A genetic algorithm for finding pulse sequences for NMR quantum computing

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Abstract

We present a genetic algorithm for finding a set of pulse sequences, or rotations, for a given quantum logic gate, as implemented by NMR. We demonstrate the utility of the method by showing that shorter sequences than have been previously published can be found for both a CNOT and for the central part of Shor’s algorithm (for \( N=15 \)). Artificial intelligence techniques like the genetic algorithm here presented have an enormous potential for simplifying the implementation of working quantum computers.

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I. INTRODUCTION

Of late the field of quantum computing has become of great interest, not least because of the possibilities of solving mathematical and physical problems either extremely difficult or impossible to compute on classical machines. There still remain, however, many obstacles to practical implementation. Some researchers have proposed the use of bulk samples at room temperature to do quantum computing: specifically, nuclear magnetic resonance (NMR) of molecules in a room temperature solution\textsuperscript{1,2,3,4}. Specific nuclear spins are the qubits. This approach has several advantages, including long coherence times for computation, ability to read out the state of each qubit spectroscopically, and ability to work at room temperature. In this implementation, the dynamics of the nuclear spins are controlled using RF pulses and delay times. However, complexity in designing a set of pulses grows rapidly with the size of the problem. The design of the pulse sequence for a given computation therefore becomes an important consideration: to find the shortest and most robust pulse sequence that implements the desired transformation. In this paper we propose a way of designing those pulse sequences, and demonstrate its utility by showing that we can increase the efficiency of the CNOT sequence by 40% and of Shor’s algorithm by 50%.

II. NMR

Over several decades Nuclear Magnetic Resonance (NMR)\textsuperscript{5,6} has been widely used as a high sensitive technique for probing impurities in materials and for identifying molecules and determining their structure and dynamics. During the last few years\textsuperscript{3,2}, the methods of NMR spectroscopy were applied to realize quantum computing experimentally. Each molecule is viewed as a single computer whose state is determined by the orientation of its spins.

Spin-1/2 nuclei are used for the purpose\textsuperscript{7}. When such a spin is subjected to a strong static magnetic field $B_0$, it can align or anti-align with this static field, similar to a classical bar magnet. These two states are labeled as a logical 0 or 1. A spin precesses at a particular resonance frequency about this static field. Each spin can be individually addressed using RF pulses tuned to its resonance frequency, provided it belongs to a different type of nucleus or one with a different chemical environment\textsuperscript{5}. By timing the duration and phase of this
pulse we can tip the spin into any direction.

We can manipulate the state of each nucleus by applying a rotating RF magnetic field at its resonance frequency. These RF pulses and the coupling between the neighboring spins provide a mechanism to realize any two-input, one-output logic gate, building blocks for computation. Two-qubit gates require an interaction between the spins. The coherence times for spin-1/2 nuclei in NMR is on the order of thousands of seconds. The switching time for a two-qubit gate can be on the order of milli-seconds. Thus several tens, hundreds or thousands of operations can be performed using NMR.

III. GENETIC ALGORITHM

The Genetic Algorithm is a model of machine learning which derives its behavior from a metaphor of the processes of evolution in nature. This is done by the creation within a machine of a population of individuals represented by chromosomes, in essence a set of character strings that are analogous to the base-4 chromosomes that we see in our own DNA. The individuals in the population then go through a process of evolution. This process leads to the evolution of populations of individuals that are better suited to their environment than the individuals that they were created from, just as in natural adaptation. The genetic algorithm is essentially a means of designing the environment and the evolution of the populations so that the desired characteristics are selected for.

At the beginning of the computation, an objective function is designed to evaluate how closely the individuals conform to the desired characteristic(s). This function, the fitness function, is designed to give graded and continuous feedback about how well an individual conforms. A number of individuals are randomly initialized. The objective function is then evaluated for these individuals. The first generation is thus produced. Individuals are selected according to their fitness for the production of offspring. In selection, the individuals producing offspring are chosen. Each individual in the selection pool receives a reproduction probability depending on their own objective value and the objective value of all other individuals in the selection pool. This fitness is used for the actual selection step afterwards.

Parents are recombined to produce offspring. Individuals with high fitness should have high probability of mating. Crossover represents a way of moving through the space of
possible solutions based on the information gained from the existing solutions. All offspring will be mutated with a certain probability. The fitness of the offspring is then computed. The offspring are inserted into the population replacing the parents, producing a new generation. This cycle is performed until the optimization criteria are reached.

IV. IMPLEMENTATION

Here we explain the actual functioning of the genetic algorithm to determine various pulse sequences which can be used to realize a CNOT gate, using 2 qubit NMR quantum computing. Previously, the CNOT gate has been realized using a single set of five pulse sequences [1]. The program which we have constructed, using genetic algorithm, finds an enormous number of pulse sequences in groups of four to realize a CNOT gate, which is a significant improvement over the already existing solution.

