Degree of Population Diversity—A Perspective on Premature Convergence in Genetic Algorithms and its Markov Chain Analysis

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Abstract—In this paper, a concept of degree of population diversity is introduced to quantitatively characterize and theoretically analyze the problem of premature convergence in genetic algorithms (GA’s) within the framework of Markov chain. Under the assumption that the mutation probability is zero, the search ability of the GA’s is discussed. It is proved that the degree of population diversity converges to zero with probability one so that the search ability of a GA decreases and premature convergence occurs. Moreover, an explicit formula for the conditional probability of allele loss at a certain bit position is established to show the relationships between premature convergence and the GA parameters, such as population size, mutation probability, and some population statistics. The formula also partly answers the questions of to where a GA most likely converges. The theoretical results are all supported by the simulation experiments.

Index Terms—Genetic algorithms, Markov chains, population diversity, premature convergence, schema.

I. INTRODUCTION

Genetic algorithms (GA’s) are search and optimization algorithms based on the principles of natural evolution [1]. In applying GA’s to solve large-scale and complex real-world problems, one of the most frequent difficulties encountered is premature convergence [2], [3]. Roughly speaking, premature convergence occurs when the population in a GA reaches such a suboptimal state that most of the genetic operators can no longer produce offspring that outperform their parents [3]. Several methods have been proposed to combat premature convergence in GA’s [4]–[7]. These include, for example, the restriction of the selection procedure, the mating procedure (e.g., more disruptive crossover operators, higher mutation rate, and local mating), and the modification of fitness assignment (e.g., scaling, fitness sharing). However, all these methods are heuristic in nature. Their effects vary with different problems and their implementation strategies need ad hoc modifications with respect to different situations.

A critical problem in studying premature convergence is the identification when it has occurred and the characterization of its extent. Srinivas and Patnaik [8], for example, use the difference between the average and maximum fitness values as a yardstick to measure premature convergence, though not a measure of genetic diversity, and vary adaptively the crossover and mutation probabilities according to the measurement. On the other hand, the term “population diversity” has been qualitatively used in many papers to study premature convergence [9]–[11]. It is widely recognized that the decrease of population diversity leads directly to premature convergence. However, so far there exists little effort in performing quantitative analysis of population diversity, let alone to use it as a tool to prevent premature convergence.

In this paper, we formally propose a concept of degree of population diversity and quantitatively characterize and theoretically analyze the problem of premature convergence in GA’s using the theory of Markov chains. Under the assumption of zero mutation probability, the search ability of GA’s (in particular, the function of the crossover operator) is discussed. It is proved that the degree of population diversity converges to zero with probability one so that the search ability of genetic algorithms decreases consistently and premature convergence necessarily occurs. The relationships between premature convergence and the GA parameters such as population size, mutation probability, and relevant population statistics are also studied in light of an explicit formula for the conditional probability of allele loss at a certain gene position. The proposed formula is also employed to partly answer the question of where a GA most likely converges to.

In Section II, we introduce the population Markov chain models for the canonical genetic algorithms (CGA’s) and present the strict probabilistic definitions of the genetic operators. With the aid of ergodic analysis of the population Markov chain, the reason why the mutation probability may be assumed to be zero when analyzing premature convergence is demonstrated. In Section III, we propose a concept of degree of population diversity and quantitatively characterize and theoretically analyze the problem of premature convergence in GA’s within the Markov chain framework. In Section IV, a series of simulation studies is employed to substantiate our theoretical investigation. We then summarize and propose some directions for further research in Section V. To facilitate discussion, we put all proofs in the Appendix.

II. CANONICAL GENETIC ALGORITHMS AND THEIR POPULATION MARKOV CHAIN

Without loss of generality, we consider the GA’s with binary string representations of length $l$ and fixed population size...
We further assume that the algorithms use proportional selection, one-point crossover, and bit mutation. Each individual in the population corresponds to an element of the space $S = \{0, 1\}^l$, which is called the individual space. The population space is denoted as $S^N$ and we call $S^2$ the parents space. For the sake of convenience, we write the population $\hat{X} \in S^N$ in both the vector and matrix forms as follows:

$$\hat{X} = (X_1, X_2, \cdots, X_N)^T = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1l} \\ x_{21} & x_{22} & \cdots & x_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{Nl} \end{pmatrix}$$

where $X_i \in S$ is the $i$th individual of $\hat{X}$, while $x_{ij}$ is the $j$th component of $X_i$. The fitness function $f: S \to \mathbb{R}^+$ can be derived from the objective function of the optimization problem by a certain decoding rule.

A CGA can, in essence, be given as follows.

**CGA**

**Step 1)** Set $k = 0$ and generate initial population $\hat{X}(0)$.

**Step 2)** Independently select $N$ pairs of individuals from the current population for reproduction.

**Step 3)** Independently perform crossover to the $N$ pairs of individuals to generate $N$ new intermediate individuals.

