International Journal Of Computer Science And Applications Vol. 1, No. 2, August 2008
ISSN 0974-1003

Convergence Analysis of Quantum Genetic Algorithm

Mehrshad Khosraviani,
Dept. of Computer Engineering & IT,
Amirkabir University of Technology (Tehran Polytechnic)
424 Hafez Ave., Tehran 15785, Iran
khosraviani@aut.ac.ir

Saadat Pour Mozafari,
Dept. of Computer Engineering & IT,
Amirkabir University of Technology (Tehran Polytechnic)
424 Hafez Ave., Tehran 15785, Iran
saadat@aut.ac.ir

Mohammad Mehdi Ebadzadeh,
Dept. of Computer Engineering & IT,
Amirkabir University of Technology (Tehran Polytechnic)
424 Hafez Ave., Tehran 15785, Iran
ebadzadeh@aut.ac.ir

ABSTRACT
It is an important and a complicated task to investigate the convergence of a new genetic algorithm based on quantum mechanics concepts including qubits and superposition of states, namely Quantum Genetic Algorithm, in the field of evolutionary computation. This paper analyzes convergence property of quantum genetic algorithm which uses its special quantum operator instead of canonical operators of classical genetic algorithms, such as crossover and mutation operators and even selection techniques. The Markov chain is a considerable part of the probability theory and stochastic processes; and one of its important applications is to model some classical evolutionary algorithms and to analyze their convergence property. In reality, inasmuch as modeling of the evolutionary algorithms in usual methods is very difficult, the finite Markov chain is used to formalize them. In here, the quantum genetic algorithm is modeled as a finite Markov chain and is shown by means of Markov chain analysis that the algorithm with preservation of the best solution in the population, will converge to the global optimum.

Categories and Subject Descriptors
G.3 [**Mathematics of Computing**]: Probability and Statistics – *Markov Processes*

General Terms
Verification

Keywords
Quantum Genetic Algorithm, Finite Markov Chain, Global Convergence

1 INTRODUCTION
Quantum computing is one of the promising new fields of the millennium and offers certain possibilities which are not present in classical computing. Although there would be significant benefit from new quantum algorithms which could solve computational problems faster than classical algorithms, to date, only a few quantum algorithms are presented [1][2][3][4].

An evolutionary computing algorithm called Quantum Genetic Algorithm (QGA) is characterized by principles of quantum computing including concepts of qubits and superposition of states, is proposed by Han and Kim in the literature [5]. The algorithm is concentrated on the quantum-inspired evolutionary computing for a classical computer. In QGA, there is not a wide spectrum of parameters and operators; however, we encounter a fastest and an effective algorithm. Han and Kim in [5][6][7] have been presented that the QGA can simplify the search process and invoke much less computation time. Practical experience indicates that QGA can sometimes find good solutions to complex problems. In optimization theory an algorithm is said to converge on the global optimum, if the global optimum can be observed in a generated sequence of solutions, eventually.

Markov chains [8][9][10] offer an appropriate model to analyze GAs and they have been used to prove their probabilistic convergence. In this paper, our proposed analysis is based on a Markov chain, by assuming the generation changes operation in a QGA is restricted to quantum gates. In this paper, we model a QGA as a finite Markov chain and then based on the concepts presented in [11][12], and prove the QGA always maintains the best solution in the population, converges with probability one to the global optimal solution.

This paper is organized as follows: first, the necessary concepts about the novel evolutionary computing algorithm, QGA, and the requisite principles of finite Markov chain for convergence analysis are presented in section 2, and in section 3, mathematical prelude to QGA is presented and then the global convergence of QGA is analyzed. And finally, some conclusions are drawn in section 4.

2 BASIC CONCEPTS

2.1 Quantum Genetic Algorithm
The description of the QGA provided here is largely based on [5], and comprehensive information and more details about it can be found in literatures [6][7].

