Optimal quantum circuit synthesis from Controlled-$U$ gates

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From a geometric approach, we derive the minimum number of applications needed for an arbitrary Controlled-Unitary gate to construct a universal quantum circuit. A new analytic construction procedure is presented and shown to be either optimal or close to optimal. This result can be extended to improve the efficiency of universal quantum circuit construction from any entangling gate. Specifically, for both the Controlled-NOT and Double-CNOT gates, we develop simple analytic ways to construct universal quantum circuits with three applications, which is the least possible.

Construction of a universal quantum circuit, i.e., a circuit that can implement any arbitrary unitary operation, is of central importance in the physical applications of quantum computation and quantum information processing. Barenco \textit{et al.} proved the celebrated result that the Controlled-NOT (CNOT) gate supplemented with single-qubit rotations is universal, which has become a de facto standard model of quantum computation. The authors have previously provided a generality beyond the standard model, namely, an analytic direct route to simulate any arbitrary two-qubit unitary operation from whatever entangling gate arises naturally in the physical applications. An extremely important further issue is the minimum applications required for a given gate to implement a universal quantum circuit. In \textsuperscript{3}, we provided an upper bound for the applications of a given entangling gate, i.e., regardless of which two-qubit gate to be implemented, we can always construct a quantum circuit with applications of the given gate not exceeding that upper bound. However, this upper bound is not tight because it may be possible to achieve universality with less applications of the given gate. For example, it was recently shown that just three applications of the CNOT gate together with local gates are universal \textsuperscript{4,5}.

The main contribution of this paper is a more general result for optimality, namely, the minimum number of applications needed for an arbitrary Controlled-Unitary (Controlled-$U$) gate to construct a universal quantum circuit. We focus on the Controlled-$U$ gates because any entangling two-qubit gate can be used at most twice to simulate a Controlled-$U$ gate \textsuperscript{5}, and these gates are then widely used as basic building blocks to construct universal quantum circuits \textsuperscript{6,7}. Our main tool to derive the minimum upper bound for any Controlled-$U$ gate is the geometric representation of nonlocal two-qubit gates developed in \textsuperscript{8}, which provides an intuitive approach to this minimum upper bound. We also obtain a near optimal construction procedure that implements a universal quantum circuit with either minimum applications of the given Controlled-$U$ gate, or one application more than the minimum, depending on the given gate. Moreover, for the CNOT and Double-CNOT (DCNOT) gate \textsuperscript{9}, we provide a simple analytic solution to simulate any two-qubit gate with at most three applications.

Preliminaries

We first briefly review some relevant background knowledge \textsuperscript{3,6,10,11,12}. Two quantum gates $U, U_1 \in SU(4)$ are called locally equivalent if they differ only by local operations: $U = k_1 U_1 k_2$, where $k_1, k_2 \in SU(2) \otimes SU(2)$. Two gates are locally equivalent if and only if they have identical Makhlin’s local invariants \textsuperscript{10}. From the Cartan decomposition on $su(4)$, any two-qubit unitary operation $U \in SU(4)$ can be written as

$$U = k_1 A k_2 = k_1 \cdot e^{c_1 \gamma^1_1 \sigma^1_1} \cdot e^{c_2 \gamma^2_2 \sigma^2_2} \cdot e^{c_3 \gamma^3_3 \sigma^3_3} \cdot k_2, \quad (1)$$

where $\sigma^1_1, \sigma^2_2, \sigma^3_3 = \sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices, and $k_1, k_2 \in SU(2) \otimes SU(2)$ are local gates. In \textsuperscript{8} we found that the local equivalence classes of two-qubit gates are in one-to-one correspondence with the points in the tetrahedron $OA_1 A_2 A_3$ shown in Fig. 14 except on its base. For a general two-qubit gate $U$ in Eq. (1), this geometric representation defines a set of parameters $c_i$ satisfying $\pi - c_2 \geq c_1 \geq c_2 \geq c_3 \geq 0$.