**Step 4)** Independently mutate the $N$ intermediate individuals to get the next generation

$$\hat{X}(k+1) = \{X_1(k+1), \cdots, X_N(k+1)\}$$

**Step 5)** Stop if some stopping criterion is met. Else, set $k = k + 1$ and go to Step 2).

From the mathematical point of view, the operators are random mappings between the spaces $S^N$, $S^2$, and $S$. They are the analogous idealized abstractions of some of the genetic mechanisms in the evolution of natural organisms. To facilitate our later analysis, we present in the following the strict probabilistic definitions of several basic operators.

a) The proportional selection operator, $T_{sel}: S^N \to S^2$, selects a couple of parents from the given population for reproduction. Given the population $\hat{X}$, the probability of selecting $(X_i, X_j) \in S^2$ as the parents is

$$P[T_{sel}(\hat{X}) = (X_i, X_j)] = \frac{f(X_i) f(X_j)}{\sum_{X \in \hat{X}} f(X) \sum_{X \in \hat{X}} f(X)} 1 \leq i \leq N, 1 \leq j \leq N.$$ (1)

b) The crossover operator, $T_{cross}: S^2 \to S$ generates an individual from the selected parents. Given the parent $X_i = (x_{i1}, \cdots, x_{il})$, $i = 1, 2$, the probability for the one-point crossover operator to generate an individual $Y$ is

$$P[T_{cross}([X_1, X_2]) = Y] = \begin{cases} \frac{k \cdot p_c}{l}, & \text{if } Y \neq X_1 \\ (1 - p_c) + \frac{k \cdot p_c}{l}, & \text{if } Y = X_1 \end{cases}$$ (2)

where $0 \leq p_c \leq 1$ is the so-called crossover probability, $k = k(X_1, X_2, \bar{Y})$ is the number of gene positions at which successful crossovers of $X_1$ and $X_2$ can generate $Y$.

**Remark 2.1:** Throughout the present paper, we only consider the two-parents-one-child crossover operator, i.e., crossing two parents will always generate only one child (which we assume to be the first offspring). Such a scheme has also been adopted by many other theoretical works on GA’s [1]. This is because only with two-parents-one-child crossover, the offspring in the next generation are conditionally independent and identically distributed. This is crucial in the derivation of some results concerning the transition probabilities of the population Markov chains of GA’s.

c) The mutation operator, $T_m: S \to S$, operates on the individual by independently perturbing each bit string in a probabilistic manner and can be specified as follows:

$$P[T_m(X) = Y] = p_m^{X \neq Y}(1 - p_m)^{|X \neq Y|}. (3)$$

Based on the genetic operators defined above, the CGA can be represented as the following iteration of populations:

$$\hat{X}(k+1) = \{T_{sel}[T_{cross}([T_{sel}(\hat{X}(k))]])], i = 1, \cdots, N\} \quad k \geq 0$$ (4)

where $(T_{sel}^i, T_{cross}^i, T_{sel}^j)$, $i = 1, \cdots, N$, are independent versions of $(T_{sel}, T_{cross}, T_{sel})$. It is easy to see that the sequence of populations $\{\hat{X}(i), k \geq 0\}$ is a time-homogeneous Markov chain with the state space $S^N$ (henceforth, it is called the population Markov chain). Similar to Rudolph [12], it can be proved that if $p_m > 0$, we have for any $\bar{Y}$, $\bar{X}$,

$$\prod_{i=1}^N P[T_m^i[T_{cross}^i(T_{sel}^i(\bar{X}))] = Y_i] > 0. (5)$$

That is, $P[\hat{X}(k+1) = \bar{Y}/\hat{X}(k) = \bar{X}] > 0$. Therefore, the population Markov chain $\{\hat{X}(i), k \geq 0\}$ is homogeneous, irreducible, and aperiodic [13]. Hence, it can reach any state infinite times with probability one regardless of the initial state. Theoretically, this means that the CGA’s will never converge and premature convergence cannot occur provided that the mutation probability is larger than zero. Practically this means that even if premature convergence can occur, it will not persist indefinitely when the mutation probability is larger than zero.

### III. Degree of Population Diversity and Its Markov Chain Analysis

In this section, we first propose and define a concept called “degree of population diversity” as a way to formalize the notion of population diversity, which has not been rigorously characterized in the literature. We then use the concept to study, in conjunction with the basic GA operators, the problem of premature convergence in CGA’s within the Markov chain framework.

**Definition 3.1:** Let $\bar{X} = (X_1, \cdots, X_N) \in S^N$ be a population. The degree of population diversity of $\bar{X}$, denoted by $\lambda(\bar{X})$, is defined as the number of the components of the vector $\sum_{i=1}^N X_i$ whose values are not equal to 0 and $N$. Accordingly, $\beta(\bar{X}) = I - \lambda(\bar{X})$ is called the degree of #ness (or, the number of lost alleles) of the population $\bar{X}$.

If we denote $\bar{X}$ in its matrix form, then $\lambda(\bar{X})$ is just the number of columns of $\bar{X}$ whose entries take on both zero and...
one as values. In particular, all the individuals of $\vec{X}$ must be identical whenever $|X| = 0$. On the contrary, $|X|$ is just the number of columns of $\vec{X}$ whose entries are either all zero or all one.

A schema $L([1])$ is a hyperplane of the individual space $S$ and can be represented as

$$L = \{X = (x_1, \cdots, x_l) \in S; x_{ik} = a_{ik}, \quad 1 \leq i_k \leq l, 1 \leq k \leq K\}$$

where $K(1 \leq K \leq l)$ is called the order of $L$, $\{i_1, \cdots, i_K\}$ are called the defining components (defining gene positions), and $\{a_{i_1}, 1 \leq k \leq K\}$ are the values of the defining components (defining alleles). To signify $L$ by its defining components and their corresponding values, we may denote $L$ as $L(a_{i_1}, \cdots, a_{i_K})$. It is obvious that a schema of order $K$ contains $2^K - K$ different individuals.

