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Review

Quantum Genetic Algorithms for Computer Scientists

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Academic Editor: Prakash Panangaden

Received: 7 July 2016; Accepted: 11 October 2016; Published: 15 October 2016

Abstract: Genetic algorithms (GAs) are a class of evolutionary algorithms inspired by Darwinian natural selection. They are popular heuristic optimisation methods based on simulated genetic mechanisms, i.e., mutation, crossover, etc. and population dynamical processes such as reproduction, selection, etc. Over the last decade, the possibility to emulate a quantum computer (a computer using quantum-mechanical phenomena to perform operations on data) has led to a new class of GAs known as “Quantum Genetic Algorithms” (QGAs). In this review, we present a discussion, future potential, pros and cons of this new class of GAs. The review will be oriented towards computer scientists interested in QGAs “avoiding” the possible difficulties of quantum-mechanical phenomena.

Keywords: quantum genetic algorithms; quantum evolutionary algorithms; reduced quantum genetic algorithm; quantum computing

1. Introduction

In the late 1980s, genetic algorithms [1] achieved enough popularity as a method of optimization and machine learning. During this decade the Nobel Prize-winning physicist Richard Feynman thought the possibility of a quantum computer, a computer that operates using the effects of quantum mechanics. However, it would have to wait some time for the emergence of the exciting idea of designing a genetic algorithm capable of running on a quantum computer. However, is this possible?

Genetic Algorithms (GAs) are search algorithms based on Darwinian natural selection and genetic mechanisms present in organisms [2]. In a simple genetic algorithm (SGA) [1], solutions are encoded in arrays that are referred as chromosomes. Usually, the algorithm begins with an initial population of chromosomes, thus the initial set of solutions, which is randomly generated. Henceforth, the algorithm evolves over and over the population in search of an optimal solution. At each generation the chromosomes in the population are evaluated before selection, obtaining their fitness f values, thus the degree of achievement or goodness of the encoded solution. Immediately after chromosomes are evaluated, the algorithm selects the “parents” or mating pool of the next generation, simulating a concept introduced by Darwin: the survival of the fittest. Once a new generation of offspring chromosomes is obtained, the algorithm simulates genetic mechanisms such as crossover and mutation. However, there are genetic algorithms based on other genetic mechanisms such as the case of bacterial conjugation [3]. These mechanisms are very important in living organisms because they are responsible for the biological variability. In the case of crossover this genetic mechanism takes place during the mating between individuals promoting the population convergence towards sub-optimal solutions present in the search space. Nevertheless, in the case of mutation this genetic mechanism involves a random change that occurs in chromosomes, pushing the population to perform a random walk through the search space. The described steps are shown in Table 1, concluding the search once the SGA meets the termination condition, i.e., the algorithm has found an optimal solution [4]. At present, GAs have many applications in optimization problems, e.g., automated design, quality control, manufacturing systems, software design, financial forecasting, robotics, etc. being widely used

in fields either economics, biology, chemistry and many others. However, from a theoretical point of view, is it possible to simulate “Darwinian evolution” in a quantum computer? In 1987 Calvin [5] coined the term “Darwin machine” to refer to a machine (analogous to a Turing machine) which returns as output the result of an iterative process similar to a GA. From a theoretical point of view the architecture of a conventional computer is adequate to implement GAs, and also to simulate from a Darwinian perspective the most important aspects of biological evolution. Consequently, whereas a digital computer can successfully simulate a Darwin machine the possibility to simulate a “Darwin quantum machine” in a quantum computer remains today a controversial question. However, what is known as “Quantum Darwinism” [6] will open up the possibility. Therefore, the Darwin’s concept of survival of the fittest could be simulated in any device capable of data manipulation based on quantum mechanical phenomena [7]. In any case, and without going into theoretical issues, since 1956 [8] when was first proposed the genetic algorithms Evolutionary Computation has made great progress. In 2002 Han [9] introduced a novel evolutionary algorithm inspired by quantum computing, growing from this date the number of publications on quantum-inspired genetic algorithms. In 2010 Ying [10] proposed that quantum computing could be used to achieve certain goals in Artificial Intelligence (AI). Over the last decade, the possibility to emulate a quantum computer has led to a new class of GAs known as “Quantum Genetic Algorithms”. In this review, we present a discussion, future potential, pros and cons of this new class of GAs, including some material presented in a lecture delivered at [11].

Table 1. Main steps of a simple genetic algorithm (SGA).

Step	
1	Randomly initialize a population $P(0)$
2	Evaluate $P(0)$
3	while (not termination condition) do
4	begin
5	$t \leftarrow t + 1$
6	Selection of parents from population $P(t)$
7	Crossover
8	Mutation
9	Evaluate $P(t)$
10	end

2. What is Quantum Computing?

One of the most striking ideas of quantum computing is that as long as a digital computer is a symbolic machine, i.e., an instruction execution engine, a quantum computer is a physical machine. This means that in a quantum computer the hardware-software duality is less obvious than in a classical computer, being the quantum circuit “hardware” itself an isolated “quantum system”. Therefore while in a digital computer a computation is given by the logical operations performed in a “symbolic system”, in a quantum computer a computation is the evolution experienced by the quantum system.

According to quantum mechanics the evolution of an isolated quantum system from an initial state to another final state, e.g., a quantum computer, is governed by the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H(t) |\psi(t)\rangle$$

where i is the imaginary number $\sqrt{-1}$ and \hbar is a constant term named “reduced Planck constant”. Planck’s constant plays the role of relating the energy in a photon to frequency, and since frequency is measured in cycles per second it is more convenient to use $\hbar = h/2\pi$. According to the mathematical expression the Schrödinger equation is a partial differential equation which “physical variable” is a state vector $|\psi(t)\rangle$ written in a somewhat special notation that we will discuss later. The $|\psi(t)\rangle$ vector depends on time and describes the state of a quantum system at time t , in this case the quantum

computational state. Since we are dealing with a differential equation, the equation also includes a rate of change or differential term, i.e., $\frac{\partial}{\partial t} |\psi(t)\rangle$. The Schrödinger equation is the holy grail of quantum computing because it characterizes the evolution of a computing state through time. The term $H(t)$ is known as “Hamiltonian operator” and somehow given the initial state $|\psi(0)\rangle$ it represents the sequence of operations performed by a quantum computer. Establishing a parallelism between quantum and digital computers we assume that quantum state $|\psi(0)\rangle$ resembles the *input* of a digital computer. An interesting point is that if we know the Hamiltonian then the Schrödinger equation can be solved, so without going into details we will denominate $U(t)$ as the solution of this equation. Hence, given an initial state $|\psi(0)\rangle$ the solution of the Schrödinger equation at time t is given by the following linear mapping in the state space:

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle$$

Therefore and according with the above reasoning we can conclude that in a quantum computer the *output* is the result of the (i) evolution of the Schrodinger equation and subsequent (ii) measurement (the meaning of measurement in quantum mechanics is introduced later). As may be seen, the equation uses for the state vector a notation that is rather unusual. The reason is because quantum mechanics has its own customized notation for classical vector and matrix operations [12]. In 1930 the theoretical physicist Paul Dirac published the book “The Principles of Quantum Mechanics” introducing the *ket* notation to refer to a column vector:

$$|V\rangle = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_i \end{pmatrix}$$

and *bra* notation to denote a row vector:

$$\langle W| = \begin{pmatrix} w_1 & w_2 & \dots & w_i \end{pmatrix}$$

Hence, the product of a bra and a ket vectors, which is written in the notation of Dirac as follows, is the ordinary inner product:

$$\langle W| V \rangle = \begin{pmatrix} w_1 & w_2 & \dots & w_i \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_i \end{pmatrix} = w_1 v_1 + w_2 v_2 + \dots + w_i v_i$$

Alternatively, the product of a ket and bra vectors, is the outer product of the two vectors:

$$|V\rangle \langle W| = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_i \end{pmatrix} \begin{pmatrix} w_1 & w_2 & \dots & w_i \end{pmatrix} = \begin{pmatrix} v_1 w_1 & v_1 w_2 & v_1 w_i \\ v_2 w_1 & v_2 w_2 & v_2 w_i \\ v_i w_1 & v_i w_2 & v_i w_i \end{pmatrix}$$

In quantum computing the elements of vectors and matrices are complex numbers but in practice we can ignore this detail.

2.1. Quantum Information

The unit of information in a quantum computer is the quantum bit or qubit, storing $|0\rangle$ and $|1\rangle$ states as well as a linear combination of both states (*superposition principle*). This linear combination represents a qubit in its “coherent state” or “quantum superposition”, i.e., $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ where α and β are the qubit amplitudes of the states $|0\rangle$ and $|1\rangle$. Amplitudes are complex numbers ($\alpha, \beta \in \mathbb{C}$) so the exact state of a qubit is specified by two complex numbers describing the particular combination of 0 and 1 in the superposition state. The normalization of the states to the unit ensures that $|\alpha|^2 + |\beta|^2 = 1$ and therefore $|\alpha|^2, |\beta|^2$ are the probabilities of finding the qubit in $|0\rangle$ or $|1\rangle$ states. According to Dirac notation such superposition is represented in vector form as follows:

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

and therefore we will represent $|0\rangle$ and $|1\rangle$ states of a qubit:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

In the realm of quantum mechanics the states of a qubit are represented geometrically in what is called as Bloch sphere. From a mathematical point of view, the state vector $|\psi\rangle$ representing the state of a qubit is defined in a space referred as Hilbert space. In a very general sense and without going into details a Hilbert space is a complex vector space with the advantage that allows us to treat a function $|\psi\rangle$ as a vector, conducting mathematical operations by the simple application of standard algebraic methods. In consequence the quantum computing state which evolution is ruled by Schrödinger equation is defined by a Hilbert space associated with a finite number of n qubits. Despite all these abstract concepts finally the definition of a universal quantum computer is close to the conceptual framework of classical computation [13].

