Towards optimization of quantum circuits

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Any unitary operation in quantum information processing can be implemented via a sequence of simpler steps - quantum gates. However, actual implementation of a quantum gate is always imperfect and takes a finite time. Therefore, seeking for a short sequence of gates - efficient quantum circuit for a given operation, is an important task. We contribute to this issue by proposing optimization of the well-known universal procedure proposed by Barenco et.al [1]. We also created a computer program which realizes both Barenco's decomposition and the proposed optimization. Furthermore, our optimization can be applied to any quantum circuit containing generalized Toffoli gates, including basic quantum gate circuits.

1 Introduction

Practical realization of quantum information processing requires ability to prepare a quantum system in a chosen state, to perform the desired operation on it and to read out the outcome via a measurement. These tasks can be carried out on a collection of two-level quantum systems - qubits. Since it is very difficult (practically impossible) to properly control simultaneous interaction among many qubits, the desired operation is usually performed as a sequence of simpler operations - quantum gates. The gate is accomplished by a temporal evolution of a system during which only few qubits interact simultaneously. The complicated operation is then built up by a sequence of quantum gates - quantum circuit containing experimentally feasible gates. In the quantum circuit model [2] the system of qubits is described as a closed quantum system. Therefore the time evolution is unitary, and each quantum gate is a unitary operator.

A set of (experimentally realizable) gates is called quantum gate library. In the rest of the paper we work with the basic-gate library [1], which contains all one qubit rotations and the Controlled-NOT (CNOT) gate. This library is universal in the sense that any unitary operation can be exactly achieved by a quantum circuit containing only finite number of gates from the basic-gate library. This universality was shown in 1995 constructively by Barenco et. al. [1]. Since that time, much effort has been made to propose a universal technique for finding an efficient quantum circuit for a general unitary operation. Many research groups focused on searching for an universal n-qubit circuit containing the lowest possible number of CNOT gates (see e.g. [3],[4],[5]). That means a circuit capable to achieve any unitary operator by tuning the circuit's one-qubit gates. The number of CNOT gates is important both, for its relation to the execution time of the circuit, and also from the point of view of complexity of its experimental implementation.

Shende, Markov and Bullock in [6] showed by dimension-counting arguments that universal n-qubit circuits have to contain at least $\frac{1}{4}(4^n - 3n - 1)$ CNOT gates. Although universal circuits with the lowest number of CNOTs are known for the special case of 2 qubits (see Refs. [6],[7],[8]), for higher number of qubits it remains

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an open problem. Furthermore, we have no guarantee that the tuning of single qubit gates corresponding to an operator realizable efficiently will lead to a straightforward simplification of the universal circuit. Therefore, universal n-qubit circuits often contain exponential number of CNOT gates (with respect to n) also for n-qubit operations realizable by a polynomial number of CNOTs. Intricacy of the simplification (optimization) of universal circuits for a chosen operator can be seen in the case of two qubit operators where the circuits with the lowest number of CNOT gates for a given operator were found by other means. On the other hand, for more than two qubits, the universal circuits are the only standard approach to find a quantum circuit for an arbitrary given operator.

In the present paper we show a simplification of the universal n-qubit circuit proposed by Barenco et.al. [1]. We tried to find, for an arbitrary given unitary operator, a quantum circuit containing the lowest possible number of CNOT gates. Barenco's decomposition utilizes the decomposition of unitary matrix into multiplication of a diagonal matrix and two-level matrices. After this decomposition one obtains a preliminary quantum circuit containing generalized Toffoli gates. These gates will be finally implemented by other constructions using basic quantum gates.

We examined some natural questions concerning generalized Toffoli gates and we propose an optimization algorithm which combines the found properties. This optimization algorithm can be applied to any quantum circuit containing generalized Toffoli gates including circuits containing basic gates. Hence, we can utilize our optimization in several stages of Barenco's decomposition. To perform Barenco's decomposition and the proposed optimization, we created a computer program (the program can be downloaded from www.quniverse.sk/people/sedlak/), which was used to estimate the efficiency of the optimization.

The rest of the paper is organized as follows. We start with a definition of the generalized Toffoli gate, which is followed by a brief sketch of Barenco's et. al. decomposition. More details about the procedure can be found in Refs. [1] and [10]. In section 3, we examine the properties of generalized Toffoli gates which are combined to create an optimization algorithm in section 4. The results obtained by the optimization algorithm are summarized in the section 5.

