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A Novel Quantum Genetic Algorithm for Continuous Function Optimization

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Abstract—In this paper, a novel quantum genetic algorithm is proposed. This algorithm compares the probability expectation of the quantum chromosome with the best binary solution to determine rotation angle of rotation gate. Different individual in population evolve with different rate to complete local search and global search simultaneously. Hε gate is used to prevent the algorithm from premature convergence. After analyzing the algorithm and its global convergence, applying this approach to the optimization of function extremum, and comparing with the simple genetic algorithm and the quantum genetic algorithm, the simulation result illustrates that the algorithm has the characteristic of quick convergence speed and high solution precision.

Introduction

Quantum genetic algorithm (QGA) is a kind of intelligent optimization algorithm based on the quantum computing and the genetic algorithm[1-4]. In 2000, Han et al. proposed genetic quantum algorithm based on quantum bits and quantum superposition properties. This algorithm takes the quantum state vector to express the genetic code, and uses the quantum rotation gates to implement the chromosome evolution. Used it for 0-1 knapsack problem, and compared with the traditional genetic algorithm, the simulation results show that the algorithm has better optimization performance. But many experiments show that the algorithm is only suited to the knapsack problem. When it is used for continuous optimization, the premature convergence occurs frequently.

In this paper, after analyzing the quantum genetic algorithm in detail, we proposed a novel quantum genetic algorithm (NQGA). The algorithm directly compared the probability expectation corresponding to the qubit with the current best binary solution to determine the rotation angle. The operator Hε gate is introduced to avoid premature convergence. Used the algorithm to solve the optimization problem of function extremum, and compared with the simple genetic algorithm and the quantum genetic algorithm, the simulation results show that the algorithm has better performance.

QGA

QGA is a kind of probability optimal algorithm based on quantum computation concept and theory. In this algorithm the smallest unit of information is qubit. A qubit may be not only in the states 0 and 1, but also in a linear superposition of the two states, The state of a qubit can be represented as

$$|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle \tag{1}$$

Where, α and β are the probability amplitudes of the states $|0\rangle$ and $|1\rangle$, and $|\alpha|^2$ and $|\beta|^2$ give the probability that the qubit will be found in the state $|0\rangle$ and $|1\rangle$ respectively. Normalization of the state to unity guarantee

$$|\alpha|^2 + |\beta|^2 = 1 \tag{2}$$

Meanwhile, each quantum bit can also use an angle θ in the phase plane to indicate uniquely.

$$|\Psi\rangle = \cos\theta|0\rangle + \sin\theta|1\rangle \tag{3}$$

Represented by n-qubits, a chromosome can represent a linear superposition of 2^n basic state probabilistically. Used the quantum rotation gates to update chromosome, we can eventually obtain the optimal solution of the problem.

NQGA

In Quantum genetic algorithm, the rotation gate is the key to determine the performance of the algorithm. In the algorithm, the rotation angle is determined through comparing the binary solution obtained by observing quantum chromosome with the best solution, but the process of obtaining binary solution was a randomness, which causes the evolution regression occur inevitably. Taking into account when the quantum chromosome is measured, the state 0 will be obtained with the probability of $|\alpha|^2$, and the 1 will be $|\beta|^2$, so that the probability expectation of the quantum bit

$$|\alpha|^2 \times 0 + |\beta|^2 \times 1 = |\beta|^2 \tag{4}$$

Therefore, we compare the probability expectation corresponded to the qubit with the best binary solution to determine the rotation angle, in turn, increase the chosen probability of the best solution. For convenience, this chromosome and its rotation gate are expressed by the angle. Considering that the probability expectation of the quantum bit can be represented in angle form as

$$\cos^2\theta \times 0 + \sin^2\theta \times 1 = \sin^2\theta \tag{5}$$

The rotation gate determined by the formula below:

$$\Delta\theta_i = (b_i - \sin^2(\theta_i)) \times r \tag{6}$$

Where b_i is the *i-th* bit of the best binary solution, and the best binary solution take the binary solutions obtained from optimal retention mechanism to ensure global convergence of the algorithm. θ_i is the angle corresponding to the *i-th* bit of the quantum chromosome, r is the adjusting factor of the rotation angle, it can be defined as