Consider an arbitrary single-qubit gate $U = \exp(i n x \sigma_x + n y \sigma_y + n z \sigma_z)$. The Controlled-$U$ operation $U_f$ derived from this gate can be written as

$$U_f = (I \otimes e^{-\gamma \gamma^1_1 \sigma^1_1}) \cdot e^{\gamma \gamma^2_2 \sigma^2_2} \cdot (I \otimes U_1), \quad (2)$$

where $\gamma = \sqrt{n_x^2 + n_y^2 + n_z^2}$, and $U_1$ is a single-qubit gate given by Proposition 3 of \textsuperscript{8}. By definition, $e^{\gamma \gamma^1_1 \sigma^1_1}$ is locally equivalent to a Controlled-$U$ gate. Therefore, without loss of generality, we can use $U_f = e^{\gamma \gamma^2_2 \sigma^2_2}$ to denote any Controlled-$U$ gate. Since $e^{(\pi - \gamma) \gamma^1_1 \sigma^1_1}$ is locally equivalent to $e^{\gamma \gamma^2_2 \sigma^2_2}$, we always take the parameter $\gamma \in (0, \frac{\pi}{2})$. Specifically, when $\gamma = \frac{\pi}{2}$, $U_f$ is equal to the CNOT gate.

Minimum upper bound for any Controlled-$U$ gate

We have previously provided an upper bound for a given entangling gate to implement a universal quantum circuit \textsuperscript{5}. For a Controlled-$U$ gate $U_f = e^{\gamma \gamma^2_2 \sigma^2_2}$, this upper bound is $6\lceil \frac{\pi}{2\gamma} \rceil$, where the ceiling function $\lceil x \rceil$ is defined as a function that rounds $x$ to the nearest integer towards infinity. This upper bound is not a tight one. We now use a geometric approach to show that the minimum upper bound for a Controlled-$U$ gate is $5\lceil \frac{\pi}{2\gamma} \rceil$. 
We now study the set of all the nonlocal gates that can be implemented by $n$ applications of $U_f$. We will first analyze the case $n \geq 3$, and then the case $n = 2$. The following theorem shows that all gates that can be simulated by $n$ (≥3) applications of $U_f$ together with local gates constitute two congruent tetrahedra in the tetrahedron $OA_1A_2A_3$, which is the geometric representation of all the nonlocal two-qubit operations.

**Theorem 1** For a Controlled-$U$ gate $U_f = e^{iγ\mathbf{σ}^1\mathbf{σ}^2}$, every gate generated by $n$ (≥3) applications of $U_f$ together with local gates is locally equivalent to a gate $e^{c_1\mathbf{σ}^1\mathbf{σ}^2}e^{c_2\mathbf{σ}^2\mathbf{σ}^3}e^{c_3\mathbf{σ}^3\mathbf{σ}^1}$, with the parameters $c_j$ satisfying either $0 ≤ c_1 + c_2 + c_3 ≤ nγ$ or $c_1 - c_2 - c_3 ≥ π - nγ$.

The proof of this theorem is mathematically complex and will be presented elsewhere. Theorem 1 tells us that all the gates that can be generated by $n$ applications of $U_f$ with local gates can be represented by two tetrahedra $OB_1B_2B_3$ and $A_1C_1C_2C_3$ in Fig. 1. Note that these two tetrahedra are congruent, and the equations describing the faces $B_1B_2B_3$ and $C_1C_2C_3$ are $c_1 + c_2 + c_3 = nγ$ and $c_1 - c_2 - c_3 = π - nγ$, respectively. These two faces are the boundaries of all those points that can be generated by $n$ applications of $U_f$.

It is clear that as $n$ grows, each of these two tetrahedra $OB_1B_2B_3$ and $A_1C_1C_2C_3$ expands with consecutive faces of each tetrahedron remaining parallel. To obtain the minimum number of applications needed for a given Controlled-$U$ gate $U_f$ to implement any arbitrary two-qubit operation, we only need to find the least integer $n$ such that the union of the two tetrahedra $OB_1B_2B_3$ and $A_1C_1C_2C_3$ can cover the whole tetrahedron $OA_1A_2A_3$ as $n$ grows. Since this is convex, we can further restrict our attention to covering all its vertices. As seen from Fig. 1, this is equivalent to the condition that one of the two tetrahedra contains the point $A_3(\frac{π}{2}, \frac{π}{2}, \frac{π}{2})$, i.e., the SWAP gate. From Theorem 1 we only require that $nγ ≥ \frac{3π}{2}$, which leads to $n = \lceil \frac{3π}{2γ} \rceil$. This provides the minimum upper bound for an arbitrary Controlled-$U$ gate to implement a universal quantum circuit, and is summarized in the following theorem.

