Initial Population Diversity Does Not Influence Performance

Pedro A. Diaz-Gomez
Computing & Technology – Cameron University
2800 W. Gore Boulevard, Lawton, Oklahoma 73505 USA
Phone:(580) 581-7934 – Fax:(580) 581-2333 – Email: pdiaz-go@cameron.edu

Dean F. Hougen
School of Computer Science – University of Oklahoma
200 Felgar Street, Room 120, Norman, Oklahoma 73019 USA
Phone: (405)325-3150 – Fax: (405)325-3150 – Email: hougen@ou.edu

Abstract - *It is widely believed that greater initial population diversity leads to improved performance in genetic algorithms. However, this assumption has not been rigorously tested previously. We put this assumption to the test on two benchmark problems and found that greater diversity did not lead to improved performance. This result will require a serious rethinking on the part of the evolutionary computation community as to why genetic algorithms sometimes perform very differently on successive applications to the same problems.*
Keywords: Performance analysis, Empirical study, Evolution dynamics, Genetic algorithms, Theory.

1 Introduction

It is a common belief that a higher diversity can help genetic algorithms (GAs) to perform better in terms of the quality of the final solution found and/or the speed with which good solutions are found [5], [16], [18], [20], [21], [25]. The primary contribution of this paper is that it shows that this belief is apparently false—we found no linear correlation between diversity and GA performance, at least within the range of diversity found in randomly generated initial populations, using standard diversity metrics in the context of two testbed problems: the one-max problem and the snake-in-the-box problem. These two problems give us two very different problems with which to test. The first has no local maxima nor even any plateaus in the fitness landscape which makes it exceedingly easy. The second has many local maxima and plateaus, which makes it quite difficult [4], [6], [23]. Because these problems are so different, yet the results of the experiments are identical, we believe our results are broadly generalizable to many problem domains encountered in evolutionary computation.

1.1 Performance

Performance in evolutionary computation can be thought of in two ways: (1) the quality of the solution found when resources are limited (if resources are unlimited, the global maximum can always be found by an effective search algorithm), and (2) the resources required to find the global maximum when resources are sufficient. Correspondingly, performance in this article has two meanings: (1) the best solution found so far during a given number of generations, and (2) the number of generations needed to reach the global maximum. Because the global maximum may not always be reached in difficult problems, we terminate the GA at a maximum of $100,000$ generations.

1.2 Diversity

As with performance, diversity can be looked at in different ways. One approach is to look at differences at the level of the gene. Another is to look at differences at the level of the entire chromosome.

Consider a binary GA (where each gene is either a 0 or a 1) in which a population is represented with a two-dimensional matrix where each row is the chromosome of a single individual and each column, then, is the alleles across individuals at each locus. In this representation, gene-level diversity can be measured by looking at each column individually. If a column has mostly 0's and very few 1's, the corresponding gene lacks diversity in this population. Similarly, if a column has mostly 1's and very few 0's, the corresponding gene also lacks diversity. Only when the column has approximately the same number of 0's and 1's is the gene-level diversity high. The diversity of the genes at each locus is then averaged over all loci to give the population average diversity at the gene level. This notion can be formalized variously as the entropy metric [12] or the Grefenstette bias [16]. In the present work, we use the entropy metric but the conclusions are identical using the Grefenstette bias.

At the chromosome level, diversity can be measured by looking at differences between entire rows [12]. Here, differences between each pair of rows can be calculated, and the average difference between pairs is then used for the population's diversity at the chromosome. Again, different formalisms are possible, such as the Hamming metric [12] where differences between rows are calculated using the well-known Hamming distance, or the neighborhood metric [12] which is based on the neighborhood concept for chromosomes [3]. In the present work, we use the Hamming metric but again the conclusions are identical using the neighborhood metric.

2 Experimental Setup

We looked for relationships between diversity and performance using two sample problems of very different difficulty levels. For each problem we generated a set of initial populations with different diversity values, ran our GA on each population and gathered performance data, then looked for correlations between initial population diversity and performance.