One of the most amazing ideas of quantum mechanics is that any attempt to measure a quantum superposition, or equivalently any interaction of the quantum system with the environment, causes the destruction of the superposition (*interference principle*). This is a natural phenomenon known in quantum physics as “collapse of wave function $|\psi\rangle$ ” and represents a major challenge in building a quantum computer. Consequently a measurement or observation of the qubit in its coherent state results in a lost of the superposition, transforming the qubit in a classic decoherent bit, i.e., 0 or 1 state. The interference principle has recently been simulated based on a new class of hybrid cellular automata [14] performing as either a quantum cellular automata (QCA) or as a classical von Neumann automata (CA).

In a quantum computer the input is stored in a quantum memory register:

$$|\psi\rangle = |\psi\rangle_1 \otimes |\psi\rangle_2 \otimes \dots \otimes |\psi\rangle_n$$

The register state is the result of Kronecker or tensor product among two or more qubits (operation that is represented with the symbol \otimes) as:

$$\begin{pmatrix} x_0 \\ x_1 \end{pmatrix} \otimes \begin{pmatrix} y_0 \\ y_1 \end{pmatrix} = \begin{pmatrix} x_0 y_0 \\ x_0 y_1 \\ x_1 y_0 \\ x_1 y_1 \end{pmatrix}$$

For instance, number 5 is represented in binary numbering system as $|101\rangle$, being the register state:

$$|5\rangle = |\psi\rangle_1 \otimes |\psi\rangle_2 \otimes |\psi\rangle_3 = |1\rangle \otimes |0\rangle \otimes |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

However, there are quantum states which cannot be written as a tensor product of two states, being known these special states as entangled states (*entanglement principle*). In this case, measurement results are dependent as it will occur at the following quantum state:

$$\frac{1}{\sqrt{2}} (|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B) = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$$

Once the information is processed by a quantum circuit, the output is the result of a measurement or observation of the qubits states resulting the collapse of wave function $|\psi\rangle$. Computation concludes once such measures have been made. In summary, in terms of computing a quantum algorithm maps an input state $|\psi(0)\rangle$ (or represented for simplicity as $|\psi\rangle_0$) onto the output or final state $|\psi(t)\rangle$ (represented as $|\psi\rangle_F$):

$$|\psi\rangle_F = U |\psi\rangle_0$$

where U (or $U(t)$, the solution of the Schrödinger equation) is referred to as “unitary evolution operator”. An important issue is that U operator can be decomposed in a sequence of q elementary quantum gates (abbreviated as Q-gates) defining these gates a quantum circuit. Q-gates perform unitary transformations on qubits, bearing in their function a resemblance with classical Boolean gates. Consequently from left to right:

$$U = U_q \cdot U_{q-1} \cdot \dots \cdot U_1$$

A quantum circuit, thus the U decomposition, represents a quantum algorithm being somehow equivalent to a classical algorithm in a digital computer. However, quantum circuits show special features allowing to a quantum computer conduct computations with a lower number of exponential operations than classical computers.

2.2. Quantum Gates

Quantum gates (Q-gates) operate on qubits undergoing unitary transformations being such operations represented by matrices. Since these unitary transformations are rotations in the Bloch sphere then Q-gates are reversible gates. The most important quantum gates that operate with a single qubit are the identity gate I and Pauli gates X , Y and Z :

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The identity gate I leaves a qubit unchanged. Pauli X gate performs a Boolean NOT operation, Pauli Y gate maps $|0\rangle \rightarrow i|1\rangle$ or $|1\rangle \rightarrow -i|0\rangle$ and Pauli Z gate changes the phase of a qubit, thus $|0\rangle \rightarrow |0\rangle$, $|1\rangle \rightarrow -|1\rangle$. For instance, let's consider the following operations between one of the above quantum gates and $|0\rangle$ or $|1\rangle$ qubit states:

$$I \cdot |0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad X \cdot |0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad Z \cdot |1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

One of the most useful Q-gates is the Hadamard or H gate. This gate is a generalization of the discrete Fourier transform which can be defined recursively for two, three or more qubits:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Let's be $|\psi\rangle$ a superposition vector:

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

multiplying the matrix H by the above vector we obtain:

$$H \cdot |\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \alpha + \beta \\ \alpha - \beta \end{pmatrix}$$

For example, if we multiply H by $|0\rangle$ we obtain:

$$H \cdot |0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

or using a different notation $\frac{1}{\sqrt{2}} |0\rangle + \frac{1}{\sqrt{2}} |1\rangle$ (Figure 1). Therefore, if we measure or observe the qubit state then we will have exactly 50% chance of seeing as 0 or 1. Similarly if now we multiply H by $|1\rangle$ we obtain:

$$H \cdot |1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

or in the alternative notation $\frac{1}{\sqrt{2}} |0\rangle - \frac{1}{\sqrt{2}} |1\rangle$ (Figure 1).

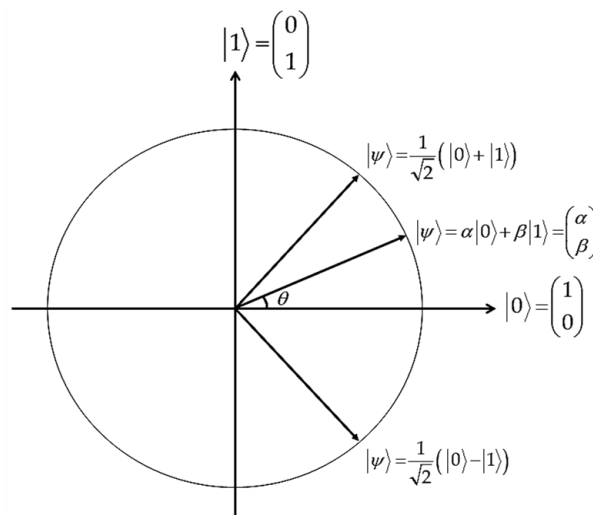


Figure 1. Qubit transformations with Hadamard gate.

One of the applications of Hadamard gate is the initialization of a quantum register. Generalizing the H gate multiplication by $|0\rangle$ to an n -qubit register that stores the value $|0^n\rangle$ results in a superposition or mixed state:

$$\frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x\rangle$$

It is interesting to note that in the case we could observe the quantum register in the above mixed state then we would see each of the 2^n binary numbers x with equal probability.

Of course, there are also Q-gates for two or more qubits operations (e.g., SWAP, CNOT, Toffoli, Fredkin gates, etc.). The SWAP gate swaps two qubits:

$$SWAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Other Q-gates exhibit the special feature of including one or more qubits controlling the operation. These gates are called *U-controlled gates*, (e.g., CNOT, Toffoli and Fredkin gates). For instance, the CNOT gate (2 qubits) performs according to truth table (Table 2) the operation $CNOT|Q1, Q2\rangle = |Q1, Q2 \oplus Q1\rangle$ (Figure 2a). Note that $*Q2 = Q2 \oplus Q1$ value is observed after performing the measurement.

Table 2. CNOT gate.

Q1	Q2	Q1	* Q2
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

* Observed after performing the measurement.

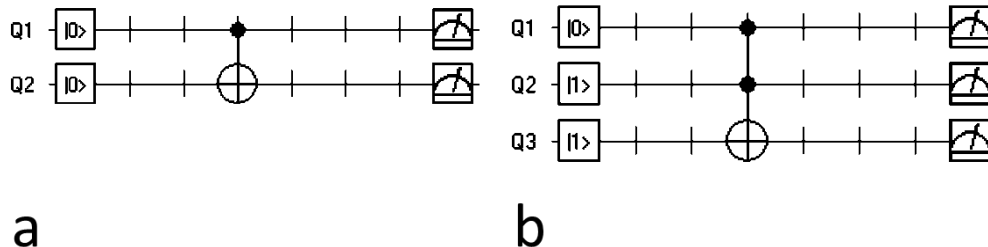


Figure 2. *U-controlled gates*. (a) CNOT gate; (b) CCNOT gate.

In contrast, Toffoli gate (3 qubits) conducts the $CCNOT|Q1, Q2, Q3\rangle = |Q1, Q2, Q3 \oplus Q1Q2\rangle$ operation (Figure 2b) according to the truth table (Table 3). The gate inverts the state of Q3 when Q1 and Q2 are set to $|1\rangle$. Note that $*Q3 = Q3 \oplus (Q1 \wedge Q2)$ value is observed after performing the measurement.

Table 3. CCNOT gate.

Q1	Q2	Q3	* Q3
0	0	0	0
0	0	1	1
0	1	0	0
0	1	1	1
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	0

* Observed after performing the measurement.

