Detecting loss of diversity for an efficient termination of EAs

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***Abstract*—Termination of Evolutionary Algorithms (EA) at its steady state so that useless iterations are not performed is a main point for its efficient application to black-box problems. Many EA algorithms evolve while there is still diversity in their population and, thus, they could be terminated by analyzing the behavior some measures of EA population diversity. This paper presents a numeric approximation to steady states that can be used to detect the moment EA population has lost its diversity for EA termination. Our condition has been applied to 3 EA paradigms based on diversity and a selection of functions covering the properties most relevant for EA convergence. Experiments show that our condition works regardless of the search space dimension and function landscape.**

***Keywords*-EA termination; EA population diversity; EA steady state**

I. Introduction

In the absence of theoretical bounds [1]–[4] on the number of Evolutionary Algorithms (EAs) runs ensuring that the minimum has been reached, termination of EAs should rely on conditions computed across iterations. Given that determining convergence to the optimum is difficult to assess in general, a most practical termination criterion should ensure that EA has reached its steady state [5].

There is a rich literature on online termination of EAs. The simplest and most extended one [6]–[8] consists in reaching a number of iterations or function evaluations. This stopping criterion is not useful by itself since the number of iterations that guarantee a steady state significantly varies across problems [6]. This has motivated the definition of alternative criteria based on either a measure derived from EA evolving population [5], [7]–[15] or the internal parameters of a particular EA algorithm [16]–[19]. In the case of EA convergence, some of the former criteria reduce the number of iterations that do not improve results anymore, provided that suitable parameters for the termination condition are given [14].

However, and up to our knowledge, existing online termination conditions have two main shortcomings for their full application to black-box problems. First, most of them have not any conditions ensuring that they terminate EA at its steady state. Second, they lack of any procedure for setting their parameters in a systematic way.

Many EA paradigms (like covariance matrix adaptation [20], differential evolution [21] or particle Swarm optimization [22]) depend on population diversity for its evolution. For this kind of algorithms, a termination condition given in terms of the rate of population diversity decrease would be useful.

This paper contributes to the termination of EAs relying on population diversity in two aspects. First, we present a formula for determining the moment a quantity has converged to its steady state. The formula is given in terms of convergence rates and only depends on two parameters. Second, we provide a statistical way to set the values for these parameters to ensure accuracy of the formula. The methodology we propose has been tested on 3 EA paradigms across 5 functions representative of the most influential landscapes for EA convergence. Results show the applicability of this methodology and also explore the variability of the formula parameters across function landscapes and EA paradigms. Results indicate that termination parameters depend on the chosen EA paradigm. The rest of the paper is organized as follows. Section II gives our numerical condition for EA termination and the statistical setting of its parameters. Section III describes the experimental setup and Section IV presents the results. Finally, conclusions and future work are given in Section V.

II. A Stopping Condition based on Steady-States

Let Q be a quantity (like EA population distribution in x-space) computed from EA current population. Assuming that EA reaches a steady state, the values of Q taken across iterations are a convergence sequence of real numbers, $(Q_k)_k$. Therefore, the natural termination condition should be stated in terms of $(Q_k)_k$ convergence. Given that a sequence is convergent if and only if it is Cauchy [23], a termination condition can be implemented by checking that the variation of $(Q_k)_k$ keeps below a threshold, ϵ_{st}, for a given number of n_{st} generations:

$$\forall i, j \in \{k, k+1, .., k+n_{st}\} \quad |Q_i - Q_j| \leq \epsilon_{st}$$

This can be formulated in terms of the range of Q in the generational interval $\{k, \ldots, k+n_{st}\}$ as:

$$Rng_{\{k,\ldots,k+n_{st}\}}(Q) = \max_{i\in\{k,\ldots,k+n_{st}\}} Q_i - \min_{i\in\{k,\ldots,k+n_{st}\}} Q_i \leq \epsilon_{st} \quad (1)$$

The EA algorithm is terminated at the first generation satisfying (1):

$$K^{Q}_{Ter} := \min_k (Rng_{\{k,\ldots,k+n_{st}\}}(Q) < \epsilon_{st}) \quad (2)$$

The number of generations, n_{st}, and the maximum variation range across them, ϵ_{st} determine how good for detecting that Q has reached a steady state the range bound (1) is. This fact can be used to set their values using the following statistical analysis [22].

