining solutions for large and difficult optimization problems. There are two major targets when improving the performance of EAs [1]. On the one hand, with the aim of reducing the computational burden involved in the use of EAs, their convergence must be as fast as possible. However, on the other hand, premature convergence must be avoided. These aims are conflicting, so the improvement in one of them might negatively influence the other one.

Premature convergence is one of the most frequent drawbacks that must be faced when using evolutionary approaches. It appears when every member of the population is in a suboptimal region and the scheme is not able to generate new individuals that are superior to their parents. For many problems, EAs might have a tendency to converge towards local optima. The likelihood of this occurrence depends on the shape of the fitness landscape [2]. The main reason for having premature convergence is that the use of finite population sizes leads to the phenomenon known as *genetic drift* [3]. Several methods have been devised to deal with premature convergence [4]. Among them, some of the most commonly used are the following:

- Restart the approach when stagnation is detected [3].
- Increase the population size with the aim of avoiding genetic drift [3].
- Apply mating restrictions as incest prevention [5], i.e., avoid the mating of individuals which are very similar. This is also known as *speciation*.
- Perform cataclysmic mutation [6]—highly disruptive mutations—when the diversity has been lost.
- Perform selection applying fitness sharing [7]. In this case, highly similar individuals are clustered and penalized by sharing the obtained fitness values among the members of the group that lie in the same niche (i.e., those that are very close from each other either in decision or in objective function space).
- Apply crowding-based selection where each offspring replaces similar individuals in the parents popula- tion [8].
- Use complex population structures, such as the island-based model [9] or the cellular approaches [10].

Multi-objective evolutionary algorithms (MOEAs) are the adaptation of EAs for dealing with multi-objective optimization problems. Several MOEAs have been proposed in the literature. Among them, the Non-dominated Sorting Genetic Algorithm II (NSGA-II) is one of the most popular ones. The optimiza- tion goal of multi-objective solvers involves multiple objec- tives [11]. First, the distance of the resulting non-dominated set to the Pareto Front should be minimized. A good distribution

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of the solutions found is also desirable. Finally, the extent of the non-dominated front should be maximized. In order to fulfill these requirements, most MOEAs try to maintain a proper diversity in the space of the objectives. Several authors have claimed that, for this reason, the use of multi-objective solvers for single-objective optimization might be helpful [12].

Multiobjectivization [13] is a method that allows the use of multi-objective solvers for dealing with single-objective optimization problems. Multiobjectivization changes the fitness landscape of the optimization problem and, therefore, it can be useful to avoid premature convergence and/or stagnation [14]. Consequently, multiobjectivization might facilitate the resolution of the considered problem. However, it can also produce a problem which is harder than the original one [15]. Multiobjectivization can be carried out following two general schemes: decomposition and aggregation. The first one is based on decomposing the original objective into several components. Then, each of the components is used as an objective. The second type of multiobjectivization is based on adding a new objective function. Such a function is used together with the original objective function. Another way of using multi-objective solvers for single-objective optimization is by considering the preservation of the diversity as an objective [12], [16]. These approaches have been referred to as multiobjectivization in some previous works [17], [18]. However, there is an important difference between this new kind of approaches and the original definition of multiobjectivization: in the new proposal, the calculation of the additional objective depends on the other individuals of the population. In order to avoid misunderstandings, the term multiobjectivization is not used in this paper to refer to this sort of scheme. Instead, the term *diversity-based multi-objective methods* is used.

Several diversity-based multi-objective methods were proposed in [18] for single-objective optimization. They are an extension of the methods proposed in [12], [16]. Basically, the genetic distance between each individual and its nearest individual is calculated, and considered as the second objective to optimize. Then, the NSGA-II is applied. Thus, individuals which are in highly populated regions are penalized. In addition, a penalization of the individuals with a very poor fitness is carried out. Results were compared with those obtained by single-objective approaches, showing the benefits of the diversity-based multi-objective schemes. In this paper, some drawbacks of such a scheme are detected and analyzed. In addition, a new scheme that overcomes such disadvantages is proposed. The main objective of the new proposal is to maintain a better diversity than the original approach, with the aim of avoiding premature convergence. The computational results show that the new scheme produces improvements in the avoidance of premature convergence. However, convergence speed has been reduced in the average case.

The rest of the paper is organized as follows. Section II presents the main diversity-based multi-objective schemes available in the literature. The main drawbacks of the previously presented methods are described in Section III. Such a section is also devoted to describe the set of modifications that have been incorporated in our proposed scheme in order to overcome the detected weaknesses. Then, our experimental validation is presented in Section IV. Finally, conclusions and some lines of future work are given in Section V.