$$r = (k / Popsize + h) \times l \tag{7}$$

Where k indicates that the *k-th* individual in the population, Popsize as population size, h and l are constants, h can avoid r in some individuals too small because of too large population, which, in turn, makes the rotation angle too small, and the evolutionary speed too slow, and by adjusting l, r can be regulated to control the convergence speed. The determination of h and l should ensure $0 < r < 1$. In the paper, h = 0.01, l = 0.01 • π. According to (7), r will vary from individual to individual. Because of different r, each individual will evolve at different speed toward the best solution. On the one hand, it can be avoided that all the quantum chromosomes always evolve toward the same goal with the same speed in the condition of the same initial state (that is, all α and β in the qubits are $1/\sqrt{2}$, and the corresponding angles are π/4), which will make the diversity between the quantum chromosome loss. On the other hand, some individuals in population that evolve faster can quickly converge to the best solution, and search in micro-space, some individuals converged slowly can search in macro-space in a long period.

To avoid premature convergence, consulting to [5], the concept of Hε gate is introduced, consider that the angle of the qubits will be always in the first quadrant in the whole evolution process, defined

$$\theta_i'' = \begin{cases} \varepsilon & \theta_i' \le \varepsilon \\ \theta_i' & \varepsilon \le \theta_i' \le \pi/2 - \varepsilon \\ \pi/2 - \varepsilon & \theta_i' \ge \pi/2 - \varepsilon \end{cases} \tag{8}$$

Where $0 < \varepsilon \ll \pi/2$, θ_i' is the qubit angle after rotating. Can be seen, Hε gate makes the angle always in the area $[\varepsilon, \pi/2 - \varepsilon]$. When $\varepsilon \to 0$, Hε gate will become a ordinary quantum rotation gate, and when $\varepsilon \to \pi/4$, the quantum gate will be out of work.

Currently, the process that using quantum genetic algorithm to solve the continuous optimization problem is to turn binary solution obtained by collapsing the quantum chromosome into real solution, and to further calculate the fitness value. But the process that turning binary solution into real solution exists the Hamming cliff problem. The quantum genetic algorithm is essentially an optimization algorithm which based on the probability distribution in the solution space, so this issue is particularly serious. Specifically as follows: When two real solutions and its fitness functions are very close, their corresponding binary solutions and the converged quantum chromosomes which represent its generation probability is very different, which results in quantum chromosome can not represents the generation probability of the solution space well. In contrast, Gray code can solve the problem well, so this coding form is adopted.

The main steps in the improved algorithm are as follows:

（1） $t = 1$, generate m initial individuals, and constitute population $\boldsymbol{Q}(t) = \{\Theta_1^t, \Theta_2^t \cdots \Theta_m^t\}$, where Θ_j^t is the *j-th* individual in the population in *t-th* generation, $\Theta_j^t = [\theta_1, \theta_2 \cdots \theta_n]$, where n is the number of quantum bits contained in each chromosome. All α and β in the qubits are taken as $1/\sqrt{2}$, and corresponding angle $\theta=\pi/4$. It means that one qubit individual Θ_j^t represents the linear superposition of all possible states with the same probability.

（2） Make p_j^t by measuring every Θ_j^t, , thus forming population $P(t)$.

（3） Evaluate each individual in $P(t)$, and compare it with the best solution to get the new best solution, if the termination condition is meeting, then terminate the algorithm.

（4） $t = t + 1$。

（5） Update $\boldsymbol{Q}(t-1)$ to generate $\boldsymbol{Q}'(t-1)$。

（6） Return（2）.