**Definition 3.2:** Let $\vec{X} = (X_1, \cdots, X_N) \in S^N$ be a population with the degree of population diversity $\lambda(\vec{X})$ and the degree of maturity $\beta(\vec{X}) = l - \lambda(\vec{X})$. Let $i_k, 1 \leq k \leq \beta(\vec{X})$ be the components at which all the individuals of $\vec{X}$ take the same values, say $a_{i_k} \in \{0, 1\}, 1 \leq k \leq \beta(\vec{X})$. We call the schema $L(a_{i_1}, \cdots, a_{i_{\beta(\vec{X})}})$ the minimum schema containing $\vec{X}$ and denote it by $L(a_{i_1}, \cdots, a_{i_{\beta(\vec{X})}}; \vec{X})$ or simply $L(\vec{X})$ if there is no confusion.

For example, consider the population $\vec{X} = \{(0011), (0010), (0111), (1010)\}$. Since the individuals of $\vec{X}$ take both zero and one at the first, third, and fourth components, the degree of population diversity of $\vec{X}$ is then $\lambda(\vec{X}) = 3$. Since all the individuals of $\vec{X}$ take the same value zero at the second component, the minimum schema containing $\vec{X}$ is $L(a_{i_2}; \vec{X}) = (**0**)$ with $a_{i_2} = 0$. By “minimum” we mean that if there is another schema $L$ that also contains $\vec{X}$, it must be true that $L(a_{i_2}; \vec{X}) \subseteq L$. It is not difficult to see that there are $2^{2-K} - 2^{K-2} - 1 = 8$ different individuals in $L(a_{i_2}; \vec{X}) = (**0**)$. To evaluate the effect of population diversity on CGA performance, we first assume that the mutation probability is zero. The following theorem characterizes the search ability of CGA’s with the mutation probability $p_m = 0$.

**Theorem 3.1:** Let $\{\vec{X}(k), k \geq 0\}$ be the population Markov chain with $p_m = 0$ and $B$ be the set of homogenous populations, i.e., $B = \{(X, X, \cdots, X); X \in S\}$. Then for each $n \geq 1$,

$$P\left\{\frac{\lambda(\vec{X})}{n} \in B | \vec{X}(0) \in B\right\} = 1.$$  (8)

**Theorem 3.2:** Let $\{\vec{X}(k), k \geq 0\}$ be the population Markov chain of a CGA with $p_m = 0$ and $B$ be the set of homogenous populations.

1) $\{\vec{X}(k), k \geq 0\}$ converges to $B$ with probability one, i.e.,

$$P\left\{\lim_{k \to \infty} \vec{X}(k) = B\right\} = 1.$$  (9)

2) The degree of diversity of the sequence of populations decreases monotonically with probability one, decreases strictly monotonically with positive probabilities, and converges to 0 with probability one. That is,

$$P\{\lambda(\vec{X}(k+1)) \leq \lambda(\vec{X}(k))\} = 1, \quad \forall k \geq 0,$$  (10)

$$P\{\lambda(\vec{X}(k+1)) < \lambda(\vec{X}(k))\} > 0, \quad \forall k \geq 0$$  (11)

$$P\left\{\lim_{k \to \infty} \lambda(\vec{X}(k)) = 0\right\} = 1.$$  (12)

**Remark 3.2:** Part a) of Theorem 3.2 has been proved earlier by Fogel [14].

**Theorem 3.2** suggests that CGA’s with $p_m = 0$ converge to homogenous populations with probability one and the convergence is monotone in terms of the degree of population diversity. The difficulty is, however, that the limiting homogenous populations may correspond to local optimal solutions, or nonextremal solutions, as well as the global optimal solutions (that is, all of the points in the individual space $S$). Hence, to show the effectiveness of CGA’s (especially that of the selection and crossover operators), the question of where a CGA most likely converges to should be answered. We now proceed to establish some explicit formulas concerning the conditional probabilities of the population Markov chain. These formulas will partly answer the above question and, on the other hand, will give a formula of the probability of allele loss at a certain gene position. In the following, we no longer assume that the mutation probability is zero. Let us first introduce some notations in the following definition:
Definition 3.3: Given a population \( \bar{X} = (X_1, \ldots, X_N) \), \( X_i = (x_{i1}, \ldots, x_{il}) \), \( i = 1, \ldots, N \), for any positive integer \( 1 \leq m \leq l \), let \( I_0^m \) and \( I_1^m \) denote the sets of indexes of all the individuals of the population \( \bar{X} \) that have, respectively, a zero or one at the gene position \( m \), that is,
\[
I_0^m = \{ i \in \{ 1, 2, \ldots, N \}; x_{im} = 0 \}
\]
and write
\[
\begin{align*}
&f_0^m(\bar{X}) = \sum_{i \in I_0^m} f(X_i), \\
&f_1^m(\bar{X}) = \sum_{i \in I_1^m} f(X_i).
\end{align*}
\]
We call
\[
\begin{align*}
a_m &= \frac{f_0^m(\bar{X})}{\sum_{j=1}^N f(X_j)}, \\
b_m &= 1 - a_m = \frac{f_1^m(\bar{X})}{\sum_{j=1}^N f(X_j)}
\end{align*}
\]
respectively, the fitness ratio of zero and one allele individuals at the \( m \)th gene position.

Theorem 3.3: Let \( \{ \bar{X}(k), k \geq 0 \} \) be the population Markov chain of a CGA, then for every \( 1 \leq m \leq l \), we have
\[
\begin{align*}
P\{ \bar{X}(1) \text{ loses allele 1 at gene } m/\bar{X}(0) = \bar{X} \} &= [a_m + (1 - 2a_m)p_m]^N, \\
P\{ \bar{X}(1) \text{ loses allele 0 at gene } m/\bar{X}(0) = \bar{X} \} &= [b_m + (1 - 2b_m)p_m]^N.
\end{align*}
\] (13)

The following corollary shows the relationship between premature convergence and the population size, the mutation probability, and the population statistics \( a_m \).

