Reversibility of Quantum Gates

We want the quantum gates to be reversible because quantum mechanics is reversible in nature. For a given quantum gate $G : X_n \to Y_n$, there exists a quantum gate $G^{-1} : Y_n \to X_n$, where X_n & Y_n are vector of n-dimensional qubits. Gates can also be called an operator, similar to a function or a mapping.

Extending classical gates

Classical gates are usually not reversible. Let us consider a few examples such as the AND gate, OR gate & bit-wise addition gates by listing their truth tables. All the following examples take two classical bits and output classical bits as the output, but they discard the original input bits.

1. AND Gate

a	b	$a \wedge b$
0	0	0
0	1	0
1	0	0
1	1	1

Table 1: AND gate truth table.

2. OR Gate

a	b	$a \vee b$
0	0	0
0	1	1
1	0	1
1	1	1

Table 2: OR gate truth table.

3. Bitwise addition Gate

a	b	$a + b$
0	0	00
0	1	01
1	0	01
1	1	10

Table 3: Bit-wise addition gate truth table.

If we look at the truth table of the AND gate in table 1 it is clear when $a \wedge b$ is 1. Both a & b have to be 1. However, there are 3 permutations of a & b, namely (0, 0), (0, 1) & (1, 0), where $a \wedge b$ is 0. However, simply looking at the value of $a \wedge b$, we cannot determine exactly what the values of a & b are. We can observe this similar pattern for the OR gate in table 2, a & b having 3 permutations of values such that $a \vee b$ is 1. For bit-wise addition in table 3 a & b has 2 permutations of values such that $a + b$ is 01.

A key aspect for an operator to be reversible is that the mapping should be one-to-one, but this is not the case with classical gates. To overcome this limitation, the number of inputs and outputs to the logic gate should be the same, and no information from the original inputs should be discarded.

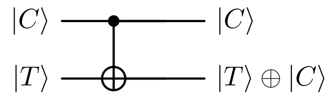

Figure 1: A CNOT gate

Making AND gates reversible

To make the AND gate reversible, we can look at the CNOT gate figure 1. Recall from the previous chapter that the control qubit $|C\rangle$ applies the XOR operation on the target qubit $|T\rangle$. Repeating the CNOT gate on the outputs of the CNOT gate gives us the qubits $|C\rangle$ & $|T\rangle$. Effectively reversing the operation of the CNOT gate.

By adding a control bit z to the set of input to the AND gates. And allowing bits x & y to pass unchanged as output, we balanced the number of inputs to the gate and outputs from the gate. The control bit z, following the CNOT gate example, is modified by XOR of z & $x \wedge y$. When computing the AND of x & y, we set the control bit z to 0, which effectively makes the output of the third bit entirely dependent on $x \wedge y$.

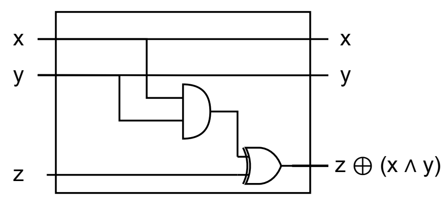

Figure 2: A Reversible AND gate

Now, repeating this reversible AND gate by taking the output in figure 2 and feeding it back into the input of another reversible AND gate will give us the output the same as the original input. In Figure figure 3, we can clearly see that x & y are unchanged throughout the computation. However, the last bit in the computation is $\{z \oplus (x \wedge y)\} \oplus (x \wedge y)$. Since the XOR operator is associative, we can re-write the bit as shown in equation 1.

$$\begin{aligned} \{z \oplus (x \wedge y)\} \oplus (x \wedge y) &= z \oplus \{(x \wedge y) \oplus (x \wedge y)\} \\ &= z \oplus 0 \\ &= z \end{aligned} \tag{1}$$

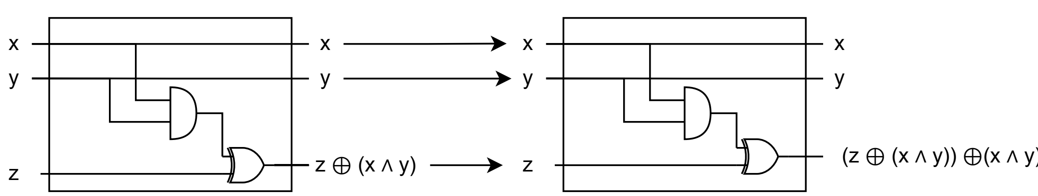

Figure 3: Chaining two reversible AND gates

Some more review of Linear Algebra Formalism

Before we proceed, we will now review some more linear algebra concepts. All of the following concepts discussed will be applicable to some n-dimensional Hilbert space $\mathcal{H}$.

Dot product

Let $\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$ & $\begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$ be some 3-dimensional $\mathcal{H}$ vectors denoted by $|\psi\rangle$ & $|\phi\rangle$ in Dirac notation respectively.

