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Numerical algorithms for use in quantum information

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Abstract

Quantum information theory is the new field of physics and electrical engineering that arose from the application of fundamental physics concepts in communications and computing. In this paper, aiming to calculate some properties of quantum communication systems and the quantum entanglement measure, for $C^2 \otimes C^2$ systems, based on relative entropy, two numerical algorithms are presented. The first one is based on the codification of the possible solution in a binary string and in the application, in that string, of an assembly algorithm, such as one used in DNA construction. The second one is the construction of a genetic algorithm where a string of density matrices and quantum gates in the reproduction stage are used. Both algorithms are used in situations where the best solution needs to be found. Numerical simulations are presented and the advantages and disadvantages of the algorithms are discussed.

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1. Introduction

Quantum information is a new area in computing and communications allowing powerful applications, without classical counterparts, like teleportation and quantum cryptography [1,2]. In this wide research area we can find very interesting problems, two examples that will be addressed in this work are: (1) The calculation of the relative entropy of entanglement. (2) Given a 4×4 unitary matrix, what is the pair of qubits that should be used at the input in order to have the maximal entanglement of the output state? Both of these problems require the search of an optimal solution. In order to solve these kind of problems we can use traditional numerical methods, like gradients' method, or numerical intelligence, like genetic algorithm or neural networks. In this paper, two algorithms based on numerical intelligence, for optimization problems in quantum information theory are proposed. The first one uses an algorithm based on the classical algorithm of construction of DNA molecules [3] to find the disentangled state that minimizes the relative entropy. The second one is the construction of a genetic algorithm in which the chromosome is a

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string of density matrices and quantum gates are used in the reproduction stage. Both algorithms are described and numerical simulations are performed. At last, the advantages and disadvantages of the algorithms are discussed.

2. Quantum entanglement measure

As mentioned earlier, the quantum relative entropy will be used to calculate the entanglement, E. This measure is equal to the von Neumann reduced entropy when applied to pure states and it is an upper bound on the distillable entanglement. It was introduced by Vedral and Plenio [4–6] and, in a short way, it can be described as follows: The entanglement of a composite quantum state Γ , a positive Hermitian matrix with unit trace, can be given by the minimal distance between it and a disentangled state:

$$E(\Gamma) = \min_{\rho \in d} D(\Gamma \| \Phi), \tag{1}$$

where d is the set of all possible disentangled state. For the distance D, not necessarily a metric, we can use the quantum relative entropy, given by [4–6]:

$$D(\Gamma \| \Phi) \equiv S(\Gamma \| \Phi) = \operatorname{Tr}(\Gamma \ln \Gamma - \Gamma \ln \Phi), \tag{2}$$

where Tr denotes the trace operation. Since we must search for the solution among all possible disentangled states, we shall use the most general formula of a disentangled state. For a bipartite state, $C_2 \otimes C_2$, the most general formula is [6]

$$\Phi = \sum_{i=1}^{16} p_i \begin{bmatrix} c^2(\theta_i) & c(\theta_i)s(\theta_i)e^{(i\xi_i)} \\ c(\theta_i)s(\theta_i)e^{(-i\xi_i)} & s^2(\theta_i) \end{bmatrix} \otimes \begin{bmatrix} c^2(\varphi_i) & c(\varphi_i)s(\varphi_i)e^{(i\phi_i)} \\ c(\varphi_i)s(\varphi_i)e^{(-i\phi_i)} & s^2(\varphi_i) \end{bmatrix},$$
(3)

where c and s are abbreviations for cosine and sine functions, respectively. The coefficients p_i are given by

$$p_{i} = \left[\sin(\psi_{i-1})\prod_{j=i}^{15}\cos(\psi_{j})\right]^{2} \quad \text{with } \psi_{0} = \pi/2$$
(4)

and the sum of all p_i s is equal to unity.

