Decomposition of quantum gates

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Abstract

A recurrence scheme is presented to decompose an n-qubit unitary gate to the product of no more than \(N(N-1)/2\) single qubit gates with small number of controls, where \(N = 2^n\). Detailed description of the recurrence steps and formulas for the number of \(k\)-controlled single qubit gates in the decomposition are given. Comparison of the result to a previous scheme is presented, and future research directions are discussed.

1 Introduction

The foundation of quantum computation [9] involves the encoding of computational tasks into the temporal evolution of a quantum system. A register of qubits, identical two-state quantum systems, is employed, and quantum algorithms can be described by unitary transformations and projective measurements acting on the state vector of the register. In this context, unitary matrices (transformations) are called quantum gates. Mathematically, a two-state quantum system has vector states \(|\psi\rangle\) in \(\mathbb{C}^2\), known as qubits. The two vectors in the standard basis \({|0\rangle, |1\rangle}\) for \(\mathbb{C}^2\) correspond to two physically measurable quantum states. An \(n\)-qubit system containing registers of \(n\)-qubits has vector states in the Euclidean space \(\mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2 = (\mathbb{C}^2)^{\otimes n}\) with basis vectors

\[|i_n \cdots i_1\rangle = |i_n\rangle \otimes \cdots \otimes |i_1\rangle, \quad i_1, \ldots, i_n \in \{0, 1\}\]

corresponding to the \(2^n\) physically measurable states.

For a single qubit, one can use quantum gates corresponding to unitary transformations to manipulate (transform) the qubit. For an \(n\)-qubit system with large \(n\), it is challenging and expensive to implement quantum gates. One often has to decompose a general quantum gate into the product of simple/elementary unitary gates which can be readily created physically. For a discussion on decomposing a unitary matrix into sets of elementary quantum gates, see, for example, [4], [5], [6], [10], and their references. By elementary linear algebra, it is known that every \(N \times N\) unitary matrix can be written as the product of no more than \(N(N-1)/2\) 2-level unitary matrices (Given’s transforms), i.e., unitary matrices obtained from the identity matrix by changing a \(2 \times 2\) principal submatrix. For example, if \(U \in M_4\) is unitary, then there are unitary matrices of the form

\[U_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad U_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad U_3 = \begin{pmatrix} * & * & 0 & 0 \\ * & * & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\]

so that \(U_1 U\) has a zero (4, 1) entry, \(U_2 U_1 U\) has zero entries at the (4, 1) and (3, 1) positions, and \(U_3 U_2 U_1 U\) has zero entries at the (4, 1), (3, 1), (2, 1) positions, and (1, 1) entry equal to one. Because \(U_3 U_2 U_1 U\) is unitary, it will be of the form \([1] \oplus \tilde{U}\) with \(\tilde{U} \in M_3\). We can then find unitary matrices of the form

\[U_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad U_5 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\]

so that \(U_5 U_4 U_3 U_2 U_1 U\) has the form \([I_2] \oplus V\) with \(V \in M_2\) and \(U_6 \cdots U_3 U_2 U_1 = I_4\). It follows that \(U = U_1^* \cdots U_6^*\).

In the context of quantum information science, not all 2-level unitary matrices are easy to implement. In this context, one considers matrices of sizes \(N = 2^n\) labeled by binary sequences \(i_n \cdots i_1 \in \{0, 1\}^n\) corresponding to the measurable quantum state \(|i_n \cdots i_1\rangle\). Then certain two level unitary matrices correspond to quantum operations
acting on the $j$th qubit provided the other qubits $|i_n\rangle, \ldots, |i_{j+1}\rangle, |i_{j-1}\rangle, \ldots, |i_1\rangle$ assume specified values in $\{0,1\}$. These are known as the fully controlled qubit gates. For example, when $n = 2$, we label the rows and columns of matrices by $00, 01, 10, 11$. There are four types of fully-controlled qubit gates:

$$(0V) : \begin{pmatrix} v_{11} & v_{12} & 0 & 0 \\ v_{21} & v_{22} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (1V) : \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & v_{11} & v_{12} & v_{13} \\ 0 & v_{21} & v_{22} & v_{23} \end{pmatrix}, \quad (V0) : \begin{pmatrix} v_{11} & 0 & v_{12} & 0 \\ 0 & 1 & 0 & 0 \\ 0 & v_{21} & v_{22} & 0 \\ 0 & v_{21} & v_{22} & 0 \end{pmatrix}, \quad (V1) : \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & v_{11} & 0 & v_{12} \\ 0 & v_{21} & 0 & v_{22} \\ 0 & v_{21} & 0 & v_{22} \end{pmatrix}$$

with the unitary $V = \begin{pmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{pmatrix} \in M_2$. In particular, a $(0V)$-gate corresponds to the unitary operator

$$a(00) + b(01) + c|01\rangle + d|11\rangle \mapsto |0\rangle V(a|0\rangle + b|1\rangle) + |1\rangle (c|0\rangle + d|1\rangle),$$

which will only change the part of the vector state with the first qubit equal to $|0\rangle$. Similarly, a $(1V)$-gate corresponds to the unitary operator

$$a(00) + b(01) + c|01\rangle + d|11\rangle \mapsto |0\rangle (a|0\rangle + b|1\rangle) + |1\rangle V(c|0\rangle + d|1\rangle),$$

which will only change the part of the vector state with the first qubit equal to $|1\rangle$. The $(V0)$-gate and $(V1)$-gate have the same physical interpretation. One can associate the 4 types of controlled qubit gates with the following circuit diagrams:

$$(0V) : \begin{array}{c} \bullet \\ \downarrow \end{array}, \quad (1V) : \begin{array}{c} \bullet \\ \downarrow \end{array}, \quad (V0) : \begin{array}{c} \bullet \\ \downarrow \end{array}, \quad (V1) : \begin{array}{c} \bullet \\ \downarrow \end{array}$$

For $n = 3$, we have fully-controlled qubit gates of the types:

$$(00V), (01V), (10V), (11V), (0V0), (0V1), (1V0), (1V1), (V00), (V01), (V10), (V11).$$

One easily extends this idea and notation to define fully-controlled gates acting on $n$-qubits.

In [14] (see also [8]), it was shown that one can decompose a quantum gate into the product of 2-level matrices corresponding to fully-controlled qubit gates. While fully-controlled qubit gates are relatively simple, it is still not easy to implement because the qubit gate $V$ can only act on the target bit after verifying that the other $(n-1)$-qubits satisfy the controlled bits. As mentioned in [14], in practice it is desirable to replace fully controlled qubit gates by qubits gates as few controls as possible. For example, when $n = 2$, the following types of unitary gates with no controls

$$(*V) : I_2 \otimes V = \begin{pmatrix} v_{11} & v_{12} & 0 & 0 \\ v_{21} & v_{22} & 0 & 0 \\ 0 & 0 & v_{11} & v_{12} \\ 0 & 0 & v_{21} & v_{22} \end{pmatrix}, \quad (V*) : V \otimes I_2 = \begin{pmatrix} v_{11} & v_{12} & 0 \\ v_{21} & v_{22} & 0 \\ 0 & 0 & v_{11} \\ 0 & 0 & v_{21} \end{pmatrix}$$

are easier to implement. Note that a $(0V)$-gate is applied on the left of a matrix $A \in M_4$, only rows $00$ and $01$ are affected. Similarly, a $(1V)$-gate will only affect the 10 and 11 gate of $A$. However, a $(*V)$-gate and $(V*)$-gate will affect all rows of $A$.