2.1 Test Problems

The one-max problem has been widely used in the literature as a classic toy problem to be studied using GAs [7], [17], [14], [26]. The problem is to find a chromosome of all ones, where fitness is simply the sum of the bits in the chromosome. This problem has the characteristic that every bit may contribute individually to the fitness value. This means that there is only one global maximum and there are no plateaus or local minima. For this reason it is a very simple but potentially useful toy problem.

The snake-in-the-box problem is to find the longest snake in a hypercube, where a *snake* is an open connected path, where each node that belongs to the path has exactly two neighbors in the path, except for the "initial" (head) and "final" (tail) nodes that have just one neighbor each. Longest snakes in hypercubes have been used in coding theory [24], digital design, and telecommunications [15]. The snake-in-the-box problem is a difficult problem with real-world applications.

2.2 Test Methods

For each problem, we randomly generate 90 populations. This provides us with a set of initial populations that have a range of diversity values. For the one-max problem, the GA is run for each initial population, and the quality of the best solution found so far is recorded every 5 generations until generation 20 and after that at each 20 generations until generation 60. For the snake-in-the-box problem, the GA is run for each initial population, and the quality of the best solution found so far is recorded every 10 generations until generation 110. Besides looking at the best solution so far, the algorithm continues until a global maximum is found or 100,000 generations, whichever comes first, recording the number of generations needed to reach the global maximum.

This procedure is repeated three times, giving us three repetitions, or *trials* of data for each problem. The data is then analyzed using the two diversity metrics and two performance metrics, for a total of eight sets of analyses.

2.3 Parameters and Parameter Justification

For both problems, the population size is 20, 2-tournament selection is used, the probability of uniform crossover is 1.0, the probability of mutation is 0.001 per bit, and a stop criterion of a maximum of 100,000 generations is used. For the one-max problem, the chromosome length is 64. The snake-in-the-box problem was tested in a 5-dimensional hypercube, i.e., the chromosome is encoded as 32 bit (2^5 bit) string.

Lobo and Goldberg [19] suggested using 100 individuals for the one-max problem with a 100 bit chromosome. As we have a 64 bit string, one might expect us to use 64 individuals in the initial population. However, we used 20 individuals in order to have a greater diversity range and to avoid a ceiling effect.[1]

Lobo and Goldberg [19] also used 2-tournament selection, a probability of uniform crossover of 1.0 and a probability of mutation of 0.0 per bit. We changed probability of mutation to 0.001 in order to help the algorithm to recover from the loss of an allele in a locus for the whole population.

[1] As expected, even with only 20 individuals in the initial population, the GA converges for the majority of initial populations by generation 80.

2.4 Data Analysis Methods

Initial testing showed no apparent curve in the diversity vs. performance graphs, so it appears appropriate to look for a linear correlation. We therefore use Pearson's correlation coefficient [8]. If $r_{XY} \approx 1.0$ then there is a strong to perfect positive linear correlation. If $r_{XY} \approx -1.0$ there is a strong to perfect negative linear correlation [8]. However, because the sampling distribution of Pearson's r is not normally distributed, it is difficult to calculate confidence intervals for it directly. Fisher's r to z' transform converts Pearson's r to Fisher's z', which *is* normally distributed and allows us to easily compute confidence intervals on our data [8]. Then z' is divided by σ (the standard deviation) to arrive at Z. Z values outside the range -1.96 to 1.96 are statistically significant at the 95% confidence level. This measure is used in this research as a strong score to show independence between diversity in the initial population and performance.

3 Experimental Results

As described in Section 2-2, two diversity metrics, two performance metrics, and two problems, give us a total of eight sets of results: (1) entropy vs. maximum so far for the one-max problem, (2) entropy vs. number of generations for one-max, (3) hamming vs. maximum so far for one-max, (4) hamming vs. number of generations for one-max, (5) entropy vs. maximum so far for snake-in-the-box, (6) entropy vs. number of generations for snake-in-the-box, (7) hamming vs. maximum so far for snake-in-the-box, and (8) hamming vs. number of generations for snake-in-the-box.

