

AN EXPLORATION MEASURE OF THE DIVERSITY VARIATION IN GENETIC ALGORITHMS

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Abstract: In this paper, a novel measure of the population diversity of a Genetic Algorithm (GA) is presented. Chromosomes diversity plays a major role for the successfully operation of a GA, since it describes the number of the different candidate solutions that the algorithm evaluates, in order to find the optimal one, in respect to a performance index, called objective function. In a well defined algorithm, the diversity of the current population should be measurable, in order to estimate the performance of the algorithm. The resulted observation, that is, the measuring of the diversity, can then be used to real-time adjust the factors that determine the chromosomes variety (P_c , P_m), during the execution of the GA. It is shown, that a simple chromosomes clustering into the search space, by using the well known *k-means* algorithm, can give a useful picture of the population's distribution. Thus, by translating the problem of finding the best solution to a GA-based problem into an iterative clustering process, and by using the scatter matrices (S_a , S_b), which describe completely the candidate's solutions topology, one could define a novel formula that gives the population diversity of the algorithm.

1 INTRODUCTION

Evolutionary Algorithms (EAs) have been used in many applications through the years, due to its stochastic mechanism for finding solutions that optimize single or multiple objective problems. Genetic Algorithms (Holland, 2001, Mitchell, 2002) are considered the most popular kind of EAs since they are characterized by a high degree of parallelism and natural behaviour.

Genetic Algorithms (GAs) are used as optimization methods to solve difficult and complex problems in a range of scientific fields, such as image processing (Mirmehdi, 1997, Papakostas, 2003), robust control (Jamshidi, 2003, Papakostas, 2004), pattern classification (Bandyopadhyay, 1995) etc. Their popularity can be justified by their ability to overcome possible local optima, and to converge

to the global solution of a problem, with high probability.

However, there are some cases in which the global optimum is quite far from the derived solution that the algorithm converged to. This undesirable situation is called *premature convergence* (Mitchell, 2002). When this phenomenon appears, the population chromosomes are all the same. In other words, the population diversity has been lost. Of course, the diversity would be also lost in the case of the algorithm converging to the global optimum. The ill-posed situation is when the diversity decreases quickly and stays to low level for many generations.

Therefore, in order to prevent this situation, it is needed to measure the diversity variation through the generations, and adjust the algorithm parameters off-line, in the initial calibration or online during the execution of the algorithm.

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In the present paper, a clustering method for exploring the distribution of the chromosomes and the scatter matrices, S_b – *between class scatter matrix* and S_w – *within class scatter matrix* of the resulted clusters for measuring the level of the current diversity, are being used.

The paper is organized as follows: the proposed method is described in section 2, by analyzing the *k-means* algorithm and the way it is used for this paper purpose, while the effectiveness of the method is examined through appropriate simulations in the third section. Finally, conclusions that may derive from the previous discussion are highlighted in the last section.

2 THE PROPOSED METHOD

The main idea of the proposed method, for measuring the population diversity of a GA, is based on viewing the process to find the optimal solution of a problem, as a clustering one. Let us consider the algorithm's chromosomes for an n -dimensional problem

$$Ch_1(x_1^1 x_2^1 x_3^1 \dots x_n^1), \dots, Ch_m(x_1^m x_2^m x_3^m \dots x_n^m)$$

where Ch_i is the i^{th} chromosome, and x_j^i is the j^{th} variable of the i^{th} chromosome. In the above formulation, the population size is equal to m .

These chromosomes can be considered as n -dimensional vectors with coordinates (x_1, x_2, \dots, x_n) , and thus can be considered as single points into the n -dimensional variable space (*search space*). To visualize these points in the search space, one can produce the scatter plot of them, as depicted in the following figure, where the points correspond to the initial population in the case of a 2-D problem.