Initially, any genetic algorithm selects an initial population of the essential characteristics from a set of values in the search space. The members of this population are called "chromosomes." In this case the characteristics are different angles and axes, since each pulse corresponds to a rotation [1]. As the possible range of angle values for this application can be anything between $\theta_0$ and $\theta_360$, we define an upper bound and a lower bound for the search space, as $\theta_360$ and $\theta_0$ respectively. Nine bits are needed to represent each angle in this search space, providing a precision of one degree. We also have a set of axes (x,y,z) to choose from. Because of the group properties of rotations, the continuum of possible axes for any single rotation can be expressed as an ordered product of rotations about the three chosen (x,y,z) axes. The genetic algorithm therefore has to choose chromosomes which represent a sequence of rotations about three possible axes for each of two qubits and for each rotation angle. At first we show how we evolve new angles from the search space and then proceed further to explain the same technique with axes.

Required mappings are done to the values to enhance the computational speed. The genetic algorithm randomly selects an angle $\theta$ and an axis $i$ from the respective search space for the angles and axes. Having done this, rotation about any axis $\alpha$, by an amount $|\alpha|$ is calculated from the following formula [11],

$$R_{\alpha}(\alpha) = \cos(\alpha/2) \cdot I - i\vec{\sigma} \cdot \hat{\sigma} \sin(\alpha/2)$$  \hspace{1cm} (1)
where $\hat{\alpha} = (\vec{\alpha} / |\vec{\alpha}|)$, $I$ is the identity matrix and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the Pauli operator. As an example, let us consider the rotation of qubits A and B about the z-axis by an amount $\alpha = |\vec{\alpha}|$:

$$R_{zAB}(\alpha) = \cos(\alpha/2) \cdot \hat{I} + i \sin(\alpha/2)S_{zAB}$$

(2)

where $S_{zAB} = \sigma_z A \otimes \sigma_z B$, with $\otimes$ the outer product, and $\sigma_z$ is

$$
\begin{pmatrix}
-1 & 0 \\
0 & 1
\end{pmatrix}
$$

where we implicitly label the rows and columns by $|0>, |1>$ and $<0|, <1|$. The rotation matrices are calculated and multiplied for the result

$$Result = R_{\vec{\alpha}_1}(\alpha_1) \cdot R_{\vec{\alpha}_2}(\alpha_2) \cdots R_{\vec{\alpha}_N}(\alpha_N)$$

(3)

The result is checked for its correctness which is the fitness function.

$$FF = Result - desired$$

(4)

For example, the CNOT gate is defined by the set of inputs with corresponding outputs, given by:

| Inputs | Outputs |
|--------|---------|
| 0 0    | 0 0     |
| 0 1    | 0 1     |
| 1 0    | 1 1     |
| 1 1    | 1 0     |

TABLE I: CNOT inputs and outputs. This is the controlled NOT because the first bit is unchanged, but the second is flipped iff the first is a 1.

This transformation is represented by the matrix

$$
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
$$
|     | 00000 | 00001 |
|-----|-------|-------|
| $P_1$ | 1010 | 0100 |
| $P_2$ | 0100 | 1010 |
| $O_1$ | 0100 | 1010 |
| $O_2$ | 1010 | 0100 |

FIG. 1: An example of the crossover procedure for producing offspring $O_1$ and $O_2$ from parents $P_1$ and $P_2$

where we implicitly label the rows and columns by the bit values of the two qubits: $|00>,|01>,|10>,|11>$ and $<00|, <01|, <10|, <11|$, each of which represents a possible input or output state. For example, the one in the third row of the matrix means that the input state $|10>$ is mapped onto the output state $<11>$.

Usually one does not get the desired output from the initial population. Hence the next step is to go for crossover. We select two chromosomes from the search space as the "parents." We have used single point crossover technique. A point for crossover is selected randomly. The first portion of the bits of the first parent is combined with the second portion of the bits to generate one new offspring and the first portion of the bits of the second parent is combined with the second portion of the bits of the first parent to generate the second new offspring. This operation is performed on all parents to produce new offspring. Figure 1 shows two parents ($P_1,P_2$) before crossover and the offspring($O_1,O_2$) after crossover. The point of crossover is randomly selected to be 5 in this example. Having generated new offspring, we perform mutation to refine or fine tune the obtained new offspring, so that the resulting offspring will have better fitness. One of the chromosomes is affected after mutation. In other words, mutation acts on one chromosome at a time. This can either be an angle or an axis depending on what we perform the mutation on. Initially we select a value $R[i]$, from the population. Two random numbers from the search space are selected and we perform a modulo operation with the mutation rate, selected earlier. If the result of the modulo function results in two identical numbers, then each bit of the value $R[i]$ is flipped. The second value from the population is selected and the same process continues until all the values in the population have gone through this process of mutation.

