Searching for a practical evidence of the No Free Lunch theorems

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Abstract. According to the No Free Lunch (NFL) theorems all blackbox algorithms perform equally well when compared over the entire set of optimization problems. An important problem related to NFL is finding a test problem for which a given algorithm is better than another given algorithm. Of high interest is finding a function for which Random Search is better than another standard evolutionary algorithm. In this paper we propose an evolutionary approach for solving this problem: we will evolve test functions for which a given algorithm A is better than another given algorithm B. Two ways for representing the evolved functions are employed: as GP trees and as binary strings. Several numerical experiments involving NFL-style Evolutionary Algorithms for function optimization are performed. The results show the effectiveness of the proposed approach. Several test functions for which Random Search performs better than all other considered algorithms have been evolved.

1 Introduction

Since the advent of the No Free Lunch (NFL) theorems in 1995 [17,18], the trend of Evolutionary Computation (EC) [9] have not changed at all, although these breakthrough theories should have produced dramatic changes. Most researchers chose to ignore NFL theorems: they developed new algorithms that work better than the old ones on some particular test problems. The researchers have eventually added:

"The algorithm A performs better than another algorithm on the considered test functions".

That is somehow useless since the proposed algorithms cannot be the best on all the considered test functions.

Moreover, most of the functions employed for testing algorithms are artificially constructed.

Consider for instance, the field of evolutionary single-criteria optimization where most of the algorithms were tested and compared on some artificially constructed test functions (most of them being known as De'Jong test problems) [9,14]. These test problems were used for comparison purposes before the birth of the NFL theorems and they are used even today (9 years later after the birth of the NFL theorems). Evolutionary multi-criteria optimization was treated in a similar manner: most of the recent algorithms in this field were tested on several artificially constructed test functions proposed by K. Deb in [3].

Roughly speaking, the NFL theorems state that all black-box optimization algorithms perform equally well over the entire set of optimization problems. Thus, if an algorithm A is better than another algorithm B on some classes of functions, the algorithm B is better than A on the rest of the functions.

As a consequence of the NFL theories, even a computer program (implementing an Evolutionary Algorithm (EA)) containing programming errors can perform better than some other highly tuned algorithms for some test functions.

Random Search (RS) being a black box search / optimization algorithm should perform better than all of the other algorithms for some classes of test functions. Even if this statement is true, there is no result reported – in the literature – of a test function for which RS performs better than all the other algorithms (taking into account the NFL restriction concerning the number of distinct solutions visited during the search). However, in [4] is presented a function which is hard for all Evolutionary Algorithms.

Instead, a lot effort is spent for proving that the No Free Lunch theorems are not true. Most researchers [4, 5, 12, 15, 16] have tried to find some classes of problems for which NFL does not hold. For instance, in [5] is shown that NFL might not hold for small problems (that have a small search space).

Three questions (on how we match problems to algorithms) are of high interest:

- For a given class of problems, what is (are) the algorithm(s) that performs (perform) better than all other algorithms?
- For a given algorithm what is (are) the class(es) of problems for which the algorithm performs best?
- Given two algorithms A and B, what is (are) the class (es) of problems for which A performs better than B?

Answering these questions is not an easy task. All these problems are still open questions and they probably lie in the class of the NP-Complete problems. If this assumption is true it means that we do not know if we are able to construct a polynomial algorithm that takes a function as input and outputs the best optimization algorithm for that function (and vice versa). Fortunately, we can try to develop a heuristic algorithm able to handle this problem.

In this paper we develop a framework for constructing test functions that match a given algorithm. More specific, given two algorithms A and B, the question is:

What the functions for which A performs better than B (and vice-versa) are?

For obtaining such functions we will use an evolutionary approach: the functions matched to a given algorithm are evolved by using an standard evolutionary algorithms ¹.

Of high interest is finding a test function for which Random Search performs better than all considered standard evolutionary algorithms. Using the proposed approach we were able to evolve such test problems ².

The paper is organized as follows: The NFL algorithm is minutely described in section 2. Test functions represented as GP trees are evolved in section 3. The fitness assignment process is described in section 3.1. The algorithms used for comparison are described in section 3.2. Several numerical experiments are carried out in section 3.3. Test functions represented as binary strings are evolved in section 4. The fitness assignment process is described in section 4.2. The algorithms used for comparison are described in section 4.3. Several numerical experiments are carried out in section 4.4.