Corollary 3.1: For the CGA's, the probability for allele loss to occur at a gene position (hence premature convergence at the gene position) decreases with the population size \( N \), and increases with \( |a_m - \frac{1}{2}| \) and \( |p_m - \frac{1}{2}| \). Particularly, for fixed \( N > 1 \), the above probability attains its minimum at \( a_m = \frac{1}{2} \) and \( p_m = \frac{1}{2} \).

Remark 3.3: Corollary 3.1 justifies the methods of scaling to prevent premature convergence. In fact, on the condition that the average fitness of the current population is not changed, scaling will make the difference between the individual fitness and the average fitness, and hence \( |a_m - \frac{1}{2}| \), even smaller.

Remark 3.4: From Theorem 3.3 and Corollary 3.1, we can see that the probability of premature convergence at a gene position is independent of the crossover probability. So the method of adapting crossover probability to prevent premature convergence presented in [8] seems to bare no theoretical support. Adapting the crossover probability can merely speed up the search of the minimum schema containing the current population.

From Theorem 3.1, we can also get the following corollary which partly answers the question of where a CGA most likely converges to.

Corollary 3.2: Let \( \{ \bar{X}(k), k \geq 0 \} \) be the population Markov chain with \( \bar{X}(0) = \bar{X} \). Denote by \( L(1) \) and \( L(0) \) the two competing schemata
\[
\begin{align*}
L(1) &= \{ X; x_{m} = 1 \}, \\
L(0) &= \{ X; x_{m} = 0 \}, \quad 1 \leq m \leq l
\end{align*}
\]
and assume that \( a_m > b_m \). Then we have
\[
P\{ \bar{X}(1) \subset L(0)/\bar{X}(0) = \bar{X} \} \geq P\{ \bar{X}(1) \subset L(1)/\bar{X}(0) = \bar{X} \}
\] (15)
and
\[
P\{ \bar{X}(1) \subset L(0)/\bar{X}(0) = \bar{X} \} \leq P\{ \bar{X}(1) \subset L(1)/\bar{X}(0) = \bar{X} \}
\] (16)

We close this section by a discussion of the relationship between the fitness ratio \( a_m \) and the degree of population diversity \( \lambda(\bar{X}) \). This relationship is indeed the very motivation for us to introduce the concept of degree of population diversity. From the proof of Theorem 3.3, we see that \( a_m \) is in fact the probability for the \( m \)th component of an individual generated from the current population to take on zero as its value. To put it in another way, let us assume that the current population is \( \bar{X}(k) \) and \( X(k+1) \) is an individual of the next generation. Then, \( a_m \) is nothing but the probability for the 0-1 random variable \( x_m(k+1) \) to take on zero as its value. The variance of \( x_m(k+1) \) is then \( a_m(1 - a_m) \). Define
\[
\lambda = \sum_{m=1}^l a_m(1 - a_m)
\]
which is a scalar characterization of the scattersness of individuals generated from the population \( \bar{X} \). Define a scalar function \( g \) as
\[
g(x) = \begin{cases} 1, & \text{if } 0 < x < 1 \\ x, & \text{if } x = 0 \text{ or } x = 1 \end{cases}
\]
then we have
\[
\lambda(\bar{X}) = \sum_{m=1}^l g(a_m)g(1 - a_m).
\]
This means that the degree of population diversity is a rough and yet easy to manipulate two-level discrete approximation of the degree of scatter of individuals generated from the population.

IV. EXPERIMENTAL RESULTS

To substantiate our theoretical results, a series of simulations was carried out to apply CGA's with parameters \( N \) (population size), \( p_m \) (mutation probability), and \( p_c \) (crossover probability) to a function optimization problem. The aim of the empirical analysis was three-fold: first, for a specific population size
and a specific mutation probability, we evaluated changes in the degree of population diversity over time (indicated by the number of function evaluations). By varying the mutation probability, we further obtained and compared the trends of changes in diversity. The same analysis was then repeated for different population sizes to examine if there were significant differences. Second, for a fixed population size, we evaluated the performance of the CGA (indicated by its ability to search for the global optimal solution) under different mutation probabilities. Third, for a fixed mutation probability, we examined the performance of the CGA with different population sizes.

Except for $p_c$, whose value was kept constant throughout, both $N$ and $p_m$ took on specified values for comparisons. The parameters of the CGA experiments were set as follows:

Population size $N = 50, 100, 200$.
Crossover probability $p_c = 0.85$.
Mutation probability $p_m = 0.000, 0.001, 0.005, 0.01, 0.50$.

The optimization problem involved the search for the global optimum of the test function, the famous Sine envelope sine wave function ([15])

$$f(x_1, x_2) = 0.5 - \frac{\sin^2 \sqrt{x_1^2 + x_2^2} - 0.5}{[1.0 + 0.001(x_1^2 + x_2^2)]^2}.$$ 

This is a rapidly varying multimodal function of two variables with $x_1 = 0$, $x_2 = 0$ as the unique global optimal solution having value $f(0, 0) = 1.0$. Each variable was encoded by 22 bits so that the string length of an individual was $l = 44$. Therefore, the maximal degree of population diversity was 44. Each experiment was repeated in 30 independent runs and the average was taken as the basis for evaluation.