2 Preliminaries

2.1 Definition of Generalized Toffoli gate $\wedge_m(A)$

The generalized Toffoli gate $\wedge_m(A)$ is an $(m+1)$–qubit gate with m control qubits $j_1, \ldots, j_m$, and one target qubit j_0. The action of the gate on computational basis vectors reads:

$$|x_1, \ldots, x_{j_0}, \ldots, x_n\rangle \rightarrow |x_1, \ldots\rangle \otimes A^{x_{j_1} \wedge \ldots \wedge x_{j_m}} |x_{j_0}\rangle \otimes |\ldots, x_n\rangle, \tag{1}$$

where A is an operator (2x2 matrix) acting on one qubit. Thus the target qubit of computational–basis vector is affected by the operator A only if all control qubits are in the state $|1\rangle$.

2.2 Brief sketch of the Barenco's decomposition

The procedure can be divided into four steps:

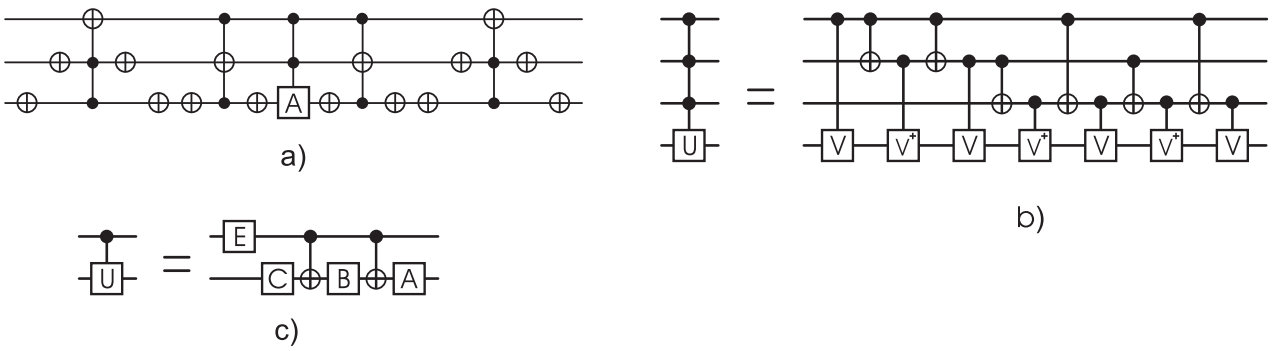


Figure 1: Examples from parts of A. Barenco et. al. decomposition.

- **Step 1 - QR decomposition.** Matrix of the chosen operator U is written as:

$$U = D^{-1}.T_{2,1}^{-1}.T_{3,1}^{-1}.T_{3,2}^{-1}\dots T_{2^n,2^n-2}^{-1}.T_{2^n,2^n-2}^{-1}, \tag{2}$$

  where D is a diagonal phase-matrix and T_{pq} are matrices acting nontrivially only in two–dimensional subspaces, which are given by pairs of computational–basis vectors.

- **Step 2 - Decomposition of matrices T_{pq} and D into generalized Toffoli gates.** General matrix T_{pq} operates on one pair of distinct computational–basis vectors. However, generalized Toffoli gate $\wedge_{n-1}(A)$ changes one pair of computational–basis vectors which differ only in one qubit. Therefore, we first use $\wedge_{n-1}(\sigma_x)$ gates and NOT gates to perform a permutation which takes the pair of computational–basis vectors given by T_{pq} to vectors differing in only one qubit. Then we apply the appropriate $\wedge_{n-1}(A)$ gate (together with some NOT gates) and finally undo the permutation. This allows to implement every matrix T_{pq}. To build the entries of diagonal matrix D, we use $\wedge_{n-1}(diag(.,.))$ gates surrounded by pairs of NOT gates. As an example, in Figure 1.a one can see the decomposition of matrix $T_{8,1}$ operating between vectors $|000\rangle$, $|111\rangle$.

- **Step 3 - Simplification of generalized Toffoli gates.** Gates $\wedge_{n-1}(A)$ are implemented by Controlled 1-qubit gates (less complicated generalized Toffoli gates $\wedge_1(V)$). As an example, Figure 1.b shows the simplification of the $\wedge_3(U)$ gate.