Analysis of Nqga and Its Convergence

Analysis of the algorithm. In the evolution process of the algorithm, each angle of qubit generates as formula:

$$\theta_i' = \theta_i + \Delta\theta_i = \theta_i + (b_i - \sin^2\theta_i) \times r \tag{9}$$

Suppose before a step of operation, the angle θ_i is in the first quadrant, that is, $0 < \theta_i < \pi/2$. Taking account that $r \in (0,1)$, when the bit of the best binary solution is 1,

$$\Delta\theta_i = (1 - \sin^2\theta_i) \times r > 0$$

$$\theta_i' = \theta_i + (1 - \sin^2\theta_i) \times r = \theta_i + \cos^2\theta_i \times r < \theta_i + \cos\theta_i$$

$$= \theta_i + \sin(\pi/2 - \theta_i) < \theta_i + \pi/2 - \theta_i = \pi/2$$

That means the angle will rotate counterclockwise toward the direction of π/2, which makes the probability that the qubit be found in 1 increase, but after rotating, the angle still less than π/2, and is in the first quadrant. When the bit of the best binary solution is 0,

$$\Delta\theta_i = -\sin^2\theta_i \times r < 0$$

$$\theta_i' = \theta_i - \sin^2\theta_i \times r > \theta_i - \sin\theta_i > 0$$

That means the angle will rotate clockwise toward the 0 direction, which makes the probability of getting 0 increase, and the angle after rotation is greater than 0, still in the first quadrant. Since in the beginning of the algorithm, all the angles of qubits in the individual are initialized to π/4, that is, in the first quadrant, then as the algorithm evolving, all the angles of qubits in the individual will always be limited to the first quadrant and the evolution direction toward the best solution. Eventually, the angles of qubits will tend to the angle 0 or π/2 of corresponding bit in the best solution, and the entire population will converge to the best solution. In the algorithm, the rotation angle is proportional to the difference between the expectation of the qubit and the corresponding binary bit of the best solution. The greater the difference, indicates the probability of collapsing the qubit to the corresponding bit of the best solution smaller, then the angle rotating toward best solution is greater, which cause the generation probability of best solution increase quickly, and the maximum of rotation angle amplitude is $|\Delta\theta_i| \approx \cos^2\varepsilon \times r$. And the smaller the difference, indicates the probability of collapsing the qubit to the corresponding bit of the best solution bigger, then the rotation angle is smaller, which can make the convergence rate slow, and maintain the global search performance of the algorithm. Because of the Hε gate, the minimum of rotation angle amplitude can be 0, and the angle converge to ε or $\pi/2-\varepsilon$.

Analysis of the convergence. In [6,7], the convergence of QGA have been analyzed, but they are all based on the quantum chromosome. Taking into account the purpose of the quantum genetic algorithm is to achieve the optimal solution, and the binary solution obtained through measuring the quantum chromosome is a kind of direct denotation of the solution we needed, and relative to the binary solution, the quantum chromosome only represents the probability distribution in the solution space, it is as an evolutionary auxiliary tool. Therefore, this paper focusing on the convergence analysis of the binary solution. Furthermore, if the best binary solution is obtained, through it, all of the quantum chromosome in the population will converge to the best solution in finite iterations. In the following we will prove that the binary solution in NQGA is globally convergent.

In [8-9], the genetic algorithm with optimal retention is an algorithm with global convergence. Based on the theory, NQGA convergence is proved in this paper. Let Φ represent the set which include all binary strings of length *n*, and all elements in the set constitute the whole binary solution space. The binary population whose size is *N* can be regarded as a point in the state space $S=\Phi^N$, its generation probability lies on the probability distribution represented by the quantum chromosome population, it is only correlated with the generation probability in previous iteration and the best binary solution, but not with every state before the last iteration, so the evolution of population can be regarded as a finite Markov chain.

Assuming in the *t-th* iteration, the *i-th* quantum chromosome in the population is $\Theta_i^t=[\theta_1^t,\theta_2^t\cdots\theta_n^t]$, which can be measured to obtain binary solution $B_i^t=[b_1^t,b_2^t\cdots b_n^t]$. After the quantum chromosome is acted by Hε gate, we can obtain the quantum chromosome of the (*t*+1)-*th* generation, $\Theta_i^{t+1}=[\theta_1^{t+1},\theta_2^{t+1}\cdots\theta_n^{t+1}]$. Then measuring the quantum chromosome, the binary solution $B_i^{t+1}=[b_1^{t+1},b_2^{t+1}\cdots b_n^{t+1}]$ can be gotten. No matter what value the *j-th* bit in the *t-th* iteration b_j^t is, the probability p^{t+1} of the bit in the (*t+1*)-*th* iteration to be 0 or 1 is satisfy $p^{t+1}\ge\sin^2\varepsilon>0$, therefore, in the evolution process, the transition probability that the population turning from any state s_i to the other state s_j satisfy $p_{ij}\ge(\sin^2\varepsilon)^{n\cdot N}>0$, that is, the probability transition matrix is strictly positive. According to [8-9], if genetic algorithm satisfies the conditions: (1) the best solution is maintained; (2) the state probability transition matrix is strictly positive, the algorithm can converge to the global optimal solution in finite generations. Consider that the algorithm we proposed take the best solution-maintained mechanism, so the method is globally convergent.