Let K^{Q}_{Ter} be the minimum iteration achieving the bound (1). By definition of a steady state, Q has reached it if the range

$$Rng(k)(Q) = \max_{i\in\{k,\ldots,k+n_{st}\}} Q_i - \min_{i\in\{k,\ldots,k+n_{st}\}} Q_i \quad (3)$$

is below ϵ_{st} for $\forall k \geq K^{Q}_{Ter}$. For each n_{st} and ϵ_{st}, this condition can be expressed by the following function:

$$X_Q := \begin{cases} 1 & \text{if } Rng(k)(Q) \leq \epsilon_{st} \quad \forall k \geq K^{Q}_{Ter} \\ 0 & \text{otherwise} \end{cases} \quad (4)$$

The function X_Q takes values in $\{0,1\}$ and taken across independent EA runs is a discrete random variable that follows a Bernoulli distribution. In this context, Q has actually reached its steady state if the probability $P(X_Q == 1) = q$ is close to 1. The proportion test:

$$\begin{array}{ll} H_0: & q \leq q_0 \\ H_1: & q > q_0 \end{array} \quad (5)$$

provides a lower bound for q with a given confidence level. The statistic for the sampling proportion follows a normal distribution $N(0,1)$ for large values of n_{samp} and p not close neither to 0 nor to 1 and is given by:

$$Z_Q = (\widehat{q} - q_0)/\sqrt{q_0(1-q_0)/n_{samp}} \backsim N(0,1)$$

for $\widehat{q} = \sum X_Q/n_{samp}$ the sampling proportion and n_{samp} the sample size. The null hypothesis H_0 is rejected if the statistic Z_Q has a p-value below α. For each ϵ_{st}, the number of generations n_{st} ensuring that Q has reached a steady state with a confidence α is given by the minimum integer such that H_0 is rejected, for the statistic Z_Q computed over EA runs.

III. Experimental Set-Up

The goal of the experiments was to validate the presented framework for terminating EA paradigms relying on diversity. We have analyzed 3 EA paradigm: Differential Evolution (DE) [21], [24], Particle Swarm Optimization (PSO) [22], [25] and Covariance Matrix Adapting Evolutionary Strategy (CMA-ES) [20], [26]. For DE we have used the 3-parameter DE/rand/1/bin scheme reported in [21]. For a real search space of dimension D, the population is randomly initialized with ND vectors. Each vector in the population is evolved by mutation and recombination operators. The mutation rate is given by a parameter $F \in [0,2]$ and the combination rate by $CR \in [0,1]$. Following the literature [24], we have chosen the following values for DE parameters: D=2, ND=20, F=0.9, CR=0.5. CMA-ES is a population-based robust local search strategy that evolves by adapting the complete covariance matrix of the normal mutation distribution. In the case of PSO an initial population of particles improve their quality measure by adapting their velocity and position, which is encoded in a simple mathematical formula. For CMA-ES and PSO we have chosen the default parameters used in [27] and [28].

The quantity measuring population diversity is the distribution of EA population in x-space given by the maximum Euclidean distance, *MxD*, of a percentage of the best individuals to the best one:

$$MxD = max_{j\in(1,\ldots,n_{best})} d(Ind_j, Ind_1)$$

for $(Ind_j)_{j=1}^{n_{best}}$ the set of the n_{best} best individuals and Ind_1 the best individual. In these experiments, we have used 30% of the best individuals [29].

We have applied this framework to 5 functions representative of the benchmark used in [9] to test 31 state-of-the-art evolutionary algorithms. The functions are clustered according to their overall properties in five groups [30]: separable, low (good) conditioning, high (bad) conditioning, multi-modal with strong global structure and with weak global structure. Moreover, the functions cover the main properties (multimodality, global structure and scalability) reported in a recent study [31] to have a high influence in the performance of EAs. In the performed experiments we have chosen the Sphere, Rosenbrock, Ellipsoidal, Rastrigin and Schwefel functions. Figure 1 shows three of these functions for dimension 2. Dependency of parameters with respect the search space dimension has been explored by considering the definition of the functions for dimensions 2, 4 and 10.

In order to account for variability across initial population, a total number of 30 runs per function have been performed. For each run 1000 EA iterations were performed in order to ensure convergence to the steady state. For each paradigm the range (3) computed for the 30 independent runs taken for the 5 test functions defines the sample of the discrete variable, X_Q. For X_Q in each of the paradigms we have applied the proportion test with $\alpha = 0.05$ and $q_0 = .9$ for the following number of generations $n_{st} = \{10, 50, 100, 200, 500\}$. For each paradigm and x-space dimension, the parameters of formula (1) best suited for its termination are the minimum number of generations that reject the proportion test.

