Lower bound on the number of Toffoli gates in a classical reversible circuit through quantum information concepts

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The question of finding a lower bound on the number of Toffoli gates in a classical reversible circuit is addressed. A method based on quantum information concepts is proposed. The method involves solely concepts from quantum information—there is no need for an actual physical quantum computer. The method is illustrated in the example of classical Shannon data compression.

In the past ten years we have witnessed the birth and explosive growth of the field of quantum information and computation. The main thrust of this new field is to study how quantum systems (such as quantum computers and quantum communication devices) can be used to solve certain mathematical problems or to improve communication capabilities. The crucial feature of this approach is that although the quantum systems themselves can be studied with pen and paper, gains are obtained only when the quantum systems are actually used in practice. The gains are due to new physical behavior unique to quantum systems and not shared by classical ones. In this Letter we take a different direction. We are not interested in using quantum systems, rather we want to use the concepts and insights gained in the study of quantum information for solving mathematical problems.

The problem we consider here concerns lower bounds on reversible classical circuits. Although reversible classical computation will probably not be realized in the foreseeable future (though increasing attention is being devoted to this issue), its study has yielded profound insights into the theory of complexity and into thermodynamics; see [1] for a review.

A reversible classical computation evaluates a function $f$ which takes $n$-bit input $\bar{x} \in \{0,1\}^n$ to $n$-bit output $f(\bar{x}) \in \{0,1\}^n$. Each particular input has its own unique output, thus $f$ is invertible. A classical circuit that evaluates $f$ can be reduced to a sequence of elementary reversible logical gates. Examples of reversible one-, two- and three-bit gates are NOT, Controlled-NOT (C-NOT) and Toffoli (Controlled-Controlled-NOT) gates. C-NOT applies NOT on the second bit only if the value of a first bit is 1; Toffoli applies NOT on the third bit only if the values of both first and second bit are 1. Reversible one- and two-bit gates do not constitute a universal set of gates. The Toffoli gate however is a universal basic gate for reversible classical computation, i.e., any reversible classical circuit can be built up from Toffoli gates [2].

Although we can build any reversible circuit out of Toffoli gates alone, an interesting conceptual question is to find the minimal number of Toffoli gates required if one allows for any number of one- and two-bit gates. The problem is interesting because Toffoli gates are, in a sense, the strongest reversible gates, and the minimal number needed tells us about the complexity of the computation itself. Furthermore, Toffoli gates require physical interaction between three bits, and are therefore more difficult to implement in practice than one- and two-bit gates, and it might be useful to minimize their use.

We formulate the problem as follows: given a reversible function $f(\bar{x})$ what is the minimum number of Toffoli gates needed to construct a circuit that will evaluate $f(\bar{x})$ for every $\bar{x}$ or only for a certain subset of $\bar{x}$.

As far as we know, a systematic approach to this problem does not exist. In this paper we use quantum information concepts to address it. In quantum information (computation) one classical bit can be encoded in two orthogonal states of a quantum system. The main idea of our method is to map the bits onto some special quantum states, and the action of the logic gates onto unitary transformations acting on these states. Then, the study of the properties of the unitary transformation that is associated with the classical reversible computation will give information about the classical circuit. The map is

$$
0 \rightarrow |0\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A |0\rangle_B + |1\rangle_A |1\rangle_B), \\
1 \rightarrow |1\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A |0\rangle_B - |1\rangle_A |1\rangle_B).
$$

(1)

The states $|0\rangle$ and $|1\rangle$, the “logical” qubits into which the classical bits are mapped, represent entangled states of two “constituent” qubits, denoted by the indexes $A$ and $B$. (Throughout this Letter we will use boldfaced fonts for the logical qubits and normal fonts for the constituent qubits.) Here the states $|0\rangle, |1\rangle$ are associated with orthogonal states of a two-level quantum system.