**Theorem 2** For an arbitrary Controlled-$U$ gate $U_f = e^{iγ\mathbf{σ}^1\mathbf{σ}^2}$, the minimum applications required to implement any arbitrary two-qubit gate together with local gates is $\lceil \frac{3π}{2γ} \rceil$.

In Fig. 2, the minimum upper bound for any Controlled-$U$ gate $U_f = e^{iγ\mathbf{σ}^1\mathbf{σ}^2}$ is shown as a function of $γ$, and depicted by thick lines. The thin lines represent the number of applications needed by a near optimal construction procedure we present below. Note that the single point at $γ = \frac{π}{2}$ with value 3 indicates that three applications of the CNOT gate with local gates suffice to implement any arbitrary two-qubit gate. The CNOT gate is therefore the most efficient gate among all the Controlled-$U$ gates.

*Near optimal universal quantum circuit*  In real physical applications, it is desirable to have a constructive procedure to implement a universal quantum circuit. At this time, there is no explicit way to construct a universal quantum circuit that exactly achieves the minimum upper bound for an arbitrary Controlled-$U$ gate $U_f$. However, we have found a construction procedure for a near optimal universal quantum circuit from an arbitrary Controlled-$U$ gate $U_f = e^{iγ\mathbf{σ}^1\mathbf{σ}^2}$ combined with loc-
The construction procedure therein takes at most \( \left\lceil \frac{\pi}{\gamma} \right\rceil \) times to simulate the third component \( e^{i\beta_1} \sigma_z \) of \( A \) (See Proposition 2, \( \text{[6]} \)). We do this in the following two steps:

1. Apply \( e^{i\beta_1} \sigma_z \) at most \( \left\lceil \frac{\pi}{\gamma} \right\rceil \) times to simulate the first two components \( e^{i\beta_2} \sigma_z \cdot e^{i\beta_2} \sigma_z \) of \( A \). (Theorem 1).

The first step follows directly from Proposition 2 in \( \text{[6]} \). The construction procedure therein takes at most \( \left\lceil \frac{\pi}{\gamma} \right\rceil \) applications when \( \gamma \in (0, \frac{\pi}{2}) \), and only two applications when \( \gamma = \frac{\pi}{2} \), i.e., for the CNOT gate. We therefore only need to realize the second step. The next theorem identifies all nonlocal gates that can be implemented by two Controlled-\( U \) gates together with local gates.

**Theorem 3** Given two Controlled-\( U \) gates \( e^{i\gamma_1} \sigma_z \) and \( e^{i\gamma_2} \sigma_z \) with \( \gamma_1, \gamma_2 \in (0, \frac{\pi}{2}) \), all the local equivalence classes of two-qubit gates that can be implemented by these two gates together with local gates can be described as \( e^{i\gamma_1} \sigma_z \cdot e^{i\gamma_2} \sigma_z \cdot e^{i\gamma_2} \sigma_z \cdot e^{i\gamma_2} \sigma_z \) with \( 0 \leq c_1 + c_2 \leq \gamma_1 + \gamma_2 \). Furthermore, we can implement such a gate by the following quantum circuit:

\[
\begin{array}{c}
\text{Apply } e^{i\gamma_1} \sigma_z \\
\text{then take } e^{i\gamma_2} \sigma_z \\
\text{and only those gates. This result was} \\
\text{also implied in } \text{[6]}. \\
\end{array}
\]