2 A NFL-style Algorithm

We define a black-box optimization algorithm as indicated by Wolpert and McReady in [17, 18].

The evolutionary model (the NFL-style algorithm) employed in this paper uses of a population consisting of a single individual. This considerably simplifies the description and the implementation of a NFL-style algorithm.

No archive for storing the best solutions found so far (see for instance *Pareto Archived Evolution Strategy* [11]) is maintained. However, we implicitly maintain an archive containing all the distinct solutions explored until the current state. We do so because only the number of distinct solutions is counted in the NFL theories. This kind of archive is also employed by Tabu Search [7, 8].

The variables and the parameters used by a NFL-style algorithm are given in Table 1.

The algorithm starts with a randomly generated solution (the current solution) over the search space. This solution is added to the archive. The following steps are executed until MAXSTEPS different solutions are explored: Generate a solution in the neighborhood of the current solution. This new solution is usually obtained by mutating the current solution. We have to ensure that the newly generated solution is different from all previously explored solutions (The algorithm that generates a solution different from all other solutions explored so far is given further in this section). We add the generated solution to the archive and it becomes the current solution which will be further explored.

The NFL-style algorithm is the following:

¹ Source code used for evolving test function is available at www.nfl.cs.ubbcluj.ro

² Test functions for which Random Search performs better than other standard Evolutionary Algorithms are available at www.nfl.cs.ubbcluj.ro

Table 1. The variables used by the NFL algorithm.

Variable	Meaning
Archive	the archive storing all distinct solutions visited by
	algorithm
$curr_sol$	the current solution (point in the search space)
new_sol	a new solution (obtained either by mutation or by
	initialization)
MAXSTEPS	the number of generations (the number of distinct
	points in the search space visited by the algo-
	rithm).
t	the number of distinct solutions explored so far

NFL-style Algorithm

An important issue concerning the NFL algorithm described above is related to the step S_6 which selects a new solution that does not belong to the Archive. This is usually done by mutating the current solution and keeping the offspring if the latter does not already belong to the Archive (The actual acceptance mechanism is minutely described in sections 3.2 and 4.3). If the offspring belongs to the Archive for a fixed number of mutations (steps) it means that the neighborhood of the current solutions could be exhausted (completely explored). In this case, a new random solution is generated and the search process moves to another region of the search space. It is sometimes possible that the generated solution to already belong to the Archive. In this case, another random solution is generated over the search space. We assume that the search space is large enough and after a finite number of re-initializations the generated solution will not belong to the Archive.

The algorithm for selecting a new solution which does not belong to the *Archive* (the step S_6) is given below:

```
SS_1. nr_mut = 0; // the number of mutations is set to 0 SS_2. Repeat SS_3. textsf new_sol = Mutate (curr_sol); SS_4. nr_mut = nr_mut + 1; SS_5. until (nr_mut = MAX_MUTATIONS) and (new_sol \notin Archive) and Accepted(new_sol); SS_6. while new_sol \notin Archive do SS_7. Initialize(new_sol); //we jump in another randomly chosen point of the search space SS_8. endwhile
```

3 Real-valued functions

Test functions represented as GP trees are evolved in this section.

3.1 Evolutionary Model and the Fitness Assignment Process

Our aim is to find a test function for which a given algorithm A performs better than another given algorithm B. The test function that is being searched for will be evolved by using Genetic Programming [10] with steady state [13].

The quality of the test function encoded in a GP chromosome is computed in a standard manner. The given algorithms A and B are applied to the test function. These algorithms will try to optimize (find the minimal value of) that test function. To avoid the lucky guesses of the optimal point, each algorithm is run 500 times and the results are averaged. Then, the fitness of a GP chromosome is computed as the difference between the averaged results of the algorithm A and the averaged results of the algorithm A. In the case of function minimization, a negative fitness of a GP chromosome means that the algorithm A performs better than the algorithm B (the values obtained by A are smaller (on average) than those obtained by B).

3.2 Algorithms Used for Comparison

We describe several evolutionary algorithms used for comparison purposes. All the algorithms described in this section are embedded in the NFL-style algorithm described in section 2. More precisely, the considered algorithms particularize the solution representation, the mutation operator, and the acceptance mechanism (the procedure *Accepted*) of the NFL algorithm described in section 2. The mutation operator is the only search operator used for exploring the neighborhood of a point in the search space.