A string of $n$ bits is mapped on the associated quantum state of $n$ qubit pairs: $x_1 x_2 \ldots x_n \rightarrow |x_1\rangle |x_2\rangle \ldots |x_n\rangle$. Any computation $x_1 x_2 \ldots x_n \rightarrow f_1(\bar{x}) f_2(\bar{x}) \ldots f_n(\bar{x})$ is mapped on the same transformation of the corresponding quantum states $|x_1\rangle |x_2\rangle \ldots |x_n\rangle \rightarrow |f_1(\bar{x})\rangle |f_2(\bar{x})\rangle \ldots |f_n(\bar{x})\rangle$. Since we consider a reversible classical computation the corresponding quantum trans-
obtained by explicitly describing an implemention of $U$ calculating the amount of entanglement required to carry out this transformation cannot be constructed solely by two-bit gates. For example the $U_{C-NOT}$ gate can be built from local C-NOT gates:

$$U_{C-NOT} = \hat{U}_C^A \otimes \hat{U}_C^B$$

as can be easily checked explicitly. Here $\hat{U}_C^A$, $\hat{U}_C^B$ is a C-NOT gate acting on the A(B) constituent qubits in the opposite direction to normal, i.e. with the second bit as the control and the first bit as the target. (Such bi-lateral transformations were considered in [3] for the purpose of density matrix purification). That the quantum equivalent of any reversible one or two-bit gates can be constructed by a similar local bi-lateral transformation can be verified explicitly. Hence, any circuit built from one or two q-bit gates is local.

We can use this property of our mapping to analyze general circuits. Given a classical reversible computation we construct the associated quantum unitary transformation $U$; if $U$ is non-local, the corresponding classical transformation cannot be constructed solely by two-bit gates. Furthermore, the amount of non-locality in $U$ gives a lower bound on the number of Toffoli gates we need.

We define $E_U$, the amount of non-locality in $U$, as the minimum amount of entanglement required to implement $U$ using only local operations and classical communication (LOCC). We denote by $E_T$ the amount of non-locality of the quantum Toffoli gate $U_T$ (we estimate $E_T$ below).

One possible implementation of $U$ is to realize the classical circuit using the non-local quantum Toffoli gates (which cost $E_T$ ebits) and the local 2-bit and 1-bit gates. Hence $U$ can be implemented using $N_T E_T$ ebits. This yields the lower bound:

$$N_T \geq E_U / E_T.$$  \hspace{1cm} (3)

We now arrive at the crucial point of the method. To determine $E_U$ may be a very complicated task - it might actually be as complicated as directly determining the required number of Toffoli gates. On the other hand, it is easier to obtain bounds on $E_T$. Upper bounds are obtained by explicitly describing an implementation $U$ and calculating the amount of entanglement required to carry out this implementation using LOCC. Equation (3) is derived from just such an upper bound.

To obtain lower bounds on $E_U$ we apply $U$ on a test state $|\Psi_{in}^{test}\rangle$:

$$U|\Psi_{in}^{test}\rangle = |\Psi_{out}^{test}\rangle,$$  \hspace{1cm} (4)

where the test state can be any arbitrary superposition of basic input states $|x_1\rangle |x_2\rangle \ldots |x_n\rangle$. We denote the amount of non-locality between A and B possessed by $|\Psi_{in}^{test}\rangle$ and $|\Psi_{out}^{test}\rangle$ by $E_{in}^{test}$ and $E_{out}^{test}$ respectively, where $E = S(Tr_A|\Psi\rangle\langle\Psi|) = S(Tr_B|\Psi\rangle\langle\Psi|)$ is the von Neumann entropy of the reduced density matrix. (Applying $U$ to the test state and computing $E_{in}^{test}$ and $E_{out}^{test}$ is straightforward). The amount of non-locality in $U$ is not less than the entanglement difference between the two states:

$$E_U \geq |E_{in}^{test} - E_{out}^{test}|.$$  \hspace{1cm} (5)

How good are these bounds on $N_T$? First of all note that any test state leads to a lower bound. However, different test states may lead to different lower bounds because the non-local content of $U$ may not be realized in full when $U$ acts on a particular state. (For example, a test state of the form $|\Psi_{in}^{test}\rangle = |x_1\rangle |x_2\rangle \ldots |x_n\rangle$ is transformed into $|\Psi_{out}^{test}\rangle = |f_1\rangle |f_2\rangle \ldots |f_n\rangle$ and leads to no increase in entanglement). Good test states can be found by either trial and error, or by systematic optimization, although it is unclear whether the method of test states can provide tight bounds on $E_U$.