- **Step 4 - Decomposition of $\wedge_1(V)$ gates into basic quantum gates.** This step finishes the decomposition by using only basic quantum gates in the circuit. The example in Figure 1.c shows the worst case decomposition of the $\wedge_1(V)$ gate into four 1-qubit gates and two CNOT gates. For some $\wedge_1(V)$ fewer gates suffice.

3 Properties of generalized Toffoli gates

By renaming qubits, each pair of generalized Toffoli gates can be drawn and denoted as shown in Figure 2. Since every linear operator is fully defined through it's action on basis vectors, we will show equality of two

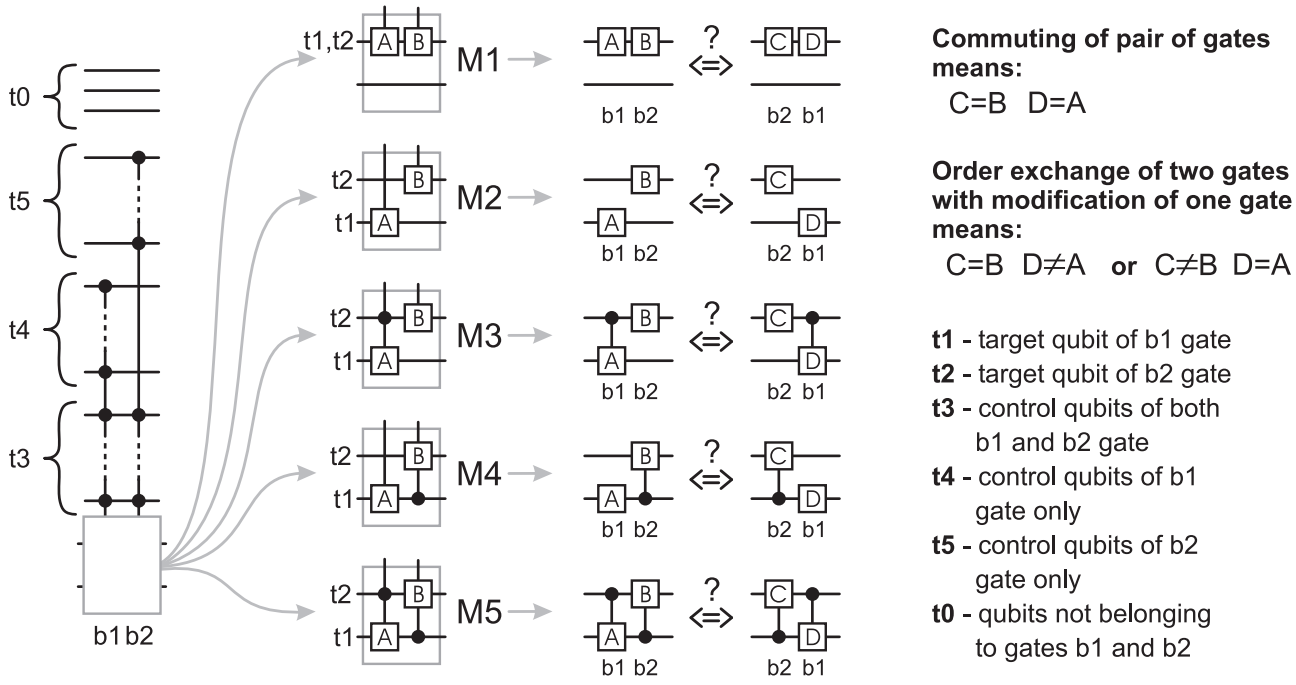


Figure 2: Examining properties of generalized Toffoli gates

operators via their action on computational–basis vectors. In what follows, the action of the gates b1,b2 is always described with respect to the computational basis.

3.1 Commutativity of pair of gates

Qubits of the type t0, t3, t4 and t5 (see definition in Figure 2) do not affect commutativity of the gates $b1 = \wedge_k(A)$ and $b2 = \wedge_l(B)$, because they control the action on qubits of the type t1, t2 in the same way in both orderings. From this property it follows that it suffices to examine the cases M1 - M5. In each of these cases the action of the gates on computational–basis vectors in both orderings yields four equations, which give constraints on entries of the 2x2 matrices A and B. In the case M1 it is obvious that the gates b1 and b2 commute if matrices A and B commute. In the case M2 the gates surely always commute. In the case M3 gates b1 and b2 commute if the matrix B is diagonal. In the case M4 the gates commute if the matrix A is diagonal. Thus we see that in the cases M3, M4 the gates b1 and b2 commute if diagonal matrix B (resp. A) is passing through the control qubit of neighbouring gate. The situation in the case M5 is a bit different, and finally it turns out that there are three ways how to fulfill the aforementioned equations: i) Both matrices A and B are diagonal, ii) $A = diag(e^{\imath\alpha}, 1)$ and no constraint on B, iii) $B = diag(e^{\imath\beta}, 1)$ and no constraint on A.