3.1 Performance on One-Max

(1) Entropy vs. maximum so far: Table I shows Pearson's coefficients for different runs until generation 40. (After generation 40 a ceiling effect is likely.) It can be observed that there is no significant linear correlation between the entropy value of the initial population and the quality of the solution for these test sets. See Figures 1 to 6 as examples of snapshots of run 1. As the Pearson's values are small, in order to see if the two variables (diversity and solution quality) have correlation zero, Z is presented in Table II, where no values are statistically significant, confirming the independence between diversity in the initial population and performance.

(2) Entropy vs. number of generations: No statistically significant correlations were discovered between

	Generation					
Trial	0	5	10	15	20	40
1	0.099	0.134	0.198	0.174	0.088	−0.066
2	−0.084	−0.122	−0.094	−0.198	−0.047	−0.128
3	−0.048	−0.087	−0.033	0.033	0.041	0.066

Table I. Pearson's Coefficients for one-max. Entropy vs. maximum so far. No significant linear correlation found.

	Generation					
Trial	0	5	10	15	20	40
1	0.93	1.26	1.87	1.64	0.82	−0.62
2	−0.79	−1.14	−0.88	−1.87	−0.44	−1.20
3	−0.45	−0.81	−0.31	0.31	0.38	0.62

Table II. Z values for one-max. Entropy vs. maximum so far. No significant linear correlation found.

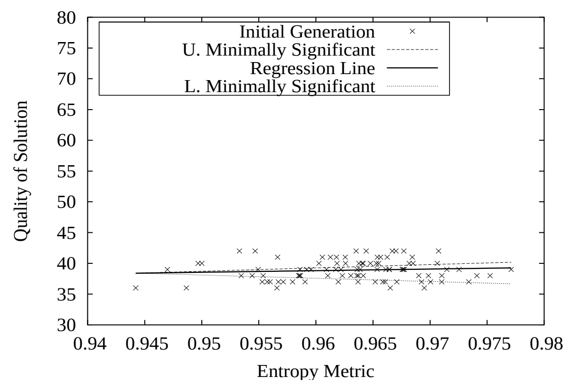

Fig. 1. Entropy vs. quality of the solution. One-max problem. Snapshot at initial generation. Trial 1. 90 Runs.

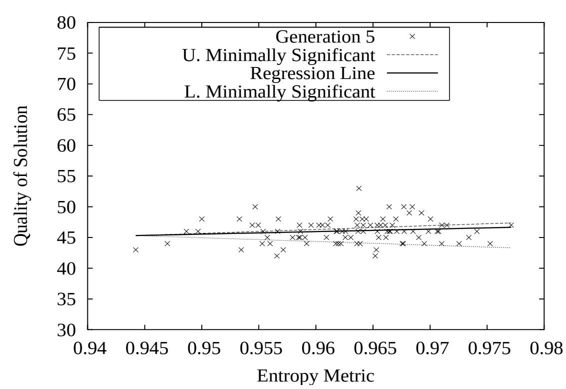

Fig. 2. Entropy vs. quality of the solution. One-max problem. Snapshot at generation 5. Trial 1. 90 Runs.

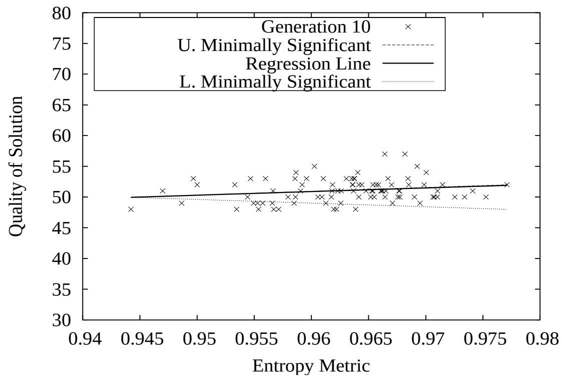

Fig. 3. Entropy vs. quality of the solution. One-max problem. Snapshot at generation 10. Trial 1. **90** Runs.