II. DIVERSITY-BASED MULTI-OBJECTIVE APPROACHES

Diversity-based multi-objective approaches for single-objective optimization are based on calculating, for each individual, an additional objective that does not depend solely on the genotype. In the rest of the paper, the original objective is referred to as fitness objective, while the additional objective is referred to as diversity objective. Several options have been proposed to define the diversity objective. In some cases, such objectives have not been a direct measure of the diversity. However, they promote the maintenance of a proper diversity in the population. Among them, some of the best well-known are the following [12]:

- Random: A random value is assigned as the diversity objective to be minimized. Smaller random values may be assigned to some low-quality individuals that would get a chance to survive.
- Inversion: In this case, the optimization direction of the fitness objective function is inverted and is used as the diversity objective. This approach highly decreases the selection pressure. In fact, every member is non-dominated, so it must be carefully applied.
- Time stamp: The diversity objective is calculated as a time stamp of each individual. Each individual in the initial population is marked with a different time stamp represented by a counter which gets incremented every time a new individual is created. From the second population all newly generated individuals get the same time stamp that is set to the population size plus the generation index. This time stamp must be minimized.

In other cases, the definitions are a direct measure of the diversity. Note that a measure of the population diversity is not required. Instead, the objective must be a measure of the diversity introduced by the individual in the population. The most popular objectives are based on calculating Euclidean distances among individuals [16]:

- DCN: The distance to the closest neighbor of the population has to be maximized.
- ADI: The average distance to all individuals of the population has to be maximized.
- DBI: The distance to the best individual of the population, i.e., the one with the lowest fitness—if we deal with a minimization problem—has to be maximized.

In other cases, the diversity objective depends on the formulation of the problem. In [17], the objective is calculated considering the distances among the behaviors of a set of robots that are evolved. Thus, the approach is very similar to the one proposed in [16], but the distances in the genotype are replaced by distances in the behavior.

An analysis considering several objective definitions was performed in [16]. It revealed the superiority of the distance-based diversity objectives. An extension of these methods was proposed in [18]. Such an extension has been considered as the starting point of this research. The scheme works as follows. The MOEA applied is the NSGA-II. The diversity objective is the DCN. However, it was modified with the aim of penalizing

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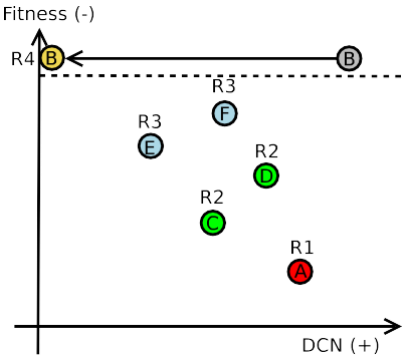


Figure 1. Behavior of NSGA-II with DCN-THR

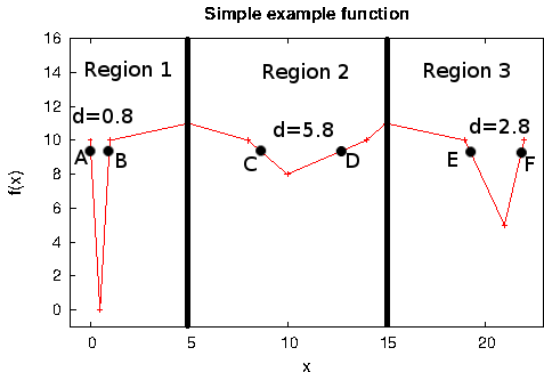


Figure 2. Simple function in which diversity maintenance problems arise

the individuals having a very low quality. In order to perform the penalization, it incorporates the use of a threshold ratio ($th \in [0, 1]$) which must be specified by the user. Such a diversity objective is named DCN-THR. Being *bestFit* the fitness value of the best individual of the population, and *shift* a value that ensures that $bestFit - shift \geq 0$ in the whole optimization process, the threshold value (v) for a minimization problem is defined as:

$$v = \frac{(bestFit - shift)}{th} + shift \quad (1)$$

The threshold ratio is used to avoid the survival of individuals with a very low quality. Figure 1 shows the behavior of DCN-THR. Each individual is represented with a circle with its tag inside. Their non-domination ranks are also shown. The diversity objective of individuals whose fitness value is higher than v (represented by a broken line) is assigned to 0. For the remaining individuals, DCN is used. As a result, individuals that cannot achieve the fixed threshold are penalized. Therefore, the aim of DCN-THR is to maintain a proper diversity among individuals with a minimum level of quality. In the case where $th = 0$, individuals are never penalized. Thus, DCN-THR with $th = 0$ has the same behavior as the DCN function. The incorporation of the threshold value provided significant benefits. The main drawback is that the proper threshold value depends on the problem to solve. However, a hyperheuristic was used to automatically control this parameter.

III. Improvement of the Diversity Preservation

The aforementioned scheme obtained high-quality solutions for a large set of single-objective optimization problems [19]. However, a subsequent analysis showed that in some executions premature convergence was arising. Although the probability of appearance was very low, it was a clear disadvantage. Thus, an analysis to detect the reasons of the emergence of the genetic drift was developed.