3. An algorithm to calculate the minimal relative entropy – CAA

In this section, it is described the classical assembly algorithm, CAA, to implement the minimization procedure required by the relative entropy of entanglement. The algorithm is based on the assembly process that is a variation of the search process, where the objective is not to find the desired solution in a database but assembly it using the available building blocks. For example, for the DNA construction the building blocks are the nucleotide bases. These bases are available in the environment and one of them is chosen randomly, if the basis chosen is good for the solution it is maintained, otherwise, it is discarded and the random choice is repeated till the DNA molecule is complete [3]. For the minimization of the relative entropy, the corresponding of the DNA molecule is a binary string, which represents a codification of the solution, and the building blocks are the bits 0 and 1. If the solution is better with the *k*th bit of the string equal to *i* (0 or 1) it is maintained, otherwise it is inverted. To code the possible solution in a binary string, each angle in (3-4) is coded in a string of 10 bits, where the string 000 (hex) corresponds to the angle 0 rad and the string 3FF (hex) corresponds to the angle 2π rad. The possible solution is formed placing the 79

strings together, in sequence, and, therefore, it has 790 bits. With this arrangement, our space of solutions has 2^{790} elements, making a brute-force method impossible, at least with the velocity of the present computers. Suppose that we are searching for a disentangled state Φ whose distance from Γ is equal to *Dist*, $S(\Gamma || \Phi) = Dist$. The algorithm to search for Γ consists of generate one random solution (string of bits) and to test, for each bit of the string, what is its best value for the solution, 0 or 1. If $|Dist - S(\Gamma || \Phi_{k=0})| \leq |Dist - S(\Gamma || \Phi_{k=1})|$, where $\Phi_{k=0(1)}$ is the density matrix obtained with the *k*th bit set equal to 0(1), then the *k*th bit of the string is set equal to 0, otherwise, it is set equal to 1. After reach the last bit of the string, the first bit is tested again and the process is repeated till the accuracy and/or time requirements are reached. The commented algorithm is shown below:

$x = \text{rand_bit_sequence}(790)$	Generates a random bit string of 790 bits
For $n = 1$ to END	END controls the accuracy of the solution and time of processing
For $k = 1$ to 790	Each bit of the solution is tested
x(k) = 0	The k th bit is set equal to 0
$\Phi_0 = \text{state_disentangled}(x)$	The matrix form is recovered from the bit string, Eqs. (2)–(4)
$\operatorname{err} 0 = Dist - S(\Gamma \Phi_0) $	The error when the k th bit is set equal to 0 is calculated
x(k) = 1	The k th bit is set equal to 1
$\Phi_1 = \text{state_disentangled}(x)$	The matrix form is recovered from the bit string, Eqs. (2)–(4)
$\operatorname{err1} = Dist - S(\Gamma \Phi_0) $	The error when the <i>k</i> th bit is made equal to 1 is calculated
if $(err0 \leq err1)$	Compare the errors when the k th bit is set equal to 0 and 1
x(k) = 0	The value of the <i>k</i> th bit is set equal to 0 if $err0 \leq err1$
else	
x(k) = 1	The value of the <i>k</i> th bit is set equal to 1 if $err1 \leq err0$
end	
end	
end	
$\Phi = \text{state_disentangled}(x)$	The matrix form is recovered from the bit string, Eqs. (2)–(4)
$E = S(\Gamma \ \Phi)$	The entanglement is made equal to the distance between \varGamma and \varPhi

In order to calculate the relative entropy of entanglement we only set Dist = 0. The crucial point for the velocity of the algorithm is the calculation of the relative entropy, (2), since it requires the calculation of the logarithm of a matrix. Any algorithm to calculate the eigenvalues and eigenvectors of matrices can be used. The first term in the right-hand side of (2) is the von Neumann entropy of Γ and it can be calculated by

$$\operatorname{Tr}(\Gamma \ln \Gamma) = \sum_{i} \mu_{i} \log(\mu_{i}), \tag{5}$$

where μ_i are the eigenvalues of Γ . The logarithm of the density matrix in the second term of the right-hand side of (2) is calculated by

$$\ln(\Phi) = C \begin{bmatrix} \ln(\varepsilon_1) & 0 & 0\\ 0 & \ddots & 0\\ 0 & 0 & \ln(\varepsilon_4) \end{bmatrix} C^{-1},$$
(6)

where ε_{1-4} are the eigenvalues of Φ and C is the matrix whose columns are the corresponding eigenvectors of Φ . When using the software MATLAB, for example, this procedure is faster than to use the log *m* function.