Another controlled gate is the Fredkin gate or CSWAP gate (3 qubits). This gate performs a controlled swap operation: if the control qubit state is equal to $|1\rangle$ then it swaps Q1 and Q2 qubits. In summary, the operations conducted by these controlled gates are represented by the following unitary matrices:

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad CCNOT = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad CSWAP = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Finally, a common element in quantum circuits is termed as oracle. It is a black box function that receives as input n qubits, performs a unitary transformation U and returns the result as output. One of its most important features is that it can measure and modify a quantum state without collapsing the state to a classical state. Furthermore, an oracle could solve a decision problem in linear time on a quantum computer. In the context of the quantum evolutionary algorithms an oracle would play the role of a classical algorithm conducting operations that are specific of a classical computer. The oracle is usually represented as U or in a more specific symbol as O .

In summary, quantum computer operations are ruled by quantum mechanics, data are qubit arrays and operations are reversible and carried out with quantum gates. Such quantum gates are represented by unitary matrices, so that operations are defined by a linear algebra in a Hilbert space. In contrast, a digital computer is governed by classical physics, data are represented by bit sequences (1010001101 ...) and operations are irreversible and performed by Boolean logic gates (AND, OR, NOT, NAND, etc.).

2.3. Quantum Algorithms and Quantum Circuits

Usually quantum algorithms (e.g., Shor's algorithm, Grover's algorithm, Deutsch's algorithm, etc.) include quantum mechanical phenomena represented in Table 4 (modified from [15]).

Table 4. Main steps of a quantum algorithm.

Step	
1	Prepare an input state
2	Apply quantum parallelism
3	Performs quantum information processing
4	Use interference to exploit the parallelism
5	Make a measure

In agreement with the main steps described above a quantum algorithm could be represented with a quantum circuit as shown in Figure 3. Thus, there is a correspondence between a quantum algorithm and quantum circuit. The circuit receives the input from the quantum register providing an output as a result of measuring or observing the state of each qubit. Once defined the ends of the circuit, several lines or cables are located in parallel between both ends, placing the quantum gates, oracle etc. (Table 5) according to the quantum algorithm. We will illustrate how a quantum circuit operates with the following example. Consider the EPR (Einstein, Podolsky and Rosen) circuit (Figure 4), one of the classic circuits in quantum computing. Based on this circuit it is possible conduct experiments of quantum teleportation, thus the transfer of quantum information based on entanglement. First, if we look at the left end of the circuit we note that in the top wire there is an H gate while the bottom wire does not have a quantum gate (or equivalently there is an I gate).

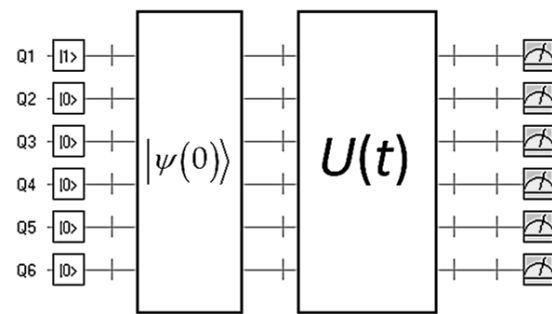


Figure 3. Quantum circuit including (from left to right) a quantum register, *input* state $|\psi(0)\rangle$, information processing step $U(t)$, and the *output* as a result of measuring or observing the state of each qubit.

Table 5. Quantum circuit gates.

Quantum Circuit Example		Symbol	Input \rightarrow Output *
Q1	$ 1\rangle$ [Circuit: Q1 line with $ 1\rangle$ box, followed by 7 vertical lines, then a meter symbol]	I	$ 1\rangle \rightarrow 1, 1.0$
Q1	$ 1\rangle$ [Circuit: Q1 line with $ 1\rangle$ box, followed by 4 vertical lines, an X box, then 3 vertical lines, then a meter symbol]	X	$ 1\rangle \rightarrow 0, 1.0$
Q1	$ 0\rangle$ [Circuit: Q1 line with $ 0\rangle$ box, followed by 4 vertical lines, a Y box, then 3 vertical lines, then a meter symbol]	Y	$ 0\rangle \rightarrow 1, 1.0$
Q1	$ 0\rangle$ [Circuit: Q1 line with $ 0\rangle$ box, followed by 4 vertical lines, a Z box, then 3 vertical lines, then a meter symbol]	Z	$ 0\rangle \rightarrow 0, 1.0$
Q1	$ 0\rangle$ [Circuit: Q1 line with $ 0\rangle$ box, followed by 4 vertical lines, an H box, then 3 vertical lines, then a meter symbol]	H	$ 0\rangle \rightarrow \begin{cases} 0, 0.5 \\ 1, 0.5 \end{cases}$
Q1	$ 0\rangle$ [Circuit: Q1 line with $ 0\rangle$ box, followed by 4 vertical lines, a CNOT gate (X on Q1, control on Q2), then 3 vertical lines, then a meter symbol]		$ 0\rangle \rightarrow 1\rangle$ $ 1\rangle \rightarrow 0\rangle$
Q1	$ 0\rangle$ [Circuit: Q1 line with $ 0\rangle$ box, followed by 4 vertical lines, a CNOT gate (X on Q1, control on Q2), then 3 vertical lines, then a meter symbol]		$ 01\rangle \rightarrow 11\rangle = 3, 1.0$
Q1	$ 1\rangle$ [Circuit: Q1 line with $ 1\rangle$ box, followed by 4 vertical lines, a CNOT gate (X on Q1, control on Q2), then 3 vertical lines, then a meter symbol]		$ 110\rangle \rightarrow 011\rangle = 3, 1.0$
Q2	$ 1\rangle$ [Circuit: Q2 line with $ 1\rangle$ box, followed by 4 vertical lines, a CNOT gate (X on Q2, control on Q1), then 3 vertical lines, then a meter symbol]		
Q3	$ 0\rangle$ [Circuit: Q3 line with $ 0\rangle$ box, followed by 4 vertical lines, a CNOT gate (X on Q3, control on Q1), then 3 vertical lines, then a meter symbol]		

* Output value and probability of being observed after performing the measurement.

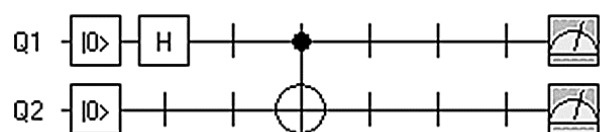


Figure 4. EPR circuit.

Since H and I are located in *parallel* lines then we perform the Kronecker product between both gates:

$$H \otimes I = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

obtaining the following matrix:

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & 1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ 1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & -1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}$$

Second, if we now look at the section of the circuit on the right side there is a $CNOT$ gate connected in series with the wire where we obtained the above matrix. Since both are connected in *series* then we carry out the inner product or multiplication between matrices, such that:

$$CNOT \cdot (H \otimes I) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}$$

obtaining the “EPR matrix” shown below:

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \end{pmatrix}$$

In practice this means that the EPR circuit is represented by the above matrix. Suppose now that EPR circuit receives as input the following vector state:

$$|Q1\rangle \otimes |Q2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

The register information will be processed by the quantum circuit simply carrying out the inner product between the EPR matrix and the vector state, obtaining a new vector:

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$

Once we obtained the above vector the output will be the result of measuring or observing the state of each qubit.

2.4. Quantum Computing in Practice

Nowadays the Canadian D-Wave Systems, Inc. is the only commercial company that offers quantum computers [16]. D-Wave One and Two models are adiabatic computers based on Washington

2048-qubit chip. According to this technology a quantum state converge to a solution based on Boltzmann probability distribution:

$$p(x_1, x_2, \dots, x_n) = \frac{1}{z} e^{-\frac{G(x_1, x_2, \dots, x_n)}{kT}}; \quad z = \sum \sum e^{-\frac{G(x_1, x_2, \dots, x_n)}{kT}}$$

Since they are adiabatic computers the best performance is obtained for continuous optimization problems. In recent years D-Wave computers have been acquired by Lockheed Martin and Google (shared with NASA) having spent a total 10–15 mill US dollars. Interestingly, although most researchers lack enough money to buy one of these models, it is feasible to emulate a quantum computer on a conventional computer. Is possible to emulate the operations and algorithms characteristic of a quantum computer using a computer with good performance. At present quantum computing emulation could be conducted applying any of the procedures listed below:

2.4.1. Q-Circuit Simulators

Quantum circuit (Q-circuit) simulators are programs including a GUI for designing and evaluating quantum circuits. Some programs—e.g., [17]—include a compiler option to design a gate to be used in larger circuits. To take the first step there are available two good Q-circuit emulators: QCAD [18], a Windows-based environment for quantum computing simulation (see Table 5 and Figure 4) and jQuantum [19], a quantum computer simulation applet.

2.4.2. Q-Programming Languages

Another possibility is the programming of a quantum algorithm using imperative programming languages oriented to quantum computing [20]. A good example of this option is QCL (Quantum Computing Language) [21]—a programming language (Figure 5) for quantum computers developed by Bernhard Ömer. QCL has been applied in a variety of problems, e.g., solving systems of nonlinear equations [22], the implementation of Bernstein-Vazirani algorithm [23], parallelization of quantum gates [24], simulation of Dijkstra's algorithm [25] and programming quantum genetic algorithms [26].

```

QCL Quantum Computation Language (32 qubits, seed 1466357188)
[0/32] 1 |0>
qcl> qureg u[1];
qcl> qureg v[1];
qcl> reset;
[2/32] 1 |0,0>
qcl> H(u);
[2/32] 0.70711 |0,0> + 0.70711 |1,0>
qcl> CNot(v,u);
[2/32] 0.70711 |0,0> + 0.70711 |1,1>
qcl> reset;
[2/32] 1 |0,0>
qcl> Not(u);
[2/32] 1 |1,0>
qcl> CNot(v,u);
[2/32] 1 |1,1>
qcl> -
  
```

Figure 5. An example of QCL program (for explanation see text).