The dot product is a type of inner product between the two vectors. The below equation shows how it is represented in the Dirac notation:

$$\begin{gathered} \begin{bmatrix} a_1 & a_2 & a_3 \end{bmatrix} \cdot \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = a_1 b_1 + a_2 b_2 + a_3 b_3 \\ \langle\psi| \cdot |\phi\rangle = \langle\psi|\phi\rangle \end{gathered} \tag{2}$$

Norm of a vector

When we are talking about a norm of a vector, we usually mean the 2-Norm or Euclidean norm or L2 norm. For a given vector $|\psi\rangle = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$. It's norm is calculated as follows:

$$\begin{aligned} \text{Norm}(\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}) &= \sqrt{a_1^2 + a_2^2 + a_3^2} \\ &= \sqrt{\langle\psi|\psi\rangle} \\ &= \||\psi\rangle\| \end{aligned} \tag{3}$$

If $\||\psi\rangle\| = 1$ then $|\psi\rangle$ is a unit vector.

Orthonormal Basis

The orthonormal basis are vectors that are linearly independent & each vector has unit length. So, if there are n orthonormal basis vectors $|b_1\rangle$, $|b_2\rangle$, .. $|b_n\rangle$. Then $\||b_1\rangle\| = \||b_2\rangle\| = ... = \||b_1\rangle\| = 1$. The dot product between all these n orthonormal basis vectors can be represented as follows:

$$\begin{gathered} \langle b_i|b_j\rangle = \delta_{i,j} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \\ \forall i, j \in \{1, 2, ..., n\} \end{gathered} \tag{4}$$

In the above equation, $\delta_{i,j}$ is the Dirac delta function which outputs 1 for a specific condition (in this case for $i = j$), otherwise it is 0.

Vector represented using Orthonormal Basis

Let's assume that we have a vector $|\psi\rangle$ and n orthonormal basis, then $|\psi\rangle$ can be expressed as:

$$\begin{aligned} |\psi\rangle &= \alpha_1|b_1\rangle + \alpha_2|b_2\rangle + ... + \alpha_n|b_n\rangle \\ &= \sum_{i=1}^{n} \alpha_i|b_i\rangle \\ &\forall i \in \{1, 2, ..., n\} \alpha_i \in \mathbb{C} \end{aligned} \tag{5}$$

In above equation, each α_i is a constant and belongs to the set of complex numbers $\mathbb{C}$.

A small exercise on dor products

Consider a 4-dimensional Hilbert space $\mathcal{H}$. Consider two vectors, $\begin{bmatrix} 0 \\ \sqrt{\frac{2}{3}} \\ 0 \\ \frac{i}{\sqrt{3}} \end{bmatrix}$ & $\begin{bmatrix} 0 \\ 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$ denoted by $|\psi\rangle$ & $|\phi\rangle$ respectively.

Now, $|\psi\rangle = \sqrt{\frac{2}{3}}|01\rangle + \frac{i}{\sqrt{3}}|11\rangle$ & $|\phi\rangle = \frac{1}{\sqrt{2}}|10\rangle + \frac{1}{\sqrt{2}}|11\rangle$.

To calculate the dot product between $|\psi\rangle$ & $|\phi\rangle$, we need to first transpose, $|\psi\rangle$. In case of real numbers, this is straightforward, but in case of complex numbers, we need also take the complex conjugate whenever we transpose a complex vector.

So, $\langle\psi| = \sqrt{\frac{2}{3}}\langle 01| + \frac{-i}{\sqrt{3}}\langle 11|$.

Now,

$$\begin{aligned}
\langle\phi|\psi\rangle &= (\sqrt{\frac{2}{3}}\langle 01| + \frac{-i}{\sqrt{3}}\langle 11|) \cdot (\sqrt{\frac{2}{3}}|01\rangle + \frac{i}{\sqrt{3}}|11\rangle) \\
&= \frac{1}{\sqrt{3}}\langle 01|10\rangle + \frac{1}{\sqrt{3}}\langle 01|11\rangle + \frac{-i}{\sqrt{6}}\langle 11|01\rangle + \frac{-i}{\sqrt{6}}\langle 11|11\rangle \\
&= 0 + 0 + 0 + \frac{-i}{\sqrt{6}} \\
&= -\frac{i}{\sqrt{6}}
\end{aligned} \tag{6}$$

Dot product of a vector using Orthonormal Basis

Following the norm sub-section & orthonormal sub-section, we have some vector, $|\psi\rangle$ with n orthonormal basis vectors, this can be expressed as follows:

$$|\psi\rangle = \alpha_1|b_1\rangle + \alpha_2|b_2\rangle + ... + \alpha_n|b_n\rangle \tag{7}$$

$$\begin{aligned}
\||\psi\rangle\|^2 &= (\alpha_1\langle b_1| + \alpha_2\langle b_2| + ... + \alpha_n\langle b_n|) \cdot (\alpha_1|b_1\rangle + \alpha_2|b_2\rangle + ... + \alpha_n|b_n\rangle) \\
&= \alpha_1^2 + \alpha_2^2 + ... + \alpha_n^2 \\
&= \sum_{i=1}^{n} \alpha_i^2
\end{aligned} \tag{8}$$