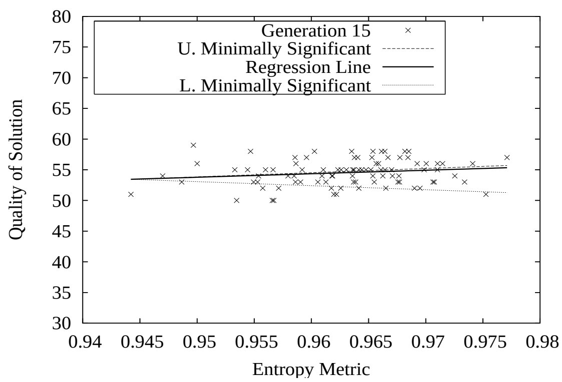

Fig. 4. Entropy vs. quality of the solution. One-max problem. Snapshot at generation 15. Trial 1. **90** Runs.

the entropy metric and the number of generations to reach the goal. The Pearson's Coefficients for the three trials were -0.106, 0.007 and -0.053 (small values) and the corresponding Z values were -0.992, 0.065 and -0.494 which are between the critical values -1.96 and 1.96. See Figure 7 for an example of the number of generations to reach a global maximum.

(3) Hamming vs. maximum so far: Table III shows the corresponding Pearson's coefficients (for the different runs) were it can be observed that there is no significant linear correlation between diversity in the initial population and the quality of the solution for these test sets. As the Pearson's values are small, in order to see if the two variables (diversity and solution quality) have correlation zero, the Fisher's coefficient is presented in Table IV, where no values are statistically significant, confirming the independence between diversity in the initial population and performance.

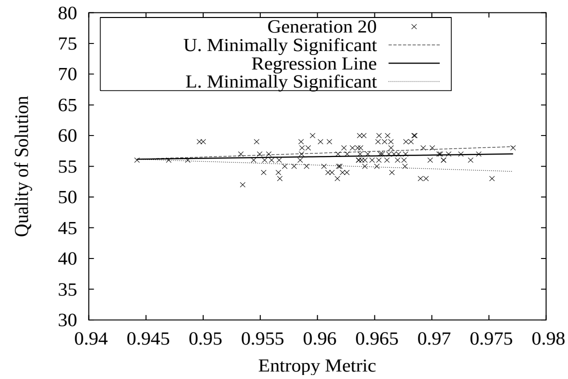

Fig. 5. Entropy vs. quality of the solution. One-max problem. Snapshot at generation 20. Trial 1. **90** Runs.

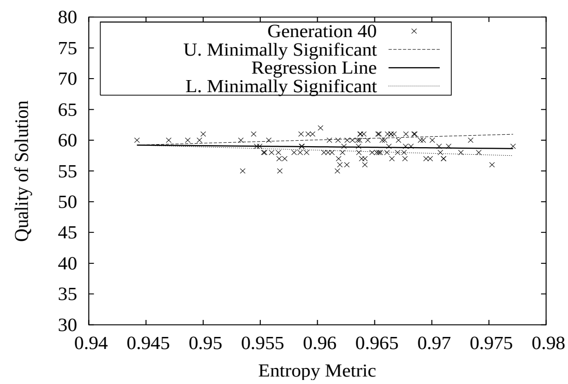

Fig. 6. Entropy vs. quality of the solution. One-max problem. Snapshot at generation 40. Trial 1. **90** Runs.

(4) Hamming vs. number of generations: For the number of generations to reach a global maximum using the Hamming metric, no statistically significant correlation was discovered. The Pearson's Coefficients for the three trials were -0.096, -0.003 and -0.052,

	Generation					
Trial	0	5	10	15	20	40
1	0.092	0.135	0.203	0.177	0.088	−0.064
2	−0.078	−0.118	−0.089	−0.196	−0.046	−0.121
3	−0.050	−0.092	−0.035	0.033	0.040	0.065

Table III. Pearson's Coefficient for the one-max problem. Hamming metric used. No linear correlation found.

	Generation					
Trial	0	5	10	15	20	40
1	0.86	1.27	1.92	1.67	0.82	−0.60
2	−0.73	−1.11	−0.83	−1.85	−0.43	−1.13
3	−0.47	−0.86	−0.33	0.31	0.37	0.61

Table IV. Fisher's Coefficient for the one-max problem. Hamming metric used. Zero correlation found.