In the example shown in Figure 5, two qubits are declared with *qureg* command: a first qubit in a register labeled as *u* and the second qubit in a register *v*. Consequently, we have implemented a quantum memory $|\psi\rangle = |u, v\rangle$. Following, using the *reset* command all qubits are forced to state zero, i.e., we reset the quantum state of the machine such that the machine state is empty $|\psi\rangle = |0, 0\rangle$. After the reset command a Hadamard function $H(u)$ is applied over *u* and returns it in a quantum superposition. Since it is only an example without practical purpose, next the example illustrates the use of $CNot(v, u)$, i.e., a controlled not gate with a target qubit *v* and a control qubit *u*. The gate mentioned flip *v* if *u* is in state one. Following, for the second time we reinitiated the quantum memory

with *reset* command. Thereafter, $Not(u)$ gate is applied to u qubit conducting a NOT operation in a similar manner to classical computing. Finally, we perform again a $CNot(v,u)$ operation.

QCL emulates a “Quantum RAM” (QRAM) model (Figure 6), thus a hybrid architecture by which a computer simultaneously performs classical and quantum operations. According to QRAM model the classical computer performs classical computing, controls the quantum register evolution and send the quantum operations to the quantum computer. The quantum computer, which is really simulated on the classic computer, conducts the initialization of the quantum register state, performs unitary transformations and measurements, sending to the classical computer the output. Even when QCL is a fairly representative programming language [27], at present there are other programming languages oriented to quantum computers [28–30].

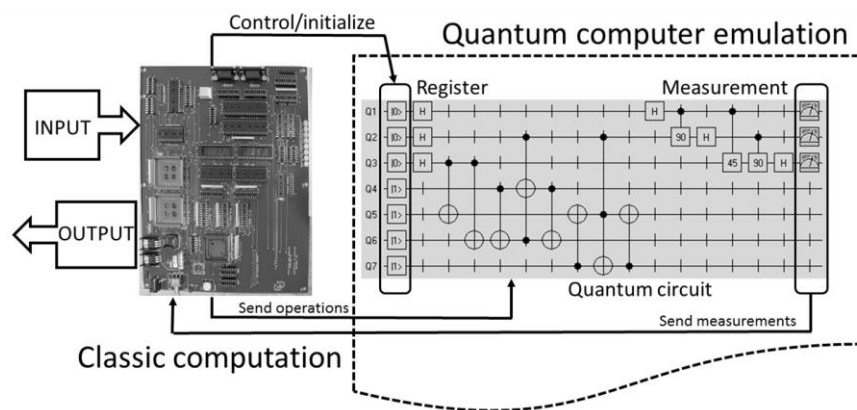


Figure 6. QRAM architecture (for explanation see text).

2.4.3. Simulated Q-Computer

Nowadays, programming on a conventional computer under a QRAM environment is the most common option. However, the program can be written in a simulated quantum computer, e.g., Google’s Quantum Computing Playground [31]. A user have accesses to a simulated GPU-accelerated quantum computer with an IDE interface and its own scripting language. The Google’s system has the ability to set quantum registers up to 22 qubits. Using a similar methodology the University of Bristol, Centre for Quantum Photonics (United Kingdom), offers an online quantum photonic chip simulator [32]: an example of quantum computing in the cloud. In this case, the program is written through an IDE showing a circuit, setting the user some photons into the input ports.

2.4.4. Do-It-Yourself: Quantum Computing with Python

Finally, in our opinion, one of the most useful approaches is to write your own program. Using a general purpose language, i.e., Python, we can efficiently implement any quantum algorithm combined with non-quantum computational procedures. Moreover, in the case of Python are available several quantum computing libraries, e.g., PyQu [33], qitensor [34], QuTiP [35], etc. In addition, SymPy [36], a Python library for symbolic computation, includes procedures to perform quantum operations.

3. Quantum Computing and Quantum Evolutionary Algorithms

Since the origins of quantum genetic algorithms (QGAs) [9] until today, lots of QGAs have been proposed in the scientific literature [37–41]. All kinds of quantum evolutionary algorithms have been successfully applied to optimization problems, such as the personnel scheduling problem [42], dynamic economic dispatch problem, e.g., in power systems [43], multi-sensor image registration [44], cryptanalysis [45], etc.

Quantum evolutionary algorithms share the main steps and features of their non-quantum counterparts. In its simplest form and adopting a QRAM architecture (Figure 6) a quantum (or quantum-inspired) evolutionary algorithm consists of the steps shown in Table 6.

Table 6. Main steps of a quantum evolutionary algorithm.

Step	Quantum Computing	Classical Computing
1	Initialize a quantum population $Q(0)$	
2	Make $P(0)$, measure of every individual $Q(0) \rightarrow P(0)$	
3		Evaluate $P(0)$
4	while (not termination condition) do	
5	begin	
6	$t \leftarrow t + 1$	
7	Update $Q(t)$ applying Q-gates: $Q(t + 1) = U(t).Q(t)$	
8	Make $P(t)$, measure of every individual $Q(t) \rightarrow P(t)$	
9		Evaluate $P(t)$
10	end	

The first step consists in the initialization of a quantum population $Q(0)$ of chromosomes. A quantum chromosome i is defined as a string of j qubits representing a quantum system $|\psi\rangle^i$ with 2^j simultaneous states:

$$\begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \dots & \alpha_j \\ \beta_1 & \beta_2 & \beta_3 & \dots & \beta_j \end{pmatrix}_i \rightarrow |\psi\rangle^i = \sum_j c_i |\psi_j\rangle$$

being the gene j , the qubit represented by vector (Figure 7):

$$\begin{pmatrix} \alpha_j \\ \beta_j \end{pmatrix} \rightarrow |\psi_j\rangle$$

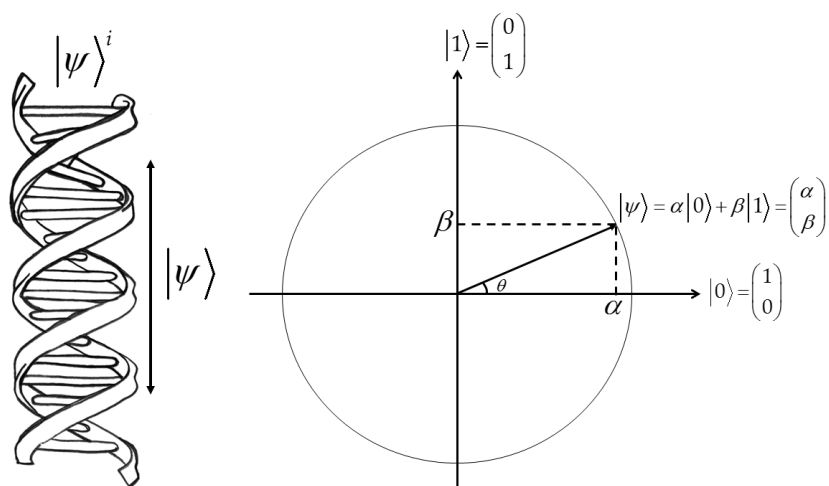


Figure 7. DNA modeled as $|\psi\rangle^i$ and gene sequence $|\psi\rangle$ represented as qubit in a superposition state.

Consequently a quantum population is defined by a set of quantum chromosomes or vectors, as shown below:

$$\begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \dots & \alpha_j \\ \beta_1 & \beta_2 & \beta_3 & \dots & \beta_j \end{pmatrix}_1 \\ \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \dots & \alpha_j \\ \beta_1 & \beta_2 & \beta_3 & \dots & \beta_j \end{pmatrix}_2 \\ \dots \\ \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \dots & \alpha_j \\ \beta_1 & \beta_2 & \beta_3 & \dots & \beta_j \end{pmatrix}_i$$

The most common technique to initialize the population is to set the value of the amplitudes of all qubits in the chromosomes to a value representing the quantum superposition of all states with equal probability. This is achieved from the product of the Hadamard matrix by the vector $|0\rangle$:

$$H \cdot |0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

obtaining a superposition vector. Subsequently to this product a phase angle θ ($0, \frac{\pi}{2}$] is randomly obtained, being the argument of the trigonometric functions or elements in the rotation matrix $U(t)$:

$$U(t) = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$$

The initialization step concludes conducting the product of the rotation matrix by the superposition vector, resulting in a pair of amplitudes (α, β) which define the state of j qubit:

$$\begin{pmatrix} \alpha_j \\ \beta_j \end{pmatrix} = \begin{pmatrix} \cos(\theta_j) & -\sin(\theta_j) \\ \sin(\theta_j) & \cos(\theta_j) \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Following, in a second step, we obtain a population $P(t)$ composed of classical chromosomes or bit strings. This population is the result of a measure or observation of qubits states in the quantum chromosomes of the population $Q(t)$. After measurement we get the classical population, such that $P(t)$ is given by a set of vectors:

$$\begin{pmatrix} x_1 & x_2 & x_3 & \dots & x_j \end{pmatrix}_1 \\ \begin{pmatrix} x_1 & x_2 & x_3 & \dots & x_j \end{pmatrix}_2 \\ \dots \\ \begin{pmatrix} x_1 & x_2 & x_3 & \dots & x_j \end{pmatrix}_i$$

Qubit observation is simulated, modelling the wave function collapse as follows:

$$\begin{cases} p(\alpha) \leq \left| \alpha_j^2 \right| & , \quad x_j = 0 \text{ (basisstate } |0\rangle) \\ p(\alpha) > \left| \alpha_j^2 \right| & , \quad x_j = 1 \text{ (basisstate } |1\rangle) \end{cases}$$

being $p(\alpha)$ a random number in the range $[0, 1)$. Assuming we are running the simulation under a QRAM architecture, this step has the purpose to create a population $P(t)$ of classical chromosomes. The aim is to conduct the fitness evaluation on a classical population using a digital computer. Otherwise, fitness evaluation on a quantum computer would produce the collapse of the quantum system destroying the superposition state. The evaluation of fitness is one of the main obstacles in the implementation of QGAs in a quantum computer.