Figure 2 shows a simple single-objective function with one decision variable. The function—which must be minimized—presents two local maxima that separate the space into three different regions. Each dot represents an individual which is alive in the current generation. It might be a member of the population or a member of the offspring. Each region is covered by two individuals, so a proper diversity has been

Algorithm 1 Proposed survivor selection scheme (DCN-THR-REF)

```
1: Best = Individual with best f(x)
2: NewPop = { Best }
3: CurrentMembers = CurrentMembers - { Best }
4: while (|NewPop| < N) do
5:     Calculate DCN-THR of CurrentMembers, considering as reference NewPop
6:     ND = Non-dominated individuals of CurrentMembers
7:     Selected = Randomly select an individual of ND
8:     NewPop = NewPop ∪ Selected
9:     CurrentMembers = CurrentMembers - {Selected}
10: end while
```

maintained. Assuming that the population size has been fixed to three individuals, the survivor selection mechanism must choose the three individuals that will pass to the next generation. In order to preserve a proper diversity, an individual of each region should be selected. Every considered individual has been assigned the same value in its fitness objective. Therefore, the diversity objective determines which members will survive. In this case, the first front consist of individuals C and D, the second front consist of individuals E and F, and the last front consist of individuals A and B. Thus, in case of using NSGA-II with the DCN or DCN-THR approach, the individuals that will survive are C, D, and E or F. Therefore, a proper diversity is not maintained since all individuals belonging to the first region are discarded. In the previous example it was assumed that every individual presents the same value in the fitness objective with the aim of simplifying the explanation. However, similar drawbacks happen even if the fitness objective is not the same for every individual.

The main reason for the improper behavior of the NSGA-II with the DCN-THR scheme is that the diversity objective is a direct measure of the diversity introduced by the individual in the current generation. As a result, performing the selection of the individuals without considering the individuals that have been previously selected to survive is not appropriate. In order to overcome such a drawback, we propose in Algorithm 1 a new survivor selection scheme (DCN-THR-REF). First, the best individual in the population, i.e., the one with the lowest objective function value—for a minimization problem—is selected. Thus, elitism is ensured in the approach. The ties are broken at random. Then, while the population is not

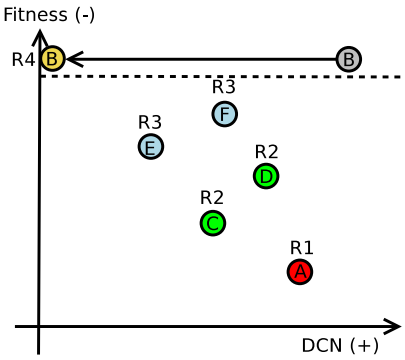


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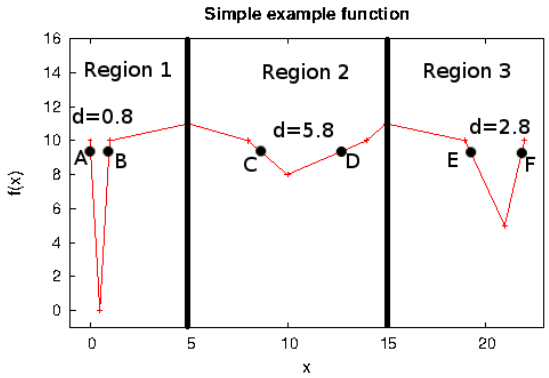


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filled with N individuals, the following steps are executed. First, the DCN-THR objective is recalculated. The calculation considers the currently selected individuals as the reference, i.e., for each pending individual, the distance to the nearest individual previously selected is calculated. Note that in order to update the objective values, the only distances that must be calculated on each step are the ones with the last selected individual. Then, considering the individuals which have not been selected, the non-dominated front is calculated. Finally, a non-dominated individual is randomly selected to survive. It is important to note that the new approach is not a deterministic model. This might also help to avoid premature convergence.

Let us consider the behavior of the new survivor selection scheme with the function in Figure 2. Since every individual has the same value for the fitness function, the first individual is randomly selected. If we assume that the first selected individual is E, then, since A is the farthest individual to E, it will be the second selected individual. Finally, the C individual will be selected because it is far enough from both A and E. Thus, an individual of each region is selected. In fact, independently of the first selected individual, the approach always selects an individual of each region.

IV. Experimental Evaluation

This section shows the experimental evaluation performed with the optimization schemes described in Section III. The models have been implemented using METCO [20] (*Metaheuristic-based Extensible Tool for Cooperative Optimization*). Tests have been run on a Debian GNU/Linux computer with four AMD R Opteron ™ (model number 6164 HE) at 1.7 GHz and 64 GB RAM. The compiler that has been used is GCC 4.6.3. The analyses have been performed with the benchmark problems F1-F11 [19]. They are a set of scalable continuous optimization problems which must be minimized. The parameter D allows setting the number of variables of the problems. In this research, the value $D = 50$ has been considered. These problems have different features and they combine different properties regarding the modality, the separability, and the ease of optimization, dimension by dimension.

