4.2 Single qubit operations

The development of our quantum computational toolkit begins with operations on the simplest quantum system of all – a single qubit. Single qubit gates were introduced in Section 1.3.1. Let us quickly summarize what we learned there; you may find it useful to refer to the notes on notation on page xxiii as we go along.

A single qubit is a vector $|\psi\rangle = a|0\rangle + b|1\rangle$ parameterized by two complex numbers satisfying $|a|^2 + |b|^2 = 1$. Operations on a qubit must preserve this norm, and thus are described by 2×2 unitary matrices. Of these, some of the most important are the Pauli matrices; it is useful to list them again here:

$$X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad Y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad Z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{4.1}$$

Three other quantum gates will play a large part in what follows, the Hadamard gate (denoted H), phase gate (denoted S), and $\pi/8$ gate (denoted T):

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}; \quad S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}; \quad T = \begin{bmatrix} 1 & 0 \\ 0 & \exp(i\pi/4) \end{bmatrix}. \tag{4.2}$$

A couple of useful algebraic facts to keep in mind are that $H = (X+Z)/\sqrt{2}$ and $S = T^2$. You might wonder why the T gate is called the $\pi/8$ gate when it is $\pi/4$ that appears in the definition. The reason is that the gate has historically often been referred to as the $\pi/8$ gate, simply because up to an unimportant global phase T is equal to a gate which has $\exp(\pm i\pi/8)$ appearing on its diagonals.

$$T = \exp(i\pi/8)\begin{bmatrix} \exp(-i\pi/8) & 0 \\ 0 & \exp(i\pi/8) \end{bmatrix}. \tag{4.3}$$

Nevertheless, the nomenclature is in some respects rather unfortunate, and we often refer to this gate as the T gate.

Recall also that a single qubit in the state $a|0\rangle + b|1\rangle$ can be visualized as a point (θ, φ) on the unit sphere, where $a = \cos(\theta/2)$, $b = e^{i\varphi}\sin(\theta/2)$, and a can be taken to be real because the overall phase of the state is unobservable. This is called the Bloch sphere representation, and the vector $(\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta)$ is called the Bloch vector. We shall return to this picture often as an aid to intuition.

Exercise 4.1: In Exercise 2.11, which you should do now if you haven't already done it, you computed the eigenvectors of the Pauli matrices. Find the points on the Bloch sphere which correspond to the normalized eigenvectors of the different Pauli matrices.

The Pauli matrices give rise to three useful classes of unitary matrices when they are exponentiated, the *rotation operators* about the $\hat{x}$, $\hat{y}$, and $\hat{z}$ axes, defined by the equations:

$$R_x(\theta) \equiv e^{-i\theta X/2} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}X = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \tag{4.4}$$

$$R_y(\theta) \equiv e^{-i\theta Y/2} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}Y = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \tag{4.5}$$

$$R_z(\theta) \equiv e^{-i\theta Z/2} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}Z = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}. \tag{4.6}$$

Exercise 4.2: Let x be a real number and A a matrix such that $A^2 = I$. Show that

$$\exp(iAx) = \cos(x)I + i\sin(x)A. \tag{4.7}$$

Use this result to verify Equations (4.4) through (4.6).

Exercise 4.3: Show that, up to a global phase, the $\pi/8$ gate satisfies $T = R_z(\pi/4)$.

Exercise 4.4: Express the Hadamard gate H as a product of R_x and R_z rotations and $e^{i\varphi}$ for some φ.

If $\hat{n} = (n_x, n_y, n_z)$ is a real unit vector in three dimensions then we generalize the previous definitions by defining a rotation by θ about the $\hat{n}$ axis by the equation

$$R_{\hat{n}}(\theta) \equiv \exp(-i\theta\, \hat{n}\cdot\vec{\sigma}/2) = \cos\left(\frac{\theta}{2}\right) I - i\sin\left(\frac{\theta}{2}\right)(n_x X + n_y Y + n_z Z), \tag{4.8}$$

where $\vec{\sigma}$ denotes the three component vector (X, Y, Z) of Pauli matrices.