In general, we can consider a $(c_0c_{n-1} \cdots c_1)$-unitary gate with $c_0, \ldots, c_1 \in \{0,1,*\}$, where only one of the terms is $V$, and the number of terms in $\{0,1\}$ is the total number of controls. For example, a $(11*0V1)$-unitary gate acting on 6-qubit states has 4 controls, and the target qubit is the fifth one.

In [14], a recurrence scheme was proposed to decompose a unitary gate as the product of controlled qubit gates with small number of controls. The purpose of this paper is to present another simple recurrence scheme, which provide an alternative choice for implementation. Moreover, the ideas and techniques in the construction may be helpful for further research in this and related problems.

Our paper is organized as follows. In Section 2, we will illustrate our scheme for the 2-qubit and 3-qubit case, and discuss how it can be extended. In Section 3, we present the general scheme with detailed description of the implementation steps and explanation of their validity. In Section 4, we obtain formulas for the number of $k$-controlled single qubit gates in the decomposition and compare our results to those in scheme in [14]. Concluding remarks and future research directions are mentioned in Section 5.
2 Two-qubit and Three-qubit cases

For an \( n \)-qubit unitary gate \( U \in M_N \) with \( N = 2^n \), we will describe a recurrence scheme for generating controlled single qubit unitary gates \( U_1, \ldots, U_r \) with \( r \leq N(N - 1)/2 \) such that \( U_r \cdots U_1 U = I_N \). Consequently, \( U = U_1^r \cdots U_1^1 \).

Our scheme is done as follows. Assume we have the reduction scheme for the \((n - 1)\)-qubit case.

**Step 1** Partition \( U \in M_n \) into a \( 2 \times 2 \) block matrix with each block lying in \( M_{N/2} \).

**Step 2** Use the scheme of the \((n - 1)\)-qubit case to help reduce \( U \) to the form \( I_{N/2} \oplus \tilde{U} \) with \( \tilde{U} \in M_{N/2} \).

**Step 3** Apply the scheme of the \((n - 1)\)-qubit case to transform \( \tilde{U} \) to \( I_{N/2} \).

In **Step 2**, we need to eliminate the nonzero off-diagonal entries of \( U \) for the first \( N/2 \) columns. We will do these elimination column by column. In each column, we first eliminate the off-diagonal entries with row indices smaller than \( N/2 + 1 \) using the scheme in the \((n - 1)\)-qubit case. Then we again use the elimination schemes of lower dimension cases to eliminate the entries with row indices larger than \( N/2 \).

**The two-qubit gate.**

In the following tables, we indicate the order of the entries to be eliminated in our scheme, and also the \((c_2c_1)\)-gates used to do the elimination.

**Column 1.**

| entries | (2,1) | (4,1) | (3,1) |
|---------|-------|-------|-------|
| gates   | \(*V*)| \(V\) | \(V\) | \(V\) |

**Column 2.**

| entries | (3,2) | (4,2) |
|---------|-------|-------|
| gates   | \(V\) | \(V\) |

**Column 3.**

| entries | (4,3) |
|---------|-------|
| gates   | \(V\) |

Here we first eliminate the \((2,1)\) entry as in the 1-qubit case. In a similar manner, annihilate the \((4,1)\) entry, treating it as the second entry of the lower left half of the first column. To keep the \((2,1)\) entry zero, we use a gate with a 1 - control in the leftmost bit. Finally we annihilate the \((3,1)\) entry with the help of the \((1,1)\) entry. In this case, we can use a control-free gate to do so. At this point, the current form of the matrix is \([1] \oplus U'\), where \(U' \in M_4\).

Then we move to the second column. We adapt the procedure of eliminating the \((4,1)\) and \((3,1)\) entries to eliminate the \((3,2)\) and \((4,2)\) entries. The gates used must not change the zero entries in the first column. After this, the matrix takes the form \(I_2 \oplus U_1\) with \(U_1 \in M_2\). We can deal with the matrix \(U_1\) as in the 1-qubit case using a \((1V)\)-gate so that the first two rows will not be affected.

**The three qubit case.**

In this case, we have 3 types of unitary gates with no control:

\((**V), (**V), (V**);\)

12 types of unitary gates with 1 control (0 or 1) and 1 target qubit:

\((0*V), (1*V), (0**V), (1**V), (**0V), (**1V), (V0*), (V1*), (**0V), (**1V), (V0), (V1);\)

and 12 types of unitary gates with 2 controls and 1 target qubit:

\((00V), (01V), (10V), (11V), (0V0), (0V1), (1V0), (1V1), (V00), (V01), (V10), (V11).\)

We execute the reduction scheme for three qubit gates as follows.
Column 1.

| entries | (2,1) | (4,1) | (3,1) | (6,1) | (8,1) | (7,1) | (5,1) |
|---------|-------|-------|-------|-------|-------|-------|-------|
| gates   | (V*)  | (V*)  | (V*)  | (V*)  | (V*)  | (V*)  | (V*)  |

Column 2.

| entries | (3,2) | (4,2) | (5,2) | (7,2) | (8,2) | (6,2) |
|---------|-------|-------|-------|-------|-------|-------|
| gates   | (V*)  | (V*)  | (V*)  | (V*)  | (V*)  | (V*)  |

Column 3.

| entries | (4,3) | (8,3) | (6,3) | (5,3) | (7,3) |
|---------|-------|-------|-------|-------|-------|
| gates   | (V*)  | (V*)  | (V*)  | (V*)  | (V*)  |

Column 4.

| entries | (7,4) | (5,4) | (6,4) | (8,4) |
|---------|-------|-------|-------|-------|
| gates   | (V*)  | (V*)  | (V*)  | (V*)  |

Column 5.

| entries | (6,5) | (8,5) | (7,5) |
|---------|-------|-------|-------|
| gates   | (V*)  | (V*)  | (V*)  |

Column 6.

| entries | (7,6) | (8,6) |
|---------|-------|-------|
| gates   | (V*)  | (V*)  |

Column 7.

| entries | (8,7) |
|---------|-------|
| gates   | (V*)  |

Remarks 2.1. Here we give some remarks about the reduction of a 3-qubit unitary gate to help illustrate our recurrence scheme and how it can be extended. The comments are numbered according to the major steps 1–3 of our scheme described in the beginning of this Section.

Step 1 We partition the $8 \times 8$ unitary matrix into 2-by-2 block matrix so that each block is $4 \times 4$.

Step 2 We consider Column 1, 2, 3, 4,

For Column 1, the elimination of $(2,1), (4,1), (3,1)$ entries will be done as in the $4 \times 4$ (2-qubit) case by changing the 2-qubit $(c_2c_1)$-gates to $(c_2c_1)$-gates in these steps.