3.2 Exchange of two gates with modification of one gate

We consider only modification of one–qubit operator(2x2 matrix) from the definition of the generalized Toffoli gate (1). We can consider the gates as not commuting, because otherwise it follows from the unitarity that neither of the gates can be modified. Let's look at exchange of gates $b1 = \wedge_k(A)$, $b2 = \wedge_l(B)$ for gates

$b2n = \wedge_l(C)$, $b1 = \wedge_k(A)$. The previous argument tells us that $B \neq C$. If the gate b1 had qubits t4, then there would exist a computational–basis vector with at least one qubit t4 in the state $|0\rangle$ and all qubits t1, t3, t5 in state $|1\rangle$ which would reveal the difference between B and C, i.e. difference between the gates b2 and b2n. Thus if we want this exchange to be possible, the gate b1 must not involve qubits t4. Gates can have the other types of qubits, because they do not enable separate action of the gate b2, and b2n. Similarly, as in the case of the commutativity of gates, it remains to examine the cases M1, M3 – M5 and to solve similar equations. The results of these technical calculations are presented in Table 1. For the completeness, the conditions for

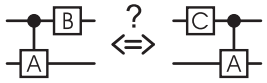
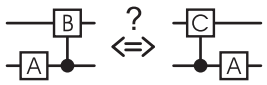
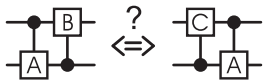
Case	Constraints on A, B	Corresponding C
M1 	no constraints	$C = A^{\dagger}.B.A$
M3 	$A = \begin{pmatrix} e^{\imath\varphi} & 0 \\ 0 & e^{\imath\varphi} \end{pmatrix}, B = \begin{pmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{pmatrix}$	$C = \begin{pmatrix} B_{00} & B_{01}e^{\imath\varphi} \\ B_{10}e^{-\imath\varphi} & B_{11} \end{pmatrix}$
M4 	It is not possible to fulfill the equations	
M5 	$A = \begin{pmatrix} e^{\imath\varphi_1} & 0 \\ 0 & e^{\imath\varphi_2} \end{pmatrix}, B = \begin{pmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{pmatrix}$	$C = \begin{pmatrix} B_{00} & B_{01}e^{\imath\varphi_2} \\ B_{10}e^{-\imath\varphi_2} & B_{11} \end{pmatrix}$

Table 1: Exchange of gates $b1 = \wedge_k(A)$, $b2 = \wedge_l(B)$ for gates $b1 = \wedge_l(C)$, $b2 = \wedge_k(A)$, which is possible only if there are no qubits t4 (see Figure 2).

exchange of gates $b1 = \wedge_k(A)$, $b2 = \wedge_l(B)$ for gates $b2 = \wedge_l(B)$, $b1n = \wedge_k(D)$ (completely analogous to the previous one) are summarized in Table 2.

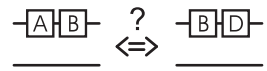
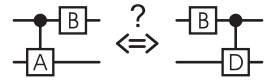
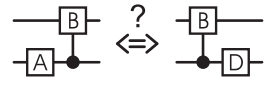
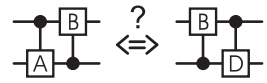
Case	Constraints on A, B	Corresponding D
M1 	no constraints	$D = B^{\dagger}.A.B$
M3 	It is not possible to fulfill the equations	
M4 	$B = \begin{pmatrix} e^{\imath\varphi} & 0 \\ 0 & e^{\imath\varphi} \end{pmatrix}, A = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix}$	$D = \begin{pmatrix} A_{00} & A_{01}e^{-\imath\varphi} \\ A_{10}e^{\imath\varphi} & A_{11} \end{pmatrix}$
M5 	$B = \begin{pmatrix} e^{\imath\varphi_1} & 0 \\ 0 & e^{\imath\varphi_2} \end{pmatrix}, A = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix}$	$D = \begin{pmatrix} A_{00} & A_{01}e^{-\imath\varphi_2} \\ A_{10}e^{\imath\varphi_2} & A_{11} \end{pmatrix}$

Table 2: Exchange of gates $b1 = \wedge_k(A)$, $b2 = \wedge_l(B)$ for gates $b1 = \wedge_l(B)$, $b2 = \wedge_k(D)$, which is possible only if there are no qubits t5(see Figure 2).