Since our experiments involve the use of stochastic algorithms, comparisons have been carried out applying the following statistical analysis, considering a significance level of 5%. First, a *Shapiro-Wilk test* is performed in order to check whether or not the values of the results follow a normal (Gaussian) distribution. If so, the *Levene test* checks for the homogeneity of the variances. If samples have equal variance, an ANOVA *test* is done. Otherwise, a *Welch test* is performed. For non-Gaussian distributions, the non-parametric *Kruskal-Wallis* test is used to compare the medians of the algorithms.

Two kinds of experiments have been performed. The first one focuses on analyzing the average behavior of the new proposed scheme. The last one focuses on analyzing the properties of the approach regarding premature convergence. For doing such an analysis, the behavior of the worst executions obtained with the scheme has been studied.

A. Analysis of the average case

In the first analysis, NSGA-II with DCN-THR and DCN-THR-REF was executed, using different values of th. Specifically, the values $th = \{0, 0.2, 0.4, 0.6, 0.8\}$ were considered. Typical values were considered for the remaining parameters of NSGA-II. The population size was fixed to 100 individuals, a mutation probability (p_m) equal to 0.02 ($\frac{1}{D}$) was considered, and the crossover operator was applied in every case ($p_c = 1$). The mutation operator adopted was polynomial-based mutation, while the crossover operator adopted was the simulated binary crossover (SBX). In every case, the parameter *shift* was fixed to -1000. This value is lower than any of the optima of the considered problems. Finally, the stopping criterion was fixed as the execution of 1×10^5 function evaluations.

Table I. Probability of selecting the best individuals

	Prob. of 10 best ind.		Prob. of 20 best ind.	
	DCN-THR	DCN-THR-REF	DCN-THR	DCN-THR-REF
F1	90.01%	79.68%	85.02%	72.17
F2	94.44%	87.73%	89.89%	83.37
F3	91.05%	86.57%	85.10%	79.37
F4	92.11%	91.04%	87.02%	86.35
F5	89.97%	79.86%	84.03%	72.42
F6	99.50%	97.12%	94.52%	92.93
F7	90.84%	84.32%	84.80%	78.04
F8	92.63%	90.24%	84.60%	85.62
F9	93.16%	90.64%	90.46%	87.37
F10	91.09%	82.52%	85.11%	74.03
F11	92.75%	90.56%	88.44%	87.79

The NSGA-II configurations have been independently run 100 times for each benchmark problem. Figure 3 shows the median obtained for each case at the end of the executions. In the cases where the differences between the results obtained with DCN-THR-REF and DCN-THR have been statistically significant, a vertical line joining their medians is shown. In most cases (F2 and F3 are the exceptions), the model that used DCN-THR-REF obtained a higher median than the model that considered DCN-THR. Moreover, in most cases, differences have been statistically significant. The reason is that maintaining a proper diversity might reduce the convergence speed of the average case. In fact, the aim of maintaining a proper diversity is not to improve the convergence speed of the average case, but to prevent the achievement of highly suboptimal results in the worst executions.

In order to better understand the reasons why the new approach presents a suboptimal behavior, the probability of survival of the best-fitted individuals has been experimentally calculated when using DCN-THR-REF and DCN-THR with $th = 0$. Table I shows the average probability of survival of the 10 best individuals, and of the 20 best individuals. In every case, the probabilities of selecting the individuals with best fitness values have been larger for the configurations that use DCN-THR than for the configurations that consider DCN-THR-REF. This means that the scheme with DCN-THR tends to focus on the best-fitted individuals, while the scheme with DCN-THR-REF performs a more diverse selection. Therefore, for the cases in which premature convergence does not arise— the majority of the executions—the selection based on DCN- THR converges faster. Other values of th were also tested. The selection probabilities highly depend on th. However, for a fixed th value, higher probabilities have appeared with DCN-THR than with DCN-THR-REF in every case.

The previous analysis has shown the superiority of the DCN-THR scheme in the average case. In order to quantify such an improvement, run-length distributions [21] (RLDs)

filled with N individuals, the following steps are executed. First, the DCN-THR objective is recalculated. The calculation considers the currently selected individuals as the reference, i.e., for each pending individual, the distance to the nearest individual previously selected is calculated. Note that in order to update the objective values, the only distances that must be calculated on each step are the ones with the last selected individual. Then, considering the individuals which have not been selected, the non-dominated front is calculated. Finally, a non-dominated individual is randomly selected to survive. It is important to note that the new approach is not a deterministic model. This might also help to avoid premature convergence.

Let us consider the behavior of the new survivor selection scheme with the function in Figure 2. Since every individual has the same value for the fitness function, the first individual is randomly selected. If we assume that the first selected individual is E, then, since A is the farthest individual to E, it will be the second selected individual. Finally, the C individual will be selected because it is far enough from both A and E. Thus, an individual of each region is selected. In fact, independently of the first selected individual, the approach always selects an individual of each region.