We then annihilate the $(6,1), (8,1)$ and $(7,1)$ entries the same way we annihilated the $(2,1), (4,1)$ and $(3,1)$ entries by treating the lower half as a $4 \times 4$ matrix. However, we have to ensure that the $(1,1)$ entry will not interact with the zero entries at the $(2,1), (3,1), (4,1)$ positions in these steps. So, we adapt the 2-qubit $(c_2c_1)$-gates to $(c_2c_1)$-gates, we will use the following rule:

$$\text{let } c_3 = 1 \text{ if } (c_2c_1) \text{ is } (V) \text{ or } (V); \text{ otherwise, let } c_3 = \ast.$$

So, a $(1 \ast V)$-gate can be used to annihilate the $(6,1)$ entry, a $(1V)$-gate can be used to annihilate the $(8,1)$ entry and a $(V\ast)$-gate to annihilate the $(7,1)$ entry. Finally, we can apply a $(V \ast \ast)$-gate to eliminate the the $(5,1)$ entry using the $(1,1)$ entry.

Note that the $(c_2c_1)$-gates used in the Column 1 satisfy $c_3, c_2, c_1 \in \{\ast, 1, V\}$ with $c_1 \neq 1$. This property will hold for the general case.

Once all off-diagonal entries in Column 1 are annihilated, we obtain a matrix of the form $[1] \oplus U'$, where $U' \in M_7$. We can proceed to Column 2.

For Column 2, we can annihilate the $(3,2)$ and $(4,2)$ entries using the scheme for annihilating the second column in the $4 \times 4$ case by changing the 2-qubit $(c_2c_1)$-gates to $(c_2c_1)$-gates in these steps.

Next, we adapt the scheme of annihilating the $(6,1), (8,1), (7,1), (5,1)$ entries to annihilate the lower half entries of the second column. Note that it is imperative that the $(6,2)$ entry be the last entry to be annihilated since it is the only entry in the lower half of the column that can be annihilated using the $(2,2)$ entry. In view of this, we will change the order of annihilation of the entries to:

$$(5,2), (7,2), (8,2), (6,2).$$
If we identify \((1, 2, \ldots, 8)\) with the binary sequences \((000, 001, \ldots, 111)\), then
\[(6, 8, 7, 5)\) corresponds to \((101, 111, 110, 100)\), and \((5, 7, 8, 6)\) corresponds to \((100, 110, 111, 101)\).

The conversion can be easily realized by

\[
(100, 110, 111, 101) = (101, 111, 110, 100) \oplus (001, 001, 001, 001) = (101 \oplus 001, 111 \oplus 001, 110 \oplus 001, 100 \oplus 001),
\]

where \(i_3j_2i_1 \oplus j_3j_2j_1\) is an entry-wise addition such that \(0 \oplus 0 = 1 \oplus 1 = 0 \oplus 1 = 1 \oplus 0 = 1\). Note that we will use a similar conversion for columns 3 and 4.

We also need to modify the \((c_3c_2c_1)\)-gates used for the annihilation of the \((6, 1), (8, 1), (7, 1)\) entries to annihilate the \((5, 2), (7, 2), (8, 2)\) entries. To accommodate the change in the order of annihilation, one must modify any control found in \(c_1\). We also have to prevent the \((1, 1)\) entries interacting with the \((2, 1), (3, 1), (4, 1)\) entries, and also prevent the \((2, 2)\) entries interacting with the \((3, 2)\) and \((4, 2)\) entries. This can be done by making sure that at least one of \(c_2\) and \(c_3\) is equal to 1. Thus, we modify \((c_3c_2c_1)\) by the following rules:

\[
\text{change } c_3 \text{ to 1 if none of } c_2, c_3 \text{ is 1; change } c_1 \text{ to 0 if } c_1 = 1.
\]

However, one sees that applying these rules will not change the \((c_3c_2c_1)\)-gates in view of the fact that \(c_1 \neq 1\). Hence we can use exactly the same set of \((c_3c_2c_1)\)-gates to eliminate the \((5, 2), (7, 2), (8, 2)\) entries of Column 2.\(^1\) Thus, we will use \((1 \ast V), (\ast 1V), (1V \ast)\) gates to annihilate the \((5, 2), (7, 2)\) and \((8, 2)\) entries, respectively.

To annihilate the \((6, 2)\) entry, we need to utilize the nonzero \((2, 2)\) entry. These two entries correspond to rows 101 and 001. This means that the target bit of the gate we need is the third bit (leftmost). Because we do not want to change the form of the upper half of the first column, we need to make sure that the target gate is not satisfied by 000 but is satisfied by 001 and 101. Thus, we use a \((V \ast 1)\)-gate. Once this is done, the matrix is now reduced to the form \(I_2 \oplus V''\) where \(V'' \in M_6\).

**For Column 3**, the \((4, 3)\) entry is annihilated using the scheme for the third column of the \(4 \times 4\) case.

Similar to the case in Column 2, we can adapt the scheme of eliminating the \((6, 1), (8, 1), (7, 1), (5, 1)\) entries to annihilate the \((8, 3), (6, 3), (5, 3), (7, 3)\) entries. The conversion \((6, 8, 7, 5)\) to \((8, 6, 5, 7)\) is done by performing

\[
(111, 101, 100, 110) = (101, 111, 110, 100) \oplus (010, 010, 010, 010)
\]

using the binary number correspondence of the indices.

We also need to modify the \((c_3c_2c_1)\)-gates used for the annihilation of the \((6, 1), (8, 1), (7, 1)\) entries to annihilate the \((8, 3), (6, 3), (5, 3), (7, 3)\) entries. In these steps, we have to prevent the \((1, 1)\) entries interacting with the \((2, 1), (3, 1), (4, 1)\) entries, the \((2, 2)\) entries interacting with the \((3, 2), (4, 2)\) entries, and the \((3, 3)\) entry interacting with the \((4, 3)\) entry. One can do this by adjusting the \(c_3\) and \(c_2\) values in the \((c_3c_2c_1)\)-gates used for the annihilation of the \((6, 1), (8, 1), (7, 1), (5, 1)\) entries by the following rules:

\[
\text{change } c_3 \text{ to 1 if } c_3 \text{ is not 1; change } c_2 \text{ to 0 if } c_2 = 1.
\]

Since \(c_3 = 1\), for \(i = 1, 2, 3, 4\), the \((i, i)\) entry will not interact with other \((k, i)\) entries for \(1 \leq k \leq 4\) and \(k \neq i\). Note that a \((c_3c_2c_1)\)-gate corresponds to a unitary matrix \(\tilde{V} \in M_8\). Changing a control bit in the position of \(c_2\) corresponds to changing \(\tilde{V}\) by a permutation similarity \(P\tilde{V}P^t\), where \(P\) corresponds to the change of the basis \([000, \ldots, 111]\) to \([010, \ldots, 101]\), here we change \([j_2j_2j_1]\) to \([j_3(j_2 \oplus 1)j_1]\). Thus, the modified \((c_3c_2c_1)\)-gates can be used for Column 3. We will give a general description of this procedure in the next section. Here, we obtain the \((1 \ast V), (10V), (1V \ast)\) gates, which can be used to annihilate the \((8, 3), (6, 3), (5, 3)\) entries.