 A_1 – real encoding (the individuals are represented as real numbers using 32 bits), Gaussian mutation with $\sigma_1 = 0.001$, the parent and the offspring compete

for survival.

 A_2 – real encoding (the individuals are represented as real numbers using 32 bits), Gaussian mutation with $\sigma_2 = 0.01$, the parent and the offspring compete for survival.

 A_3 – binary encoding (the individuals are represented as binary strings of 32 bits), point mutation with $p_m = 0.3$, the parent and the offspring compete for survival.

 A_4 – binary encoding (the individuals are represented as binary strings of 32 bits), point mutation with $p_m = 0.1$, the parent and the offspring compete for survival.

3.3 Numerical Experiments

Several numerical experiments for evolving functions matched to a given algorithm are performed in this section. The algorithms used for comparison have been described in section 3.2.

The number of dimensions of the space is set to 1 (i.e. one-dimensional functions) and the definition domain of the evolved test functions is [0, 1].

The parameters of the GP algorithm are given in Table 2.

Table 2. The parameters of the GP algorithm used for numerical experiments

Parameter	Value
Population size	50
Number of generations	10
Maximal GP tree depth	6
Function set	$F = \{+, -, *, sin, exp\}$
Terminal set	$T = \{x\}$
Crossover probability	0.9
Mutation	1 mutation / chromosome
Runs	30

The small number of generations (only 10) has been proved to be sufficient for the experiments performed in this paper.

Evolved functions are given in Table 3. For each pair (A_k, A_j) is given the evolved test function for which the algorithm A_k performs better than the algorithm A_j . The mean of the fitness of the best GP individual over 30 runs is also reported.

From Table 3 it can be seen that the proposed approach made possible the evolving of test functions matched to the most of the given algorithms. The

Table 3. The evolved test functions

Algorithms	Evolved Test Function	Averaged fitness
(A_1, A_2)	$f_1(x) = 0.$	0
(A_2, A_1)	$f_2(x) = -6x^3 - x.$	-806.03
(A_3, A_4)	$f_3(x) = x - 2x^5.$	-58.22
(A_4, A_3)	$f_4(x) = -4x^8.$	-34.09
(A_2, A_4)	$f_5(x) = 0.$	0
(A_4,A_2)	$f_6(x) = -6x^3 - x.$	-1601.36

results of these experiments give a first impression of how difficult the problems are. Several interesting observations can be made:

The GP algorithm was able to evolve a function for which the algorithm A_2 (real encoding with $\sigma=0.01$) was better then the algorithm A_1 (real encoding with $\sigma=0.001$) in all the runs (30). However, the GP algorithm was not able to evolve a test function for which the algorithm A_1 is better that the algorithm A_2 . In this case the function f(x)=0 (where both algorithms perform the same) was the only one to be found. It seems to be easier to find a function for which an algorithm with larger "jumps" is better than an algorithm with smaller "jumps" than to find a function for which an algorithm with smaller "jumps" is better than an algorithm with larger "jumps".

A test function for which the algorithm A_4 (binary encoding) is better than the algorithm A_2 (real encoding) was easy to find. The reverse (i.e. a test function for which the real encoding algorithm A_2 is better than the binary encoded algorithm A_4) has not been found by using the GP parameters considered in Table 2.

4 Binary-valued functions

Test functions represented as binary strings are evolved in this section. We employed the binary-strings representation for the test functions because in this way we can evolve any function without being restricted to a given set of operators.

4.1 Prerequisite

Our analysis is performed in the finite search space X [17]. The space of possible "cost" values, Y, is also finite. We restrict our analysis to binary search spaces. This is not a hard restriction since all other values can be represented as binary strings. Thus $X = \{0,1\}^n$ and $X = \{0,1\}^m$.

An optimization problem f is represented as a mapping $f: X \mapsto Y$.

The set $F = Y^X$ denotes the space of all possible problems. The size of F is $|Y|^{|X|}$.

In our experiments n = 16 and m = 8. Thus $|X| = 2^{16} = 65536$ and $|Y| = 2^8 = 256$. The number of optimization problems in this class is $|Y|^{|X|} = 256^{65536} \approx 10^{157826}$.