A third step consists in the population update applying Q-gates, thus:

$$Q(t + 1) = U(t).Q(t)$$

From a theoretical point of view the evolution of the population is governed by Schrödinger's equation, being Q-gates the operators that play the role of the "genetic mechanisms" transforming chromosomes. Since evolution takes place in a complex vector space, i.e., a Hilbert space, such transformations are unitary transformations. Thus, let U be a unitary matrix, e.g., a rotation matrix, then it will be a unitary transformation if it holds that $U.U' = I$.

In the following section we describe the most characteristic quantum genetic operators.

3.1. Quantum Genetic Operators

At present there are several proposed quantum genetic operators performing genetic operations on quantum chromosomes. It is important to note that in the scientific literature sometimes these operators are termed indifferently like "interference gates" which can confuse the reader. In this review, we have renamed the operators, indicating between parentheses the term interference when in the literature such term is used in reference to such operator.

3.1.1. Qubit (Interference) Rotation Gate

Although there are several updating operators the most characteristic is the interference or rotation Q-gate. The rotation operator or quantum interference is defined as a gate $U(t)$:

$$U(t) = \begin{pmatrix} \cos(\delta\theta_j) & -\sin(\delta\theta_j) \\ \sin(\delta\theta_j) & \cos(\delta\theta_j) \end{pmatrix}$$

Applying this operator the evolution of a population is the result of a process of unitary transformations. In particular, rotations approximating the state of chromosomes to the state of the optimum chromosome in the population. Thus, this gate amplifies or decreases the amplitude of qubits or genes according to the chromosome with maximum fitness $f \left(x_1 \ x_2 \ x_3 \ \dots \ x_j \right)_i^{\text{maximum}}$. Consequently, the evolution of the quantum state is guided by the best individual (Figure 8):

$$\begin{pmatrix} \alpha_j^{t+1} \\ \beta_j^{t+1} \end{pmatrix} = \begin{pmatrix} \cos(\delta\theta_j) & -\sin(\delta\theta_j) \\ \sin(\delta\theta_j) & \cos(\delta\theta_j) \end{pmatrix} \begin{pmatrix} \alpha_j^t \\ \beta_j^t \end{pmatrix}$$

being $\begin{pmatrix} \alpha_j^t \\ \beta_j^t \end{pmatrix}$ and $\begin{pmatrix} \alpha_j^{t+1} \\ \beta_j^{t+1} \end{pmatrix}$ the amplitudes of the j qubit before and after the updating, respectively. In general, the rotation angle is obtained according to the following expression:

$$\delta\theta = sg(\alpha_j, \beta_j) \Delta\theta_j$$

where $sg(\alpha_j, \beta_j)$ and $\Delta\theta_j$ represent the direction and rotation value, respectively. Note that rotation value plays the role of an "evolution rate". Consequently, we should avoid too high or too low values. The values of these parameters are summarized in a look-up table (Table 7), comparing the fitness of the current chromosome $f(x_j)$ with the fitness of the best individual $f(b_j)$.

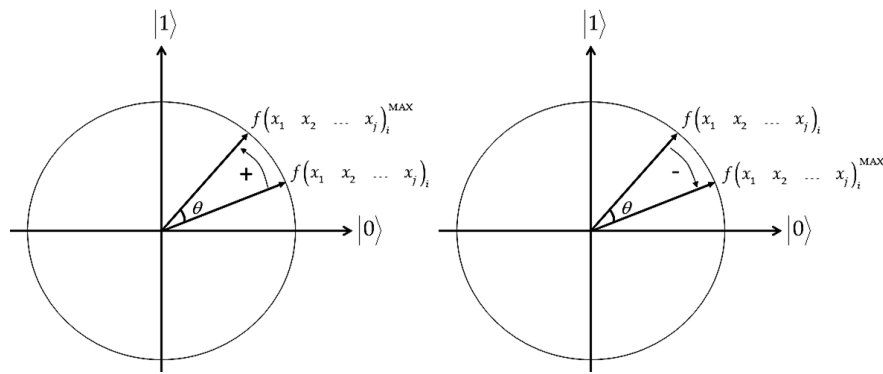


Figure 8. Rotation gate (for explanation see text).

Table 7. Lookup table of the rotation angle (δ is the angle step).

x_j	b_j	$f(x_j) \geq f(b_j)$	$\Delta\theta_j$	$sg(\alpha_j \beta_j)$			
				$\alpha_j \beta_j > 0$	$\alpha_j \beta_j < 0$	$\alpha_j = 0$	$\beta_j = 0$
0	0	False	0	-	-	-	-
0	0	True	0	-	-	-	-
0	1	False	δ	+1	-1	0	± 1
0	1	True	δ	-1	+1	± 1	0
1	0	False	δ	-1	+1	± 1	0
1	0	True	δ	+1	-1	0	± 1
1	1	False	0	-	-	-	-
1	1	True	0	-	-	-	-

A disadvantage of rotation operator is that the look-up table depends on the optimization problem, which affects the algorithm performance. Therefore the values in the table should be set according to the optimization problem: e.g., knapsack problem [46–49], OneMax problem [47], benchmark functions (i.e., De Jong, six-peaks and many-peaks functions) [50]. However, there is a standard table (Table 7) that is usually useful in many optimization problems [51]. In Table 7 δ is the angle step, having an effect on convergence speed, such that a very large value causes the population converges or diverges very quickly with respect to a local optimum. Unfortunately quantum genetic algorithm performance depends on look-up table values [48], being a general criterion to set δ values between 0.1π and 0.005π . One common solution is to use an adaptive strategy [37]. For example, suppose we define a range between 0.005π and 0.05π . In this example and according to [52] $\Delta\theta_j$ is changed as:

$$\Delta\theta_j = 0.005\pi + (0.05\pi - 0.005\pi) \frac{|f(x_j) - f(b_j)|}{\max(f(x_j), f(b_j))}$$

Note that rotation operator plays the role of the selection operator in SGA. In a classical SGA the selection operator simulates Darwinian natural selection, enhancing populations by promoting individuals with better fitness and punishing those with poorer performance. However, in QGA selection pressure is replaced by a change of all individuals towards the best individual. Therefore, when population is updated with the rotation operator the population converges to the fitter states, but usually QGAs are trapped in local optima undergoing premature convergence. In order to avoid this problem sometimes quantum genetic algorithms include either roulette or elite selection. For instance, a QGA with a selection step is used in an improved K-means clustering algorithm [53]. In fact, there are more extreme approaches such as [54] where a QGA includes selection and simulated annealing avoiding premature convergence. In other cases a selection step is included without resorting to operators commonly used in SGAs. Such is the case of a semiclassical genetic algorithm [55] where

a selection operator seeks for the maximum fitness individual by means of a quantum approach, in particular using a variant of the Grover's search algorithm.

According to [56] given the following determinant:

$$A = \begin{bmatrix} \alpha_b & \alpha_j \\ \beta_b & \beta_j \end{bmatrix}$$

it is interesting to note that when $x_j \neq b_j$ (Table 7), e.g., $x_j = 1$ and $b_j = 0$, and $A \neq 0$ then the direction of the rotating angle is $-\text{sgn}(A)$. Otherwise, thus when ($A = 0$) the direction of the rotating angle can be either positive or negative.