Finally, to annihilate the \((7, 3)\) entry, we use the \((3, 3)\) entry. Hence, the target bit of the gate we need is the leftmost bit. To avoid changing the form of the first and second columns, we need to use controls that are not satisfied by 000 and 001 but is satisfied by 010 and 110. Thus, we use the gate \((V1\ast)\).

\(^1\)As we will see, the same phenomenon will hold for columns 3 and 4, and also for the general case.
For Column 4, we need not do anything about the first four entries at this point.

We will adapt the scheme for the (6, 1), (8, 1), (7, 1), (5, 1) entries to annihilate the (7, 4), (5, 4), (6, 4), (8, 4) entries. The conversion (6, 8, 7, 5) to (7, 5, 6, 8) is done by performing

$$(110, 100, 101, 111) = (101, 111, 110, 100) \oplus (011, 011, 011, 011)$$

using the binary number correspondence of the numbers.

We adjust the $(c_3c_2c_1)$-gates used for the (6, 1), (8, 1), (7, 1) entries to annihilate the (7, 4), (5, 4), (6, 4) entries as follows,

change $c_3$ to 1 if $c_3$ is not 1; for $i = 1, 2$, change $c_i$ to 0 if $c_i = 1$.

Note that column 4 is associated to the binary sequence 011.\(^2\) We will obtain the $(1 \ast V), (10V), (1V \ast)$ gates, which can be used to annihilate the (7, 4), (5, 4), (6, 4) entries.\(^3\) Finally use a $(V11)$-gate to annihilate the (8, 4) entry using the (4, 4) entry while avoiding any change in the form of the first three columns.

**Step 3** Note that after Column 4 is dealt with, the matrix takes the form $I_4 \oplus V'$ where $V' \in M_4$. We can then use the scheme for the 2-qubit case to transform $V'$ to $I_4$. However, to avoid changing the form of the first four columns, we need to extend the $(c_2c_1)$-gates used in the $4 \times 4$ case to $(1c_2c_1)$-gates for the remaining steps. This explains the tables for columns 5 to 7.

## 3 General Scheme

In this section, we present the general recurrence scheme for the annihilation of the off-diagonal entries of an $n$-qubit unitary gate by adapting the reduction scheme of the $(n - 1)$-qubit case. We will carry out **Steps 1 – 3** described at the beginning of Section 2. As illustrated in the 3-qubit case and explained in Remark 2.1, **Step 2** of the scheme requires some careful attention. For each column $\ell = 1, \ldots, N/2$ with $N = 2^n$, we can always annihilate the off-diagonal entries in the upper half of column $\ell$ using the scheme for annihilating the first column for an $(n - 1)$ qubit unitary gate. One only needs to change a $(c_2c_1)$-gate to a $(\ast c_{n-1} \cdots c_1)$-gate.

For the lower half of column $\ell$, we have to refine **Step 2** to the following steps.

**Step 2.1** For column 1, use the reduction scheme for an $(n - 1)$-qubit to eliminate the off-diagonal entries in the upper half of the column by changing the $(c_{n-1} \cdots c_1)$-gates used in the $(n - 1)$-qubit gate case to $(\ast, c_{n-1}, \ldots, c_n)$-gates in these steps.

Next, we apply the same scheme to eliminate the entries in the lower half except for the $(N/2 + 1, 1)$ entry, which will be eliminated last. This is done by changing the $(c_{n-1} \cdots c_1)$-gates in the $(n - 1)$-qubit case to $(c_n \cdots c_1)$-gates, where

$$c_n = \begin{cases} 1 & \text{none of } c_{n-1}, \ldots, c_1 \text{ equals 1,} \\ \ast & \text{otherwise.} \end{cases} \quad (1)$$

The $(c_n \cdots c_1)$-gate constructed in this way will ensure that the $(1, 1)$ entry will not interact with $(2, 1), \ldots, (N/2, 1)$ entries when we annihilate the $(N/2 + j, 1)$ entry for $j = 2, \ldots, N/2$ because $1 \in \{c_n, \ldots, c_1\}$. Finally, apply a $(V \ast \cdots \ast)$-gate to annihilate the $(N/2 + 1, 1)$ entry.

An easy inductive argument will verify that the $(c_n \cdots c_1)$-gates used in Column 1 satisfy $c_n, \ldots, c_1 \in \{\ast, 1, V\}$ with $c_1 \neq 1$.

The annihilation steps of Column 1 can be summarized in the following.

\(^2\) As we will see in the next section, we always adjust the gates according to the the binary sequence associated to the column index.

\(^3\) Note also that the $(c_3c_2c_1)$-gates are the same as those used in Column 3 before the final step. We will also explain this in the next section.
Procedure 2.1

Suppose in the \((n - 1)\) - qubit case, the off-diagonal entries in the first column are eliminated in the order of

\[(b_1,1),\ldots, (b_{N/2-1},1) \text{ by } C_1 - \text{gate,} \ldots, C_{N/2-1} - \text{gate.}\]

Eliminate the entries in the upper half of the Column 1 in the order of

\[(b_1,1),\ldots, (b_{N/2-1},1) \text{ by } (\ast C_1) - \text{gate,} \ldots, (\ast C_{N/2-1}) - \text{gate.}\]

For \(C = (c_{n-1} \ldots c_1)\) let \(G(C) = (c_n c_{n-1} \ldots c_1)\) with \(c_n\) satisfying (1).

Eliminate the entries in the lower half of the column in the order of

\[(d_1,1),\ldots, (d_{N/2-1},1) \text{ by } G(C_1) - \text{gate,} \ldots, G(C_{N/2-1}) - \text{gate,}\]

where \(d_i = b_i + N/2\) for \(i = 1,\ldots, N/2 - 1,\) and eliminate the \((N/2 + 1, 1)\) entry by a \((V \ast \ast \ast) - \text{gate.}\)

Step 2.2 For column \(\ell\) with \(2 \leq \ell \leq N/2,\) we can use the same scheme as that of the \((n - 1)\)-qubit case to eliminate the off-diagonal entries in the upper half. Then we can adapt the scheme for eliminating the entries in the lower half of Column 1 to other columns. To this end, we need to modify

(a) the order of the elimination of the entries in the lower half so that the last entry in the lower half will be eliminated by the \((\ell, \ell)\) entry.

(b) the control gates used to do the elimination so that

(b.i) they will not affect the zero entries obtained in the previous steps; and

(b.ii) they will annihilate the entries in the order prescribed in (a).