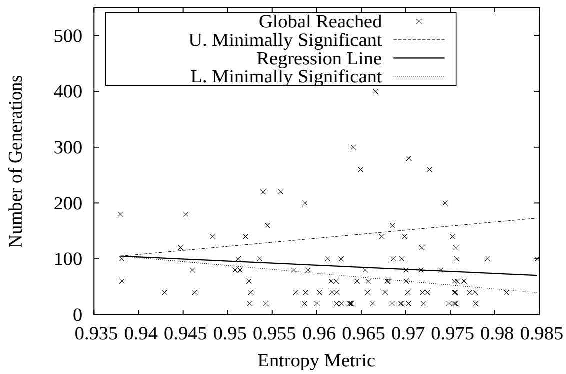

Fig. 7. Entropy metric vs. number of generations to reach the global maximum. One-max problem. **90** Runs.

Trial	Generation 0	10	20	30	40	80
1	−0.068	−0.014	−0.008	−0.017	−0.022	−0.011
2	0.185	−0.115	−0.115	−0.186	−0.143	−0.097
3	−0.015	−0.047	−0.003	0.045	0.028	0.103

Table V. Pearson's Coefficients for the Snake-in-the-box problem. Entropy metric. No linear correlation found.

and the corresponding Z values were -0.898, -0.028 and -0.485 which shows that diversity and solution quality are independent.

3.2 Performance on Snake-in-the-box

(5) Entropy vs. maximum so far: No statistically significant positive correlation between the entropy metric and the quality of the solution was discovered as shown by the Pearson's Coefficients and Z values in Tables V and VI respectively. However, a single value that seems to indicate a statistically significant *negative* correlation was found at generation 110, trial number 2, with a Pearson's Coefficient of -0.227 and a Z value of -2.15. (See Section 4 for an analysis of this result.)

(6) Entropy vs. number of generations: No statistically significant correlation between the entropy metric and the number of generations to reach a global maximum was found. The Pearson's coefficient was -0.209 and the corresponding Z value was -1.14.

Trial	Generation 0	10	20	30	40	80
1	−0.64	−0.13	−0.07	−0.16	−0.21	−0.10
2	1.75	−1.08	−1.08	−1.76	−1.34	−0.91
3	−0.14	−0.44	−0.03	0.42	0.26	0.96

Table VI. Fisher's Coefficients for the Snake-in-the-box problem. Entropy metric. No linear correlation found.

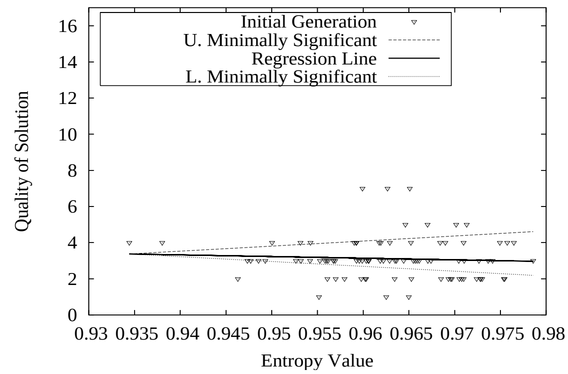

Fig. 8. Entropy vs. quality of the solution. Snake-in-the-box Problem. Trial 1. Snapshot at initial generation. **90** Runs.

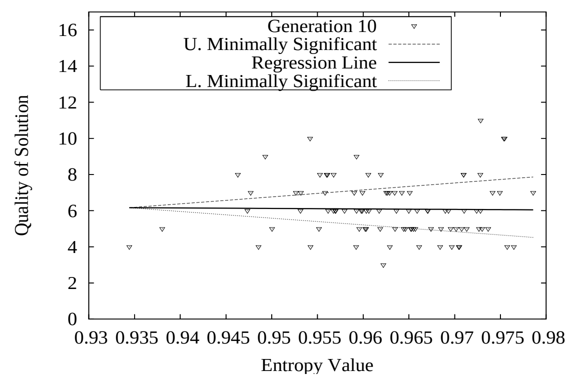

Fig. 9. Entropy vs. quality of the solution. Snake-in-the-box Problem. Trial 1. Snapshot at generation 10. **90** Runs.