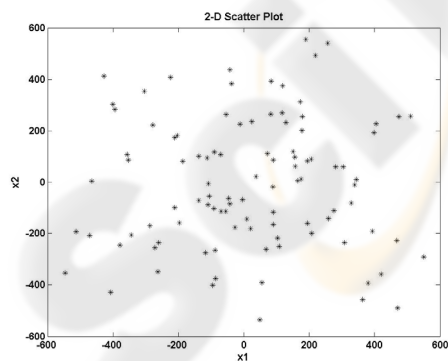


Figure 1: 2-D scatter plot of the initial algorithm's population

Assuming that the above figure represents the location of the initial population of the algorithm,

during the operation of the GA all the chromosomes tend to converge to the same point of the search space. As the algorithm converges to an optimum (global or local), the form of the scatter plot will be similar to the one of Figure 2.

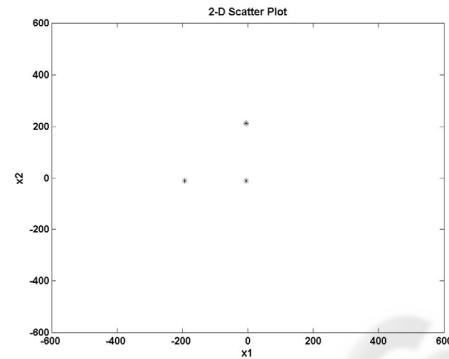


Figure 2: 2-D scatter plot of the final algorithm's population

As can be seen in Figure 2, the diversity of the final population has significantly decreased over the generations, since there are only three different chromosomes. If the solution given by the algorithm is the global optimum, then the diversity reduction is acceptable. However, in most of the cases where the problem to be solved is quite complex, the global optimum is unknown. It is therefore desirable to keep the diversity in high levels during the optimization procedure, in order to explore the search space as much as possible. Such a strategy can guarantee the suitability of the current solution, by high probability.

In the current work, a clustering method is applied, in order to investigate the location of the entire population inside the variable space, and the diversity of the population is measured by means of the scatter matrices of the resulted chromosome clusters.

In the next section a brief description of the *k-means* clustering algorithm, is taking place, while the proposed diversity measure is defined, later.

2.1 *k-means* Algorithm

Clustering methods have many applications in the engineering science, where data analysis is involved. In the following, a short definition, of what *clustering* stands for, is presented.

Definition 1. *Clustering of a given data set, in N-dimensional space, is the process that partitions these data into a number of groups (clusters) by means of a similarity or dissimilarity metric (Fukunaga, 1990).*

One of the most used clustering algorithms is the *k-means* one (Looney, 1997), which can be described in the following steps:

Step 1: Choose K initial cluster centers, C_1, C_2, \dots, C_k .
 Step 2: Classify each point of the data set to a cluster according to the following statement: point x belongs to cluster i^{th} with center C_i , if

$$\|x - C_i(t)\| \leq \|x - C_j(t)\|, \forall i, j = 1, 2, \dots, K, i \neq j$$

Step 3: Compute the new cluster centers according to

$$C_i(t+1) = \frac{1}{N_i} \sum_{x \in C_i} x, i = 1, 2, \dots, K$$

where N_i is the number of points belong to the i^{th} cluster.

Step 4: If $C_i(t+1) = C_i(t)$, for $i = 1, 2, \dots, K$, then algorithm is terminated, otherwise goes to step 2.

It must be noted, that the initialization of the cluster centers, play major role to the performance and the fast convergent of the algorithm.

In the proposed method, the *k-means* algorithm is applied in each generation to cluster the population chromosomes. In our approach, two essential assumptions about this algorithm have been made:

Assumption 1: *The initial number K of the cluster centers are chosen to be equal to the population size.*

Assumption 2: *In each iteration of the *k-means* algorithm, the empty clusters are being discarded.*

Assumption 1 is being justified by Remark 1 of the next section, while assumption 2 is made to prevent the increasing of the clusters number, by keeping the empty ones, which stay empty until the end of the algorithm.

2.2 Diversity Measure

Once the clustering is applied on each generation of the GA, a number of clusters are obtained. The number and the relative location of these clusters can be used to measure the diversity of the algorithm.

A high diversity is presented by a population which covers the search space as much as possible,

while the low diversity is presented by a population with all chromosomes being the same. These main concepts can be declared by Remark 1 and 2 respectively, in terms of clustering.