We remap angles which exceed $\angle 360$ to maintain a 9-bit length, by using the mapping
function given below

\[ r[i] = r[i] \times ((max - min)/(2^L - 1)) \]  

(5)

where \( r[i] \) is an array of integers representing the angles, \( max \) is the maximum value \( r[i] \) can hold from the search space, \( min \) is the minimum value \( r[i] \) can take from the search space, and \( L \) is the maximum number of bits used to represent the \{\( r[i] \)\}. We have thus mapped the angles which exceed 360 to any value between 0 and 360.

Having evolved a new set of values, rounding of the angles is performed in the same manner as it was done for the initial population. Now that we have found new angles we repeat the same procedure for the axes. In this case, the axes are allowed to crossover and the new generation just obtained is made to undergo mutation. Mutation can be defined as a method to fine tune the results obtained as a result of crossover. With these initial values derived, the fitness function is calculated as shown above in equation (3), and then the result is checked for correctness using equation (4). If the result is a zero, then the pulse sequence we have found can be used to realize a CNOT gate. If we get any other value, then the entire process of crossover, mutation and rounding of the angles followed by the crossover and mutation of the axes and evaluating the fitness function is performed. This process continues until a correct result is found.

V. RESULTS

A. CNOT

We have realized a CNOT gate using pulse sequences with just 3 rotations thus increasing the efficiency by 40% from the earlier techniques which used 5 rotations. The two solutions found are given in Table 2.

|   | \( R_zB(270) \) | \( R_{xzAB}(90) \) | \( R_xA(90) \) |
|---|----------------|----------------|------------|
| 1 | \( R_xA(90) \) | \( R_zB(270) \) | \( R_{xzAB}(90) \) |

TABLE II: Sample pulse sequences found by the genetic algorithm, with 3 rotations, whose ordered product produces the CNOT matrix. Each pulse corresponds to a rotation \( R_{\vec{a}}(\alpha) \).
B. Shor’s Algorithm

Since its discovery [12] by Peter Shor in 1994, this algorithm for factorizing large numbers using a quantum computer has generated a large amount of interest [13], not least because of its potential to render ineffective the RSA algorithm. Chuang and co-workers [2][4] have shown a way to implement this algorithm for N=15 with the NMR system: a sequence of steps whose core is two successive CNOT gates, $CNOT_{\text{AB}}$ and $CNOT_{\text{AC}}$. As our genetic algorithm has increased the efficiency of the implementation of CNOT from 5 rotations to 3, the efficiency of Shor’s has increased from 10 to 6. But can we do still better? We decided to simulate the product of the CNOT gates, which is the matrix

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

Where we implicitly label the rows and columns again by the values of bits A, B, and C, i.e, $|000>$, $|001>$, $|010>$, $|011>$, $|100>$, $|101>$, $|110>$ and $<000|$, $<001|$, $<010|$, $<011|$, $<100|$, $<101|$, $<110|$, $<111|$. The program found two solutions of only 5 rotations, which is an improvement of 50%. They are listed in Table 3.

|   | $R_{xA}(90)$ | $R_{xC}(250)$ | $R_{xCA}(160)$ | $R_{zxBC}(90)$ | $R_{xzAB}(260)$ |
|---|-------------|-------------|-------------|-------------|-------------|
| 1 | $R_{xzAB}(80)$ | $R_{xA}(80)$ | $R_{zB}(190)$ | $R_{xC}(105)$ | $R_{zB}(190)$ |

TABLE III: Sample pulse sequences found by the genetic algorithm, with 5 rotations, whose ordered product produces the product matrix $CNOT_{\text{AB}} CNOT_{\text{AC}}$, the core calculation of Shor’s algorithm for N=15. Each pulse corresponds to a rotation $R_{\vec{a}}(\alpha)$. 


VI. CONCLUSIONS AND FUTURE DIRECTIONS

We have devised a new algorithm to genetically determine the pulse sequence necessary to realize a given quantum gate. Our program largely simplifies the design of pulses and realizes a CNOT gate using a pulse sequence with just three rotations. This is an improvement in efficiency of 40%. The efficiency of the Shor’s algorithm implementation has been improved by 50% for the N=15 case.

It should be noted that while the pulse sequences found are shorter, they may not necessarily be easier to implement. Several of the sequences found require interactions of types, like xz, which may not be easily accessible experimentally. This would depend on the specific spin system being used.

It should also be noted that the product of the two CNOT gates forms the core of Shor’s algorithm only for the N=15 case. For a different factorization a completely different sequence of CNOT and Toffoli gates may be necessary; however, it only underscores the usefulness of an AI approach, that one would need to find different sequences of gates and therefore different sequences of pulses for each factorization calculation.

In practice, NMR quantum computing is more than simply designing a pulse sequence off line and then implementing it exactly as simulated. Any experimental setup inevitably contains factors and effects which no simulator, simplified as it must be, can take into consideration. Artificial intelligence techniques like the genetic algorithm are potentially powerful tools for the simplification of experimental quantum computing. The scientist constantly must twiddle with variables like the pulse widths to tune the system to the desired output; in principle, this could be done online with a genetic algorithm or neural network taking the scientist’s place to find the optimal values for the variables.

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