IV. Experimental Evaluation

This section shows the experimental evaluation performed with the optimization schemes described in Section III. The models have been implemented using METCO [20] (*Metaheuristic-based Extensible Tool for Cooperative Optimization*). Tests have been run on a Debian GNU/Linux computer with four AMD ® Opteron ™ (model number 6164 HE) at 1.7 GHz and 64 GB RAM. The compiler that has been used is GCC 4.6.3. The analyses have been performed with the benchmark problems F1-F11 [19]. They are a set of scalable continuous optimization problems which must be minimized. The parameter D allows setting the number of variables of the problems. In this research, the value $D = 50$ has been considered. These problems have different features and they combine different properties regarding the modality, the separability, and the ease of optimization, dimension by dimension.

Since our experiments involve the use of stochastic algorithms, comparisons have been carried out applying the following statistical analysis, considering a significance level of 5%. First, a *Shapiro-Wilk test* is performed in order to check whether or not the values of the results follow a normal (Gaussian) distribution. If so, the *Levene test* checks for the homogeneity of the variances. If samples have equal variance, an ANOVA *test* is done. Otherwise, a *Welch test* is performed. For non-Gaussian distributions, the non-parametric *Kruskal-Wallis* test is used to compare the medians of the algorithms.

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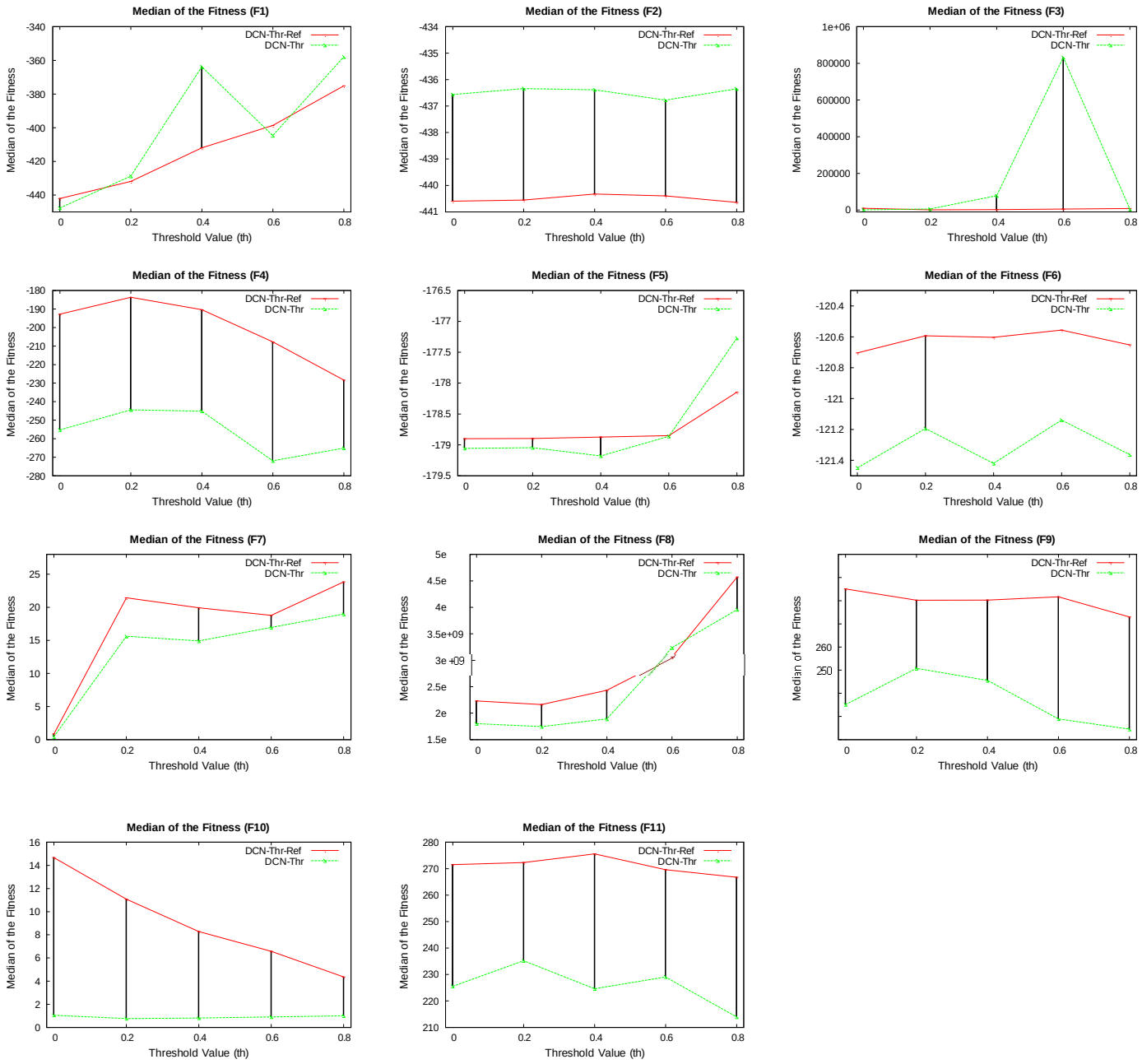