Quantum Genetic Algorithm (QGA) is based on the quantum computing concepts including qubits and superposition of the two states. This algorithm uses a notable representation that is based on the concepts of qubits which are in quantum mechanics. A qubit may be in '1' state, '0' state, or in any superposition of the two. So, the state of a qubit can be presented as

$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where $|\alpha|^2$ and $|\beta|^2$ gives the probability that the qubit will be found in '0' state and '1' state, respectively and so, $|\alpha|^2 + |\beta|^2 = 1$. So, the qubit is defined with a pair of numbers, (α, β) and consequently, a qubit individual is represented as a string of qubits. In (1), an individual of m qubits is instantiated as

$$\begin{bmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_m \\ \beta_1 & \beta_2 & \cdots & \beta_m \end{bmatrix}, \quad (1)$$

where $|\alpha_i|^2 + |\beta_i|^2 = 1$, $i = 1, 2, \cdots, m$. The advantages of this representation are its ability to represent any linear superposition of states. This genetic algorithm with the representation in (1) has a better characteristic of population diversity than the other genetic algorithms.

QGA is a probabilistic algorithm similar to other genetic algorithms and it also maintains a population of n qubit individuals at generation t in $Q(t) = \{q_1^t, q_2^t, \ldots, q_n^t\}$, where q_j^t is a qubit individual defined as

$$q_j^t = \begin{bmatrix} \alpha_{j1}^t & \alpha_{j2}^t & \cdots & \alpha_{jm}^t \\ \beta_{j1}^t & \beta_{j2}^t & \cdots & \beta_{jm}^t \end{bmatrix}, \quad (2)$$

where m is the number of qubits, i.e., the string length of the qubit individual, and $j = 1, 2, \cdots, n$.

Figure 1 shows the QGA procedure, and its overall structure is explained in the following:

```
begin
    t ← 0
    initialize Q(t)
    make Pop(t) by observing Q(t) states
    evaluate Pop(t)
    store the best solution among Pop(t)
    while (not termination-condition) do
    begin
        t ← t+1
        make Pop(t) by observing Q(t-1) states
        evaluate Pop(t)
        update Q(t) using quantum gate
        store the best solution among Pop(t) and
B(t-1)
    end
```

Figure 1. Procedure of Quantum Genetic Algorithm

A quantum gate, $U(t)$, is defined as

$$U(t) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}, \quad (3)$$

where θ is a rotation angle.

The quantum gates that are defined as (3), are the rotation operators and their angels contribute to the convergence time; and also, these gates has a reversibility property and can be represented as unitary operators acting on qubit basis states. Like was said before, the quantum gate $U(\theta_i)$ is employed to update a qubit individual q_j^t as a novel genetic operator. The pair of number, (α_i, β_i) of *i*-th qubit is updated as follows:

$$\begin{bmatrix} \alpha_i' \\ \beta_i' \end{bmatrix} = \begin{bmatrix} \cos(\theta_i) & -\sin(\theta_i) \\ \sin(\theta_i) & \cos(\theta_i) \end{bmatrix} \cdot \begin{bmatrix} \alpha_i \\ \beta_i \end{bmatrix}. \quad (4)$$

The magnitude of θ_i has been effect on the speed of convergence, but if is too big, the solutions may diverge or converge prematurely to local optimum. In literature [6][7] is recommended that the magnitude of θ_i are ranging from 0.001π to 0.1π, although they depend on the problems. Additionally, sign of θ_i determines the direction of convergence.

2.2 Finite Markov Chain

A finite Markov chain describes a probabilistic trajectory over a finite state space. The probability $p_{ij}(t)$ is of transition probability from i to j at step t. If the transition probabilities are independent from t, the Markov chain is said to be homogenous. The transition probabilities of a homogenous finite Markov chain can be expressed in a transition matrix $P = \{p_{ij}\}$; For each entries, $p_{ij} \in [0,1]$.