Hadamard Basis

Let us consider a 2 dimensional standard hadamard basis, then the following equation shows us the two orthonormal basis.

$$\begin{aligned}
|+\rangle &= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\
|-\rangle &= \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)
\end{aligned} \tag{9}$$

Let us try to express orthonormal basis vectors $|0\rangle$ & $|1\rangle$ as a linear combination of hadamard basis vectors as shown in the following equation. If we simply add $|+\rangle$ & $|-\rangle$, we can eliminate $|1\rangle$ from the expression, thus giving us the value of $|0\rangle$. Similarly, if we subtract $|0\rangle$ & $|1\rangle$, we can eliminate $|0\rangle$ from the expression.

$$\begin{aligned}
|0\rangle &= \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) \\
|1\rangle &= \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)
\end{aligned} \tag{10}$$

Let us consider an example of a vector $\begin{bmatrix} \frac{1}{\sqrt{5}} \\ i\sqrt{\frac{4}{5}} \end{bmatrix}$. Now, using the Dirac notation, we can express it as $\frac{1}{\sqrt{5}}|0\rangle + i\sqrt{\frac{4}{5}}|1\rangle$. By substituting using previous equation, we can express our vector in hadamard basis as shown in below equation.

$$\begin{aligned}
&\frac{1}{\sqrt{5}}|0\rangle + i\sqrt{\frac{4}{5}}|1\rangle \\
&= \frac{1}{\sqrt{5}}\{\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)\} + i\sqrt{\frac{4}{5}}\{\frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)\} \\
&= \frac{1}{\sqrt{10}}|+\rangle + \frac{1}{\sqrt{10}}|-\rangle + i\sqrt{\frac{2}{5}}|+\rangle - i\sqrt{\frac{2}{5}}|-\rangle \\
&= (\frac{1}{\sqrt{10}} + i\sqrt{\frac{2}{5}})|+\rangle + (\frac{1}{\sqrt{10}} - i\sqrt{\frac{2}{5}})|-\rangle
\end{aligned} \tag{11}$$

Outer Product

In contrast to inner product, we will show how an outer product operation is calculated, let's consider $\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$ & $\begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$ be some 3-dimensional $\mathcal{H}$ vectors denoted by $|\psi\rangle$ & $|\phi\rangle$ in Dirac notation respectively.

$$\begin{gathered}
\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} \cdot \begin{bmatrix} b_1 & b_2 & b_3 \end{bmatrix} = \begin{bmatrix} a_1 \cdot b_1 & a_1 \cdot b_2 & a_1 \cdot b_3 \\ a_2 \cdot b_1 & a_2 \cdot b_2 & a_2 \cdot b_3 \\ a_3 \cdot b_1 & a_3 \cdot b_2 & a_3 \cdot b_3 \end{bmatrix} \\
|\psi\rangle \cdot \langle\phi| = |V| \\
|\psi\rangle\langle\phi| = |V|
\end{gathered} \tag{12}$$

Operators

In our previous chapter, we looked at NOT gate, CNOT gate. We represented them as matrices that, when multiplied by vectors, transformed these vector qubits. In certain areas of mathematics & physics, these are called operators. These operators are also termed reversible gates or unitary matrices. These operators can be represented as a linear combination of outer product of vectors.

Let us have another look at some gates, more specifically their representation as an operator & an outer product of vectors.

NOT Gate / Operator

Recall that NOT Gate had the form of $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. We can express this as a linear combination of outer products of orthonormal vectors $|0\rangle$ & $|1\rangle$.

$$\begin{aligned}
\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} &= \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \\
&= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \end{bmatrix} \\
&= |0\rangle\langle 1| + |1\rangle\langle 0|
\end{aligned} \tag{13}$$

Strange Gate / Operator

Let us have a new type of gate /operator S. The S operator flips the sign of the qubit such that $S|1\rangle = |-1\rangle$ & $S|0\rangle = |0\rangle$. Following intuition, we had when developing the NOT operator. For the $|0\rangle$ qubit, its value remains unchanged, indicating that the first entry in the 2×2 matrix is 1 followed by 0. But for the last entry, it should be -1, and for the third entry, it should be 0 as only the sign of $|1\rangle$ qubit is flipped.

Following the above intuition, we can write S as follows:

$$
\begin{aligned}
S &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \\
&= |0\rangle\langle 0| - |1\rangle\langle 1|
\end{aligned} \tag{14}
$$