3.1.2. Quantum Mutation (Inversion) Gate

In imitation of SGAs there is also available a quantum version of the classic mutation operator [57]. The gate performs an inter-qubit mutation of the j th qubit, swapping the amplitudes with the quantum Pauli X gate:

$$U(t) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

resulting in:

$$\begin{pmatrix} \beta_j^{t+1} \\ \alpha_j^{t+1} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha_j^t \\ \beta_j^t \end{pmatrix}$$

3.1.3. Quantum Mutation (Insertion) Gate

This gate [57,58] reminds the biological mechanism for chromosome insertion. Chromosome insertion means that a chromosome segment has been inserted into an unusual position on the same or different chromosome. The quantum version of this genetic mechanism involves the permutation or swap between two randomly chosen qubits (left qubit, right qubit). For example, suppose that given the following chromosome we choose randomly the first and third qubits:

$$\begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \dots & \alpha_j \\ \beta_1 & \beta_2 & \beta_3 & \dots & \beta_j \end{pmatrix}$$

once applied the insertion operator, we get the new chromosome:

$$\begin{pmatrix} \alpha_3 & \alpha_2 & \alpha_1 & \dots & \alpha_j \\ \beta_3 & \beta_2 & \beta_1 & \dots & \beta_j \end{pmatrix}$$

3.1.4. Quantum Crossover (Classical) Gate

Quantum crossover [57] is simulated resembling the classical recombination algorithm used in SGAs but operating with amplitudes. However, whereas the quantum version of mutation could be implemented on a quantum computer, there are theoretical reasons preventing this with crossover. Nevertheless, and despite the theoretical limitations, the quantum version of classical crossover operator is applied in many practical optimization problems. In these cases a solution is searched using a quantum evolutionary "inspired" approach. Following, the operator is illustrated for the case of one point crossover. In this example if the cut point is randomly chosen, e.g., a point between first and second positions, then an exchange of chromosomal segments occurs:

$$\begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \dots & \alpha_j \\ \beta_1 & \beta_2 & \beta_3 & \dots & \beta_j \end{pmatrix}_m$$

$$\begin{pmatrix} \alpha'_1 & \alpha'_2 & \alpha'_3 & \dots & \alpha'_j \\ \beta'_1 & \beta'_2 & \beta'_3 & \dots & \beta'_j \end{pmatrix}_n$$

resulting the following recombinant chromosomes:

$$\begin{pmatrix} \alpha_1 & \alpha'_2 & \alpha'_3 & \dots & \alpha'_j \\ \beta_1 & \beta'_2 & \beta'_3 & \dots & \beta'_j \end{pmatrix}_{m^*}$$

$$\begin{pmatrix} \alpha'_1 & \alpha_2 & \alpha_3 & \dots & \alpha_j \\ \beta'_1 & \beta_2 & \beta_3 & \dots & \beta_j \end{pmatrix}_{n^*}$$

3.1.5. Quantum Crossover (Interference) Gate

The present quantum operator [59] performs crossover by recombining according to a criterion based on drawing diagonals. In consequence, all individuals interfere with each other resulting the offspring. Consider the following example. When the crossover is performed with the next six chromosomes:

$$\begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} & \alpha_{14} & \alpha_{15} & \alpha_{16} \\ \beta_{11} & \beta_{12} & \beta_{13} & \beta_{14} & \beta_{15} & \beta_{16} \end{pmatrix}_1$$

$$\begin{pmatrix} \alpha_{21} & \alpha_{22} & \alpha_{23} & \alpha_{24} & \alpha_{25} & \alpha_{26} \\ \beta_{21} & \beta_{22} & \beta_{23} & \beta_{24} & \beta_{25} & \beta_{26} \end{pmatrix}_2$$

$$\begin{pmatrix} \alpha_{31} & \alpha_{32} & \alpha_{33} & \alpha_{34} & \alpha_{35} & \alpha_{36} \\ \beta_{31} & \beta_{32} & \beta_{33} & \beta_{34} & \beta_{35} & \beta_{36} \end{pmatrix}_3$$

$$\begin{pmatrix} \alpha_{41} & \alpha_{42} & \alpha_{43} & \alpha_{44} & \alpha_{45} & \alpha_{46} \\ \beta_{41} & \beta_{42} & \beta_{43} & \beta_{44} & \beta_{45} & \beta_{46} \end{pmatrix}_4$$

$$\begin{pmatrix} \alpha_{51} & \alpha_{52} & \alpha_{53} & \alpha_{54} & \alpha_{55} & \alpha_{56} \\ \beta_{51} & \beta_{52} & \beta_{53} & \beta_{54} & \beta_{55} & \beta_{56} \end{pmatrix}_5$$

$$\begin{pmatrix} \alpha_{61} & \alpha_{62} & \alpha_{63} & \alpha_{64} & \alpha_{65} & \alpha_{66} \\ \beta_{61} & \beta_{62} & \beta_{63} & \beta_{64} & \beta_{65} & \beta_{66} \end{pmatrix}_6$$

we obtain the following first and second recombinant chromosomes:

$$\begin{pmatrix} \alpha_{11} & \alpha_{22} & \alpha_{33} & \alpha_{44} & \alpha_{55} & \alpha_{66} \\ \beta_{11} & \beta_{22} & \beta_{33} & \beta_{44} & \beta_{55} & \beta_{66} \end{pmatrix}_{1^*}$$

$$\begin{pmatrix} \alpha_{21} & \alpha_{32} & \alpha_{43} & \alpha_{54} & \alpha_{65} & \alpha_{16} \\ \beta_{21} & \beta_{32} & \beta_{43} & \beta_{54} & \beta_{65} & \beta_{16} \end{pmatrix}_{2^*}$$

3.2. A Canonical Classification of Quantum Evolutionary Algorithms

In order to summarize this review as much as possible, most of the quantum evolutionary algorithms have been grouped into two major classes: Quantum Genetic Algorithms (QGAs) and Hybrid Genetic Algorithms (HGAs). Since there is no agreement on terminology, different names are used interchangeably: Quantum Evolutionary Algorithms (QEAs), Quantum-Inspired Evolutionary Algorithms (QIEAs), etc. Anyway, in general a QGA includes the main steps shown in Table 8. Likewise an HGA comprises the main steps set out in Table 9.

Table 8. Main steps of a QGA.

Step	Quantum Computing	Classical Computing
1	Initialize a quantum population $Q(0)$	
2	Make $P(0)$, measure of every individual $Q(0) \rightarrow P(0)$	
3		Evaluate $P(0)$
4	while (not termination condition) do	
5	begin	
6	$t \leftarrow t + 1$	
7	Rotation Q-gate	
8	Mutation Q-gate	
9	Make a measure $Q(t) \rightarrow P(t)$	
10		Evaluate $P(t)$
11	end	

Table 9. Main steps of an HGA.

Step	Quantum Computing	Classical Computing
1	Initialize a quantum population $Q(0)$	
2	Make $P(0)$, measure of every individual $Q(0) \rightarrow P(0)$	
3		Evaluate $P(0)$
4	while (not termination condition) do	
5	begin	
6	$t \leftarrow t + 1$	
7	Rotation Q-gate	
8	Crossover operator	
9	Mutation Q-gate	
10	Make a measure $Q(t) \rightarrow P(t)$	
11		Evaluate $P(t)$
12	end	

4. Towards True Quantum Evolutionary Algorithms

QGA and HGA algorithms can be considered as classical optimization methods inspired by the principles of quantum computing. Programs implementing such methods can be executed on a digital computer, without this implying practical or theoretical difficulties. At present one of the challenges in Quantum Artificial Intelligence is the design of true quantum evolutionary algorithms and therefore of programs that in the future can run on a quantum computer. However, some problems arise when we translate the main steps of a SGA to the quantum version. This is a paradoxical situation because a SGA bears a resemblance to Grover's quantum algorithm: SGAs are parallel search methods although this feature is not implemented in their usual applications. One of the main problems with QGA and HGA algorithms [60] is to find a method to perform measurements of the population of individuals but without collapsing the superposition state of chromosomes. Furthermore, [60] notes that to date a key issue not addressed is how to implement in a quantum computer a crossover operator. Whereas mutation could be easily conducted in a quantum computer, i.e., using a Pauli X gate, it is unclear how to carry out crossover using for this purpose quantum mechanical phenomena.

One of the most interesting ideas is proposed in 2006 by [61,62] taking the first steps in the implementation of a genetic algorithm on a quantum computer. The authors of these papers proposed a true quantum evolutionary algorithm, which was termed as Reduced Quantum Genetic Algorithm (RQGA). The algorithm consists of the main steps described below (Table 10).

Table 10. Main steps of a RQGA.

Step	Quantum Computing
1	Initialize a superposition of all possible chromosomes
2	Evaluates fitness with operator F
3	Apply Grover's algorithm
4	Ask to the oracle O
5	Apply Grover's diffusion operator G
6	Make a measure

In the first place, the algorithm begins preparing a superposition of all individuals, i.e., N , or chromosomes of population $Q(t)$:

$$|\psi\rangle^{Q(t)} = \frac{1}{\sqrt{N}} \sum |\psi\rangle_i$$

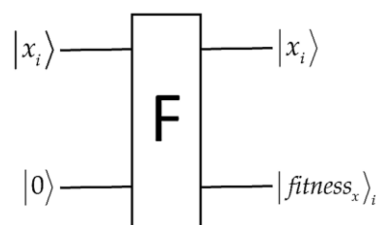
Therefore, all individuals are represented by only one individual quantum register. That is, the entire population is represented by a single chromosome in a superposition state:

$$\begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \dots & \alpha_j \\ \beta_1 & \beta_2 & \beta_3 & \dots & \beta_j \end{pmatrix}_i = c_0 |00\dots 00\rangle + c_1 |00\dots 01\rangle + \dots + c_{2^n-2} |11\dots 01\rangle + c_{2^n-1} |11\dots 11\rangle$$

One of the key steps of RQGA is the correlation between the individual quantum register $|x\rangle_i$ and a fitness quantum register $|fitness_x\rangle_i$:

$$|\psi\rangle_i = |x\rangle_i \otimes |fitness_x\rangle_i$$

From a formal point of view, we have a fitness quantum gate F which evaluates the fitness of individuals (Figure 9). In 2008 [63], a similar idea is also applied to other version of a true quantum evolutionary algorithm which was termed as Quantum Genetic Optimization Algorithm (QGOA).