Because there were populations that did not reach a global maximum in the $100,000$ generations, our data here is divided into two data samples— the populations that reach the goal (17 points as in Figure 14) and the ones that do not. The Pearson's Coefficients are for the populations in which the goal was reached. To see if there is a correlation between diversity and reaching the goal within $100,000$ generations, a logistic regression test was applied. This gives a p value of 0.0075 for the best ξ^2 model value, i.e., the model cannot adequately fit the data. Therefore, there is no correlation between diversity in the initial population and reaching the goal within $100,000$ generations.

(7) Hamming vs. maximum so far: No statistically significant correlation between the entropy metric and the quality of the solution was discovered as the Pearson's coefficients and Z values show in Tables VII and VIII, except for the second run generation 110,

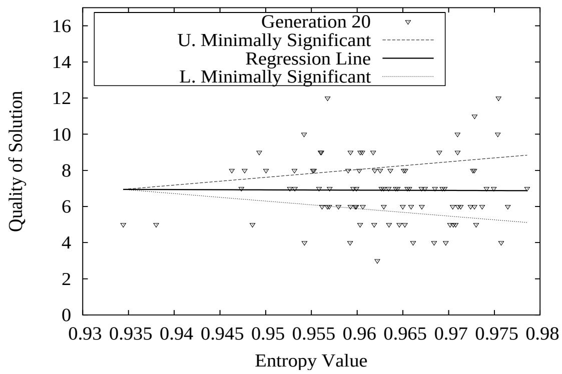

Fig. 10. Entropy vs. quality of the solution. Snake-in-the-box Problem. Trial 1. Snapshot at generation 20. **90** Runs.

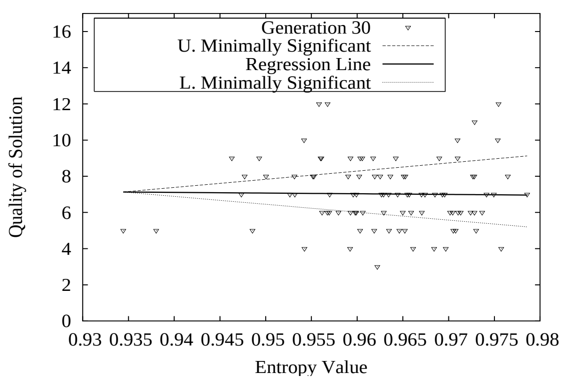

Fig. 11. Entropy vs. quality of the solution. Snake-in-the-box Problem. Trial 1. Snapshot at generation 30. **90** Runs.

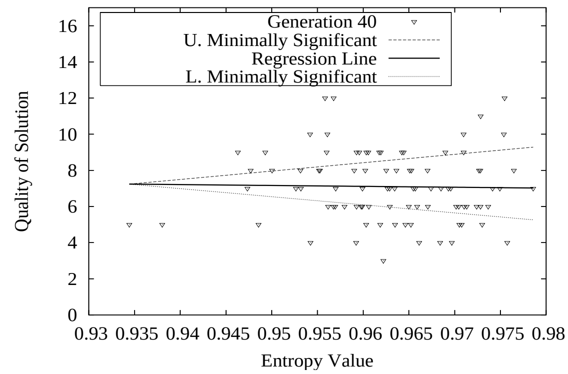

Fig. 12. Entropy vs. quality of the solution. Snake-in-the-box Problem. Trial 1. Snapshot at generation 40. **90** Runs.

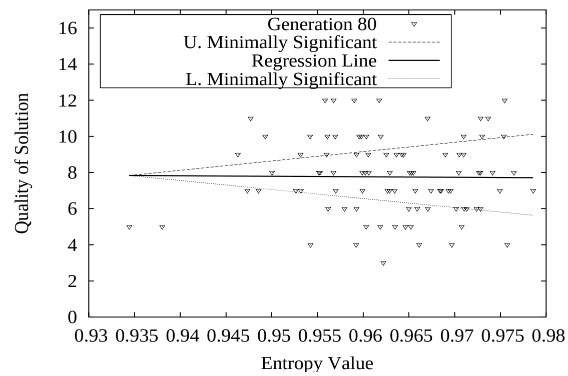

Fig. 13. Entropy vs. quality of the solution. Snake-in-the-box Problem. Trial 1. Snapshot at generation 80. **90** Runs.

which shows a statistically significant *negative* correlation (see Section 4 for analysis).