Remark 1: *The highest diversity appears when each chromosome constitutes the center of a cluster with one member, the chromosome itself and they are equally spaced, with maximum permit able distance over the search space (Figure 3).*

Remark 2: *The lowest diversity appears when all the chromosomes of the population are the same. This means that there is one cluster with all the chromosomes being the center (Figure 4).*

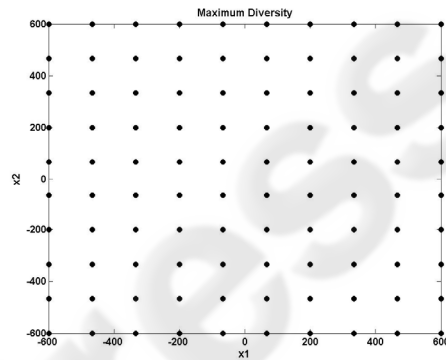


Figure 3: 2-D Maximum Diversity, by optimal chromosomes arrangement

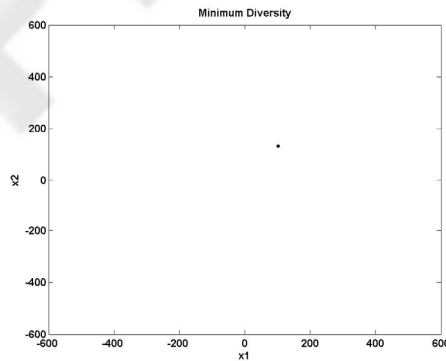


Figure 4: 2-D Minimum Diversity

The above figures correspond to the extreme situations a GA can be found. In practice, the algorithm, never presents the diversity illustrated in Figure 3, but it begins with a random chromosomes arrangement (Figure 1) and it decreases its diversity generation by generation. When, the algorithm terminates, its diversity looks like this of Figure 2, or this of Figure 4 for full convergence.

To measure these variations of the chromosomes diversity, the scatter matrices S_w and S_b (Fukunaga, 1990), are used, when the clustering has finished.

Between clusters scatter matrix S_b , describes how the data clusters, obtained by clustering, are distributed along the search space, and can be calculated by using the following equation

$$S_b = \sum_{i=1}^K (m_i - m)(m_i - m)^T$$

where K is the number of clusters obtained from k -means algorithm, m_i is the mean value of the chromosomes belong to cluster i , and m the mean value of the entire population.

Within clusters scatter matrix, S_w , measures the distribution of the chromosomes inside the clusters that they belong, and is described by the equation

$$S_w = \sum_{i=1}^K \sum_{j=1}^{N_j} (Ch_j - m_i)(Ch_j - m_i)^T$$

where N_j is the number of chromosomes belonging to the cluster i and Ch_j the j^{th} chromosome. The remaining symbols are the same as in S_b .

In the previous equations the quantities are vectors in \mathfrak{R}^n , according to the problem's dimensionality.

Keeping in mind the above definitions of the scatter matrices, Remark 1 and 2, can be restated as Remark 3 and 4, below

Remark 3: High diversity occurs when the between clusters scatter matrix S_b , takes its optimal value for a number of clusters equal to the population size, and simultaneously the within clusters scatter matrix S_w , is zero.

Remark 4: Low diversity occurs when the between clusters scatter matrix S_b , is zero meaning that the number of clusters is equal to one, and simultaneously the within clusters scatter matrix S_w , is zero.

Remark 5 is a direct consequent of the above remarks:

Remark 5: All the intermediate cases are characterized by random values of S_b , S_w and number of clusters.

In order to represent the situations described by Remark 1 and 2, by a measurable quantity, the following measure diversity is introduced.

$$\text{Diversity} = \log(\text{tr}(S_b)^{N_{cl}} + 1) + \log(\text{tr}(S_w) + 1)$$

where N_{cl} is the number of clusters obtained by the clustering algorithm and $\text{tr}()$ the trace of the matrix .

This measure takes high values as N_{cl} and $\text{tr}(S_b)$ increases, while $\text{tr}(S_w)$ decreases, thus the Remark 3 is satisfied.

The minimum value of this measure appears in the case presented in Figure 4, and is equal to zero, since $S_b=0$, and $S_w=0$.

The above measure has been applied to explore the diversity of the population, which is being used to optimize a benchmark function, over the generations.