**Figure 9.** Fitness quantum gate.

In a second step the algorithm searches for the maximum fitness:

$$|fitness_x\rangle_i^{\max}$$

In the late 1990s, [64] proposed a quantum algorithm for searching the maximum value among N values. Once the operator F is applied, RQGA searches for the maximum fitness value based on the Grover's search algorithm [65]. This is one of the most popular quantum algorithms oriented to search in an unstructured database. Without going into details on this algorithm, RQGA performs the following two steps. First, given a register with a set of fitness values an oracle O is designed to mark all the kets:

$$|\psi\rangle_i$$

having a fitness value greater than a cutoff value:

$$O|\psi\rangle^{Q(t)} = (-1)^{f(x)} |\psi\rangle^{Q(t)}$$

such that:

$$f(x) = \begin{cases} 1, & \text{if } |fitness_x\rangle_i = |fitness_x\rangle_i^{\max} \\ 0, & \text{otherwise} \end{cases}$$

Secondly, the algorithm concludes applying Grover's diffusion operator G . This operator aims at finding the marked states, i.e., $f(|fitness_x\rangle_i) = 1$:

$$|\psi\rangle^{Q(t)} = G |\psi\rangle^{Q(t)}$$

Finally, making a measure in $|\psi\rangle^{Q(t)}$ the chromosome with maximum fitness is obtained. All these steps are summarized in the quantum circuit shown in Figure 10.

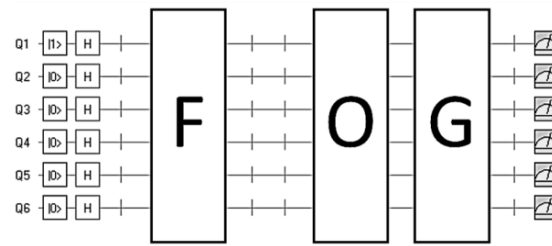


Figure 10. Quantum circuit representing the RQGA.

5. Simulation Experiments

In this review, we illustrate how to implement the above quantum genetic algorithms, using a simple optimization problem. The goal is to find the value of x within the range $0 \leq x \leq 15$ that maximizes the value of the benchmark function shown below:

$$f(x) = \left| \frac{x - 5}{2 + \sin(x)} \right|$$

The $f(x)$ function has an optimum reached with $x = 11$, thus 1011 in binary numbering system. Since in the experiments $f(x)$ is multiplied by 100, the maximum fitness is equal to 599.9941. QGA, HGA and RQGA codes were written in Python 3.4.4 language and they can be downloaded from [66–68]. In the simulation experiments conducted with QGA we defined three experimental protocols: QGA in the absence of mutation (QGA1), QGA setting population and qubit mutation probabilities equal to 0.01 (QGA2) and QGA setting these parameters to lower values, in particular equal to 0.001 (QGA3). In HGA one-point crossover probability was set equal to 0.75, also conducting three kinds of experiments: simulation experiments in the presence of mutation, i.e., setting population and qubit mutation probabilities equal to 0.01 (HGA2) and setting these parameters to 0.001 (HGA3). As in the previous experiments with QGA we also conducted simulation experiments without mutation (HGA1). The simulation experiments conducted with above quantum genetic algorithms were compared with a non-quantum simple genetic algorithm (SGA). The SGA code can be downloaded from [69]. In this latter algorithm the one-point crossover probability was equal to 0.75 and the population and bit mutation probabilities were both equal to 0.01. Simulations were performed for 150 generations, with a population size of 50 chromosomes. Thereafter, we performed five experimental replicates with each of the above algorithms. Next, from each experimental replicate we selected the average fitness values from the last 10 generations. Finally, for each of the algorithms a total of 50 values (5 replicates \times 10 fitness averages) was collected in a single sample. Statistical analysis [70] of the seven samples (SGA, HGA1, HGA2, HGA3, QGA1, QGA2 and QGA3) was accomplished using the statistical package STATGRAPHICS Centurion XVII version 17.1.12 (Statpoint Technologies, Inc. Warrenton, VA, USA).

6. Results

The obtained results show how the classical algorithm SGA has greater performance than the quantum versions of the genetic algorithm (Figure 11). In fact, SGA is the only evolutionary algorithm that achieves the maximum value of fitness, i.e., 599.9941 (Figure 12). The Kruskal-Wallis test (Table 11) shows with a p -value equal to zero that there are statistically significant differences among medians at the 95.0% confidence level. Compared to each other the algorithms we conclude that SGA differs significantly from HGA and QGA. The HGA algorithm without mutation (HGA1) differs significantly from HGA with mutation (HGA3), whereas there are not significant differences among the QGA protocols. One possible explanation for the better performance of SGA could be the mechanism that drives evolution. That is, in QGA and HGA evolution is the result of unitary transformations, particularly rotations approximating the state of chromosomes to the state of the optimum chromosome with maximum fitness. Since this procedure is repeated generation after generation the result is a fast convergence to local optima, taking place a phenomenon of local trapping. A general strategy to improve QGA performance consists of using minor enhancements of the algorithm. For instance, including new operators, e.g., a quantum disaster [56], perturbation [71] or other “customized” algorithms [72]. In many cases, these operators are only useful in highly specific applications, e.g., in Bioinformatics specific quantum operators (ResidueBlockShuffle, GapBlockShuffle, BlockMove, etc.) were devised by their authors [73] in a problem of multiple sequence alignment.

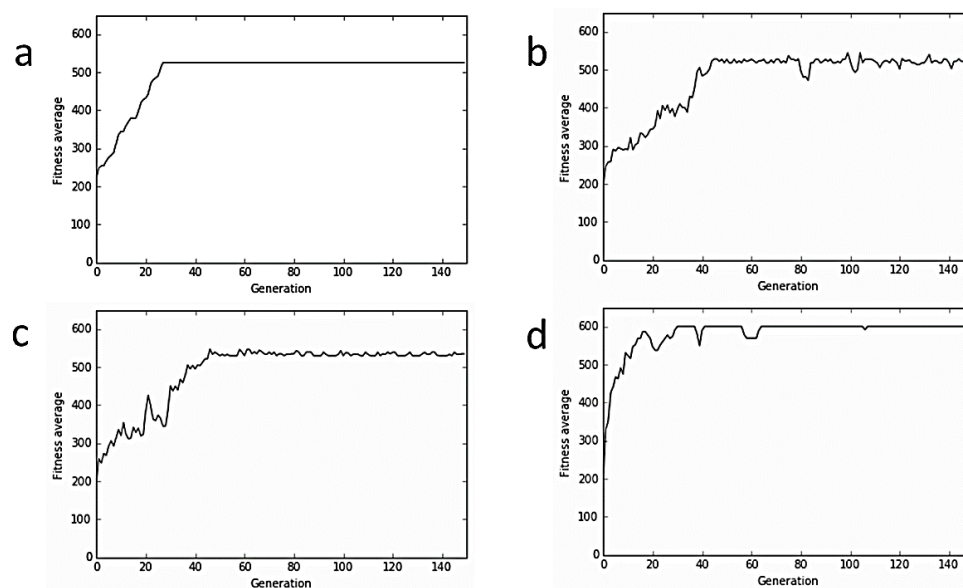


Figure 11. Representative performance graph obtained in the benchmark function optimization experiments conducted with (a) Quantum genetic algorithm (QGA); (b) Hybrid genetic algorithm (HGA) with mutation; (c) Hybrid genetic algorithm (HGA) without mutation; (d) Simple genetic algorithm (SGA).

Table 11. Kruskal-Wallis test.

Algorithm	Sample Size	Mean Rank
SGA	50	325.5
HGA1	50	119.12
HGA2	50	111.52
HGA3	50	202.98
QGA1	50	151.3
QGA2	50	184.38
QGA3	50	133.7

Statistic = 161.425; p -value = 0.0.

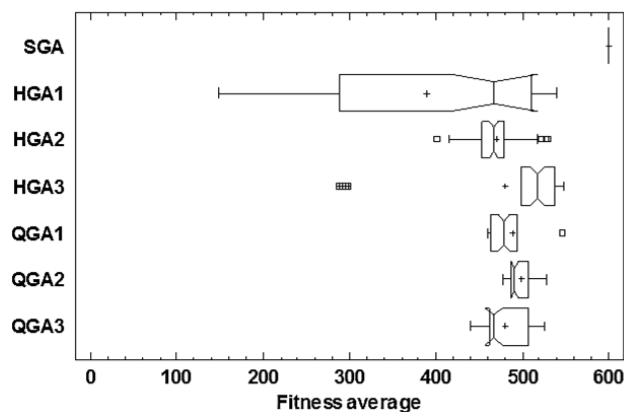


Figure 12. Notched Box-and-Whisker Plots, one boxplot per evolutionary algorithm showing the medians (notches) and means (crosses) of the fitness [70]. Squares indicate outliers (unusual fitness values).

Therefore, we could conclude that in quantum evolutionary algorithms evolution (or optimization) is the result of a rotation quantum gate, which introduces an interference phenomenon. Thus, individuals are adjusted or modified to be more similar to the best individual in the population. Consequently, the population is subjected to a lower Darwinian selection pressure. However, in SGA once individuals are evaluated the algorithm simulating selection (e.g., wheel parents selection operator) will replace the old population $P(t)$ with a new population $P(t + 1)$ of individuals. Since individuals are selected according to their fitness values we are evolving a population of solutions via Darwinian evolution but with a greater selection pressure than QGA and HGA. Hence, SGA replaces obsolete strategies by innovative strategies represented by the offspring. Likewise, when crossover is included as a step in HGA algorithm, its performance usually improves approaching to SGA.