4. Simulations using the CAA

In order to test the CAA we will calculate the entanglement of the Werner states [6,7], the family of states introduced by Horodecki [8], and some mixed states chosen randomly. The results are compared with the results obtained by the genetic algorithm, GA, presented in [9] and the entanglement of formation [10], since it is an upper bound for the entanglement of two-qubit bipartite states. The Werner states are defined by

$$W = F|\psi^{-}\rangle\langle\psi^{-}| + \frac{1-F}{3}(|\psi^{+}\rangle\langle\psi^{+}| + |\phi^{-}\rangle\langle\phi^{-}| + |\phi^{+}\rangle\langle\phi^{+}|),$$

$$\tag{7}$$

$$|\phi^{\pm}\rangle = (1/\sqrt{2})(|00\rangle \pm |11\rangle), \quad |\psi^{\pm}\rangle = (1/\sqrt{2})(|01\rangle \pm |10\rangle),$$
(8)

$$W = F \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.5 & -0.5 & 0 \\ 0 & -0.5 & 0.5 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \frac{1 - F}{3} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0.5 & 0.5 & 0 \\ 0 & 0.5 & 0.5 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$
(9)

where the states in (8) form the Bell's basis and the states $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$ form the standard basis. The parameter *F*, belonging to the interval [0.25, 1], is called fidelity. In Fig. 1 we can see the minimal relative entropy, S_g , for Werner states, with *F* varying in the interval [0.5, 1], obtained by the GA of [9], taking the average of the curves for 500, 700 and 1200 generations. The entanglement of Werner states using the CAA is presented in Fig. 2. In this figure, E_F (dashed line) is the entanglement of formation and *S* (dotted line) is the minimal relative entropy. Moreover, the minimal relative entropy is fitted by a polynomial of degree 5 (continuous line). The curves in Figs. 1 and 2 are in good agreement with the curve presented in [6]. Let us consider now the family of states introduced by Horodecki [8]:

$$\Gamma = q|\Psi_1\rangle\langle\Psi_1| + (1-q)|\Psi_2\rangle\langle\Psi_2|,\tag{10}$$



Fig. 1. Average curve (500, 700 and 1200 generations) for the entanglement of Werner states, using relative entropy (S_g) calculated by a GA, versus fidelity (F).



Fig. 2. Entanglement of Werner states versus fidelity (F): entanglement of formation (E_F , dashed line), relative entropy (S, dotted line) calculated by CAA and polynomial of degree 5 (continuous line).

$$|\Psi_1\rangle = a|00\rangle + \sqrt{1 - a^2}|11\rangle,\tag{11}$$

$$|\Psi_2\rangle = a|10\rangle + \sqrt{1 - a^2}|01\rangle,\tag{12}$$

where 0 < q, a < 1. The density matrix (10) in the standard basis is

$$\Gamma = \begin{bmatrix} qa^2 & 0 & 0 & qa\sqrt{1-a^2} \\ 0 & (1-q)(1-a^2) & (1-q)a\sqrt{1-a^2} & 0 \\ 0 & (1-q)a\sqrt{1-a^2} & (1-q)a^2 & 0 \\ qa\sqrt{1-a^2} & 0 & 0 & q(1-a^2) \end{bmatrix}.$$
(13)

In Fig. 3 it is shown the entanglement of formation (dashed line), E_F , the relative entropy of entanglement using the GA of [9] (small dots), S_g , and the relative entropy of entanglement based on the relative entropy using the CAA (large dots), S. In this simulation it was used a = 0.75 and q varying in the interval (0, 1). As can be seen in Fig. 3, the entanglement of formation and both relative entropies have the same behavior but, as expected, the former is larger than the others. Further, we can also see a good agreement between the curves obtained by the GA and the CAA. In the last simulation, shown in Fig. 4, 100 mixed states were choose randomly [11,12] and, for these states, the entanglement of formation, E_F , and relative entropy, S, were calculated using Wooter's equation and the CAA, respectively. As can be observed in Fig. 4, both, E_F and S, have roughly the same behavior. Furthermore, as expected the entanglement of formation is always larger than relative entropy (all points are below the line $E_F = S$).

5. Advantage and disadvantage of the CAA

The main advantage of the CAA is its very easy implementation despite the large number of parameters involved, 79. It is not as fast as the gradient method used in [6] but, for the same accuracy, it is faster than the genetic algorithm proposed in [9]. The CAA presented in Section 3 is a first-order algorithm, in the sense that only one bit is tested per time. Higher-order CAA algorithms can be easily implemented considering two or more bits per time. This can improve the accuracy but it will also increase the time of processing. For



Fig. 3. Entanglement of Horodecki states versus q (a = 0.75): entanglement of formation (E_F , dashed line), relative entropy (S_g , small dots) using GA and relative entropy (S, large dots) using CAA.



Fig. 4. Entanglement of formation ($E_{\rm F}$) versus relative entropy of entanglement (S) using CAA, for 100 mixed states chosen randomly.

two-qubit bipartite mixed states, the first-order CAA algorithm has shown good results. For pure states chosen randomly, in a not presented simulation, the maximal error $|S_{vN} - S|$ was close to 0.02, where S_{vN} is the von Neumann entropy of each partial state.