Figure 3. Median of the fitness obtained with different threshold values

have been used. They show the relationship between success ratios and number of evaluations. Success ratio is defined as the probability of achieving a certain quality level. Table II shows the percentage of evaluations that are saved by using DCN- THR, considering a success ratio of 50%. The quality level has been fixed as the highest median obtained by DCN-THR or DCN-THR for each threshold value in 1×10^5 evaluations. The negative values indicate that DCN-THR-REF obtained a better performance. For each problem, data for the threshold value that obtained the best median is shown in boldface. In the average case, the number of extra evaluations required by DCN-THR-REF is considerable.

Table II. PERCENTAGE OF SAVED EVALUATIONS BY NOT USING THE REFERENCE

	$Th = 0$	$Th = 0.2$	$Th = 0.4$	$Th = 0.6$	$Th = 0.8$
F1	20%	-5%	-40%	5%	-17.5%
F2	-17.5%	-17%	-17.5%	-15%	-17.5%
F3	30%	-22.5%	-27.5%	-27.5%	5%
F4	32.5%	35%	32.5%	37.5%	27.5%
F5	25%	25%	30%	2.5%	-25%
F6	35%	40%	45%	40%	35%
F7	17.5%	25%	28.20%	7.89%	40%
F8	10%	10%	12.5%	-2.5%	12.5%
F9	35%	23.07%	27.5%	37.5%	30%
F10	45%	42.5%	37.5%	32.5%	22.5%
F11	30%	32.5%	37.5%	30%	32.5%