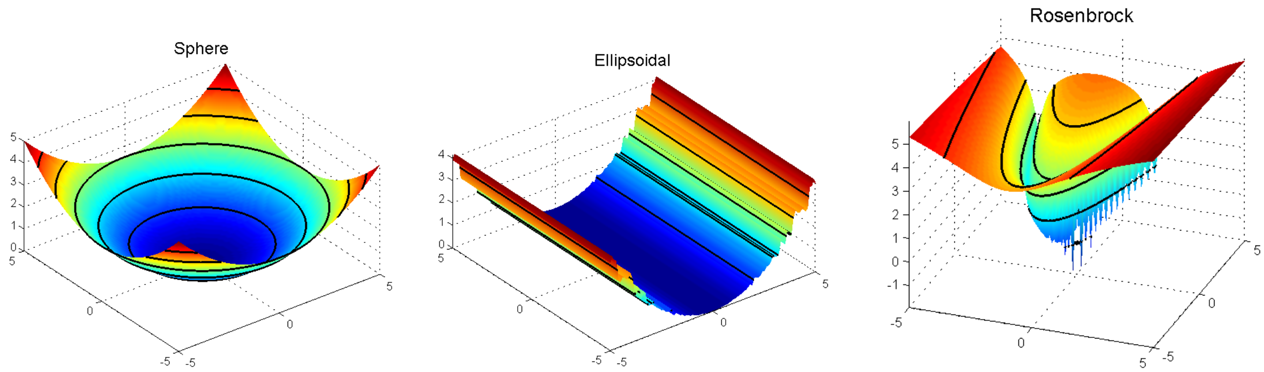


Figure 1. Representative benchmark test functions.

IV. Results and Discussion

Tables I, II, III report the results of the proportion test for DE, PSO and CMA, respectively. using $\epsilon_{st} = 10^{-1}$ for the computation of the range formula. Each table reports results across the selected number of generations (columns) and x-space dimension (rows). We report the hypothesis test result (1 for null hypothesis rejection, 0 for not rejection), the test p-value and the sampling proportion.

For the 2D case a minimum number of generations could be achieved for all paradigms. For dimension 4, our range formula fails to detect PSO steady state and for dimension 10 the proportion of detected steady states is below 0.9 for all n_{st} and paradigms. An analysis of the profiles of population diversity across iterations shows that failures arise from a number of iterations insufficient for reaching steady states of some particular functions. These cases are Rosenbrock, Schwefel for DE, Schwefel for PSO and Rosenbrock for CMA. These functions have a landscape showing a poor EA convergence rate at least for the chosen parameters for each paradigm and would require more iterations. Figure 2 shows the profiles of MxD for one of the failing cases in comparison to the always convergent Sphere.

Given that our methodology only applies in case EA has reached its steady state, the proportion test has been applied removing the above functions failing to do so. Further, in order to explore the impact of ϵ_{st}, X_Q was computed using $\epsilon_{st} = 10^{-1}$ and $\epsilon_{st} = 10^{-2}$. Tables IV, V and VI show the results obtained for DE, PSO and CMA.

For low dimensions (up to 4) the number of generations required for termination remains unchanged across ϵ_{st} for the 3 methods considered. For higher dimensionality, PSO is the only method that has the same behavior regardless of ϵ_{st}. DE and CMA present a variability in the number of generations that should be further investigated (see Section V). It is worth noticing that PSO termination is also stable across dimensions and, for low dimensionality, DE as well. This is not the case for CMA, for which termination generation seems to increase across dimensionality.

There are several interesting conclusions that can be derived from our experiments. For the PSO paradigm, convergence to steady states is apparently unchanged across the dimension of the search space. For low dimensions, this also holds for DE. In such cases, the number of generations required to terminate EA can be kept relatively low and, thus, termination based on population diversity is computationally efficient. For the CMA paradigm, loss of diversity drops as the dimension increases and, thus, it requires a higher number of generations for ensuring termination at the steady state.

The dependency of parameters across paradigms illustrates that the choice of the quantity used for EA termination is linked to EA internal mechanisms and, thus, its selection is at the very core of the methods used as termination criteria. In this context, loss of population diversity seems to be a good candidate for PSO and DE (at least for low dimensions), but might nor be the most appropriate one for CMA.

The dependency between ϵ_{st} and function landscape will be further investigated.

V. Future Work

Termination of EA in black-box applications is still an open issue. This work presents a 2-parameter criterion together with statistical tools for adjusting parameters optimal values. Our criterion can be used to detect loss of diversity for EA termination. We have applied our method to 3 EA paradigms (DE, PSO and CMA) and 5 representative test functions up to dimension 10. Experiments show that the tools presented constitute an appealing basis for the definition of a general framework for EA termination criteria analysis. However, more research is needed in order to fully validate our framework as a solid methodology for the implementation of termination strategies.