(8) Hamming vs. number of generations: No statistically significant correlation between the Hamming metric and the number of generations to reach a global maximum was discovered as the Pearson's coefficients and Z values of 0.125 and 1.172 were obtained which are not statistically significant.

Again, some populations did not reach the global maximum in $100,000$ generations or fewer, so the logistic regression test was applied. This gives a p value of 0.0039 for the best ξ^2 model value, i.e., the model cannot adequately fit the data. Therefore, there is no correlation between the two sets.

4 Analysis

This paper tested the hypothesis that says in its general form:

$$\text{If } V(P_A) \geq V(P_B) \text{ then } X(G, P_A) \geq X(G, P_B), \quad (1)$$

	Generation					
Trial	0	10	20	30	40	80
1	-0.068	-0.011	-0.005	-0.015	-0.020	-0.009
2	0.187	-0.116	-0.119	-0.191	-0.148	-0.103
3	-0.013	-0.049	-0.005	0.044	0.027	0.100

Table VII. Pearson's Coefficients for the Snake-in-the-box problem. Hamming Metric. No linear correlation found.

	Generation					
Trial	0	10	20	30	40	80
1	-0.64	-0.10	-0.05	-0.14	-0.19	-0.08
2	1.76	-1.09	-1.11	-1.80	-1.39	-0.96
3	-0.12	-0.46	-0.048	0.41	0.25	0.94

Table VIII. Fisher's Coefficients for the Snake-in-the-box problem. Hamming Metric. No linear correlation found.

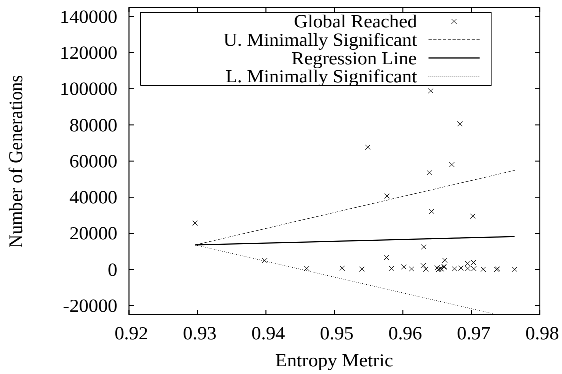

Fig. 14. Entropy metric vs. number of generations to reach the global maximum. $100,000$ Generations. Snake-in-the-box Problem. **90** Runs.

where $V(P)$ is the diversity of population P and $X(G, P)$ is the expected performance of a genetic algorithm G with population P. Expected performance is measured as the expected solution quality of the best solution found so far after a given number of generations or the expected number of function evaluations to obtain a global maximum.

Two problems, two diversity metrics, and two performance metrics were used, for none of the specific cases tested was a strong correlation between diversity and performance found using as test statistics the Pearson's coefficient and the Fisher's r to z transform.

The Pearson's coefficient R_{XY} gives a positive, negative, or no linear relationship between two variables [8]. For the particular research, the two variables are diversity and performance of a GA. If $R_{XY} \approx 1.0$ then there is a strong to perfect positive linear correlation, and if $R_{XY} \approx -1.0$ there is a strong to perfect negative linear correlation [8]. No one of those values was reached for any of the specific hypothesis as can be seen in Tables I, III, V, and VII. However, to be more certain about the independence of the two variables the Fisher's r to z transform was applied, the results of which are in Tables II, IV, VI, and VIII. In all cases the correlation was almost zero, and in one case, a small negative correlation was found (it occurs in the second run at generation 110 with the Pearson value of -0.227). Because no result returns a statistically significant outcome, we are not concerned with false positives of multiple comparison test, and the conclusion remains that there is no direct linear correlation between diversity and performance.[2]