To achieve (a) and (b), identify \(k \in \{1,\ldots, 2^n\}\) with the binary sequence \(\overline{k}_n \ldots \overline{k}_1 \in \{0 \ldots 0,\ldots, 1 \ldots 1\}\) so that

\[k = \sum_{j=1}^{n} \overline{k}_j 2^{j-1} + 1.\]

For (a), if we annihilate the entries in the lower half of Column 1 in the order of \((d_1,1),\ldots, (d_{N/2},1),\) then we will annihilate the entries in the lower half of column \(\ell\) in the order of

\[(d_1 \oplus \ell, \ell),\ldots, (d_{N/2} \oplus \ell, \ell),\]

where the binary sequence of \(d_j \oplus \ell\) is obtained by entry-wise addition \(\oplus\) (without carried digits) of the two binary sequences of \(d_j\) and \(\ell\) such that \(0 \oplus 0 = 1 \oplus 1 = 0\) and \(0 \oplus 1 = 1 \oplus 0 = 1.\)\(^4\) Note that \(d_{N/2} = N/2 + 1,\) and hence \(d_{N/2} \oplus \ell = N/2 + \ell,\) so that \((N/2 + \ell, \ell)\) is the last entry in the lower half of Column \(\ell\) to be eliminated.

For (b), suppose \(2^{m-1} < \ell \leq 2^m\) with \(m \in \{1,\ldots, n-1\}\) and \(\ell = \sum_{j=1}^{n} \overline{\ell}_j 2^{j-1} + 1.\) We adjust the \((c_n \ldots c_1)\)-gate used to annihilate the \((d_i,1)\) entry with \(N/2 + 1 \leq d_i < N\) to the \((\tilde{c}_n \ldots \tilde{c}_1)\)-gates for annihilating the \((d_i \oplus \ell, \ell)\) entry as follows, where

\[
\tilde{c}_j = \begin{cases} 1 & \text{if } j = n \text{ and none of } c_n, \ldots, c_{m+1} \text{ is 1,} \\
0 & \text{if } 1 \leq j \leq m \text{ and } c_j = \overline{\ell}_j = 1, \\
c_j & \text{otherwise.} \end{cases}
\]

\(^4\) For instance, the binary form of \(f_2(d_i)\) is the sum of (using \(\oplus\)) the binary sequence \(0 \ldots 01\) and the binary form of \(d_i;\) the binary form of \(f_3(d_i)\) is the sum of the binary sequence \(0 \ldots 010\) and the binary form of \(d_i;\ldots,\) and the binary form of \(f_{N/2}(d_i)\) is the sum of the binary sequence \(01 \ldots 1\) and the binary form of \(d_i.\)
Because at least one of \(\hat{c}_n, \ldots, \hat{c}_{m+1}\) is 1, for \(1 \leq j \leq 2^m\) the \((j,j)\) entries will not interact with other \((k,j)\) entry with \(1 \leq k \leq N/2\) and \(k \neq j\).

Note also that a \((c_n \cdots c_1)\)-gate with \(c_n, \ldots, c_1 \in \{*, 0, 1, V\}\) corresponding to the unitary matrix

\[
\tilde{V} = I_N + V_n \otimes \cdots \otimes V_1,
\]

where

\[
V_i = \begin{cases} 
0 \otimes 0 & \text{if } c_i = 0, \\
1 \otimes 1 & \text{if } c_i = 1, \\
V - I_2 & \text{if } c_i = V, \\
I_2 & \text{if } c_i = *.
\end{cases}
\]

For the \((c_n \cdots c_1)\)-gates used in the first columns, we have \(c_n, \ldots, c_1 \in \{*, 1, V\}\) with \(c_1 \neq 1\). So, changing the 1-control in the \(c_1\) position whenever \(\hat{\ell}_i = 1\) in our rule is equivalent to applying a unitary similarity transform to change \(\tilde{V}\) to \(P_{\ell}^T V P_{\ell}\), where \(P_{\ell}\) is the permutation matrix changing the basis \([|j_n \cdots j_1\rangle : j_r \in \{0,1\}\} \) to \([|\tilde{j}_n \cdots \tilde{j}_1\rangle : \tilde{j}_r \in \{0,1\}\} \), where \(\tilde{\ell}_n \cdots \tilde{\ell}_1\) is the binary number corresponding to \(\ell\).

So, the modified gates can be used to annihilate \((d_1 \oplus \ell, \ell)\) entries for \(j = 1, \ldots, N/2-1\). After that, only the \((\ell, \ell)\) and \((N/2 + \ell, \ell)\) entries are nonzero in column \(\ell\). We annihilate the \((N/2 + \ell, \ell)\) entry using the \((V\hat{c}_{n-1} \cdots \hat{c}_{1})\)-gate to ensure that the annihilation in these steps will not affect the zero entries in the previous steps, where \((\hat{c}_{n-1} \cdots \hat{c}_{1})\) is obtained from the binary sequence correspondence \((\tilde{\ell}_{n-1} \cdots \tilde{\ell}_1)\) of \(\ell\) by changing all 0 terms to \(*\).

Note also that except for the last step one will always get the same set of \((c_n \cdots c_1)\)-gates for the elimination of the lower half of the entries in Columns \(2k-1\) and \(2k\) because the modification in (2) will have the same effects in these columns. This follows from the fact that the \((c_n \cdots c_1)\)-gates for Column 1 satisfy \(c_n, \ldots, c_1 \in \{*, 1, V\}\) with \(c_1 \neq 1\).

The annihilation steps of Column \(\ell\) can be summarized in the following.

---

**Procedure 2.2**

Suppose in the \((n-1)\) – qubit case, the off-diagonal entries in Column \(\ell\) are eliminated in the order of

\[(a_1, \ell), \ldots, (a_{N/2-\ell}, \ell) \quad \text{by} \quad D_1 - \text{-gate,} \ldots, D_{N/2-\ell} - \text{-gate.}\]

For the \(n\) – qubit case, eliminate the entries in the upper half of the column in the order of

\[(a_1, \ell), \ldots, (a_{N/2-1}, \ell) \quad \text{by} \quad (*D_1) - \text{-gate,} \ldots, (*D_{N/2-\ell}) - \text{-gate.}\]

For \(C = (c_{n-1} \cdots c_1)\) let \(G_{\ell}(C) = (\hat{c}_{n-1} \cdots \hat{c}_1)\) satisfy (2), and let \(d_1\) and \(G(C_i)\) be defined as in Procedure 1.1.

Eliminate the entries in the lower half of the column in the order of

\[(d_1 \oplus \ell, \ell), \ldots, (d_{N/2+\ell, \ell}) \quad \text{by} \quad G_{\ell}(G(C_1)) - \text{-gate,} \ldots, G_{\ell}(G(C_{N/2-1})) - \text{-gate;}
\]

eliminate the \((N/2 + \ell, \ell)\) entry by a \((V\hat{c}_{n-1} \cdots \hat{c}_1)\) – gate, where \((\hat{c}_{n-1} \cdots \hat{c}_1)\) is obtained from the binary sequence correspondence \((\tilde{\ell}_{n-1} \cdots \tilde{\ell}_1)\) of \(\ell\) by changing all 0 terms to \(*\).