3.3 Conditions for merging two gates into one

First of all, we will examine the circumstances under which two generalized Toffoli gates form an identity. This will enable us to formulate conditions of merging two generalized Toffoli gates into one. We consider the gates $b1 = \wedge_k(A)$ and $b2 = \wedge_l(B)$, both different from the identity. The gates b1 and b2 must not involve the qubits t4 and t5, because they involve action of either the gate b1 or b2 on some subspace of the Hilbert space, where we see their difference from the identity. It suffices to examine the cases M1 – M5 (see Figure 2), because the gates b1 and b2 act nontrivially only on computational-basis vectors with all qubits of the type t3 in the state $|1\rangle$ and do not modify the qubits other than t1 and t2. So in each case we write down the transformation carried out by the gates b1, b2 and require it to be the identity. The resulting constraints on elements of the matrices A and B are presented in Table 3. Obviously, if we have two neighbouring generalized Toffoli gates

Case	Constraints on A, B
M1	$A.B = 1$
M2	$A = 1.e^{\imath\varphi}, B = 1.e^{-\imath\varphi}$
M3	$A = diag(e^{-\imath\varphi}, e^{-\imath\varphi}), B = diag(1, e^{\imath\varphi})$
M4	$A = diag(1, e^{\imath\varphi}), B = diag(e^{-\imath\varphi}, e^{-\imath\varphi})$
M5	$A = diag(1, e^{\imath\varphi}), B = diag(1, e^{-\imath\varphi})$

Table 3: Two generalized Toffoli gates $b1 = \wedge_k(A)$ and $b2 = \wedge_l(B)$ form the identity if they don't have qubits of the type t4, t5 (see Figure 2) and fulfill these constraints.

which form identity, we remove them from the circuit. Also, if we have two such neighbouring gates $b1 = \wedge_k(A)$ and $b2 = \wedge_l(B)$, which do not form the identity only because either of the matrices A or B does not fulfill the constraints from Table 3, it is possible to simplify the circuit. It suffices to suitably divide the gate b1 or b2 as shown in Figure 3a) and to remove the pair of gates forming the identity. This finally leads us to merging the two gates into one.

3.4 Exchange of two gates with help of one additional gate

During the Barenco's decomposition we work with circuits, where NOT gates act on control qubit of a neigbouring generalized Toffoli gate $\wedge_m(\sigma_X)$. These pairs of gates do not commute and their order cannot be exchanged even when we modify one of them. This is the reason why we generalized the well known CNOT identity shown in Figure 3.b. Our generalization is depicted in Figure 3.c, where matrices A, B are not arbitrary, but restricted as we will describe below. In the case there are no qubits t4, the requirement of equality of transformations performed by circuits from Figure 3.c only tells us that the matrix A must have vanishing diagonal elements. But if qubits t4 are present, then we must fulfill also the condition $B = B^\dagger$, because only gates b2, and b2n act on computational–basis vectors with at least one qubit t4 in the state $|0\rangle$.