An advantage of the quantum genetic algorithms is that they require fewer chromosomes than SGA. Under a theoretical realm in a “true” quantum genetic algorithm, i.e., RQGA, we can consider that the population is made up of a single chromosome in a state of superposition. Although this fact may be bizarre at first sight, it is not from the perspective of quantum mechanics. Moreover, the algorithm RQGA demonstrates that using quantum computing the genetic search strategy becomes unnecessary (Figure 13): evolution takes place in a single generation.

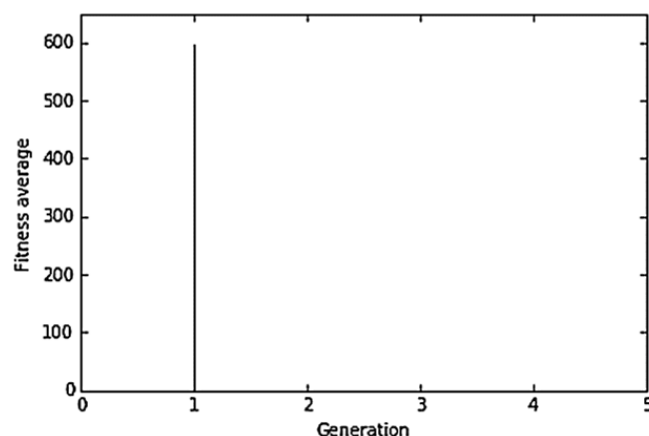


Figure 13. Performance graph obtained in the benchmark function optimization experiment conducted with RQGA, a true quantum genetic algorithm based on Grover’s algorithm.

In order to illustrate above idea let us consider the results we have obtained once the RQGA program was executed on a “quantum computer”. First, the program creates the superposition state:

[illegible]

In second place, the oracle O marks the maximum fitness of $|\psi\rangle$:

[illegible]

such that when $O|\psi\rangle^{Q(t)} = (-1)^{f(x)}|\psi\rangle^{Q(t)}$ is applied we obtain the superposition shown below:

$$\begin{pmatrix} 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ -0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \end{pmatrix}$$

This second step is repeated a given number of iterations. The Grover's maximum number of iterations is calculated as:

$$\frac{\pi}{4}\sqrt{2^n}$$

being n the number of qubits or length of the quantum chromosome, thus $n = 4$ in the example of the function described in Section 5. Repeating the second step resulted in:

$$\begin{pmatrix} 0.1875 \\ 0.1875 \\ 0.1875 \\ 0.1875 \\ 0.1875 \\ 0.1875 \\ 0.1875 \\ 0.1875 \\ 0.1875 \\ 0.1875 \\ 0.1875 \\ -0.6875 \\ 0.1875 \\ 0.1875 \\ 0.1875 \\ 0.1875 \end{pmatrix}$$

In third and last place the Grover's diffusion operator G finds the chromosome in $|\psi\rangle^{Q(t)}$ with a marked state. Therefore, performing the following operation $|\psi\rangle^{Q(t)} = G |\psi\rangle^{Q(t)}$ the result is:

$$\begin{pmatrix} 0.078125 \\ 0.078125 \\ 0.078125 \\ 0.078125 \\ 0.078125 \\ 0.078125 \\ 0.078125 \\ 0.078125 \\ 0.078125 \\ 0.078125 \\ 0.078125 \\ 0.953125 \\ 0.078125 \\ 0.078125 \\ 0.078125 \\ 0.078125 \end{pmatrix}$$

Finally, making a measure in $|\psi\rangle^{Q(t)}$ we get the state that points to chromosome with maximum fitness:

[illegible]

In other words, in the present example we have 15 possible chromosomal states represented as:

[illegible]

Consequently, since RQGA algorithm found the state $|11\rangle$ then according to Table 12 the optimum chromosome is $|1011\rangle_{11}$ with fitness $|599\rangle_{11}$.

Table 12. Chromosomal states.

State	$ x\rangle_i$	$ fitness_x\rangle_i$
$ 0\rangle = \dots$	$ 0000\rangle_0$	$ 250\rangle_0$
$ 1\rangle = \dots$	$ 0001\rangle_1$	$ 140\rangle_1$
$ 2\rangle = \dots$	$ 0010\rangle_2$	$ 103\rangle_2$
$ 3\rangle = \dots$	$ 0011\rangle_3$	$ 93\rangle_3$
$ 4\rangle = \dots$	$ 0100\rangle_4$	$ 80\rangle_4$
$ 5\rangle = \dots$	$ 0101\rangle_5$	$ 0\rangle_5$
$ 6\rangle = \dots$	$ 0110\rangle_6$	$ 58\rangle_6$
$ 7\rangle = \dots$	$ 0111\rangle_7$	$ 75\rangle_7$
$ 8\rangle = \dots$	$ 1000\rangle_8$	$ 100\rangle_8$
$ 9\rangle = \dots$	$ 1001\rangle_9$	$ 165\rangle_9$
$ 10\rangle = \dots$	$ 1010\rangle_{10}$	$ 343\rangle_{10}$
$ 11\rangle = \dots$	$ 1011\rangle_{11}$	$ 599\rangle_{11}$
$ 12\rangle = \dots$	$ 1100\rangle_{12}$	$ 478\rangle_{12}$
$ 13\rangle = \dots$	$ 1101\rangle_{13}$	$ 330\rangle_{13}$
$ 14\rangle = \dots$	$ 1110\rangle_{14}$	$ 300\rangle_{14}$
$ 15\rangle = \dots$	$ 1111\rangle_{15}$	$ 377\rangle_{15}$

7. Future Directions

Over the next years the incorporation of quantum computing in Artificial Intelligence will lead to a fast development of related research areas, e.g., machine learning, as a consequence of an increased execution speed and effectiveness of the algorithms. For instance [74] report an experimental implementation of a quantum support vector machine algorithm for an optical character recognition problem. In the experiments, they implemented a 4 qubit processor using the NMR technique with ^{13}C -iodotrifluoroethylene and a spectrometer at 306 K. Furthermore, in the future we will achieve the physical realization [75] of 50–100 qubits and therefore the hardware to build a quantum computer. At present, it is possible to experience with a 5 qubits quantum computer via a cloud computing platform and run experiments, such is the case of IBM's quantum processor [76]. However, today, even when QGAs are inspired by principles of quantum computing they are eventually executed on a classical computer. In our opinion this scenario will change once we achieve the design and implementation of a RQGA on a quantum computer. Consequently, this will accelerate research on quantum evolutionary algorithms designing higher-order QGA [77], QGAs with entanglement [78] or hybridizing QGAs with the quantum version of optimization algorithms, e.g., artificial bee colony [79], cuckoo search [58], etc. The leap from emulation to the actual implementation of quantum algorithms is a big step that should be accompanied by a good training of future computer scientists on the fundamentals of quantum mechanics [80]. The result of these changes will be a dramatic increase of the applications of quantum evolutionary algorithms, either on specific problems, e.g., the analysis of cancer microarray data [81] or in classical engineering optimization problems [82]. Moreover, it is also expected an increase in the number of applications in the field of Artificial Intelligence, e.g., the N-Queens problem [83], and even in the field of Artificial Life [84]. In the future quantum computing may also have a profound influence on Darwinism [85], transforming our vision of life on Earth. However, until these advancements occur we must exploit the advantages that provides us the current software and hardware technologies, e.g., designing more efficient QGAs with the support of CUDA (from NVIDIA) platform and the Matlab Graphic Processing Unit (GPU) library [86].

8. Conclusions

In this paper, we survey the main concepts in quantum computing and quantum evolutionary computation. In recent years, the possibility to emulate a quantum computer has led to a new class

of GAs, i.e., QGAs. At present, in this class of algorithms research is splitted between two trends or flavors. On the one hand, some researchers are “inspired” by quantum mechanics developing a new class of GAs. In this case, the researcher does not intend in the near future to run the algorithm in a quantum computer. The aim is to solve an optimization problem on a digital computer, either to test a novel improvement or hardware technology in the QGA, or solve real-world problems using a novel class of algorithm instead classical GAs. In our opinion, at present this is the main trend in research on QGAs. On the other hand, in recent years there has arisen a line of research that explores the possibility to design a “true” QGA, so that in the future the algorithm can be run on a quantum computer. According to the way of thinking we have followed through this paper, we believe that this last line of research may have a profound influence on Artificial Intelligence and Artificial Life as well as in disciplines such as Biology.

Acknowledgments: I would like to express my special thanks of gratitude to Dr. Gabriela Ochoa at the Department of Computing Science and Mathematics, University of Stirling, Scotland, for her advice and comments about my research work during my stay in the summer of 2015. R. Lahoz-Beltra was supported by a grant PRX14/00319 from Ministerio de Educación, Cultura y Deporte (Spain) through the program “Estancias de movilidad de profesores e investigadores seniores en centros extranjeros de enseñanza superior e investigación, incluido el Programa Salvador de Madariaga 2014”.

Conflicts of Interest: The author declares no conflict of interest.

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