A more important restriction is due to the fact that Eq. (3) can be far from tight. This is because when implementing the classical circuit some of the Toffoli gates may increase the entanglement whereas others may decrease it. Thus there may be more efficient ways of implementing $U$ than realizing the classical circuit. For instance if $U$ acts on states composed of $n$ logical qubits, then $E_U \leq 2n$, because one can always implement $U$ by teleporting Alice’s qubits to Bob, letting Bob implement $U$ locally, and teleporting Alice’s qubits back to her. This shows that our method can only provide bounds that grow linearly in $n$. On the other hand it is known that for some problems of classical reversible computation the number of Toffoli gates grows exponentially and for these problems our method is very inefficient. Nevertheless we expect that in many cases the number of Toffoli gates will grow linearly with, or as a fractional power of, $n$. Bounding the actual power may give an interesting - indeed, sometimes fundamental - insight.

Let us now consider the case of the Toffoli gate itself and prove the basic fact that classical Toffoli gates cannot be built from reversible two-bit gates. We will do this by showing that under our map the quantum equivalent of the Toffoli gate is non-local. Specifically we will obtain the upper and lower bounds

$$1 \leq E_T \leq 2.$$  \hspace{1cm} (6)

Note that it is not essential for our method to find the exact value of $E_T$ since in general we are interested only
in the scaling of the number of Toffoli gates with the size of the problem.

The lower bound $E_T \geq 1$ is obtained by showing that under our map the quantum Toffoli gate is capable of producing at least one ebit of entanglement. Consider the test state

$$|\Psi_{in}^{test}\rangle = \frac{1}{2}(|0\rangle_1|0\rangle_2|0\rangle_3 + |1\rangle_1|0\rangle_2|0\rangle_3 + |0\rangle_1|1\rangle_2|0\rangle_3$$

$$-|1\rangle_1|1\rangle_2|1\rangle_3) = \frac{1}{\sqrt{2}}(|001\rangle_A|001\rangle_B + \frac{1}{2\sqrt{2}}(|000\rangle_A|000\rangle_B$$

$$+ |010\rangle_A|010\rangle_B + |100\rangle_A|100\rangle_B - |110\rangle_A|110\rangle_B),$$

where the third logical bit is the target of the Toffoli gate. After acting with $U_T$ on $|\Psi_{in}^{test}\rangle$ we obtain

$$|\Psi_{out}^{test}\rangle = \frac{1}{2}(|0\rangle_1|0\rangle_2|0\rangle_3 + |1\rangle_1|0\rangle_2|0\rangle_3 + |0\rangle_1|1\rangle_2|0\rangle_3$$

$$-|1\rangle_1|1\rangle_2|1\rangle_3) = \frac{1}{2\sqrt{2}}(|000\rangle_A|000\rangle_B + |001\rangle_A|001\rangle_B$$

$$+ |010\rangle_A|010\rangle_B + |100\rangle_A|100\rangle_B + |111\rangle_A|111\rangle_B$$

$$+ |011\rangle_A|011\rangle_B - |101\rangle_A|101\rangle_B - |110\rangle_A|110\rangle_B - |111\rangle_A|111\rangle_B).$$

The Schmidt coefficients are found to be $\alpha_1 = \{1, 1, 1, 1, 1, 1, 0, 0, 0\}$ and $\beta_1 = \{1, 1, 1, 1, 1, 1, 0, 0, 0\}$ respectively. Hence $E_{in}^{test} = 2$ ebits and $E_{out}^{test} = 3$ ebits and $E_T \geq 1$. (In passing we note that the quantum Toffoli gate cannot be implemented without classical communication: if such an implementation were possible it would violate relativistic causality).