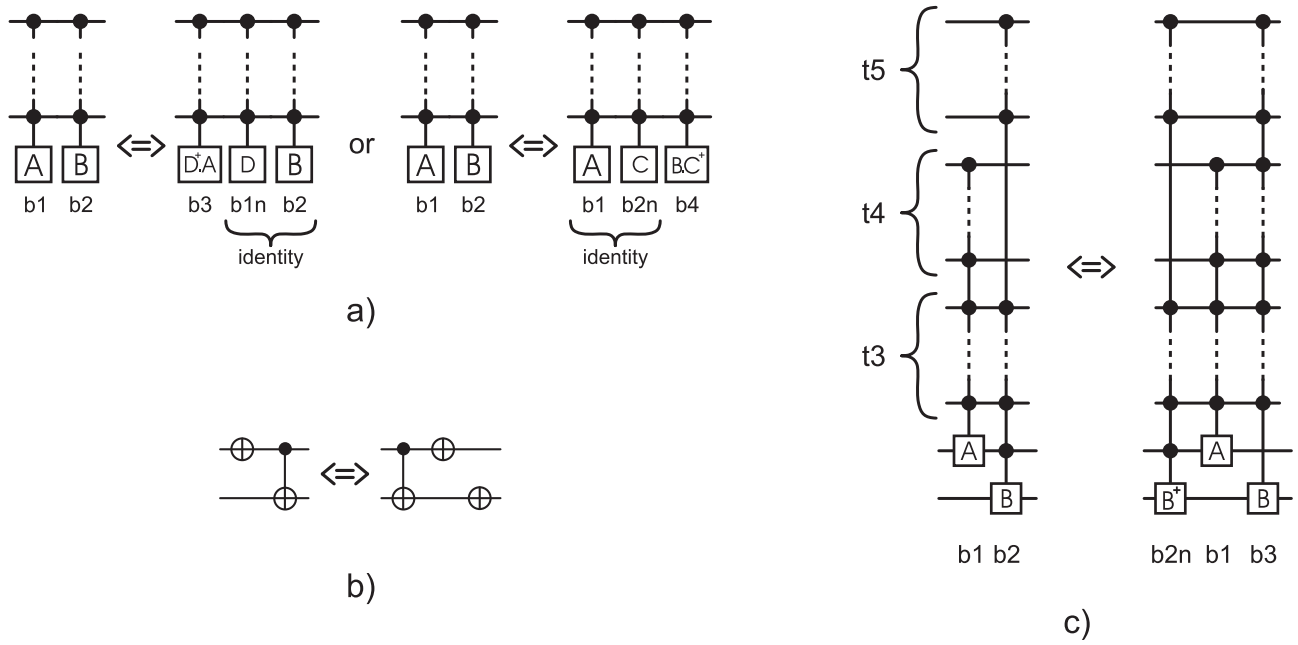


Figure 3: Circuit identities. The one from c) holds if matrix A has vanishing diagonal elements.

4 Optimization algorithm

The main idea of our approach to an optimization of quantum circuits containing generalized Toffoli gates is based on using the properties of $\wedge_k(.)$ gates described above. We drag the selected gate to the left until we merge it with a neighbouring gate or we are not able to drag it further. After that, we try the same to the right and then select another gate, and repeat the whole procedure. We do these steps, until the number of gates in the circuit is decreasing. We perform the dragging as follows: If gates commute we exchange them, otherwise we try to exchange them while modifying one of them. If it is not possible to use any of these options, we use exchange of two gates with the help of one additional gate, but only if there are no qubits t4 (see Figure 3.c). In addition, we use it only once before we succeed in merging the gates. This guarantees that the number of gates in the circuit will not grow. In case we use an exchange of two gates with the help of one additional gate, the number of gates in the circuit will be the same, but one generalized Toffoli gate will have less control qubits, which leads to less basic gates in subsequent steps of Barenco's decomposition.

5 Results

Due to the fact that Barenco's et. al. decomposition [1] leads to quantum circuits containing hundreds of gates even in the case of 3-qubit operations, it is not possible to perform the decomposition and the proposed optimization by hand. This reason stimulated us to create a computer program which realizes both Barenco's decomposition and optimization algorithm proposed in this paper. We can show analytically that, in the worst case of a 2-qubit operation, our optimization improves Barenco's decomposition to obtain circuit containing 10 CNOTs instead of 20 CNOTs. However, it is known that three CNOTs suffice to implement any 2-qubit

	Decomposition			
Number of qubits n	A. Barenco's	A.Barenco's **+ Our optimization**	NQ	CS
2	20	10	3	4
3	576	379	21	26
4	8000	6278	105	118
5	91520	76208	465	494

Table 4: The Number of CNOT gates in the circuits produced by various decompositions for the generic unitary operator.

operation, therefore we see that the proposed optimization is only a partial one. We examined the efficiency of our optimization for different subsets of operators acting on various numbers of qubits numerically. Our approach starts by randomly generating the operator with known upper bound on number of CNOTs needed for its implementation. This is done by computing the operation corresponding to a circuit build from that number of CNOTs and randomly picked 1-qubit gates. Then we decompose this operator by Barenco's et. al. decomposition with/without our optimization. We did this several times and evaluated the results. One would expect that the number of CNOTs in the circuit created by Barenco's decomposition with our optimization will strongly depend on the operator we are decomposing. We have found out that, except for the operators generated by circuits containing artificially chosen 1-qubit gates, each decomposition with the proposed optimization leads to a circuit with exactly the same number of CNOT gates (for the chosen number of qubits). This is caused by a redundancy in the blocks of generalized Toffoli gates, which our optimization is not able to remove in generic cases. For a more quantitative overview see Table 4. This table also shows comparison with the NQ [4] and the CS [5] decompositions, which are the best performing universal decompositions in the worst case of unitary operators. The asymptotic number of CNOT gates used by Barenco's decomposition to implement any n–qubit unitary is $O(n^3 4^n)$. Our numerical investigation suggests that the asymptotics may be the same also with using the proposed optimization. The NQ and CS decompositions are more efficient in general (creating roughly $1/2 \times 4^n$ CNOT gates in the worst case of a unitary operator), because their procedure contains steps which systematically remove a part of the redundancy introduced in previous steps.