The simulation results of changes in diversity over time are summarized in Figs. 1–3, which depict the variations of the average degree of population diversity with respect to population size and CGA performance, we observe in Table I and Figs. 4 and 5 that the larger the population size, the more notable is the effect of the mutation probability on the algorithm’s performance (Fig. 5). In addition, though the performance of the CGA with 0.5 mutation probability is not very bad (Fig. 4), the convergence rate is obviously slower than the case of a lower mutation probability, e.g., $p_m = 0.005$ and $p_m = 0.01$.

To summarize, the experimental results reveal that the impact of population size on the CGA’s performance is more favorable than that of the mutation probability. For example, as shown in Table I, the performance of the CGA with $N = 200$ and $p_m = 0.000$ is better than that of the CGA with $N = 50$ and $p_m = 0.005$. All these theoretical and empirical results suggest that a more effective method to maintain the degree of population diversity to prevent premature convergence is to increase the population size instead of adopting a high mutation rate.

V. CONCLUSION

We have introduced in this paper a concept of degree of population diversity, and quantitatively characterized and theoretically analyzed the problem of premature convergence in CGA’s using the theory of Markov chain. Under the assumption that the mutation probability is zero, we have proved that the degree of population diversity converges to zero with probability one so that the search ability of a genetic algorithm decreases over time, resulting in premature convergence. An explicit formula for the conditional probability of allele loss at a certain gene position has been established to show relationships between premature convergence and the CGA parameters—population size $N$, mutation probability $p_m$, and population statistics $a_m$. The formula also partly answers the question of where a genetic algorithm most likely converges to. A series of simulations have also been conducted to validate our theoretical analysis. We conclude that to prevent premature convergence, increase in population size tends to play a more important role than the variation of the mutation probability. Any effort in varying the crossover probability, unlike what has been suggested by some research in the literature, has no contribution in avoiding premature convergence.

For further research, we at least can pursue the following two lines of investigation:

1) Use the degree of population diversity as a quantitative measure to prevent premature convergence by adaptively varying population size and mutation probability. Some optimization procedures can also be explored to improve performance.

2) The degree of population diversity presented in this paper is exclusively based on the genotype of the population. Resorting to Theorem 3.3 of the present paper, as has been outlined at the end of Section III, it is
Fig. 1. The convergence curves of population diversity as functions of the number of function evaluations with different mutation probabilities $p_m$ and fixed population size $N = 50$.

Fig. 2. The convergence curves of population diversity as functions of the number of function evaluations with different mutation probabilities $p_m$ and fixed population size $N = 100$. 
Fig. 3. The convergence curves of population diversity as functions of the number of function evaluations with different mutation probabilities $p_m$ and fixed population size $N = 200$.

Fig. 4. The convergence curves of the optimal value found by GA's, as functions of the number of function evaluations, with different mutation probabilities $p_m$ and fixed population size $N = 50$. 
possible to introduce a more involving concept of degree of population diversity based on both genotype and its corresponding fitness.

**APPENDIX**

1) Proof of Theorem 3.1:

a) Let $Y = (y_1, y_2, \ldots, y_l) \in \mathbb{I}[a_{i_1}, \ldots, a_{i_\beta(X_0)}; X_0]$ and

$$X_0 = (X_1, X_2, \ldots, X_N)^T = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1l} \\ x_{21} & x_{22} & \cdots & x_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{Nl} \end{pmatrix}.$$ 

Since the degree of population diversity of $X_0$ is $\lambda(X_0)$, we may suppose that the first $\beta(X_0)$ components of the individuals in $X_0$ take the same bit value, i.e.,

$$x_{ij} = y_j, \quad 1 \leq i \leq N, \quad 1 \leq j \leq \beta(X_0).$$

By the definition of degree of population diversity, for each $1 + \beta(X_0) \leq j \leq l$, there is an individual $X_i$ in $X_0$ such that its $j$th component $x_{ij}$ equals to $y_j$.

We now proceed with the method of induction. Consider first the case of $\lambda(X_0) = 2$. We have

$$x_{ij} = y_j, \quad 1 \leq i \leq N, \quad 1 \leq j \leq l - 2.$$ 

So there are $1 \leq p, \ q \leq N, \ p \neq q$, so that $x_{pq} = y_{l-1}$ and $x_{qy} = y_l$. Let $Z = (Z_1, \ldots, Z_N)$ be a population such that $Z_i = X_i (i \neq p)$ and that $Z_p$ is the individual generated by crossing the two individuals $X_p, X_q$ at the $l$th component, i.e.,

$$Z_p = [x_{p1}, x_{p2}, \ldots, x_{pl-1}, x_{ql}] = (y_1, \ldots, y_l) = Y.$$ 

By the definition of the selection operator and crossover operator, we get

$$P\{Y \in X(1)/X(0) = X(0)\} \geq P\{X(1) = Z/X(0) = X(0)\} \geq \prod_{j \neq p} \left[ \frac{f^2(X_j)}{\sum_{j=1}^N f(X_j)} \right]^2 \frac{p_c}{l} \left[ \sum_{j=1}^N f(X_j) \right]^2 \geq 0.$$ 

This proves the case of $\lambda(X_0) = 2$. 

Fig. 5. The convergence curves of the optimal value found by GA’s, as functions of the number of function evaluations, with different mutation probabilities $p_m$ and population size $N$. (a) $p_{m1} = 0.0001$. (b) $p_{m2} = 0.001$. (c) $p_{m3} = 0.005$. (d) $p_{m4} = 0.010$. 