Since the second step of the procedure is indeed equivalent to implementing any gate in the triangle \( OA_1A_2 \), we can now realize it by using Theorem 1. From a given Controlled-\( U \) gate \( U_f = e^{i\gamma_1} \sigma_z \) by \( n \) applications of \( U_f \). We then take \( \gamma_1 = n \gamma \) and \( \gamma_2 = m \gamma \). From Theorem 1 to ensure that \( e^{i\gamma_1} \sigma_z \cdot e^{i\gamma_2} \sigma_z \cdot e^{i\gamma_2} \sigma_z \cdot e^{i\gamma_2} \sigma_z \) can simulate any gate in the triangle \( OA_1A_2 \), we only require that the shaded area in Fig. 3 covers the point \( A_2 \). This is equivalent to \( (m + n) \gamma \geq \pi \), whence \( m + n = \left\lceil \frac{\pi}{\gamma} \right\rceil \). We can therefore choose any positive integers \( m \) and \( n \), as long as they satisfy this equality. Moreover, the parameters \( \beta_1 \) and \( \beta_2 \) of the local gates can be determined by solving Eq. (3). Hence we can explicitly simulate any nonlocal gate \( e^{i\beta_1} \sigma_z \cdot e^{i\beta_2} \sigma_z \) by applying the Controlled-\( U \) gate \( U_f = e^{i\beta_1} \sigma_z \) at most \( \left\lceil \frac{\pi}{\gamma} \right\rceil \) times.

Combining these two steps together, for a given Controlled-\( U \) gate \( U_f = e^{i\beta_1} \sigma_z \), the constructive approach presented above needs at most \( \left\lceil \frac{\pi}{\gamma} \right\rceil + \left\lceil \frac{\pi}{\gamma} \right\rceil \) applications for the case \( \gamma \in (0, \frac{\pi}{2}) \), or 4 applications for the case \( \gamma = \frac{\pi}{2} \), to implement any arbitrary two-qubit operation. In Fig. 2 the upper bound of this construction procedure is shown as thin lines. It is evident that our procedure is near optimal — it implements a universal quantum circuit with either minimum possible applications of \( U_f \), or one more than the minimum.

In \( \text{[6]} \) we provided an upper bound of \( 6\left\lceil \frac{\pi}{\gamma} \right\rceil \) applications for an arbitrary Controlled-\( U \) gate \( U_f \). Since \( \left\lceil \frac{\pi}{\gamma} \right\rceil + \left\lceil \frac{\pi}{\gamma} \right\rceil \leq 6\left\lceil \frac{\pi}{\gamma} \right\rceil \), it is clear that the construction procedure presented here is more optimal. Furthermore, since \( U_f \) is a basic building block for implementing a universal quantum circuit from arbitrary entangling gate, we also obtain a much more efficient route to this more general goal. \( \text{[2, 3, 6, 7]} \).

**Universal quantum circuit from three CNOT or DC-NOT gates** The explicit construction procedure presented above requires four applications of the CNOT gate to implement any arbitrary two-qubit gate. From Theorem 1 we know that the minimum upper bound for the CNOT gate is three (see also Fig. 2). Since the CNOT
gate with local gates are widely adopted as the standard model of universal quantum computation, it is especially important to find an attractive construction with a minimum number of applications. Recent work has provided constructions with three applications of CNOT [4, 5]. We have found the following simple analytic route to construct a universal quantum circuit from three applications with three applications of CNOT [4, 5]. We then developed simple analytic ways for both the CNOT gate with local gates.

Proposition 1 The following quantum circuit is locally equivalent to a generic nonlocal gate $A = e^{-\frac{i}{\hbar} \sigma_1^x \sigma_2^x + \frac{i}{\hbar} \sigma_1^y \sigma_2^y} e^{-\frac{i}{\hbar} \sigma_1^z \sigma_2^z}$:

![Quantum Circuit Diagram]

Proof: By direct algebraic computation, we can show that Makhlin’s local invariants [10] of the above quantum circuit are identical to those of the nonlocal gate $A$ (See Eq. (25) in [3]). Therefore this quantum circuit implements the nonlocal gate $A$.

Moreover, we have a similar result for the DCNOT gate, which is defined as the quantum gate performing the operation: $|m\rangle \otimes |n\rangle \rightarrow |n\rangle \otimes |m \oplus n\rangle$ [8]. It is easy to prove that the DCNOT gate is locally equivalent to the gate $e^{-\frac{i}{\hbar} \sigma_1^x \sigma_2^x + \frac{i}{\hbar} \sigma_1^y \sigma_2^y} e^{-\frac{i}{\hbar} \sigma_1^z \sigma_2^z}$, which corresponds to $A_{2}(\frac{\pi}{2}, \frac{\pi}{2}, 0)$ in Fig. 1. Note that this is not a Controlled-U gate.