Exercise 4.5: Prove that $(\hat{n}\cdot\vec{\sigma})^2 = I$, and use this to verify Equation (4.8).

Exercise 4.6: (Bloch sphere interpretation of rotations) One reason why the $R_{\hat{n}}(\theta)$ operators are referred to as rotation operators is the following fact, which you are to prove. Suppose a single qubit has a state represented by the Bloch vector $\vec{\lambda}$. Then the effect of the rotation $R_{\hat{n}}(\theta)$ on the state is to rotate it by an angle θ about the $\hat{n}$ axis of the Bloch sphere. This fact explains the rather mysterious looking factor of two in the definition of the rotation matrices.

Exercise 4.7: Show that $XYX = -Y$ and use this to prove that $XR_y(\theta)X = R_y(-\theta)$.

Exercise 4.8: An arbitrary single qubit unitary operator can be written in the form

$$U = \exp(i\alpha)R_{\hat{n}}(\theta) \tag{4.9}$$

for some real numbers α and θ, and a real three-dimensional unit vector $\hat{n}$.

1. Prove this fact.
2. Find values for α, θ, and $\hat{n}$ giving the Hadamard gate H.
3. Find values for α, θ, and $\hat{n}$ giving the phase gate

$$S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}. \tag{4.10}$$

An arbitrary unitary operator on a single qubit can be written in many ways as a combination of rotations, together with global phase shifts on the qubit. The following theorem provides a means of expressing an arbitrary single qubit rotation that will be particularly useful in later applications to controlled operations.

Theorem 4.1: (**Z-Y decomposition for a single qubit**) Suppose U is a unitary operation on a single qubit. Then there exist real numbers α, β, γ and δ such that

$$U = e^{i\alpha}R_z(\beta)R_y(\gamma)R_z(\delta). \tag{4.11}$$

Proof
Since U is unitary, the rows and columns of U are orthonormal, from which it follows that there exist real numbers α, β, γ,and δ such that

$$U = \begin{bmatrix} e^{i(\alpha-\beta/2-\delta/2)} \cos \frac{\gamma}{2} & -e^{i(\alpha-\beta/2+\delta/2)} \sin \frac{\gamma}{2} \\ e^{i(\alpha+\beta/2-\delta/2)} \sin \frac{\gamma}{2} & e^{i(\alpha+\beta/2+\delta/2)} \cos \frac{\gamma}{2} \end{bmatrix}. \tag{4.12}$$

Equation (4.11) now follows immediately from the definition of the rotation matrices and matrix multiplication. □

Exercise 4.9: Explain why any single qubit unitary operator may be written in the form (4.12).

Exercise 4.10: (**X-Y decomposition of rotations**) Give a decomposition analogous to Theorem 4.1 but using R_x instead of R_z.

Exercise 4.11: Suppose $\hat{m}$ and $\hat{n}$ are non-parallel real unit vectors in three dimensions. Use Theorem 4.1 to show that an arbitrary single qubit unitary U may be written

$$U = e^{i\alpha} R_{\hat{n}}(\beta) R_{\hat{m}}(\gamma) R_{\hat{n}}(\delta), \tag{4.13}$$

for appropriate choices of α, β, γ and δ.

The utility of Theorem 4.1 lies in the following mysterious looking corollary, which is the key to the construction of controlled multi-qubit unitary operations, as explained in the next section.

Corollary 4.2: Suppose U is a unitary gate on a single qubit. Then there exist unitary operators A, B, C on a single qubit such that $ABC = I$ and $U = e^{i\alpha} AXBXC$, where α is some overall phase factor.