Definition 1: A square matrix $A: n \times n$ is said to be

Nonnegative, if $a_{ij} \geq 0$ for all $i, j = 1, 2, \cdots, n$

Positive, if $a_{ij} > 0$ for all $i, j = 1, 2, \cdots, n$

Primitive, if there exists a $k \in N$ such that A^k is positive.

Reducible, if matrix A can be transformed into the form (with square matrix C and T) by applying the same permutations to rows and columns: $\begin{bmatrix} C & 0 \\ R & T \end{bmatrix}$

Stochastic, if $\sum_{j=1}^{n} a_{ij} = 1$ for all $i = 1, 2, \cdots, n$

Definition 2: Let $Z_t = \max\{f(\theta_k(t)) \mid k = 1, 2, \cdots, n\}$ be a sequence of random variables representing the best fitness within a population presented by individual k at step t. One of the classes of genetic algorithms converge to the global optimum, if and only if

$$\lim_{t\to\infty} P\left\{Z_t = f^*\right\} = 1, \tag{5}$$

where $f^* = \max\left\{ f\left(\theta\right) \mid \theta \in B^m\right\}$ is the global optimum of objective function; and B^m is contained all the solution possibilities in search space.

Theorem 1: [10][11] P is a primitive stochastic matrix. Then P^k converges as $k\to\infty$ to a positive stable stochastic matrix $P^\infty = 1' p^\infty$, where $p^\infty = p^0 \cdot \lim_{k\to\infty} P^k = p^0 P^\infty$ has nonzero entries and is unique regardless of initial distribution.

Theorem 2: [10][11] $P = \begin{bmatrix} C & 0 \\ R & T \end{bmatrix}$ is reducible stochastic matrix, where $C: m\times m$ is primitive stochastic matrix and $R, T \neq 0$. Then

$$P^\infty = \lim_{k\to\infty} \begin{bmatrix} C^k & 0 \\ \sum_{i=0}^{k-1} T^i R C^{k-i} & T^k \end{bmatrix} = \begin{bmatrix} C^\infty & 0 \\ R^\infty & 0 \end{bmatrix}, \tag{6}$$

is a stable stochastic matrix with $P^\infty = 1' p^\infty$, where $p^\infty = p^0 P^\infty$ is unique regardless of the initial distribution, and p^∞ satisfies: $p_i^\infty > 0$ for $1 \le i \le m$ and $p_i^\infty = 0$ for $m < i \le n$.

3 ANALYSIS OF THE QGA

The QGA can be described as Markov chain: The state of its Markov model depends only on the genes of the individuals so that the state space is $S = B^{m.n}$, where n denotes the population size and m is the number of genes (qubits) of the solution. State space, S, is defined based on the qubit individuals, $Pop(t)$. Each element of this state space can be regarded as an integer number in representation. Contrary to us knows about the canonical genetic algorithms (GAs), it must be noted that in QGA, the intermediate transitions is not caused by the selection and the other genetic operators. Primary operator of the QGA is the quantum gate $U(t)$.

Lemma 1: Markov chain model of QGA is non-homogeneous, but it's possible to extract the homogeneous part from the main one.

Proof: Suppose the quantum gate in (3); if its rotation angles are not zero, it could change the transition probability matrix in each generation. The transition probability at generation t supposed to be

$$p(t) = \xi(t)\, p(t-1), \tag{7}$$

where $\xi(t)$ is the increasing rate of the transition probability $p(t)$, $0 < p(t) \le 1$ and $1 < \xi(t) \ll \frac{1}{p(t)}$ for $t > 1$. In [7], is considered that

$$\xi = 1 + \frac{\delta}{p(0)}, \tag{8}$$

where $0 < \delta \ll p(0)$, so we will have

$$P(t) \approx \left(1 - p(0)\right)^{t-1} \xi^{t-1} p(0). \tag{9}$$

Concerning (8), and with respect to $0 < \delta \ll p(0)$, we can see $\xi \to 1$, and subsequently $\lim_{k\to\infty} \xi^k \approx 1$. □

Now we have two parts, ξ and $p(0)$, which are non-homogeneous and homogeneous, respectively. Incidentally, $p(t)$ is positive.