6. Genetic algorithm using density matrices and quantum gates

Genetic algorithm is a computational technique based on the evolution of the species [13]. A possible solution of the problem is coded in a binary string, called chromosome. An initial population of chromosomes is created (randomly) and processed by natural operators: natural selection (by tournament), reproduction (*crossover*: exchange of parts of the binary string between chromosomes; and *mutation*:

inversion of one of the bits of the binary string; for both, the position where the exchange and inversion takes place is chosen randomly) and evaluation of the fitness (how good the solution is). With these rules, the good features of one solution can be transmitted to the next generation of chromosomes and better solutions can be found. Natural selection and reproduction are probabilistic stages and, hence, a genetic algorithm is a random process. This technique has been used successfully in several kinds of problems, where the search of a minimal or a maximal value is necessary, even when local minima (or maximal) are present. A natural generalization of a binary string is a string of density matrices. Hence, it is possible to use the structure of a genetic algorithm having a sequence of density matrices as a chromosome and using quantum operations in the reproduction in order to find the best solution in some problems of quantum information. Let us suppose that we have a problem and its solution is a set of density matrices: $\rho_1\rho_2\rho_3\rho_4\rho_5\rho_6\rho_7\rho_8\rho_9\cdots\rho_N$. For example, given a unitary matrix (4 × 4) what are the two density matrices, $\rho_1\rho_2$, used at the input, that maximize the entanglement of the output total state? The first step to solve a given problem is creating, randomly, an initial population of chromosomes. This population will be used in two procedures: reproduction and measurement. The reproduction consists of two steps: mutation and crossover. Mutation consists in the application of a single-qubit gate (unitary matrix 2×2) in a density matrix chosen randomly in the string, as shown in Fig. 5. After the mutation, the kth density matrix of the chromosome, ρ_k , is changed by the density matrix $U\rho_k U^+$. Single-qubit gates like Not, Pauli's gates, Hadamard or any other 2×2 unitary gates can be tested. For the crossover, two-qubit gates like CNOT, SWAP or any other 4×4 unitary matrix can be used. The diagram in Fig. 6 shows the crossover process. As can be seen in Fig. 6, the *i*th density matrices of the chromosomes children are $Tr_b(U\rho_i^1 \otimes \rho_i^2 U^+)$ and $\operatorname{Tr}_a(U\rho_i^1\otimes\rho_i^2U^+)$ where ρ_i^1 and ρ_i^2 are the *i*th density matrices at the chromosomes parents.

The entropy of the states at the output of U operator shown in Fig. 6 is always equal or larger than the entropy of the input states. After several runs of the algorithm the partial output states tend to the maximally mixed state 1/2I, where I is the identity matrix. In this case the unitary operations become ineffective. In order to decrease the mean entropy of the solution and avoid the presence of several maximally mixed states in a chromosome, a measurement is performed in some states chosen randomly. The measurement is realized using the operators $M_1 = |0\rangle\langle 0|$ and $M_2 = |1\rangle\langle 1|$. If the state ρ is measured, then the possible states after the measurement are $\rho_1 = M_1\rho M_1^+/p_1$ and $\rho_2 = M_2\rho M_2^+/p_2$, where p_1 and p_2 are their probabilities of occurrence, given by $p_1 = \text{Tr}(M_1^+M_1\rho)$ and $p_2 = \text{Tr}(M_2^+M_2\rho)$. Hence, during the measurement stage, according to the result of a random choice obeying the values of the probabilities p_1 and p_2 , the state ρ is changed by ρ_1 or ρ_2 .



Fig. 5. Mutation in the QGA.



Fig. 6. Crossover in the QGA.

7. Simulations using the genetic algorithm with quantum gates

Given a unitary matrix U (4×4) what is the pair of density matrices that, when applied at the input, provides the total output state with maximal entanglement? Mathematically: given U which are ρ_a and ρ_b that maximizes $E_F[U\rho_a \otimes \rho_b)U^+]$, where E_F is the entanglement of formation? In order to solve this problem, a population of chromosomes of two density matrices was created. The crossover was performed applying the quantum gates CNOT and SWAP, while the mutation was performed applying the quantum gates Hadamard, Z and Not. The result was compared with a classical genetic algorithm used to solve the same problem. A hundred simulations using the same U matrix was performed and each simulation had 500 runs (generations). The unitary matrix used was chosen randomly from the ensemble of all unitary matrices with the natural Haar measure on the group U (4) [12]:

$$U = \begin{bmatrix} -0.12308344431670 - 0.21650705747456i & -0.93898257589479 + 0.10890455948802i \\ -0.05871429648377 + 0.70901965092325i & -0.18766503177980 + 0.01600920722546i \\ 0.55307259224604 + 0.353928146555348i & -0.21809264972165 + 0.02024356381571i \\ 0.01090951857969 + 0.02335557705909i & 0.11875617059208 - 0.09433889138392i \\ -0.13551362257148 - 0.07013508375196i & 0.11284621053497 + 0.09170354289840i \\ -0.02384441200722 - 0.04148307342058i & -0.59489237790140 + 0.31966070211182i \\ 0.02665771466643 - 0.02213183681701i & 0.05065731565752 - 0.71909996068915i \\ -0.98652282021661 & -0.00358235261998 - 0.05561058249039i \end{bmatrix}.$$
(14)

Both algorithms, hereafter named by CGA (binary chromosome) and QGA (using density matrices), reached good results, entanglement close to 1. In Fig. 7 it is shown the average value of the entanglement, over the 100 simulations, for each run. As can be seen, the QGA was always better than the CGA. Fig. 8 shows, for the same 100 simulations, in which runs the best result was found. The number of generations needed to find the best result was lower for the QGA.

Another problem where the QGA can be useful is in the calculation of the relative entropy of entanglement. In Fig. 9 it is shown the entanglement of formation and the relative entropy for 100 pure states chosen randomly. According to (3–4), a CGA was used to find the best set of p_i s and a QGA was used to



Fig. 7. Evolution of the average entanglement (over 100 simulations using the same unitary matrix) of the algorithms CGA and QGA for 500 generations.



Fig. 8. Generation in which the best result was found for CGA and QGA, for 100 simulations using the same unitary matrix.



Fig. 9. Entanglement of formation (E_F) versus relative entropy of entanglement (S) using QGA, for 100 pure states chosen randomly.

find the best set of density matrices. The stop criterion used was the error, $|E_f - S|$, lower than 0.01. As can be seen in Fig. 9, the results obtained by the QGA are in good agreement with the analytical result, since the points almost lie on the line $S = E_F$.

8. Advantage and disadvantage of using genetic algorithm with density matrices and quantum gates

The main disadvantage is the fact that we have to handle a vector of matrices instead of vector of integer numbers. Obviously this requires more computer memory and the algorithm is a bit more complex. On the other hand, no codification is needed and this simplifies the input and output of data. Another important point is that, in the simulations presented, the reproduction stage was very effective, since the best results were found in a low number of generations. Particularly, the mutation is very effective since it changes one density matrix for another one. This may not happen when we change only one bit in a whole binary string. For a codification decimal-to-binary, using 10 bits per parameter, if the mutation changes one of the least significant bits, it will be very few effective. Because of this, a high mutation rate (0.25) was used in the problems solved. At last, the algorithm can be easily modified to treat problems of higher dimension. All that we have to do is to change the dimension of the matrices of the chromosomes and the unitary matrices of the reproduction stage.

9. Conclusions

We explained, briefly, the quantum entanglement measure based on relative entropy. Following, we proposed an algorithm based on the classical algorithm of DNA construction as an alternative method to search the disentangled state that is in the minimal distance, in the sense explained in the text, from the state whose entanglement we want to measure. The computer program showed results that agree with results presented in the literature and it can be used as a tool for numerical studies of quantum communication systems, based on quantum entanglement, or to find properties of quantum entanglement. On the other hand, a genetic algorithm based on a string of density matrices and reproduction using quantum operations, QGA, opens new possibilities to solve problems of quantum information where the search of a minimal or a maximal value is necessary. The QGA implemented showed good precision, robustness and easy implementation. The main disadvantage is its low velocity, as happen for all kind of genetic algorithms. At last, working with Wooter's equations for the entanglement of formation the sum (3) can be reduced to four terms, reducing significantly the number of unknown parameters. However, this is true only for two-qubit bipartite states. There is still another possibility, once any two-qubit bipartite state has 15 unknown variables, it is possible to produce bipartite states varying only 27 parameters (3 are real numbers and 12 are complex numbers) and using the Wooter's equation (or even the Peres-Horodecki criterion) to discard the entangled states produced. However, since it is important to keep the structure of program easily modifiable for higher dimension and multipartite system, none of those possibilities was exploited here.

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