Experiment

To verify its performance, NQGA is used for the optimization of function extremum, and compared with the simple genetic algorithm (SGA) and quantum genetic algorithm (QGA). Below five functions are used.

(1) Sphere function

$$F_1=10-\sum_{i=1}^{5}(x_i-5)^2 \tag{10}$$

Where $1\le x_i\le10$. The global maximum point is x_i=5, and the global maximum is 10. When the optimization result is more than 9.99, the algorithm is considered to be convergent.

(2) Schwefel' Problem 1.2 function

$$F_2=10-\sum_{i=1}^{5}(\sum_{j=1}^{i}x_j)^2 \tag{11}$$

Where ∣ x_i ∣ ≤10. The global maximum point is x_i=0, and the global maximum is 10. When the optimization result is more than 9.99, the algorithm is considered to be convergent.

(3) Rosenbrock function

$$F_3 = 10 - (100(x_2 - x_1^2)^2 + (x_1 - 1)^2) \tag{12}$$

Where ∣ x_i ∣ ≤5.12. The global maximum point is x_i=1, and the global maximum is 10. When the optimization result is more than 9.99, the algorithm is considered to be convergent.

(4) Shekel's foxholes function

$$F_4 = \frac{1}{500} + \sum_{j=1}^{25} \frac{1}{j + \sum_{i=1}^{2} (x_i - a_{ij})^6} \tag{13}$$

Where ∣ x_i ∣ ≤65.536. The global maximum point is x_i=-32, and the global maximum is 1.002. When the optimization result is more than 1, the algorithm is considered to be convergent.

(5) Sinc function

$$F_5 = \frac{\sin\left(\sum_{i=1}^{5} |x_i - 5|\right)}{\sum_{i=1}^{5} |x_i - 5|} \tag{14}$$

Where 1≤x_i≤10. The global maximum point is x_i=5, and the global maximum is 1. When the optimization result is more than 0.99, the algorithm is considered to be convergent.

All functions are optimized 50 times by NQGA, QGA, SGA, respectively. In these three algorithms, the population size is set to 30, the maximum number of iteration is 500, and the mutation probability Pm is 0.01, and the crossover probability Pc in SGA is 0.8. The optimization results are shown in Table 1-5 and Figs.1-5.

Table I. Optimization Results Of Function F1

Algorithm	Best result	Average result	Worst result	Convergence times
SGA	9.9999	9.8237	9.2461	17
QGA	9.9999	9.9916	9.7414	47
IQGA	10.0000	10.0000	9.9999	50

Table II. Optimization results of function f2

Algorithm	Best result	Average result	Worst result	Convergence times
SGA	10.0000	9.9660	9.2187	43
QGA	9.9976	9.9370	9.4572	8
IQGA	10.0000	9.9938	9.9585	44

Table III. Optimization results of function f3

Algorithm	Best result	Average result	Worst result	Convergence times
SGA	10.0000	9.6893	9.0000	9
QGA	10.0000	9.9901	9.8678	40
NQGA	10.0000	9.9974	9.9628	46

Table IV. Optimization results of function f4

Algorithm	Best result	Average result	Worst result	Convergence times
SGA	1.0020	0.8297	0.0853	23
QGA	1.0020	0.8976	0.7092	18
IQGA	1.0020	1.0020	1.0020	50

Table V. Optimization results of function f5

Algorithm	Best result	Average result	Worst result	Convergence times
SGA	1.0000	0.4567	0.1284	10
QGA	0.9999	0.9919	0.8956	43
IQGA	1.0000	1.0000	0.9999	50