A limitation of this study is that we have only considered 5 functions up to dimension 10 with a number of EA runs that fall shortly to achieve steady states for some cases. We are aware that to fully generalize results more functions and iterations should be considered. This is a

Table I
OPTIMAL NUMBER OF TERMINATION GENERATIONS FOR DE

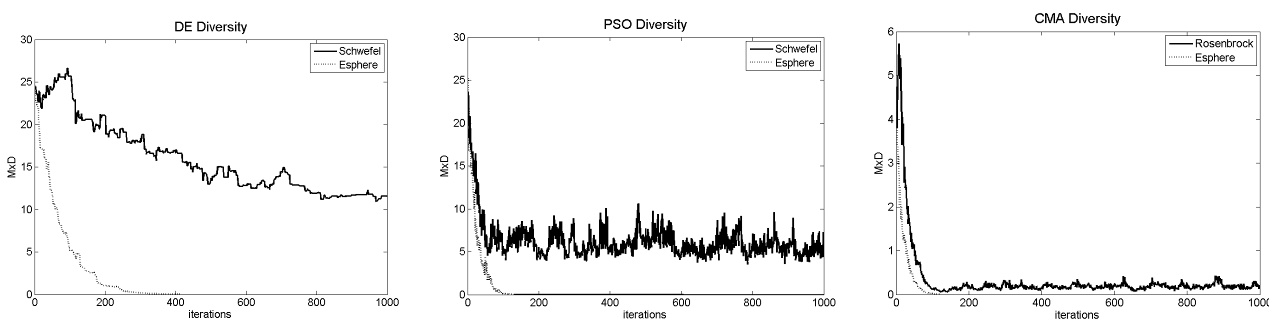
	Null Hypothesis Rejection					$p-value$					Sampling Proportion q				
	10	50	100	200	500	10	50	100	200	500	10	50	100	200	500
dim 2	0	1	1	1	1	1.0	2.2e-05	2.2e-05	2.2e-05	2.2e-05	0.55	1	1	1	1
dim 4	0	0	0	1	1	1.0	0.9	0.13	2.0e-04	2.0e-03	0.23	0.77	0.89	0.97	0.94
dim 10	0	0	0	0	0	1.0	1.0	1.0	0.8	1.0	0	0.32	0.50	0.53	0.33

Table II
OPTIMAL NUMBER OF TERMINATION GENERATIONS FOR PSO

	Null Hypothesis Rejection					$p-value$					Sampling Proportion q				
	10	50	100	200	500	10	50	100	200	500	10	50	100	200	500
dim 2	0	1	1	1	1	1.0	2.0e-004	2.2e-05	2.2e-05	2.2e-05	0.75	0.97	1	1	1
dim 4	0	0	0	0	0	1.0	0.9	0.9	0.9	1.0	0.59	0.77	0.77	0.77	0.74
dim 10	0	0	0	0	0	0.3	0.2	0.2	0.8	0.7	0.52	0.87	0.88	0.88	0.83

Table III
OPTIMAL NUMBER OF TERMINATION GENERATIONS FOR CMA

	Null Hypothesis Rejection					$p-value$					Sampling Proportion q				
	10	50	100	200	500	10	50	100	200	500	10	50	100	200	500
dim 2	1	1	1	1	1	0.01	2.2e-05	2.2e-05	2.2e-05	2.2e-05	0.95	1	1	1	1
dim 4	0	1	1	1	1	0.8	2.2e-05	2.2e-05	2.2e-05	2.2e-05	0.82	1	1	1	1
dim 10	0	0	0	0	0	1.0	1.0	1.0	0.5	0.2	0.34	0.65	0.70	0.86	0.88



(a) (b) (c)

Figure 2. Loss of population diversity across iterations for DE, (a), PSO, (b) and CMA, (c).

Table IV
IMPACT OF ϵ_{st} IN DE TERMINATION

	Null Hypothesis Rejection					$p-value$					Sampling Proportion q				
$\epsilon_{st} = 10^{-1}$	10	50	100	200	500	10	50	100	200	500	10	50	100	200	500
dim 2	0	1	1	1	1	0.98	$7.8e-04$	$7.8e-04$	$7.8e-04$	$7.8e-04$	0.83	1	1	1	1
dim 4	0	1	1	1	1	1	0.0025	0.0025	0.0025	$7.8e-04$	0.47	0.99	0.99	0.99	1
dim 10	0	0	0	1	0	1.0	1.0	0.36	0.039	1	0.00	0.63	0.91	0.96	0.66
	Null Hypothesis Rejection					$p-value$					Sampling Proportion q				
$\epsilon_{st} = 10^{-2}$	10	50	100	200	500	10	50	100	200	500	10	50	100	200	500
dim 2	0	1	1	1	1	0.14	$7.8e-04$	$7.8e-04$	$7.8e-04$	$7.8e-04$	0.93	1	1	1	1
dim 4	0	1	1	1	1	0.52	0.007	0.0025	0.0025	$7.8e-04$	0.61	0.98	0.99	0.99	1
dim 10	0	0	0	0	0	1	0.5	0.75	0.07	0.25	0.0	0.59	0.82	0.94	0.33

matter of computational resources, time and an efficient parallel implementation and it is our top issue in our to-do list.