---

\footnote{For example, for Column 2 we change \((c_n \cdots c_1)\) to \(G_2(c_n \cdots c_1)\) by changing only \(c_1\) and \(c_n\) because 2 corresponds to \(0 \cdots 01\), and \((\hat{c}_n \cdots \hat{c}_1) = (V \cdots \cdots 1)\); for Column 3, we change \((c_n \cdots c_1)\) to \(G_3(c_n \cdots c_1)\) by changing only \(c_2\) and \(c_n\) because 3 corresponds to \(0 \cdots 01\), and \((\hat{c}_n \cdots \hat{c}_1) = (V \cdots \cdots 1)\); for Column 4, we change \((c_n \cdots c_1)\) to \(G_4(c_n \cdots c_1)\) by changing only \(c_1, c_2\) and \(c_n\) because 4 corresponds to \(0 \cdots 01\), and \((\hat{c}_n \cdots \hat{c}_1) = (V \cdots \cdots 11)\).}
Several remarks concerning Procedures 1 and 2 are in order.

1. In Column 1, it is easy to determine the order of the entries to be eliminated and the \((c_n \cdots c_1)\)-gates used.

2. For the lower half of Column \(\ell\) with \(2 \leq \ell \leq N/2\), we change the order of entries to be eliminated to \((d_1 \oplus \ell, d_2 \oplus \ell, \ldots, d_{N/2} \oplus \ell, \ell)\), and change the \((c_n \cdots c_1)\)-gates to \(G_\ell(c_n \cdots c_1)\)-gates.

3. The \((c_n \cdots c_1)\)-gates used in Column 1 satisfy \(c_n, \ldots, c_1 \in \{*, 1, V\}\) with \(c_1 \neq 1\).

4. The \((c_n \cdots c_1)\)-gates used to eliminate the entries in the lower half of Column \(2k - 1\) and \(2k\) are always the same before the last step, for \(k = 1, \ldots, N/4\).

5. The \((c_n \cdots c_1)\)-gates used in the last steps of Columns 1, \ldots, \(N/2\) satisfy \(c_n = V\), and \((c_{n-1} \cdots c_1)\) is obtained from the binary sequences \((0 \cdots 0), \ldots, (1 \cdots 1)\) of length \(n - 1\) by replacing 0 with *.

The recurrence scheme easy to do. Even the most non-trivial steps of adapting the procedures of eliminating the entries in the lower half of the first column to other columns are quite straightforward. We illustrate this for the case \(n = 4\).

**Four qubit case, lower left block**

|        | entries | binary | gates |
|--------|---------|--------|-------|
| Col 1, steps 8-15 | (10,1) | 0101 | 1**V **1V |
|        | (12,1) | 0100 | **1V **1V |
|        | (11,1) | 0100 | 1**V **1V |
|        | (14,1) | 1101 | 1*1V 1V |
|        | (16,1) | 1111 | 10*V 1V |
|        | (15,1) | 1110 | 101V 1V |
|        | (13,1) | 1100 | 101V 1V |
|        | (9,1)  | 1000 | 101V 1V |

| Col 2, steps 7-14 | (9,2)  | 0100 | 1**V **1V |
|        | (11,2) | 0100 | 1**V **1V |
|        | (12,2) | 1010 | 1**V **1V |
|        | (13,2) | 1100 | 1**V **1V |
|        | (15,2) | 1110 | 1**V **1V |
|        | (16,2) | 1111 | 1**V **1V |
|        | (14,2) | 1100 | 1**V **1V |
|        | (10,2) | 1000 | 1**V **1V |

| Col 3, steps 6-13 | (12,3) | 1011 | 1**V **1V |
|        | (10,3) | 1001 | 1**V **1V |
|        | (9,3)  | 1000 | 1**V **1V |
|        | (16,3) | 1110 | 1**V **1V |
|        | (14,3) | 1111 | 1**V **1V |
|        | (13,3) | 1101 | 1**V **1V |
|        | (15,3) | 1100 | 1**V **1V |
|        | (11,3) | 1000 | 1**V **1V |

| Col 4, steps 5-12 | (14,4) | 1101 | 1**V **1V |
|        | (16,4) | 1100 | 1**V **1V |
|        | (15,4) | 1101 | 1**V **1V |
|        | (13,4) | 1100 | 1**V **1V |
|        | (14,4) | 1110 | 1**V **1V |
|        | (12,4) | 1111 | 1**V **1V |
|        | (10,4) | 1100 | 1**V **1V |
|        | (9,4)  | 1000 | 1**V **1V |

| Col 5, steps 4-11 | (16,5) | 1110 | 1**V **1V |
|        | (15,5) | 1111 | 1**V **1V |
|        | (10,5) | 1111 | 1**V **1V |
|        | (11,5) | 1101 | 1**V **1V |
|        | (12,5) | 1100 | 1**V **1V |
|        | (9,5)  | 1000 | 1**V **1V |
|        | (13,5) | 1000 | 1**V **1V |

| Col 6, steps 3-10 | (15,6) | 1111 | 1**V **1V |
|        | (16,6) | 1110 | 1**V **1V |
|        | (9,6)  | 1111 | 1**V **1V |
|        | (11,6) | 1100 | 1**V **1V |
|        | (12,6) | 1101 | 1**V **1V |
|        | (10,6) | 1100 | 1**V **1V |
|        | (14,6) | 1100 | 1**V **1V |

| Col 7, steps 2-9 | (14,7) | 1111 | 1**V **1V |
|        | (13,7) | 1110 | 1**V **1V |
|        | (12,7) | 1110 | 1**V **1V |
|        | (10,7) | 1111 | 1**V **1V |
|        | (9,7)  | 1110 | 1**V **1V |
|        | (11,7) | 1110 | 1**V **1V |
|        | (17,7) | 1110 | 1**V **1V |

| Col 8, steps 1-8 | (13,8) | 1111 | 1**V **1V |
|        | (14,8) | 1110 | 1**V **1V |
|        | (11,8) | 1111 | 1**V **1V |
|        | (9,8)  | 1111 | 1**V **1V |
|        | (10,8) | 1111 | 1**V **1V |
|        | (12,8) | 1111 | 1**V **1V |
|        | (16,8) | 1111 | 1**V **1V |
4 Total Number of Controls and Comparison to a Previous Study

The following theorem gives the formula for the number $g_n^k$ of $k$-controlled qubit gates used in the recurrence scheme of our decomposition for a unitary matrix $U \in M_{2^n}$, where $k = 0, 1, \ldots, n - 1$.