Each test problem in this class can be stored in a string of 65536 * 8bits = 512Kb.

Within this huge search space we will try to find test problems for which a given algorithm A is better than another given algorithm B.

4.2 Evolutionary Model and the Fitness Assignment Process

Our aim is to find a test function for which a given algorithm A performs better than another given algorithm B. The test function that is being searched for will be represented as strings over the $\{0,1\}$ alphabet as described in section 4.1.

The algorithm used for evolving these functions is a standard steady state [13] Evolutionary Algorithm that works with a binary encoding of individuals [1, 2]. Each test problem in this class can be stored in a string of 65536*8bits = 512Kb.

The most important aspect of this algorithm regards the way in which the fitness of an individual is computed.

The quality of the test function encoded in a chromosome is computed as follows: The given algorithms A and B are applied to the test function. These algorithms will try to optimize (find the minimal value of) that test function. To avoid the lucky guesses of the optimal point, each algorithm is run 100 times and the results are averaged. Then, the fitness of a chromosome encoding a test function is computed as the difference between the averaged results of the algorithm A and the averaged results of the algorithm B.

In the case of function minimization, a negative fitness of a chromosome means that the algorithm A performs better than the algorithm B (the values obtained by A are smaller (on average) than those obtained by B).

4.3 Algorithms Used for Comparison

We describe several evolutionary algorithms used for comparison purposes. All the algorithms described in this section are embedded in the NFL algorithm described in section 2. More precisely, the considered algorithms particularize the solution representation, the mutation operator, and the acceptance mechanism (the procedure *Accepted*) of the NFL algorithm described in section 2.

All algorithms are derived from (1+1) ES and can be described as follows:

- (i) Individuals are represented as binary strings over the search space X.
- (ii) Mutation operator is the only search operator used for exploring the neighborhood of a point in the search space.
- (iii) The parent and the offspring compete for survival.

The number of mutations / chromosome is a parameter of the compared algorithms. The range for this parameter is 1 up to chromosome length. If the number of mutations / chromosome is equal to the chromosome length, the considered algorithm will behave like Random Search.

Since the number of mutations / chromosome is different from algorithm to algorithm we denote by B_k the NFL-style Algorithm that performs k mutations / chromosome.

4.4 Numerical Experiments

Several numerical experiments for evolving functions matched to a given algorithm are performed in this section. The algorithms used for comparison have been described in section 4.3.

The parameters of the algorithm used for evolving test functions are given in Table 4.

Table 4. The parameters of the algorithm used for evolving test functions

Parameter	Value					
Population size	10					
Number of generations	10					
Crossover type	Uniform					
Crossover probability	0.9					
Mutation type	Point mutation					
Mutation probability	0.01					
Chromosome length	65536*8 bits					
Runs	30					

The small number of generations (only 10) has been proved to be sufficient for the experiments performed in this paper.

Results are given in Table 5. For each pair (B_k, B_j) is given the average (over 30 runs) of best fitness scored by an individual (encoding a test function) for which the algorithm B_k performs better than the algorithm B_j .

Table 5 shows that the proposed approach made possible the evolving of test functions matched to all given algorithms (all fitness values are negative). The results of these experiments give a first impression of how difficult the problems are. Several interesting observations can be made:

In the first row of data (corresponding to the algorithm B_1) the average fitness decrease from -95 (for the pair (B_1, B_2)) to -284 (for the pair (B_1, B_{16})). Knowing that a negative value of the fitness means that the algorithm B_1 is better than the algorithm B_k we may infer that is more easy to find a function for which an algorithm performing 1 mutation/chromosome is better than an algorithm performing 16 mutations/chromosome (the algorithm B_{16} which is actually behaves like Random Search) than to find a test function for which an algorithm performing 1 mutation/chromosome is better than an algorithm performing 2 mutations/chromosome.

If we take a look at each row of data after the cells in the first diagonal we can see that the values have an descending tendency. This means that is easier

Table 5. Fitness of the best individual in the last generation. Results are averaged over 30 independent runs.