Another interesting topic to be further investigated is the variability of the number of generations n_{st} under different configurations in functions, as well as, the dependency

Table V
IMPACT OF ϵ_{st} IN PSO TERMINATION

	Null Hypothesis Rejection					$p-value$					Sampling Proportion q				
$\epsilon_{st} = 10^{-1}$	10	50	100	200	500	10	50	100	200	500	10	50	100	200	500
dim 2	0	1	1	1	1	0.63	0.0025	$7.8e-04$	$7.8e-04$	$7.8e-04$	0.89	0.99	1	1	1
dim 4	0	1	1	1	1	0.99	0.0025	0.0025	0.0025	0.039	0.80	0.99	0.99	0.99	0.96
dim 10	0	1	1	1	1	0.54	0.0025	$7.8e-04$	$7.8e-04$	$7.8e-04$	0.63	0.99	1	1	1
	Null Hypothesis Rejection					$p-value$					Sampling Proportion q				
$\epsilon_{st} = 10^{-2}$	10	50	100	200	500	10	50	100	200	500	10	50	100	200	500
dim 2	0	1	1	1	1	0.92	0.0025	$7.8e-04$	$7.8e-04$	$7.8e-04$	0.85	0.99	1	1	1
dim 4	0	1	1	1	1	1.0	0.0025	0.0025	0.0025	0.0039	0.77	0.99	0.99	0.99	0.97
dim 10	0	1	1	1	1	0.57	0.0025	$7.8e-04$	$7.8e-04$	$7.8e-04$	0.66	0.99	1	1	1

Table VI
IMPACT OF ϵ_{st} IN CMA TERMINATION

	Null Hypothesis Rejection					$p-value$					Sampling Proportion q				
$\epsilon_{st} = 10^{-1}$	10	50	100	200	500	10	50	100	200	500	10	50	100	200	500
dim 2	1	1	1	1	1	0.0075	$1.3e-04$	$1.3e-04$	$1.3e-04$	$1.3e-04$	0.96	1	1	1	1
dim 4	0	1	1	1	1	0.11	$1.3e-04$	$1.3e-04$	$1.3e-04$	$1.3e-04$	0.93	1	1	1	1
dim 10	0	0	0	1	1	1.0	0.98	0.27	$4.1e-04$	$1.3e-04$	0.5	0.84	0.92	0.99	1
	Null Hypothesis Rejection					$p-value$					Sampling Proportion q				
$\epsilon_{st} = 10^{-2}$	10	50	100	200	500	10	50	100	200	500	10	50	100	200	500
dim 2	1	1	1	1	1	$4.1e-04$	$1.3e-04$	$1.3e-04$	$1.3e-04$	$1.3e-04$	0.99	1	1	1	1
dim 4	0	1	1	1	1	0.38	$1.3e-04$	$1.3e-04$	$1.3e-04$	$1.3e-04$	0.90	1	1	1	1
dim 10	0	0	1	1	1	0.45	0.27	$1.3e-04$	$1.3e-04$	$1.3e-04$	0.53	0.91	0.99	1	1

on other parameters involved in the computation of the termination condition. In the first case, it would be of interest to determine the variability of generations across landscapes and dimensions, in order to check if the diversity criterion is still useful. Although a preliminary study [29] suggests that the parameters involved in the computation of the quantity selected for measuring diversity (in particular the percentage of best individuals used for computing MxD) is not a critical issue, at least for DE, its influence should be further explored. Finally, the impact that the accuracy, ϵ_{st}, required by the application has on the number of generations, and, thus, EA executions requires a deeper study, especially for high dimensions. Variability under different conditions, can be assessed with ANOVA test using functions and dimensions properties for inter-group variability. In the case of absence of normality and/or homoscedasticity a non-parametric test would be used.

Finally a comparison to existing methods for adaptive termination of EAs should be carried out in order to determine the relevance of the presented approach. Still, this preliminary work constitutes a first new effort in the use of statistical analysis as a tool for termination of EA algorithms and illustrates their potential for analyzing the behavior of EA algorithms.

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