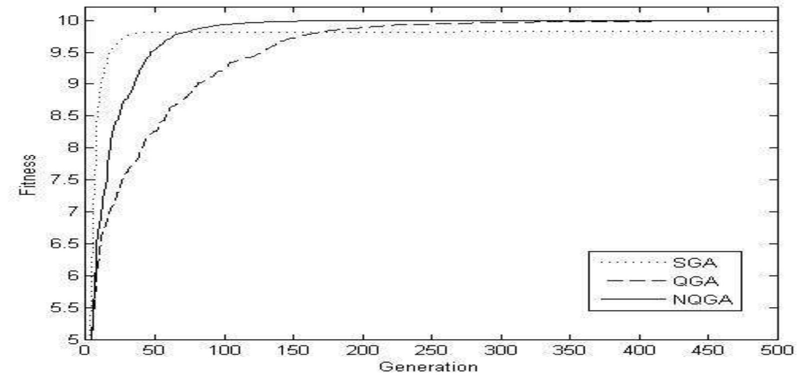

Figure 1. Performance varying curves of function F1

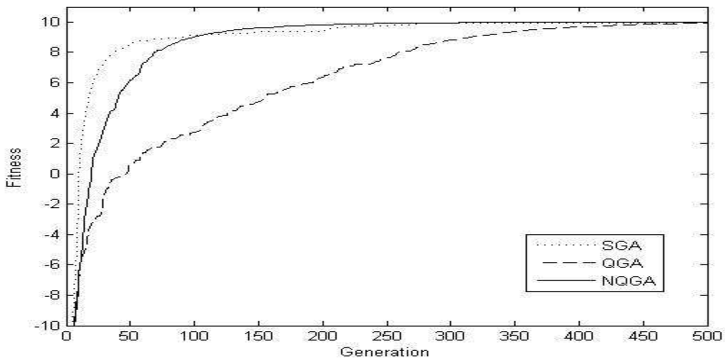

Figure 2. Performance varying curves of function F2

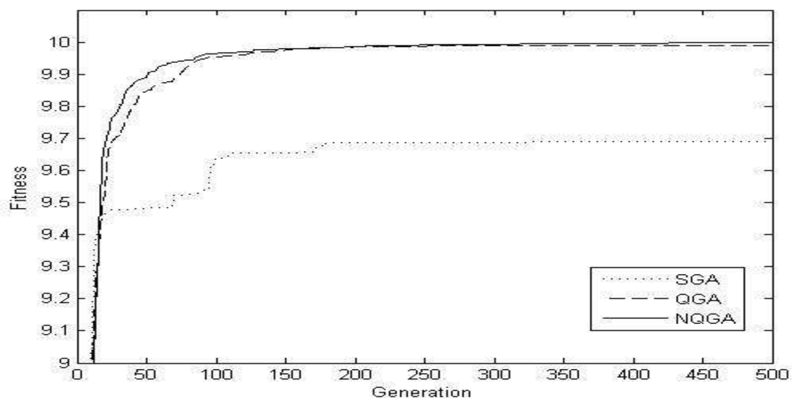

Figure 3. Performance varying curves of function F3

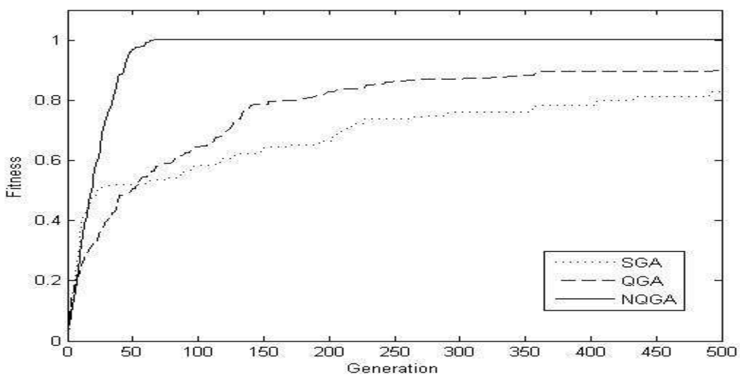

Figure 4. Performance varying curves of function F4

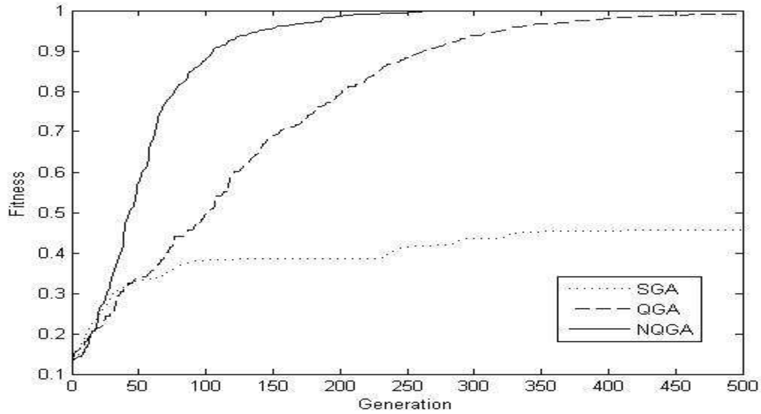

Figure 5.Performance varying curves of function F5

Can be seen from the simulation result, when being used in the optimization of function extremum, the search capability and convergence speed of NQGA are all superior to that of the other two algorithms. It can obtain the global best solution fast and steadily.

Conclusion

Through analyzing the defects existed in the quantum genetic algorithm, a novel quantum genetic algorithm is proposed. After analyzing the algorithm and its convergence, applying this approach to the optimization of function extremum, the simulation result illustrates that the algorithm is superior to SGA and QGA in both convergence speed and solution precision.

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References

[1] Narayanan A, Moore M. Quantum-inspired genetic algorithms[C]. Proc of IEEE Int Conf on Evolutionary Computation. Nagoya: IEEE Press, 1996: 61-66.

[2] Han K H, Kim J H. Genetic quantum algorithm and its application to combinatorial optimization problems[C]. Proc of the 2000 IEEE Congress on Evolutionary Computation. Piscataway: IEEE Press, 2000, 7: 1354-1360.

[3] Han K H, Kim J H. Quantum-inspired evolutionary algorithm for a class of combinatorial optimization[J]. IEEE Trans on Evolutionary Computation, 2002, 6(6):580-593.