To obtain the upper bound $E_T \leq 2$ we will describe explicitly a method for realising the quantum map of the Toffoli that requires 2 ebits. Consider three pairs of qubits on which we are going to apply $U_T$, where the states $|\Phi\rangle_1$, $|\Psi\rangle_2$ are control and $|\Theta\rangle_3$ is a target (see Fig. 1). It is convenient to analyze in parallel the cases where $|\Phi\rangle_1$ is $|0\rangle_1$ or $|1\rangle_1$. The two parties start by performing local Hadamard rotations $H_{A(B)}$ (acting as $H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, $H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$) of $A_1$ and $B_1$ of the first pair, obtaining

$$|0\rangle_1 \rightarrow |0'\rangle_1 = \frac{1}{\sqrt{2}}(|0\rangle_1^A|0\rangle_1^B + |1\rangle_1^A|1\rangle_1^B),$$

$$|1\rangle_1 \rightarrow |1'\rangle_1 = \frac{1}{\sqrt{2}}(|0\rangle_1^A|1\rangle_1^B + |1\rangle_1^A|0\rangle_1^B).$$

Then the parties proceed by performing local Toffoli gates on their particles, which can be written as

$$U^{A(B)}_T = |0\rangle_1|0\rangle_2 \otimes I_3 + |1\rangle_1|1\rangle_2 \otimes U_{23},$$

where $U_{23}$ is a local C-NOT between particles 3 and 2 (with particle 3 as the control and particles 2 as the target). As a result the initial states evolve to:

$$|0'\rangle_1|\Psi\rangle_2|\Theta\rangle_3 \rightarrow \frac{1}{\sqrt{2}}(|0\rangle_1^A|0\rangle_1^B + |1\rangle_1^A|1\rangle_1^B|U_{23}^A|U_{23}^B|\Psi\rangle_2|\Theta\rangle_3, $$

$$|1'\rangle_1|\Psi\rangle_2|\Theta\rangle_3 \rightarrow \frac{1}{\sqrt{2}}(|0\rangle_1^A|1\rangle_1^B|U_{23}^A|U_{23}^B|\Psi\rangle_2|\Theta\rangle_3. $$

Next they swap the states of $A_1$ and $B_1$. This operation utilizes two ebits and can be performed using two ordinary teleportations in both directions. This yields

$$\frac{1}{\sqrt{2}}(|0\rangle_1^A|0\rangle_1^B + |1\rangle_1^A|1\rangle_1^B|U_{23}^A|U_{23}^B|\Psi\rangle_2|\Theta\rangle_3, $$

$$\frac{1}{\sqrt{2}}(|0\rangle_1^A|0\rangle_1^B + |1\rangle_1^A|1\rangle_1^B|U_{23}^A|U_{23}^B|\Psi\rangle_2|\Theta\rangle_3. $$

Next, they perform $|\Phi\rangle$ again. The resulting states are

$$|0'\rangle_1|\Psi\rangle_2|\Theta\rangle_3$$

and

$$|1'\rangle_1|U_{23}^A|U_{23}^B|\Psi\rangle_2|\Theta\rangle_3. $$

Finally, they apply $H_A$ and $H_B$ again and obtain

$$|0\rangle_1|\Psi\rangle_2|\Theta\rangle_3$$

and

$$|1\rangle_1|U_{23}^A|U_{23}^B|\Psi\rangle_2|\Theta\rangle_3. $$

As we have already noted, two local C-NOT transformations are equivalent to a nonlocal C-NOT transformation. Thus, from the last expression it follows that a nonlocal C-NOT is applied on pairs 2 and 3 (with pair 2 as the control and pair 3 as the target) if and only if the state of the first pair is $|1\rangle$. Thus this protocol implements the nonlocal Toffoli gate and utilizes two ebits, which are needed to swap two states in the intermediate stage. Due to linearity of quantum mechanics all these arguments will hold also in the case of arbitrary superposition of initial states.