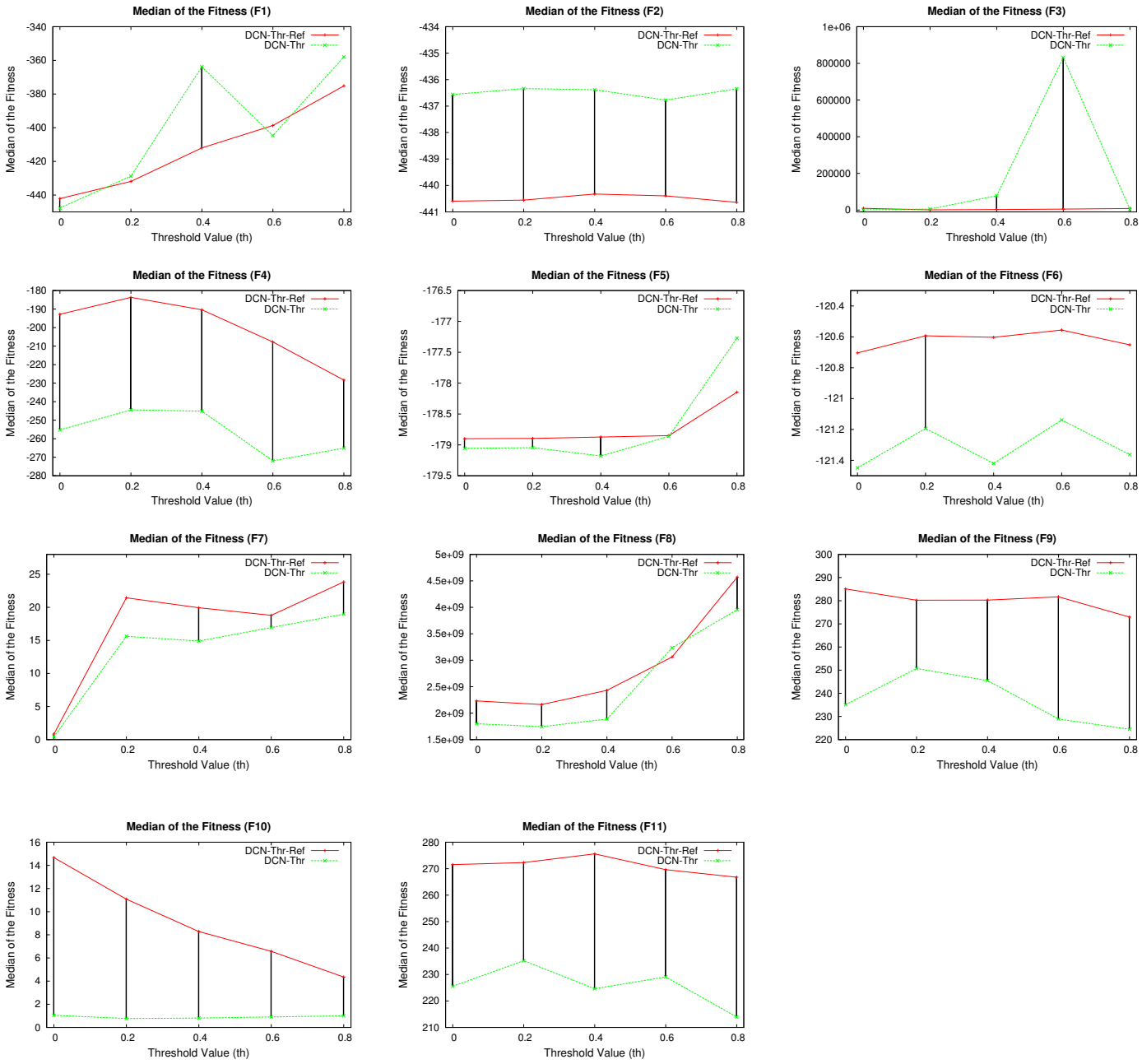


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F5	25%	25%	**30%**	2.5%	-25%
F6	**35%**	40%	45%	40%	35%
F7	**17.5%**	25%	28.20%	7.89%	40%
F8	10%	**10%**	12.5%	-2.5%	12.5%
F9	35%	23.07%	27.5%	37.5%	**30%**
F10	45%	**42.5%**	37.5%	32.5%	22.5%
F11	30%	32.5%	37.5%	30%	**32.5%**