![Fig. 5](image-url)
Suppose that the theorem is valid for $\lambda(\bar{X}_0) = m - 1$. Consider the case of $\lambda(\bar{X}_0) = m$. Then, we have

$$x_{ij} = y_j, \quad 1 \leq i \leq N, \; 1 \leq j \leq l - m$$

and there exists $1 \leq i_0 \leq N$ such that $x_{i_0d} = y_d$. Let $\bar{Z}(1) = (Z_1, \ldots, Z_N)$ be a population such that $Z_{i_0} = X_{i_0}$ and $Z_i = [x_{i1}, x_{i2}, \ldots, x_{i(j-1)}, x_{iod}], \quad i \neq i_0$.

It is easy to see that $\lambda[Z(1)] = m - 1$ and $Y \in \mathbf{L}[y_1, y_2, \ldots, y_{l-m}, y_d; \bar{Z}(1)]$. And hence

$$P\left\{\bar{X}(1) = \bar{Z}(1)/\bar{X}(0) = X_0\right\}$$

$$\geq \prod_{i \neq i_0} \left\{ \frac{f(X_i)f(\bar{X}_0)}{\sum_{j=1}^{N} f(X_j)} \right\}^2 \cdot \frac{p_c}{l} \cdot \left\{ \frac{\sum_{j=1}^{N} f(X_j)}{\sum_{j=1}^{N} f(X_j)} \right\}^{n^*}$$

$$> 0.$$  \hfill (18)

By the assumption and homogeneity of the Markov chain $\{\bar{X}(k), k \geq 0\}$, there is a $n^* > 0$ such that

$$P\left\{Y \in \bar{X}(n^* + 1)/\bar{X}(1) = \bar{Z}(1)\right\} > 0.$$  \hfill (19)

Let $n = n^* + 1$, we get

$$P\left\{Y \in \bar{X}(n)/\bar{X}(0) = X_0\right\}$$

$$\geq P\left\{Y \in \bar{X}(n^* + 1)/\bar{X}(1) = \bar{Z}(1)\right\}$$

$$\cdot P\left\{\bar{X}(1) = \bar{Z}(1)/\bar{X}(0) = X_0\right\}$$

$$> 0.$$  \hfill (20)

Thus, the theorem is valid for the case $\lambda(\bar{X}_0) = m$. The proof of the first part of Theorem 3.1 is completed.

b) We write $\bar{X} \in \mathbf{L}[a_1, \ldots, a_{\lambda(\bar{X}_0)}; \bar{X}_0]$ to express that each individual of $\bar{X}$ belongs to the schema $\mathbf{L}[a_{i_1}, \ldots, a_{i_{\lambda(\bar{X}_0)}}; \bar{X}_0]$ so that all the individuals of $\bar{X}$ have the same values at the components $i_1, \ldots, i_{\lambda(\bar{X}_0)}$. Therefore, neither selection operator nor crossover operator can change the values at these components of the individuals in the population. So, for each $Y \in \mathbf{L}[a_{i_1}, \ldots, a_{i_{\lambda(\bar{X}_0)}}; \bar{X}_0]$, we have

$$P\left\{\bar{X}(k + 1) \in \mathbf{L}[a_{i_1}, \ldots, a_{i_{\lambda(\bar{X}_0)}}; \bar{X}_0]/\bar{X}(k) = Y\right\} = 1.$$  

To simplify the notation, let us write $\mathbf{L}$ for

$$\mathbf{L}[a_{i_1}, \ldots, a_{i_{\lambda(\bar{X}_0)}}; \bar{X}_0].$$

By the Markovian property, we get

$$P\left\{\bar{X}(n) \in \mathbf{L}/\bar{X}(0) = X_0\right\}$$

$$\geq \sum_{\bar{Y}(1) \in \mathbf{L}} \cdots \sum_{\bar{Y}(n) \in \mathbf{L}} P\left\{\bar{X}(1) = \bar{Y}(1)/\bar{X}(0) = X_0\right\}$$

$$\cdot P\left\{\bar{X}(2) = \bar{Y}(2)/\bar{X}(1) = \bar{Y}(1)\right\} \cdots$$

$$P\left\{\bar{X}(n) = \bar{Y}(n)/\bar{X}(n-1) = \bar{Y}(n-1)\right\}$$

$$= 1.$$  \hfill (21)

Since $Y \in \bar{X}(n)$ implies $\bar{X}(n) \notin \mathbf{L}$, we have

$$P\left\{Y \in \bar{X}(n)/\bar{X}(0) = X_0\right\} = 0.$$  \hfill (22)

This completes the proof.

2) Proof of Lemma 3.1: For any homogeneous population $\bar{X} \in \mathbf{B}$ and nonhomogeneous population $\bar{Y} \notin \mathbf{B}$, it follows from Theorem 3.1b) that $P\{\bar{X}(n) = \bar{Y}/\bar{X}(0) = \bar{X}\} = 0$. And hence

$$P\left\{\bar{X} \in \mathbf{B}/\bar{X}(0) \in \mathbf{B}\right\}$$

$$= 1 - P\left\{\bar{X}(n) \notin \mathbf{B}/\bar{X}(0) \in \mathbf{B}\right\}$$

$$= 1 - \sum_{\bar{Y} \notin \mathbf{B}} P\{\bar{X}(n) = \bar{Y}, \bar{X}(0) \in \mathbf{B}\}/P\{\bar{X}(0) \in \mathbf{B}\}$$

$$= 1 - \sum_{\bar{Y} \notin \mathbf{B}} \sum_{\bar{X} \in \mathbf{B}}$$

$$P\left\{\bar{X}(n) = \bar{Y}/\bar{X}(0) = \bar{X}\right\} \cdot P\{\bar{X}(0) = \bar{X}\}$$

$$P\{\bar{X}(0) \in \mathbf{B}\}$$

$$= 1.$$  \hfill (23)