6 Summary

Finding an efficient quantum circuit for a given n-qubit operation is an important task in the quantum circuit model of computation. Few universal procedures performing this task were proposed, but their efficiency (the number of created CNOT gates) is very often known only for the worst case of n-qubit unitary operators. However, it is believed that interesting operations might require only polynomial number of CNOT gates with respect to the number of qubits. Hence, it is very important to know the performance of such universal procedures on this kind of operators. Therefore, we proposed an optimization of the universal procedure by

Barenco et. al., and examined it's efficiency on the operators realizable by a small number of CNOT gates. To perform this task we created a computer program performing Barenco's procedure together with the proposed optimization. The results show that this procedure is in general not as efficient as the NQ and CS decompositions and still leaves some redundancy in the created circuit. On the other hand, our optimization is not restricted to be used only with Barenco's decompositon and can be aplied on any quantum circuit containing generalized Toffoli gates which include circuits containing basic quantum gates. This can be useful once we have some basic gate circuit corresponding to unitary operator we are decomposing. Our optimization can also be useful in situations when the quantum algorithm is given as a sequence of efficient sub-circuits performing the sub-tasks. A very similar idea to our optimization was proposed and extended to a slightly more general framework by D. Maslov, G. W. Dueck and D.M. Miller in [11]. It's not possible to correctly compare their numerical results to ours, since they work with different gate library containing one–qubit gates, controlled–NOT gate, and controlled-sqrt-of-NOT gate. But roughly we can say that the portion of the gates removed in the particular examples they present is very similar to the portion of gates our optimization removes in the case of Barenco's decomposition. All published optimizations of quantum circuits are based on exchanging sequences of gates for shorter ones doing precisely the same thing. To propose a better optimization strategies it seems that we probably need to understand more deeply what is computed in the considered part of the circuit.

ACKNOWLEDGMENTS

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[1] A. Barenco et.al.,"Elementary gates for quantum computation", Physical Review A, March 22, 1995 (AC5710)

[2] D. Deutsch, "Quantum computational networks", Proc. R. Soc. London A 425, 73 (1989).

[3] M. Möttönen, J. Vartiainen,V. Bergholm and M. Salomaa,"Quantum Circuits for General Multiqubit Gates", Physical Review Letters **93**, 130502 (2004)

[4] V. Shende, S. Bullock and I. Markov, "Synthesis of Quantum Logic Circuits", IEEE Transactions on Computer-Aided Design **25** no. 6 pg. 1000 (2006)

[5] V. Bergholm, J. Vartiainen, M. Möttönen and M.Salomaa, "Quantum circuits with uniformly controlled one-qubit gates", Phys. Rev. A **71**, 052330(2005)

[6] V. Shende, I. Markov and S. Bullock, "Minimal Universal Two-Qubit controlled-NOT-based Circuits", Physical Review A **69**, 062321 (2004)

[7] F. Vatan and C. Williams, "Optimal Quantum Circuits for General Two-Qubit Gates", Physical Review A **69**, 032315 (2004)

[8] G. Vidal and C.Dawson, "Universal quantum circuit for two-qubit transformations with three controlled-NOT gates", Phys. Rev. A **69**, 010301(2004)

[9] V. Shende, S. Bullock and I. Markov, "Recognizing small-circuit structure in two-qubit operators", Physical Review A **70**, 012310 (2004)

[10] M. Nielsen and I. Chuang, "Quantum Computation and Quantum Information", Cambridge University Press (2000)

[11] D. Maslov, G. W. Dueck and D.M. Miller, "Quantum Circuit Simplification and Level Compaction", Proceedings of the conference on Design, Automation and Test in Europe - Volume 2 1208 - 1213 (2005), arXiv:quant-ph/0604001 (2004)