To conclude, from Eqs. (3) we obtain the following lower bound on the number $N_T$ of Toffoli gates required to carry out a computation

$$N_T \geq \frac{|E_{out}^{test} - E_{in}^{test}|}{2}. $$

We illustrate this result on the example of Shannon data compression. We were led to consider this particular example by our research in multi-particle entanglement compression [3]. In fact, this is how we discovered this method in the first place.
The method of classical compression of \( n \)-bit source-string of 0’s and 1’s, where \( p \) is the probability of each bit to be equal 1, is based on the fact that the most probable (typical) strings, generated by the source will contain \( np \) ones when \( n \) is large \( \left( \frac{n}{np} \right) \). If \( p \neq \frac{1}{2} \) then the Shannon entropy of the source \( H(p) \) is smaller than 1 and the number of typical strings, \( 2^{nH(p)} \), is less than the total number of strings \( 2^n \). Thus, a message generated by the source can be compressed to a shorter message.

We consider a ”Shannon compressor” - a classical reversible circuit which receives as input an \( n \) bit string which contains \( np \) ones (i.e. a typical string) and outputs a compressed version of the string in which only the first \( \log \left( \frac{n}{np} \right) \approx nH(p) \) bits carry information and the other \( n(1 - H(p)) \) redundant bits are set to some standard sequence, e.g. to all 0’s:

\[
x_1x_2...x_n \rightarrow f_1f_2...f_n0_{nH+1}...0_n. \tag{10}
\]

Our goal is to find a lower bound on the number of Toffoli gates needed to build the ”Shannon compressor”. We take the initial test state to be the uniform superposition of states with \( np \) ones:

\[
|\Psi_{test}^{in}\rangle = N \sum_{x_i \in \{0,1\}, \sum x_i = np} |x_1\rangle|x_2\rangle...|x_n\rangle,
\]

where \( N = \left( \frac{n}{np} \right)^{-1/2} \). The output state is:

\[
|\Psi_{test}^{out}\rangle = N \sum_{f_i \in \{0,1\}} |f_1\rangle|f_2\rangle...|f_n\rangle|0_{nH+1}\rangle...|0_n\rangle.
\]

For fixed value of \( p \) we can calculate the entanglement of \( |\Psi_{test}^{in}\rangle \) and \( |\Psi_{test}^{out}\rangle \). The entanglement \( E_{test}^{out} \) is easy to calculate: it equals the number of output redundant pairs, i.e. \( E_{test}^{out} = n(1 - H(p)) \). We have calculated \( E_{test}^{out} \) using a combination of analytical and numerical techniques which will be described in \ref{7}. Fig. \ref{fig:entanglement_vs_n} presents our results for \( p = 0.8 \). A linear dependance of \( E_{test}^{in} - E_{test}^{out} \) on \( n \) is obtained. Thus, the number of Toffoli gates needed to perform Shannon compression grows at least linearly with \( n \). For instance for \( p = 0.8 \) we need at least \( 0.2332n \) Toffoli gates. Inspired by our numerical result, Buhrman has found, using a completely different technique, an analytical proof of this lower bound \ref{7}.

In summary we have addressed the problem of evaluating the number of Toffoli gates needed to perform classical reversible computations. We have proposed a method based on quantum information concepts in which strings of classical bits are mapped into sequences of special non-local quantum states and classical reversible computations are mapped onto unitary transformations of these quantum states. The nonlocal properties of these transformations provide information about the classical reversible computation. In particular, if the unitary transformation is nonlocal then the corresponding classical reversible circuit cannot be built solely from one- and two-bit gates. The amount of non-locality possessed by the unitary transformation associated with any classical reversible computation provides a lower bound on the number of Toffoli gates needed for this computation.

As an example we considered classical Shannon compression and calculated the amount of non-locality of the associated unitary transformation. According to our numerical results, the lower bound on the number of Toffoli gates grows linearly with the size of the string \( n \). Thus quantum methods can provide fundamental insights about classical computation.

We hope that our approach may prove useful for other problems concerning classical reversible computation.

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