Results for specific cases tested in this paper showed an independence between diversity in the initial population and performance of GAs. If diversity alone is not impacting performance of GAs, then what could be the factor or factors in the input that could be impacting performance? As it has been highlighted, population size is an important parameter to be set when working with GAs [18], [2], [1], [16], [20], [22]. So, we return to the empirical study in [11] where it was found empirically a positive correlation between population size and performance. However, population size as addressed in [11] carried a change in diversity,[3] and this fact lead us to hypothesize that the factor that was impacting performance was diversity. What, then, is the implication of the negative result obtained for hypothesis as in Equation 1? Possibly that diversity and population size together are factors that impact performance or that population size alone is a factor that is influencing performance. But, what about other factors? We need to consider not only the input, but the process that is in between the input and the output. As the algorithm iterates, usually the diversity measure is decreasing. If decreasing in diversity leads to a value near of zero quite soon, it is possible that a premature convergence occurs with poor quality [18], [5], [20], [16]. This is one of the difficulties when working with GAs—due to the interdependence of parameters, a change in one parameter can impact the whole result [13].

5 Conclusions & Future Work

The general hypothesis tested in this paper points out the relationship between diversity in the initial population and the quality of the possible solution. The results of these specific hypotheses showed no direct correlation between diversity and the quality of the solution, nor for the number of generations to reach the global maximum, for the one-max function and the snake-in-the-box problem in a 5-dimensional hypercube, using the set of parameters as in Section 2-2. This result goes against the common belief that diversity in the initial population (using wide used definitions of diversity) influences directly the performance of GAs [18], [5], [20], [16], [21], [25]. This does not mean that diversity

[2]The only case of a Pearson's value of -0.227 and Fisher's value of -2.15 does not change the conclusion in the sense that, this value could occur by chance, and contrary of what it was expected, a higher diversity value returned a lower outcome.

[3]Usually increasing population size carries an increase in diversity in terms defined in [11].

in the initial population is not important, but different as in the empirical study in [11], in Equation 1, population size is constant and diversity is the independent variable that could impact the performance GAs.

The rejection of this hypothesis lead us to think that maybe, it is not diversity alone but the increasing of the population size that could help sometimes in the performance of GAs as is shown in [11]. However, population size and diversity cannot be considered isolated from the rest of parameters, and specifically it is quite important to measure how diversity changes as the algorithm iterates. If diversity decreases quite soon then it is expected that the algorithm is going to converge prematurely. The parameter that could have a strong relation with diversity is selection pressure [18]. If selection pressure is high then it is expected that the GA is going to choose the more fit individuals, and in consequence it is going to converge prematurely [18]. If, on the contrary, selection pressure is quite low, then it is possible that the algorithm is going to expend a lot of computations to converge or it may diverge because of the lack of selection pressure [18]. It should be highlighted that the selection pressure used, for testing the eight cases presented in Section 3, was previously used by [19] ($S_p = 2$) in testing the one-max function and by [9], [10] in testing the snake-in-the-box problem in 4 and 8-dimensional hypercubes.

This paper tested the independence between diversity in the initial population and performance for GAs, this does not mean that diversity in the initial population is not important, but that diversity in conjunction with other factor(s) should be considered. Population size plays a role here in the sense that usually increasing the population size carries an increase in the initial diversity and a better performance is usually obtained [20], [11]. Selection pressure by other hand is the parameter that is decreasing diversity as the algorithm iterates in finding a possible solution, this means that, not only initial diversity could be considered, but how diversity is "consumed" as the algorithm goes on is quite important to consider too. With the two metrics considered in this research, the crossover operator is not influencing diversity values, but it is exploring other areas of the search space and for end is influencing the performance of GAs. The Mutation operator certainly influence diversity in the population, but how such influence affects the performance of GAs is a difficult problem topic of research nowadays [22]. Population diversity and its relation with fitness is important to considered too as addressed by [5] it is important to understand the improving of fitness by controlling diversity. Future research then in areas like the relationship between diversity and selection pressure; mutation probability and diversity; selection pressure, diversity and mutation/crossover probability, diversity and fitness could be accomplished.

In conclusion, diversity cannot be seen alone in the initial population as a factor influencing performance in GAs, but in conjunction with the rest of parameters: selection pressure, crossover and mutation, that are responsible for exploring new regions of the search space, fitness function and the stop criteria, where diversity itself can be used as a measure of stopping.

6 Acknowledgments

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