Theorem 4.1. 1. $g_n^0 = n$

2. $g_n^{n-1} = \begin{cases} 1 & \text{if } n = 1 \\ 4 & \text{if } n = 2 \\ 7 + (n - 3) & \text{if } n \geq 3 \end{cases}$

3. $g_n^k = g_{n-1}^k + g_{n-1}^{k-1} + \binom{n-1}{k}$ for all $3 \leq k < n - 1$

4. $g_n^1 = n(n-1)(2^{n-2} + 1)$ for all $n \geq 2$

5. $g_n^2 = \frac{1}{3}(4^n - 4) - 2^n(n - 1) + \frac{n(n-1)(n-2)}{2}$ for all $n \geq 3$

Note that $\sum_{k=0}^{n-1} g_n^k = 2^{n-1}(2^n - 1) = N(N-1)/2$. By convention $g_1^0 = 1$. In general, if $n > 1$,$$
 g_n^k = A_n^k + B_n^k + C_n^k + D_n^k,$$

where $A_n^k$ is the number of $g_n^k$ gates used to annihilate entries in the upper left block of the matrix, $B_n^k$ is the number of $g_n^k$ gates used to annihilate entries of the lower half of columns $1, \ldots, 2^{n-1}$ excluding the entries of the form $\left(\frac{N}{2} + \ell, \ell\right)$. The number $C_n^k$ is the number of $g_n^k$ gates used to annihilate entries $(\frac{N}{2} + \ell, \ell)$, where $\ell \in \{1, \ldots, 2^{n-1}\}$. Finally $D_n^k$ is the number of $g_n^k$ gates used to annihilate the lower right block entries of the matrix. For example, we saw in section 2 that

$g_2^0 = 2 = 1 + 0 + 1 + 0$ and $g_2^1 = 4 + 0 + 2 + 1 + 1$

and $g_3^0 = 3 = 2 + 0 + 1 + 0$, $g_3^1 = 18 = 4 + 10 + 2 + 2$, and $g_3^2 = 0 + 2 + 1 + 4$

Remarks 4.2. Immediately, we can see the following recursive properties.

1. $A_n^k = g_n^{k-1}$ for $k \in \{0, \ldots, n-2\}$ and $A_n^{n-1} = 0$ as illustrated in tables 2 and 3.

2. $D_n^k = g_n^{k-1}$ for $k \in \{1, \ldots, n-1\}$ and $D_n^0 = 0$ as seen from table 2 and 5.

3. $C_n^k = \binom{n-1}{k}$ for $k \in \{0, \ldots, n-1\}$, because $C_n^k$ is the number of column indices $\ell$, with $1 \leq \ell \leq 2^{n-1}$, such that the binary sequence of $\ell$ of length $n$ has exactly $k$ digits equal to 1.

4. Observe that the gate $G_i = \mathcal{G}(C_i)$, $1 \leq i \leq \frac{N}{2} - 1$, in table 1 has exactly one 1-control. All other gates accounted for by $B_n^k$ are obtained from the $G_i$’s via the transformation $G_\ell$, for $2 \leq \ell \leq \frac{N}{2}$. But notice that $G_i(G_j)$ either has the same number of controls as $G_j$ or has one more control than $G_j$. Hence $B_n^k = 0$ for $k > 2$ and $B_n^2 + B_n^2 = 2^{n-1}(2^{n-1} - 1)$.

Let us observe the recursive scheme for the first column (see Table 1). The following lemma can be proven inductively from this scheme.

Lemma 4.3. If

\[ i = 2^{s_1-1} + \sum_{m=1}^{j} (2^{s_m-1} - 1), \text{ where } 1 \leq s_1 < s_2 < \cdots < s_j \leq n - 1 \text{ and } 1 \leq j \leq n - 1 \]

then

\[ b_i = 1 + \sum_{m=1}^{j} 2^{s_{m-1}}, \text{ and } \quad C_i = (\ast \ast \cdots \ast c_{s_2} \ast \cdots \ast c_{s_1} \ast \cdots \ast), \quad (3) \]

where $(c_{s_2}, c_{s_1}) = (\ast, V)$ when $j = 1$, otherwise $(c_{s_2}, c_{s_1}) = (1, V)$.

Lemma 4.4. Let $G_1, \ldots, G_{N/2-1}$ be as in remark 4.2.4. Suppose $G_i$ is a $(c_{i_1} \cdots c_{i_1})$-gate. Then the following holds

\[ \#\{i : c_{ik} = 1\} = \begin{cases} n - 1 & \text{when } k = n, \\ 2^{n-k-1}(k-1) & \text{otherwise}. \end{cases} \]
Lemma 4.5. Proof of Theorem 4.1

We want to know how many of the gates used to annihilate entries of column \( 2 \). Let us look at the gates used to annihilate entries of column \( \ell \in \{1, \ldots, \frac{N}{2} \} \) that contribute to \( B^1_n \).

Lemma 4.5. Let \( 2^{m-1} < \ell \leq 2^m \) with \( 1 \leq m \leq n-1 \) and \( G_1, \ldots, G_{\frac{N}{2}-1} \) be as in Lemma 4.4. Then

\[
\# \{i | \text{G}_\ell (G_i) \text{ has exactly one control} \} = \begin{cases} 
\frac{n-1}{2^n} + 1 & \text{if } m = n-1, \\
(n-1) + \sum_{k=m+1}^{n-1} 2^{n-k-1}(k-1) & \text{otherwise.}
\end{cases}
\]

Proof. If \( 2^{m-1} < \ell \leq 2^m \), then \( \ell = \sum_{j=1}^{m} j \cdot 2^{j-1} + 1 \). Recall that \( G_\ell (G_i) \) has exactly one control if \( G_i = (c_m, \ldots, c_1) \) has one 1-control in \( \{c_{(m+1)}, \ldots, c_n\} \). Thus

\[
\# \{i | \text{G}_\ell (G_i) \text{ has exactly one control} \} = \sum_{k=m+1}^{n} \# \{i | c_{ik} = 1 \}
\]

The conclusion follows from Lemma 4.4.

Proof of Theorem 4.1

1. A control-free gate can only be utilized in Column 1. This is because when we transform the matrix to the form \([1] \oplus U'\), the succeeding gates must make sure that the first row does not interact with other rows. As mentioned in Lemma 4.3 and illustrated in Table 1, these gates with no control are the gates that annihilate the entries of the form \((1 + 2^{m-1})\) for \( m \in \{1, \ldots, n\} \). Indeed \( g_0 = n \).

2. We have shown that \( g_0^1 = 1, g_2^1 = 4 \) and \( g_3^1 = 7 \). From Remark 4.2 we deduce that \( g_n^{a-1} = \binom{n-1}{a-1} + g_{n-1}^{a-2} \) for all \( n \geq 4 \) and hence

\[
g_n^{a-1} = 1 + g_{n-1}^{a-2} = (n-3) + g_3 = (n-3) + 7.
\]

3. Now, assume \( n-1 > k \geq 3 \). From Remark 4.2, we get \( g_k = g_{k-1}^{k-1} + \binom{n-1}{k} + 0 + g_{k-1}^{k-1} \).