3) Proof of Theorem 3.2:

a) Let $P(\bar{X}, \bar{Y}) = P(\bar{X}(k+1) = \bar{Y}/\bar{X}(k) = \bar{X})$. For each $\bar{X} = (X_1, \ldots, X_N) \in S^N$, we have

$$P(\bar{X}, \mathbf{B}) := \sum_{\bar{Y} \in \mathbf{B}} P(\bar{X}, \bar{Y})$$

$$\geq \sum_{i=1}^{N} P\{\bar{X}(k+1) = (X_1, \ldots, X_i)/\bar{X}(k) = \bar{X}\}$$

$$\geq \sum_{i=1}^{N} \left\{ \frac{f^2(X_i)}{\left[ \sum_j f(X_j) \right]^2} \right\}^{N} > 0.$$  \hfill (24)

Let $a = \inf_{\bar{Y} \in \mathbf{B}} P(\bar{Y}, \mathbf{B})$, then $0 < a < 1$. If $\bar{X}(0) \in \mathbf{B}$, it follows from Lemma 3.1 that $\bar{X}(n) \in \mathbf{B}$ for any $k \geq 1$. So the part a) of Theorem 3.2 is valid.

Now assume that $\bar{X}(0) \notin \mathbf{B}$ and define

$$T = \inf \{k \geq 1; \bar{X}(k) \in \mathbf{B}\}.$$


For any $k \geq 1$, we get
\[
P\{T = k\} = \sum_{\bar{y}_1, \ldots, \bar{y}_{k-1} \in \mathcal{B}} P(\bar{X}, \bar{Y}_1)P(Y_1, \bar{Y}_2) \ldots P(Y_{k-2}, \bar{Y}_{k-1})P(Y_{k-1}, \mathcal{B}) \leq (1 - \alpha)^{k-1}.
\]
It follows that $E(T) = \sum_{k=1}^{\infty} kP\{T = k\} < +\infty$, where $E(T)$ is the expectation of the random variable $T$. And hence $P\{T < +\infty\} = 1$. From Lemma 3.1 and the definition of $T$ we know that $\lim_k \bar{X}(k) \in \mathcal{B}$ whenever $T < +\infty$. Therefore, we get $P\{\lim_k \bar{X}(k) \in \mathcal{B}\} = 1$ as what we intend to prove.

b) Denote by $L(\bar{X})$ the minimal schema containing $\bar{X}$. By virtue of the formula of total probability, we have
\[
P\{\lambda[\bar{X}(k+1)] \leq \lambda[\bar{X}(k)]\}
= \sum_{X(k+1) \in L(\bar{X}) \times L(\bar{X})} \ldots \times L(\bar{X})/\lambda(\bar{X}(k)) = \bar{X}\}P\{\bar{X}(k) = \bar{X}\}
= 1
\]
which proves (10). Since for each $\bar{X} \in S^N$,
\[
P\{\lambda[\bar{X}(k+1)] < \lambda[\bar{X}(k)]/\lambda(\bar{X}(k)) = \bar{X}\}
= P\{\lambda[\bar{X}(k+1)] \leq \lambda[\bar{X}(k)] - 1/\lambda(\bar{X}(k)) = \bar{X}\}
\geq P\{\lambda[\bar{X}(k+1)] = 0/\lambda(\bar{X}(k)) = \bar{X}\}
\geq \left\{ \frac{f^2(X_i)}{\sum_{i=1}^{N} f(X_i)} \right\}^N > 0
\]
then an application of the formula of total probability yields the desired result (11).

To get (12), it should be observed that $\lambda(\bar{Y}) = 0$ for each $\bar{Y} \in \mathcal{B}$. It follows that $\lim_k \lambda[\bar{X}(k)] \in \mathcal{B}$ implies $\lim_k \lambda[\bar{X}(k)] = 0$, and hence, $P\{\lim_k \lambda[\bar{X}(k)] = 0\} = 1$. The proof is completed.