Theorem 3: The transition matrix of QGA with transition probability $p(t)$ is primitive.

Proof: It follows by lemma 1 that $p(t)$ is positive. Since every positive matrix is primitive, the proof is completed. □

Theorem 4: The QGA with parameter ranges as in Theorem 3 is an ergodic Markov chain with, i.e., there exists an unique limit distribution for the states of the chain with nonzero probability to be in any state at any time regardless of initial distribution.

Proof: This corollary is understood from Theorem 1 and 3. □

Theorem 5: [10][11] In an ergodic Markov chain, the expected transition time between initial state i and any other state j is finite regardless of the state i and j. □

This paper introduces a strategy that with the preservation of the best individual, gives the global convergence proof. The population of Markov chain description is enlarged by an additional best solution. The best individual is preserved in left and top position of the new matrix and is not affected by the quantum gate and resultant transition probability. It is simply copied to the next generation with probability one. The cardinality of the state space grows from $2^{n.m}$ to $2^{(n+1).m}$.

The extended transition matrix for $p^+(0)$ can be expressed as follows:

$$p^+(0) = \begin{bmatrix} p(0) & & & \\ & p(0) & & \\ & & \ddots & \\ & & & p(0) \end{bmatrix}, \tag{10}$$

The copy operation is presented by upgrade matrix $Upgr$ which upgrades an intermediate state containing an individual better than its last generation's best individual if the current generation includes the higher fitness individual. Let $newbest = \arg\max\left\{ f\left(\theta_k(i)\right) \mid k = 1, 2, \cdots, n\right\}$ represents the individual with highest fitness at state i excluding the last generation's best individual. If fitness of the new best individual is better then the last generation's best individual, the state is being changed and $upgr_{ij} = 1$, otherwise $upgr_{ii} = 1$. In other words, a state either becomes upgraded or remains unaltered. Therefore, the upgrade matrix can be written as

$$Upgr = \begin{bmatrix} upgr_{1,1} & & & \\ upgr_{2,1} & upgr_{2,2} & & \\ \vdots & \vdots & \ddots & \\ upgr_{2^m,1} & upgr_{2^m,2} & \cdots & upgr_{2^m,2^m} \end{bmatrix} \quad (11)$$

Size of the transition probability matrix and upgrade matrix, $p^+(0)$ and $Upgr$ is $2^{n.m} \times 2^{n.m}$, possessing the same structure. This paper assumes that the optimization problem only has one global point. Then $upgr_{1,1}$ is a unit matrix whereas all matrices $upgr_{i,i}$ with $i \geq 2$ are unit matrices with some zero diagonal entries.

Theorem 6: The QGA with parameter ranges as in Theorem 3 that is maintaining the best solution over time converges to the global optimum.

Proof: The final transition matrix for QGA, after applying two last steps in **while** loop in Fig. 1 ("*update* $Q(t)$ *using quantum gate*" and "*store the best solution among* $Pop(t)$"), can be written as

$$\begin{bmatrix} p(0) & & & \\ & p(0) & & \\ & & \ddots & \\ & & & p(0) \end{bmatrix} \cdot \begin{bmatrix} upgr_{1,1} & & & \\ upgr_{2,1} & upgr_{2,2} & & \\ \vdots & \vdots & \ddots & \\ upgr_{2^m,1} & upgr_{2^m,2} & \cdots & upgr_{2^m,2^m} \end{bmatrix} = \begin{bmatrix} I & 0 \\ R & T \end{bmatrix} \quad (12),$$

where I is a quadratic unit matrix describing the absorbing states, R describes movement from transient to absorbing states and T describes the movement among transient states. In fact, sub-matrix I represents the transition probability for states containing a globally optimal state. Since this sub-matrix is a primitive stochastic matrix and $R \neq 0$, Theorem guarantees that the probability of staying in any non-global optimal state converges to zero and the probability of being in any global optimal state converges to one, so that the limit of $P\{Z_t = f^*\}$ converges to one after $t \to \infty$.Since (5) is satisfied and under lemma 1, the non-homogeneity part of the algorithm is limited, is drawn the global convergence property proof of the QGA. □

So far, the convergence analysis of the QGA has been completed and QGA converges on the optimal solution.