The simulations being presented in the next section, establish the novel diversity measure, a significant measure to investigate and visualize the variety of the algorithm population.

3 SIMULATION RESULTS

The experimental results presented here, justify the usefulness of the proposed diversity measure, in supervising the progress of a GA.

The previous figures are generated by the optimization of a known benchmark function, the Griewangk's function (Digalakis2000). This function has the following form for two variables

$$f = 1 + \sum_{i=1}^2 \left(\frac{x_i^2}{4000} \right) - \prod_{i=1}^2 \left(\cos \left(\frac{x_i}{\sqrt{i}} \right) \right) \\ - 600 \leq x_i \leq 600$$

Griewangk's function is multimodal, but the location of the minima are regularly distributed, as illustrated in Figure 5,

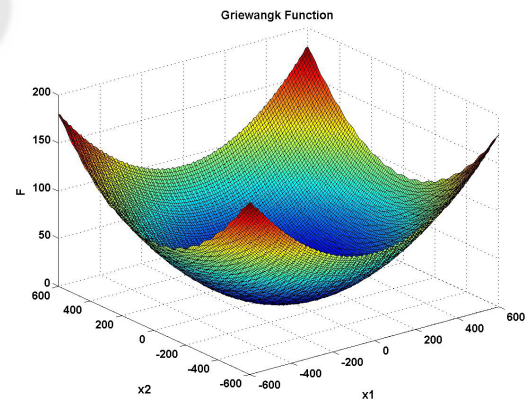


Figure 5: Griewangk's function for 2 dimensions

The algorithm used for these experiments is configured according to the following Table 1.

Table 1: GA Parameters

Population Size	100	Crossover Probability (P_c)	0.8
Selection Method	SUS	Mutation Probability (P_m)	0.01
Generations 100			

The simulations are based on the observations of the minimization process of the above function, using a simple real-valued GA. During the execution, the population diversity in each generation is measured by using, the previously introduced formula.

Let us investigate the progress of the GA, in optimizing the Griewangk's function. The algorithm starts with a random population and diversity measure, as depicted in Figure 6.

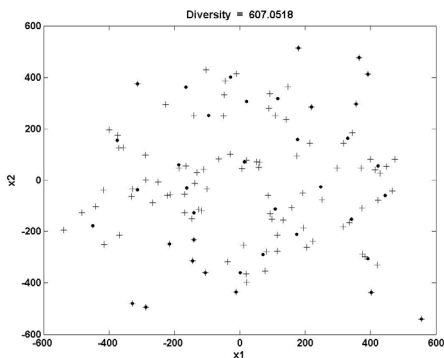


Figure 6: Initial population with Diversity = 607.0518

As the above figure shows, the cluster centers (dots) and the chromosomes (plus signs) cover a large area of the search space, and thus they provide high diversity measure.

In Figure 7, the scatter plot of the 30th generation's population is presented.

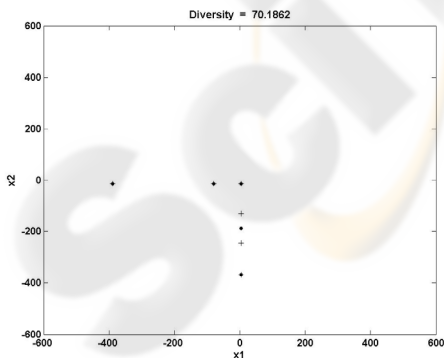


Figure 7: 30th generation's population Diversity = 70.1862

It is obvious from the above Figures 6-7, that the diversity of the population has been lost, after 30

generations. If the minimum has been reached, the goal has been achieved. In the specific case, the minimum after 30 generations is 0.5115, quite far from the global minimum, which is 0.

Thus, the measured diversity can be useful in changing the crossover and mutation probabilities, in order to converge to the global minimum.