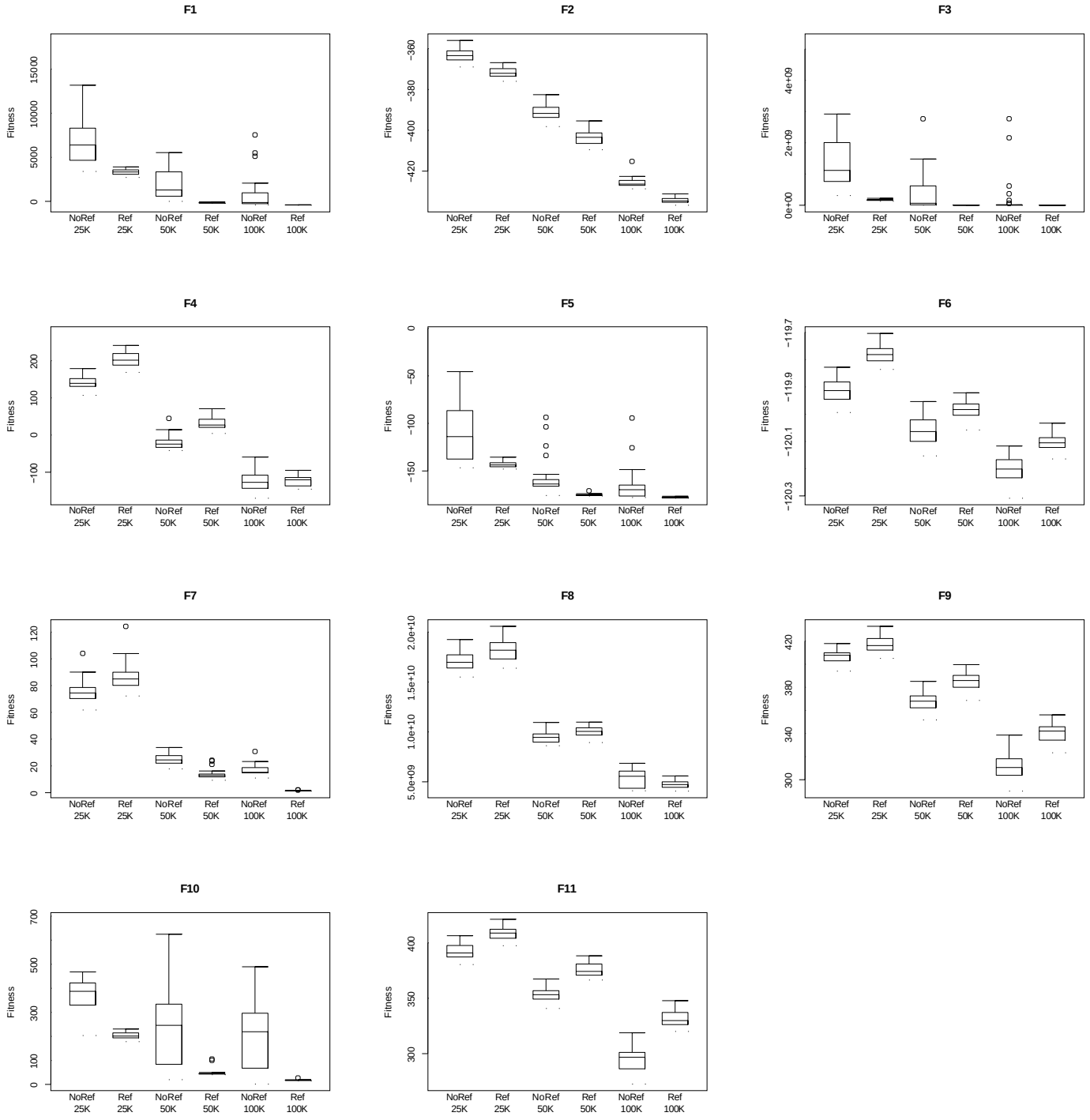


Figure 4. Boxplots of the worst-behaved executions

B. Analysis of the worst case

In the second analysis, the worst-case behavior of the previous considered approaches has been studied. For each problem, the threshold value that performed the best with DCN-THR has been used. In order to perform the analysis, each configuration was executed 3.000 times. The executions were gathered in groups of 100 executions, and the worst of each group was stored. Thus, a set of 30 results for each configuration and benchmark problem was taken into account. The obtained data represents the worst results that are obtained with a 1% of probability.

Figure 4 shows the boxplots of the fitness values obtained by using DCN-THR, and DCN-THR-REF. Three different stop criteria have been considered: 2.5×10^4, 5×10^4, and 1×10^5

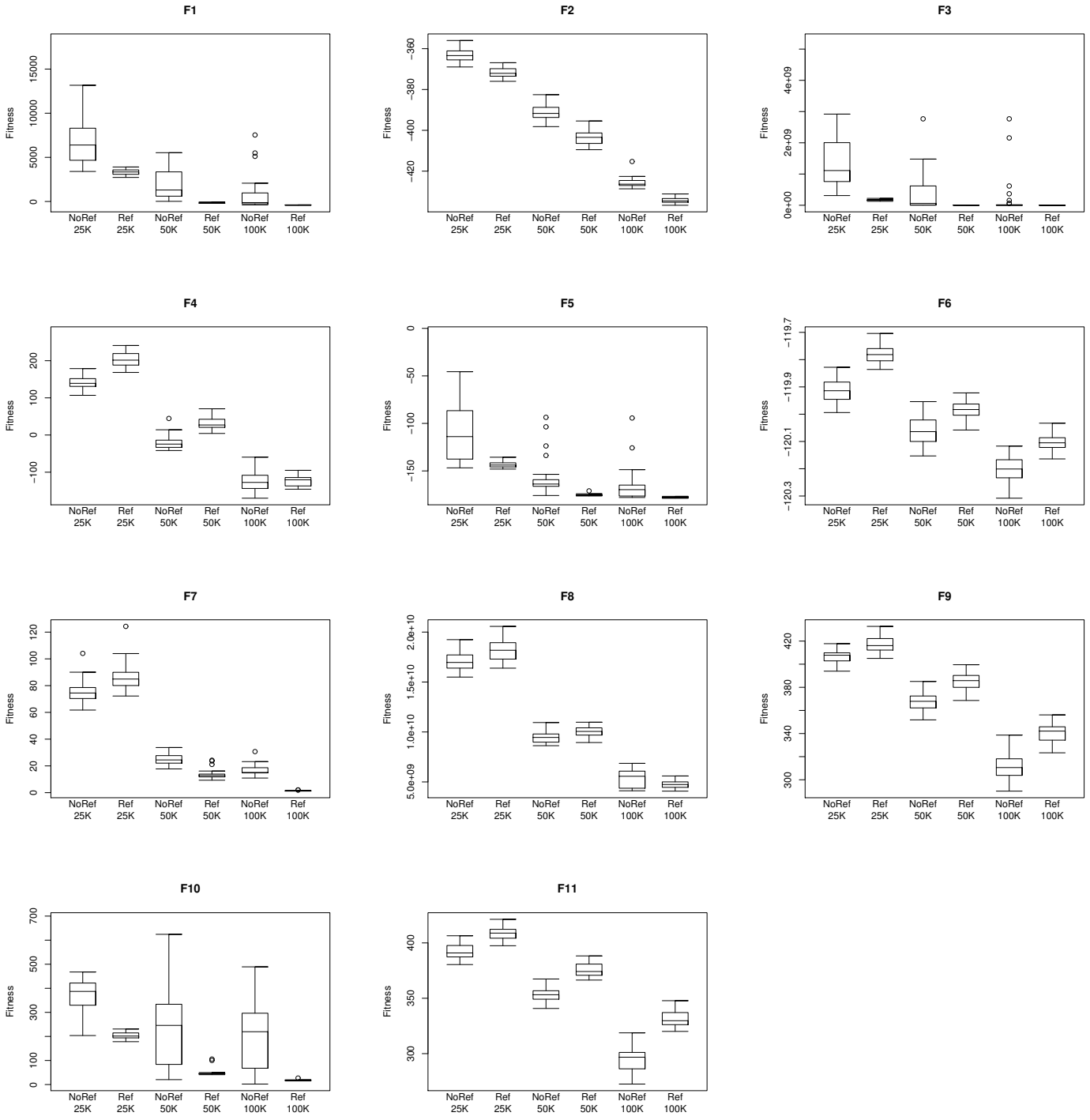


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