4 CONCOLUSION

Canonical genetic algorithms apply special crossover, mutation and selection operators. These operators will add computation time and be prone to destroy the promising segments of the individuals. Whereas, Quantum Genetic Algorithm applies its special operator based on quantum computing concepts, namely quantum gate and additionally, a qubit individual include the superposition of states.

Convergence can be also obtained with the qubit representation. Each of the qubits constituting an individual converges to a single state and the property of diversity disappears gradually. That means the qubit representation is able to possess the two characteristics of exploration and exploitation, simultaneously.

In this paper, we formalized the QGA as a finite Markov chain and its convergence analysis has been studied based on the properties of Markov chain.

Although non-homogeneity is the intimate property of this algorithm, but in this paper, we revealed that the QGA converge to the global optimum by extraction of the two incongruous parts (non-homogeneity and homogeneity) and surveying of those separately.

In the last section, we investigated the global convergence of QGA satisfied its homogenous Markov chain and proved this algorithm is converged on the global optimum with probability one.

5 REFERENCES

[1] P. W. Shor, "Algorithms for Quantum Computation: Discrete Logarithms and Factoring," in Proceedings of the 35th Annual Symposium on Foundations of Computer Science, pp. 124-134, 1994.

[2] P. W. Shor, "Quantum Computing," Documenta Mathematica, vol. Extra Volume ICM, pp. 467-486, 1998.

[3] L. K. Grover, "A Fast Quantum Mechanical Algorithm for Database Search," in Proceedings of the 28th ACM Symposium on Theory of Computing, pp. 212-219, 1996.

[4] L. K. Grover, "Quantum Mechanical Searching," in Proceedings of 1999 Congress on Evolutionary Computation, pp. 2255-2261, 1999.

[5] K.-H. Han and J.-H. Kim, "Genetic Quantum Algorithm and its Application to Combinatorial Optimization Problem," in Proceeding of the 2000 Congress on Evolutionary Computation, Piscataway, NJ: IEEE Press, vol. 2, pp. 1354-1360, July 2000.

[6] K.-H. Han and J.-H. Kim, "Quantum-inspired Evolutionary Algorithm for a class of Combinatorial Optimization," IEEE Transactions on Evolutionary Computation, Piscataway, NJ: IEEE Press, vol. 6, no. 6, pp. 580-593, December 2000.

[7] K.-H Han, Quantum-inspired Evolutionary Algorithm, Ph.D. dissertation, Department of Electrical Engineering and Computer Science, Korea Advanced Institute of Science and Technology, Daejeon, Korea, 2003.

[8] V. G. Kulkarni, Modeling and Analysis of Stochastic Systems, London: Chapman & Hall, 1995.

[9] A. Leon-Garcia, Probability and Random Processes For Electrical Engineering, New Jersey: Prentice Hall, 2007.

[10] M. Iosifescu, Finite Markov Processes and Their Applications, Chichester: Wiley, 1980.

[11] G. Rudolph, "Convergence Analysis of Canonical Genetic Algorithms," IEEE Transactions on Neural Network, vol. 5, no. 1, pp. 96-101, 1994.

[12] D. Xiaoming, Z. Runmin, S. Rong, f. Rui and H. Shao, "Convergence Properties of Non-Crossover Genetic Algorithm," in Proceeding of the 4^{th} World Congress on