Figure 8, shows the variation of the diversity through the generations

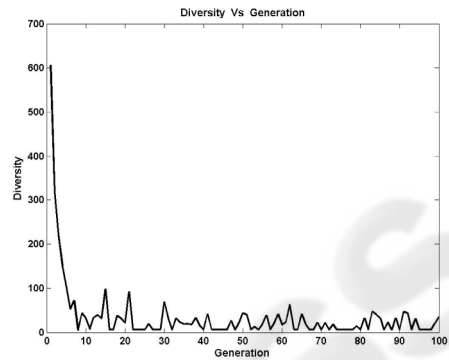


Figure 8: Diversity variation of the algorithm ($P_m=0.01$)

For the rest of the generations, the diversity is varied in low levels, decreasing the probability to find the global optimum. If the diversity stays in high levels this probability is increased.

Therefore, the diversity measure proposed in this paper seems to have the ability to describe the evolution of the algorithm's population.

It is very interesting to investigate, the behaviour of the algorithm in terms of the diversity, by changing the crossover and mutation probabilities P_c and P_m , respectively.

Figure 9, presents the diversity variation, for $P_m=0.1$.

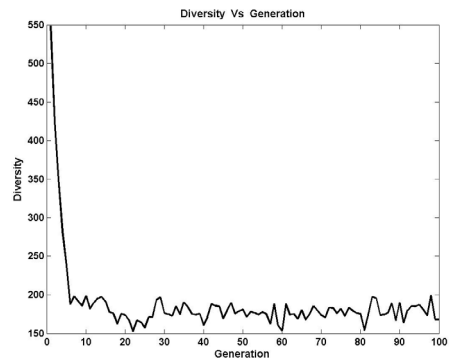


Figure 9: Diversity variation of the algorithm ($P_m=0.1$)

Mutation probability (P_m) controls the appearance of the search space points that might have not been presented before. In other words, it manages to generate all the possible search space points, by some probability. Thus, it tries to keep the

diversity in high levels, a fact that is proved by the form of the diversity variation of Figure 9. As, can be seen from this figure, the diversity fluctuates between 100 and 200, while in the case of $P_m=0.01$, it varies between 5 and 50.

On the other hand, crossover probability (P_c), defines the probability by which the chromosomes interchange their information, in order to produce better individuals. This probability is changed to 0.5, in the initial algorithm and the measured diversity is drawing in Figure 10.

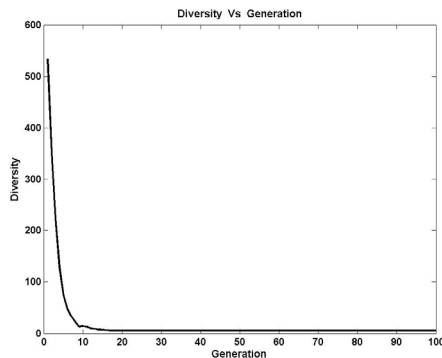


Figure 10: Diversity variation of the algorithm ($P_c=0.5$)

Crossover probability determines the population diversity, by a high degree, as displayed in Figure 10, since a reduction of the crossover probability has led to premature convergence.

It must be noted that, each one of these experiments is executed for 100 times, and the mean diversity has been presented in the above figures. Additionally, Figures 9 and 10 have been obtained by applying only one of the operators (crossover, mutation) each time, during the algorithm execution.

These simulations demonstrates, that the behaviour of the GA and the impact the crossover and mutation probabilities have, can be represented by the diversity measure introduced in this paper.

4 CONCLUSIONS

An innovative formula, which measures the diversity of GA's population, has been introduced in the previous sections. The diversity measure is based on the statistical quantities that describe the chromosome clusters obtained by applying the *k-means* algorithm to the chromosomes population.

The resulted measurement can be used to calibrate the GA by choosing the appropriate crossover P_c and mutation P_m probabilities. Additionally this measurement will be useful in adjusting the probabilities on-line during the

execution of the algorithm, in order to keep the diversity in high levels.

Appropriate experiments have shown that the proposed measure describes the evolution of the algorithm's population. This measure can also be used to any population-based algorithm, since it uses the statistical properties of the population's distribution over the search space.

Future work must be carried out in order to use this measure to adaptively adjust the crossover and mutation probabilities. Additional experiments with more complex optimization problems such as Neural Networks training by using GAs must be done. The training phase of a Neural Network is a process that is quite blind, because the only measure that one may have is the approximation error, and due to the high dimensionality the investigation of the weights evolution is not possible.

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