[4] Han K H, Kim J H. On Setting the Parameters of Quantum-inspired Evolutionary Algorithm for Practical Applications[C] Proc of the 2003 Congress on Evolutionary Computation. IEEE Press, 2003, 12: 178-184.

[5] Han K H, Kim J H. Quantum-inspired evolutionary algorithms with a new termination criterion, H_ε gate, and two-phase scheme[J]. IEEE Trans on Evolutionary Computation, 2004, 8(2):156-169.

[6] Yang Jun-an, Li Bin, Zhuang Zhen-quan,et al. Quantum genetic algorithm and its application research in blind source separation. MINI-MICRO SYSTEMS. 2003, 24(8):1518-1523.

[7] Yang Shu-yuan, Jiao Li-cheng, Liu Fang. The quantum evolutionary algorithm. CHINESE JOURNAL OF ENGINEERING MATHEMATICS, 2006, 23(2):235-246.

[8] Dai Xiaoming, Sun Rong, Zou Runming, et al. Global Convergence Analysis of Non-Crossover Genetic Algorithm and Its Application to Optimization. Journal of Systems Engineering and Electronics, 2002, 13 (2): 84-91.

[9] Günter Rudolph. Convergence Analysis of Canonical Genetic Algorithms. IEEE Trans on Neural Networks, 1994, 5(1):96-101.

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DOI References
[3] Han K H, Kim J H. Quantum-inspired evolutionary algorithm for a class of combinatorial optimization[J]. IEEE Trans on Evolutionary Computation, 2002, 6(6): 580-593.
10.1109/TEVC.2002.804320
[5] Han K H, Kim J H. Quantum-inspired evolutionary algorithms with a new termination criterion, Hε gate, and two-phase scheme[J]. IEEE Trans on Evolutionary Computation, 2004, 8(2): 156-169.
10.1109/TEVC.2004.823467
[9] Günter Rudolph. Convergence Analysis of Canonical Genetic Algorithms. IEEE Trans on Neural Networks, 1994, 5(1): 96-101.
10.1109/72.265964