Proposition 2 The following quantum circuit is locally equivalent to a generic nonlocal gate $A = e^{-\frac{i}{\hbar} \sigma_1^x \sigma_2^x + \frac{i}{\hbar} \sigma_1^y \sigma_2^y} e^{-\frac{i}{\hbar} \sigma_1^z \sigma_2^z}$:

![Quantum Circuit Diagram]

This proposition can also be proved by direct algebraic computation of Makhlin’s invariants, as for Proposition 1.

Conclusion In summary, we have found the minimum upper bound to construct a universal quantum circuit from any Controlled-U gate together with local gates. This minimum upper bound depends only on the single Controlled-U parameter $\gamma$, as shown in Fig. 2. It shows that among all the Controlled-U gates, the CNOT gate is the most efficient, a fact not evident from the previous upper bound result in [3]. A new explicit construction of universal quantum circuits from a given Controlled-U gate was provided and shown to be close to optimal, i.e., it implements a universal quantum circuit with either minimum applications, or one more than the minimum. For the CNOT gate, this gives four applications, which is one more than optimal and than other recent results [4, 7]. We then developed simple analytic ways for both the CNOT and DCNOT (not a Controlled-U) gate to construct universal quantum circuits with exactly three applications, which is the least possible.

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APPENDIX. PROOF OF THEOREM

Proof: A general two-qubit quantum circuit that consists of two Controlled-\(U\) gates \(e^{\gamma_1 \frac{1}{2} \sigma_z^1 \sigma_z^2}\) and \(e^{\gamma_2 \frac{1}{2} \sigma_z^1 \sigma_z^2}\) together with local gates can be described as

\[
e^{\gamma_1 \frac{1}{2} \sigma_z^1 \sigma_z^2} \cdot (k_1 \otimes k_2) \cdot e^{\gamma_2 \frac{1}{2} \sigma_z^1 \sigma_z^2}.
\]

(A.4)

Recall that the local gates \(k_1\) and \(k_2\) can be written in Euler’s ZYZ decomposition as:

\[
k_1 = e^{\alpha_1 i \sigma_z} \cdot e^{\beta_1 i \sigma_x} \cdot e^{\gamma_1 i \sigma_z},
\]

\[
k_2 = e^{\alpha_2 i \sigma_z} \cdot e^{\beta_2 i \sigma_x} \cdot e^{\gamma_2 i \sigma_z}.
\]

(A.5)

Substituting Eq. (A.5) into Eq. (A.4), and taking into account the fact that \(\sigma_z^1\) and \(\sigma_z^2\) both commute with \(\sigma_z^1\sigma_z^2\), we obtain the following quantum circuit that is locally equivalent to Eq. (A.4):

We want to find all the nonlocal gates that can be generated by the above quantum circuit by tuning the parameters \(\beta_1\) and \(\beta_2\) of the local gates. Following the procedure in [14], we find that Makhlin’s local invariants for this quantum circuit are

\[
g_1 = \cos r_1 \cos r_2 - \sin r_1 \sin r_2 \cos \beta_1 \cos \beta_2,
\]

\[
g_2 = 0,
\]

\[
g_3 = 2(\cos \beta_1 + \cos \beta_2)^2 \sin^2 \gamma_1 \sin^2 \gamma_2 + 2 \cos \gamma_1 + 2 \cos \gamma_2 - 1
\]

\[
- 4 \cos \beta_1 \cos \beta_2 \sin \gamma_1 \sin \gamma_2 \cos (\gamma_1 - \gamma_2).
\]

(A.6)

From [8], we know that these Makhlin’s invariants can also be written as functions of the parameters \(c_j\) in the geometric representation:

\[
g_1 = \cos c_1 \cos c_2 \cos c_3,
\]

\[
g_2 = \sin c_1 \sin c_2 \sin c_3,
\]

\[
g_3 = 2(\cos^2 c_1 + \cos^2 c_2 + \cos^2 c_3) - 3.
\]

(A.7)