4) Proof of Theorem 3.3: We only prove (13) and the proof of (14) is similar. Let $x_{i}(j)$ be the $j$th component of the $i$th individual of $\bar{X}(1)$ and $Y = (y_1, \ldots, y_l)$ the random individual generated by the selection and crossover operator from $\bar{X}(0)$. Then, for each $i$
\[
P\{x_{im}(1) = 0/\bar{X}(0) = \bar{X}\}
= P\{y_m = 0/\bar{X}(0) = \bar{X}\} \cdot (1 - p_m)
+ P\{y_m = 1/\bar{X}(0) = \bar{X}\} \cdot p_m
= P\{y_m = 0/\bar{X}(0) = \bar{X}\} \cdot (1 - p_m)
+ \left(1 - P\{y_m = 0/\bar{X}(0) = \bar{X}\}\right) \cdot p_m.
\]
By the definition of the selection and crossover operators, we get
\[
P\{y_m = 0/\bar{X}(0) = \bar{X}\}
= \sum_{i, j \in I^m} \frac{f(X_i)f(X_j)}{\sum_{i=1}^{N} f(X_i)} \frac{l - m}{l}
+ \sum_{i \in I^m} \sum_{j \in I^m} \frac{f(X_i)f(X_j)}{\sum_{i=1}^{N} f(X_i)} \frac{m(1 - p_c)}{l}
+ \sum_{i \in I^m} \sum_{j \in I^m} \frac{f(X_i)f(X_j)}{\sum_{i=1}^{N} f(X_i)} \frac{mp_c}{l}
= \left[ \sum_{i \in I^m} f(X_i) \right]^2 \frac{N}{\sum_{i=1}^{N} f(X_i)}
+ \sum_{i \in I^m} \frac{f(X_i)}{\sum_{i=1}^{N} f(X_i)} \frac{m(1 - p_c)}{l}
= a_m^2 + a_m(1 - a_m)
= a_m.
\]
The four terms in the right hand side of the second equation correspond to the four possible events of selection and crossover all of which result in an individual with the $m$th component being zero. The first one is that the $m$th components of the selected parents are both zero and crossover is arbitrary and immaterial. The second and third terms correspond to the situation that the first parent is selected with the $m$th component zero and the second parent has one at the $m$th component. The difference is that the second term corresponds to the case that the crossover point is selected after the $m$th component and crossover either occurs or does not occur (i.e., having crossover or not is immaterial), while the third one is the situation where the crossover point is before the $m$th component and crossover does not take place. The fourth term captures the case that the first parent has one at its $m$th component and the second parent has zero at the same position, and crossover occurs with the crossover point being selected before the $m$th component.

Therefore, for each $i$
\[
P\{x_{im}(1) = 0/\bar{X}(0) = \bar{X}\} = a_m(1 - p_m) + (1 - a_m)p_m
= a_m + (1 - 2a_m)p_m.
\]
Since the $N$ individuals of $\bar{X}(1)$ are independently generated with the same manner, we get

$$P\left\{\bar{X}(1) \text{ loses allele 1 at gene } m/\bar{X}(0) = \bar{X}\right\}$$

$$= P\left\{x_m(1) = 0, \ 1 \leq i \leq N/\bar{X}(0) = \bar{X}\right\}$$

$$\prod_{i=1}^{N} P\left\{x_m(1) = 0/\bar{X}(0) = \bar{X}\right\}$$

$$= [a_m + (1 - 2a_m)p_m]^N.$$

This completes the proof.

5) Proof of Corollary 3.1: From Theorem 3.3, we know that

$$P\left\{\bar{X}(1) \text{ loses an allele at gene } m/\bar{X}(0) = \bar{X}\right\}$$

$$= [a_m + (1 - 2a_m)p_m]^N + [b_m + (1 - 2b_m)p_m]^N$$

$$= [a_m + (1 - 2a_m)p_m]^N + [1 - a_m - (1 - 2a_m)p_m]^N$$

$$:= f(a_m, p_m, N), \quad (21)$$

Since 0 $\leq a_m + (1 - 2a_m)p_m \leq 1$ for each $a_m$ and $p_m$, the function $f(a_m, p_m, N)$ decreases with $N$.

We write $a = a_m + (1 - 2a_m)p_m$ to simplify the notation. The partial differential of $f(a_m, p_m, N)$ with respect to $a_m$ can be given as

$$\frac{\partial f}{\partial a_m} = Na^{N-1}(1 - 2p_m) - N(1 - a)^{N-1}(1 - 2p_m)$$

$$= N(1 - 2p_m)[a^{N-1} - (1 - a)^{N-1}].$$

It can be shown that, for each $0 \leq a_m \leq 1$, $\partial f/\partial a_m \leq 0$ whenever $0 \leq a_m \leq \frac{1}{2}$ and $\partial f/\partial a_m \geq 0$ whenever $\frac{3}{2} \leq a_m \leq 1$. That is to say that $f(a_m, p_m, N)$ is decreasing when $a_m \leq \frac{1}{2}$ and increasing when $a_m \geq \frac{3}{2}$. It follows that the probability for an allele loss to occur at a gene position increases with $[a_m - \frac{1}{2}]$. Similarly, we can prove that the probability for allele loss to occur at a gene position increases with $[p_m - \frac{1}{2}]$.

Solving the equations $\partial f/\partial a_m = 0$ and $\partial f/\partial p_m = 0$, we get an unique solution $p_m = \frac{1}{2}$, $a_m = \frac{1}{2}$. Hence, for fixed $N$, $f(a_m, p_m, N)$ takes its minimum at $p_m = \frac{1}{2}$ and $a_m = \frac{1}{2}$. The proof is completed.

6) Proof of Corollary 3.2: It is obvious that $\bar{X}(1) \subset L(0)$ [or $\overline{X}(1) \subset L(1)$] if and only if $\bar{X}(1)$ lose the allele 1 (respectively 0) at gene $m$. So

$$P\left\{\bar{X}(1) \subset L(0)/\bar{X}(0) = \bar{X}\right\} = f(a_m + (1 - 2a_m)p_m)^N$$

$$P\left\{\bar{X}(1) \subset L(1)/\bar{X}(0) = \bar{X}\right\} = f(b_m + (1 - 2b_m)p_m)^N.$$

If $a_m > b_m$, simple calculation shows that

$$a_m + (1 - 2a_m)p_m > b_m + (1 - 2b_m)p_m$$

if $0 \leq p_m < \frac{1}{2}$

$$a_m + (1 - 2a_m)p_m < b_m + (1 - 2b_m)p_m$$

if $\frac{1}{2} < p_m \leq 1$.

The corollary then follows.

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