Proof
In the notation of Theorem 4.1, set $A \equiv R_z(\beta)R_y(\gamma/2)$, $B \equiv R_y(-\gamma/2)R_z(-(\delta+\beta)/2)$ and $C \equiv R_z((\delta-\beta)/2)$. Note that

$$ABC = R_z(\beta)R_y\left(\frac{\gamma}{2}\right) R_y\left(-\frac{\gamma}{2}\right) R_z\left(-\frac{\delta+\beta}{2}\right) R_z\left(\frac{\delta-\beta}{2}\right) = I\,. \tag{4.14}$$

Since $X^2 = I$, and using Exercise 4.7, we see that

$$XBX = XR_y\left(-\frac{\gamma}{2}\right) XXR_z\left(-\frac{\delta+\beta}{2}\right) X = R_y\left(\frac{\gamma}{2}\right) R_z\left(\frac{\delta+\beta}{2}\right). \tag{4.15}$$

Thus

$$AXBXC = R_z(\beta)R_y\left(\frac{\gamma}{2}\right) R_y\left(\frac{\gamma}{2}\right) R_z\left(\frac{\delta+\beta}{2}\right) R_z\left(\frac{\delta-\beta}{2}\right) \tag{4.16}$$

$$= R_z(\beta)R_y(\gamma)R_z(\delta)\,. \tag{4.17}$$

Thus $U = e^{i\alpha}AXBXC$ and $ABC = I$, as required. □

Exercise 4.12: Give A, B, C, and α for the Hadamard gate.

Exercise 4.13: (Circuit identities) It is useful to be able to simplify circuits by inspection, using well-known identities. Prove the following three identities:

$$HXH = Z; \quad HYH = -Y; \quad HZH = X. \tag{4.18}$$

Exercise 4.14: Use the previous exercise to show that $HTH = R_x(\pi/4)$, up to a global phase.

Exercise 4.15: (Composition of single qubit operations) The Bloch representation gives a nice way to visualize the effect of composing two rotations.

(1) Prove that if a rotation through an angle β_1 about the axis $\hat{n}_1$ is followed by a rotation through an angle β_2 about an axis $\hat{n}_2$, then the overall rotation is through an angle β_{12} about an axis $\hat{n}_{12}$ given by

$$c_{12} = c_1 c_2 - s_1 s_2 \, \hat{n}_1 \cdot \hat{n}_2 \tag{4.19}$$

$$s_{12}\hat{n}_{12} = s_1 c_2 \hat{n}_1 + c_1 s_2 \hat{n}_2 - s_1 s_2 \, \hat{n}_2 \times \hat{n}_1 \,, \tag{4.20}$$

where $c_i = \cos(\beta_i/2)$, $s_i = \sin(\beta_i/2)$, $c_{12} = \cos(\beta_{12}/2)$, and $s_{12} = \sin(\beta_{12}/2)$.

(2) Show that if $\beta_1 = \beta_2$ and $\hat{n}_1 = \hat{z}$ these equations simplify to

$$c_{12} = c^2 - s^2 \, \hat{z} \cdot \hat{n}_2 \tag{4.21}$$

$$s_{12}\hat{n}_{12} = sc(\hat{z} + \hat{n}_2) - s^2 \, \hat{n}_2 \times \hat{z} \,, \tag{4.22}$$

where $c = c_1$ and $s = s_1$.

Symbols for the common single qubit gates are shown in Figure 4.2. Recall the basic properties of quantum circuits: time proceeds from left to right; wires represent qubits, and a '/' may be used to indicate a bundle of qubits.

Hadamard	$-\boxed{H}-$	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Pauli-X	$-\boxed{X}-$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y	$-\boxed{Y}-$	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z	$-\boxed{Z}-$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Phase	$-\boxed{S}-$	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$	$-\boxed{T}-$	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$

Figure 4.2. Names, symbols, and unitary matrices for the common single qubit gates.

4.3 Controlled operations

'If A is true, then do B'. This type of *controlled operation* is one of the most useful in computing, both classical and quantum. In this section we explain how complex controlled operations may be implemented using quantum circuits built from elementary operations.