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	B_{11}	B_{12}	B_{13}	B_{14}	B_{15}	B_{16}
B_1	-	-95	-53	-19	-102	-69	-79	-108	-151	-214	-182	-192	-159	-246	-259	-284
B_2	-331	-	-132	-119	-195	-177	-197	-163	-192	-230	-254	-284	-261	-291	-313	-356
B_3	-454	-283	-	-122	-196	-179	-171	-234	-264	-293	-236	-319	-317	-324	-315	-333
B_4	-495	-332	-168	-	-176	-159	-190	-185	-248	-259	-327	-321	-330	-421	-334	-374
B_5	-496	-309	-164	-132	-	-125	-198	-151	-266	-244	-285	-250	-259	-346	-364	-338
B_6	-555	-286	-169	-126	-180	-	-175	-163	-200	-243	-197	-284	-276	-340	-364	-351
B_7	-531	-358	-198	-140	-149	-138	-	-159	-199	-250	-207	-230	-262	-272	-306	-345
B_8	-513	-323	-196	-159	-160	-140	-174	-	-202	-220	-217	-259	-289	-311	-291	-328
B_9	-538	-338	-201	-156	-138	-145	-153	-150	-	-204	-197	-237	-271	-306	-312	-315
B_{10}	-526	-336	-190	-190	-156	-134	-149	-151	-131	-	-188	-187	-245	-228	-274	-292
B_{11}	-528	-321	-210	-161	-169	-136	-147	-131	-156	-190	-	-245	-248	-275	-294	-325
B_{12}	-602	-296	-224	-191	-145	-148	-121	-148	-122	-166	-115	-	-205	-234	-262	-287
B_{13}	-493	-331	-193	-127	-152	-136	-125	-167	-143	-182	-154	-164	-	-226	-238	-236
B_{14}	-544	-345	-210	-181	-174	-149	-117	-137	-125	-158	-123	-147	-158	-	-175	-218
B_{15}	-543	-298	-212	-150	-128	-103	-109	-89	-126	-148	-153	-181	-150	-195	-	-202
B_{16}	-583	-329	-234	-151	-144	-129	-108	-83	-115	-134	-147	-158	-129	-161	-173	-

to beat an algorithm performing more mutations than to beat an algorithm performing less mutations / chromosome.

In the first column the values have a descending trend, too. This means that in the space of test functions it is more easy to find a test function for which an algorithm performing 16 mutations/chromosome is better an algorithm performing 1 mutation/chromosome than to find a test function for which an algorithm performing 2 mutations/chromosome is better an algorithm performing 1 mutation/chromosome. This results can be explained by the fact that B_1 and B_{16} are very different whereas B_1 and B_2 are very similar is more difficult to find test problems for which two very similar algorithms perform significantly different.

The lowest value in Table 5 is -583 and it corresponds to pair (B_{16}, B_1) . This means that finding a function for which an algorithm performing 16 mutations/chromosome is better than an algorithm performing 1 mutation/chromosome was the easiest operation. This suggests a rugged fitness landscape of the evolved test function. In order to confirm this hypothesis we have analyzed the landscape of the evolved test functions (30 functions obtained in 30 runs) for the pair (B_{16}, B_1) . Each test function was considered as having 1 real-valued variable over the interval [0, 65535]. The average number of peaks (a point is considered as being a peak (local or global optimum) if its left and right values are higher than its value) of the evolved test functions was 23127 (out of 65536 points). This suggests an highly rugged landscape.

5 Conclusions and Further Work

In this paper, a framework for evolving test functions that are matched to a given algorithm has been proposed. The proposed framework is intended to provide a practical evidence for the NFL theories. Numerical experiments have shown the efficacy of the proposed approach: test functions for which Random Search performs better than all other considered evolutionary algorithm have been successfully evolved.

Further research will be focused on the following directions:

- (i) Proving that the evolved test problems are indeed hard for the considered Evolutionary Algorithms.
- (ii) Comparing other evolutionary algorithms for single and multiobjective optimization. Several test functions matched to some classical algorithms (such as standard GAs or ES) for function optimization will be evolved. In this case the problem is much more difficult since the number of distinct solutions visited during the search process could be different for each algorithm.
- (iii) Evolving difficult test instances for algorithms used for solving other real-world problems (such as TSP [2], symbolic regression [10], classification etc).
- (iv) Finding the set (class) of test problems for which an algorithm is better than the other.

Acknowledgment

The source code for evolving test functions matched to a given algorithm and all the evolved functions described in this paper are available at www.nfl.cs.ubbcluj.ro.

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