4. When \( n = 2 \), we know that that \( g_2^1 = 4 = 2(2-1)(2^0 + 1) \).

Now, assume \( n > 2 \). From Remark 4.2, \( g_n^1 = g_{n-1}^1 + B_n^1 + \binom{n-1}{a-1} + \sum_{a=1}^{n-1} g_{n-1}^{a-1} \). Let us look at the summing definition \( B_n^1 \). From Remark 4.2.4, Column 1 contributes \( \frac{N}{2} = 2^{n-1} - 1 \) gates to \( B_n^1 \). From Lemma 4.5, we deduce that

\[
B_n^1 = (2^{n-1} - 1) + 2^{n-2}(n-1) + \sum_{a=1}^{n-1} \sum_{k=0}^{n-2} 2^{n-k-1}(k-1)
\]

Thus \( g_n^1 = g_{n-1}^1 = 2(n-1) + 2^{n-3}(n+3)(n+2)(n-1) \). Using a telescoping sum, we get

\[
g_n^1 = g_2^1 + \sum_{m=2}^{n} [2(m-1) + 2^{m-3}(m+3)(m+2)(n-1)].
\]

5. If \( n = 3, g_3^1 = 7 = \frac{1}{3}(4^3 - 4) - 2(3-1) + \frac{3+4}{2} \). Now, assume \( n > 3 \). From Remark 4.2 and equation (4),

\[
g_n^2 = g_{n-1}^2 + g_{n-1}^1 + \binom{n-1}{2} + 2^{n-1}(2^{n-1} - 1) - 2^{n-3}(n+2)(n-1).
\]

Then

\[
g_n^2 - g_{n-1}^2 = (2^{n-3} + 1)(n-1)(n-2) + \frac{(n-2)(n-1)}{2} + 2^{n-1}(2^{n-1} - 1) - 2^{n-3}(n+2)(n-1)
\]

And hence

\[
g_n^2 = g_3^2 + \sum_{m=4}^{n} [2^{m-1}(2^{m-1} - m) + \frac{3}{2}(m-2)(m-1)]
\]

\[
= \frac{1}{3}(4^n - 4) - 2^n(n-1) + \frac{n(n-1)(n-2)}{2}.
\]
In [14], the Gray code basis was utilized to achieve the same goal of this paper. Let us denote the total number of gates with \( k \) controls in the decomposition scheme presented in [14] by \( g_n^k \). The recursion formula presented in the said study is
\[
g_n^k = g_n^{k-1} + g_{n-1}^{k-1} + \max(2^{n-2}, 2^k) + (2^{2n-k-2} - 2^{n-2}) \quad (\text{for } k \geq 1)
\]
with the conditions that \( g_n^0 = 2^{n-1} \) and \( g_n^0 = 0 \) for all \( n \). Let us compare values for small \( n \).

| \( n \) | \( g_n^k \) | \( g_n^k / g_n^0 \) | \( g_n^k / g_n^1 \) | \( g_n^k / g_n^2 \) | \( g_n^k / g_n^3 \) | \( g_n^k / g_n^4 \) | \( T_1(n) / T_2(n) \) |
|------|--------|----------------|----------------|----------------|----------------|----------------|----------------|
| 1    | 1 / 1  | -              | -              | -              | -              | 0 / 0          | 4 / 4          |
| 2    | 2 / 2  | 4 / 4          | -              | -              | -              | 4 / 4          | 4 / 4          |
| 3    | 3 / 4  | 18 / 14        | 7 / 10         | -              | -              | 32 / 34        | 180 / 196      |
| 4    | 4 / 8  | 60 / 50        | 48 / 40        | 8 / 22         | -              | 880 / 960      |                |
| 5    | 5 / 16 | 180 / 186      | 242 / 154      | 60 / 94        | 9 / 46         | 880 / 960      |                |

Here, \( T_1(n) \) (respectively, and \( T_2(n) \)) is the total number of controls in the decomposition of a unitary \( U \in M_{2^n} \) using the scheme in this paper (respectively, the scheme in [14]). Starting from \( n = 3 \), we get a small advantage in our decomposition and because both methods are recursive, the discrepancy becomes large as \( n \) gets larger. For example, \( T_2(10) - T_1(10) = 30,720 \).

In Figure 1, we plot the difference between \( T_2 \) and \( T_1 \) for \( n \) from 1 to 50. We use the log scale in the \( y \)-axis.

![Figure 1](image.png)

5 Concluding Remarks and Future Research

In this paper, we present a recurrence scheme for generating controlled single qubit unitary gates \( U_1, \ldots, U_r \) with \( r \leq N(N - 1)/2 \) such that \( U_r \cdots U_1 U = I_N \). Consequently, \( U = U_1^\dagger \cdots U_r^\dagger \). We have the following.

Recurrent scheme

**Step 1** Partition \( U \in M_n \) into a \( 2 \times 2 \) block matrix with each block lying in \( M_{N/2} \), where \( N = 2^n \).

**Step 2** Use the scheme of the \((n - 1)\) - qubit case to help reduce \( U \) to the form \( I_{N/2} \oplus \tilde{U} \) with \( \tilde{U} \in M_{N/2} \).

**Step 2.1** For Column 1, use Procedure 2.1 in Section 3.

**Step 2.2** For Column \( \ell \) with \( 2 \leq \ell \leq N/2 \), use Procedure 2.2 in section 3.

**Step 3** Apply the scheme of the \((n - 1)\) - qubit case to transform \( \tilde{U} \) to \( I_{N/2} \).

It is worth noting that one can actually describe the entire recursive scheme in terms of the steps used to eliminate the off-diagonal entries of the first column as follows.

- We first generate the \((c_n \cdots c_1)\)-gates for eliminating the off-diagonal entries:
  
  For \( n = 1 \) use \( V \) to eliminate the \((2,1)\) entry; for \( n > 1 \) modify the \((c_{n-1} \cdots c_1)\)-gates to \((c_{n-1} \cdots c_1)\)-gates to eliminate the off-diagonal entries in upper half of Column 1 in the \( n\)-qubit case, and \( G(c_{n-1} \cdots c_1)\)-gates to eliminate the entries in the lower half.

- Once, we have the \((c_n \cdots c_1)\)-gates for Column 1, we can modify them to eliminate the off-diagonal entries for the leading \( 2^n \times 2^n \) blocks for \( m = 1, \ldots, n \), using Steps 2.1 and 2.2 described in Section 3.
We give recursive formulas for the number of controlled single qubit gates needed in the decomposition. The total number of controls used in our scheme is less than that in [14].

For future research, it might be interesting to design other recurrence schemes, which are easy to implement and use even less controls. Moreover, there might be other optimality criteria depending on the physical implementation of qubits. One may take this into consideration and assign a cost $w_k$ for implementing $k$-controlled single qubit gates, and then study the optimal decomposition by minimizing the cost instead of number of controls.

Matlab programs for the decomposition using our scheme is posted at http://ckixx.people.wm.edu/mathlib.html. The program decomposition.m displays the order of entries to be annihilated, the $(c_n c_{n-1} \cdots c_1)$-gate used and the single qubit gate $V \in M_2$ used for the controlled gates. One types $[U,A,x,y,controls,num,V]=decomposition(n)$; in the command line, where $n$ is the number of bits and the program will prompt for the user to either choose to create a random unitary matrix or input the unitary matrix manually. The variable $U$ is the unitary matrix being decomposed. The variable $A$ is an array of strings that describe the form of the gate, and $(x,y)$ are the row and column indices arranged according to their order of annihilation. The variable $controls$ gives the total number of controls used and $num$ is the number of nontrivial unitary controlled gates used. The variable $V$ is the product of the controlled gates and hence, must always equal to the identity matrix. This is used to help the user check that the decomposition is correct. The matlab program gatecount.m counts the total number of controls in our scheme and that of [14].

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After the first version of this manuscript was put on arXiv, the following related references [1, 3, 4, 6, 10, 11] came to our attention.

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