To find the corresponding point \([c_1, c_2, c_3]\) of this quantum circuit in the geometric representation, we only need to equate Eqs. (A.6) and (A.7), and thereby obtain:

\[
c_3 = 0,
\]

\[
\cos c_1 \cos c_2 = \cos r_1 \cos r_2 - \sin r_1 \sin r_2 \cos \beta_1 \cos \beta_2,
\]

\[
\cos^2 c_1 + \cos^2 c_2 = (\cos \beta_1 + \cos \beta_2)^2 \sin^2 \gamma_1 \sin^2 \gamma_2 + \cos^2 \gamma_1 + \cos^2 \gamma_2
\]

\[
- 2 \cos \beta_1 \cos \beta_2 \sin \gamma_1 \sin \gamma_2 \cos (\gamma_1 - \gamma_2).
\]

(A.8)

After some algebraic derivations, we obtain the following equations for the tuning parameters \(\beta_1\) and \(\beta_2\):

\[
\cos \beta_1 + \cos \beta_2 = \sqrt{\cos^2 c_1 + \cos^2 c_2 - \cos^2 \gamma_1 - \cos^2 \gamma_2 + 2(\cos \gamma_1 \cos \gamma_2 - \cos c_1 \cos c_2) \cos (\gamma_1 - \gamma_2)}
\]

\[
\cos \beta_1 \cos \beta_2 = \frac{\cos \gamma_1 \cos \gamma_2 - \cos c_1 \cos c_2}{\sin \gamma_1 \sin \gamma_2}
\]

(A.9)

It is clear that \(\cos \beta_1\) and \(\cos \beta_2\) can be viewed as two roots of the following quadratic equation:

\[
f(x) = \sin \gamma_1 \sin \gamma_2 x^2 + (\cos^2 c_1 + \cos^2 c_2 - \cos^2 \gamma_1 - \cos^2 \gamma_2
\]

\[
+ 2(\cos \gamma_1 \cos \gamma_2 - \cos c_1 \cos c_2) \cos (\gamma_1 - \gamma_2)) \frac{1}{2} x + \cos \gamma_1 \cos \gamma_2 - \cos c_1 \cos c_2 = 0
\]

(A.10)

Since \(\gamma_1, \gamma_2 \in (0, \frac{\pi}{2})\), we have \(\sin \gamma_1 \sin \gamma_2 > 0\). To guarantee the existence of two roots in the interval \([-1, 1]\), we need the following three conditions to be satisfied: \(f(1) \geq 0\), \(f(-1) \geq 0\), and \(\Delta \geq 0\), where \(\Delta\) is the discriminant of
quadratic equation. It is not hard to see that the first two conditions \( f(1) \geq 0 \) and \( f(-1) \geq 0 \) are equivalent to the following inequality:

\[
(sin \gamma_1 \sin \gamma_2 + \cos \gamma_1 \cos \gamma_2 - \cos c_1 \cos c_2)^2 \geq \cos^2 c_1 + \cos^2 c_2 - \cos^2 \gamma_1 - \cos^2 \gamma_2
+ 2(\cos \gamma_1 \cos \gamma_2 - \cos c_1 \cos c_2) \cos(\gamma_1 - \gamma_2). \tag{A.11}
\]

After some algebraic derivations, Eq. (A.11) can be simplified to \( \sin^2 c_1 \sin^2 c_2 \geq 0 \), which always holds true. Therefore, the conditions \( f(1) \geq 0 \) and \( f(-1) \geq 0 \) are automatically satisfied for any parameters \( \beta_1 \) and \( \beta_2 \). For the third condition, we have

\[
\Delta = (\cos c_1 \cos(\gamma_1 + \gamma_2) - \cos c_2)^2 - \sin^2(\gamma_1 + \gamma_2) \sin^2 c_1. \tag{A.12}
\]

To ensure \( \Delta \geq 0 \), we only need that \( 0 \leq c_1 + c_2 \leq \gamma_1 + \gamma_2 \). Therefore, all the local equivalence classes that can be generated by these two Controlled-\( U \) gates and local gates can be described as \( e^{c_1 \sigma_1^z} e^{c_2 \sigma_2^z} \), where \( 0 \leq c_1 + c_2 \leq \gamma_1 + \gamma_2 \).