Notes 8.370/18.435 Fall 2022

Lecture 3 Prof. Peter Shor

Last time, we started talking about quantum mechanics. We mentioned the principle that: *Isolated quantum systems evolve unitarily.* That is, for an isolated system (one that does not interact with its environment), there is a unitary matrix U_t such that if we let the system alone for time t, $|\,\Psi_t\rangle = U_t\,|\,\Psi_0\rangle$, where the initial state of the system is $|\,\Psi_0\rangle$ and ehe final state of the system is $|\,\Psi_t\rangle$.

Unitary matrices U are the complex analog of rotation matrices, also called orthogonal matrices; they take unit length complex vectors to unit length complex vectors. A matrix is unitary if and only if $U^\dagger U = I$. (An equivalent condition is $UU^\dagger = I$.) Here $U^\dagger$ is the complex conjugate transpose of U (also called the *Hermitian transpose*). We mentioned three specific unitary matrices last time, the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We discussed the representation of spin-$\frac{1}{2}$ states on the Bloch sphere, and we looked at the actions of the Pauli matrices on the Bloch sphere, these being 180° rotations around the x-, y-, and z-axes, respectively. .

Today, we'll be talking about how unitary matrices arise in quantum mechanics, and then talk more about the Bloch sphere and rotations on the Bloch sphere.

So suppose you want to build a quantum computer, and you want to implement a unitary matrix U. What do you do? There's no magic incantation that takes the state directly from $|\,\psi\rangle$ to $U\,|\,\psi\rangle$. In fact, quantum unitary evolution can only changes quantum states continuously, and not in discrete jumps.

To explain how to implement a unitary gate, first I need to say something about quantum mechanics. Quantum mechanics assumes that isolated systems evolve according to Schödinger's equation,

$$i\hbar \frac{d}{dt}\,|\,\psi(t)\rangle = H\,|\,\psi(t)\rangle\,.$$

Here $\hbar$ is a very small physical constant, $|\,\psi(t)\rangle$ is the quantum state at time t, and H is a Hamiltonian—a Hermitian[1] matrix, to be exact, which can be associated with a Hermitian quadratic form that takes the quantum state as input and outputs its energy.

If we assume that H is constant, we can solve this equation:

$$|\,\psi(t)\rangle = e^{-iHt/\hbar}\,|\,\psi(0)\rangle$$

Let's assume that the eigenvectors of H are $|\,\xi_1\rangle$, $|\,\xi_2\rangle$, $\ldots$, $|\,\xi_d\rangle$, with λ_i be the eigenvalue corresponding to $|\,\xi_i\rangle$. What the above equation means is that if the intial state $|\,\psi(0)\rangle$ is $\sum_i \alpha_i\,|\,\xi_i\rangle$, then

$$|\,\psi(t)\rangle = \sum_i e^{-\lambda_i t/\hbar} \alpha_i\,|\,\xi_i\rangle\,.$$

[1] A Hermitian matrix is one that satisfies $M = M^\dagger$.

We're not actually going to be using Schrödinger's equation until much later in the course. I'm introducing it now to give you some idea as to how you might implement unitary gates in practice, and to motivate the next thing I'll be talking about, which is three one-qubit gates which are rotations of the Bloch sphere by an angle θ. These are

$$\begin{aligned} R_x(\theta) &= e^{-i\theta\sigma_x/2}, \\ R_y(\theta) &= e^{-i\theta\sigma_y/2}, \\ R_z(\theta) &= e^{-i\theta\sigma_z/2}, \end{aligned}$$

What are these rotations? We have $R_z(\theta) = e^{-i\theta\sigma_z/2}$. To exponentiate a diagonal matrix, we can simply exponentiate each of the elements along the diagonal This gives

$$R_z(\theta) = e^{-i\theta\sigma_z/2} = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix} = e^{-i\theta/2} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}.$$

You can check that if $\theta = \pi/2$, this is a rotation of a $\pi/2$ angle around the z-axis (multiplied by a global phase) and if $\theta = \pi$, this is a rotation of π around the z-axis (again multiplied by a global phase). So this gives us rotations around the z axis of an arbitrary angle.

To compute $R_y(\theta)$, we could diagonalize it to get $D = U^\dagger R_y(\theta) U$, and then exponentiate D to get $R_y(\theta) = U e^D U^\dagger$. We will compute it using a different method, to show how this method works. What we do is use a Taylor expansion.

$$e^{-i\theta\sigma_y/2} = I - i\frac{\theta}{2}\sigma_y - \frac{1}{2}\left(\frac{\theta}{2}\right)^2 \sigma_y^2 + i\frac{1}{3!}\left(\frac{\theta}{2}\right)^3 \sigma_y^3 + \frac{1}{4!}\left(\frac{\theta}{2}\right)^4 \sigma_y^4 - i\frac{1}{5!}\left(\frac{\theta}{2}\right)^5 \sigma_y^5 + \dots$$

Since $\sigma_y^2 = I$, we have

$$\begin{aligned} e^{-i\theta\sigma_y/2} &= I - i\frac{\theta}{2}\sigma_y - \frac{1}{2}\left(\frac{\theta}{2}\right)^2 I + i\frac{1}{3!}\left(\frac{\theta}{2}\right)^3 \sigma_y + \frac{1}{4!}\left(\frac{\theta}{2}\right)^4 I \dots \\ &= I\left(1 - \frac{1}{2}\left(\frac{\theta}{2}\right)^2 + \frac{1}{4!}\left(\frac{\theta}{2}\right)^4 - \dots\right) - i\sigma_y\left(\frac{\theta}{2} - \frac{1}{3!}\left(\frac{\theta}{2}\right)^3 + \frac{1}{5!}\left(\frac{\theta}{2}\right)^5 - \dots\right) \\ &= I\cos\frac{\theta}{2} - i\sigma_y \sin\frac{\theta}{2} \end{aligned}$$

But $-i\sigma_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, so we see that

$$e^{-i\theta\sigma_y/2} = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix},$$

which we see is a rotation in the $x - z$ plane. Looking at its action on the states of the Bloch sphere, it rotates the Bloch sphere around the y-axis by an angle of θ.

We can similarly see that

$$e^{-i\theta\sigma_x/2} = \begin{pmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix},$$

Now that we have $R_y(\theta)$ and $R_z(\theta)$, we can perform any one-qubit unitary by applying

$$R_z(\theta_3)R_y(\theta_2)R_z(\theta_1).$$

To see this, let us visualize what this does to the Bloch sphere. We first rotate the Bloch sphere by an angle of θ_1 around the north pole. The second rotation moves the north pole down to an arbitrary longitude. Finally, by applying $R_z(\theta_3)$, we can move the north pole to end up at an arbitrary latitude. Combined, these give an arbitrary rotation of the Bloch sphere. See the figure

Figure 1: Performing an arbitrary rotation by using three rotations, around the z-axis, the y-axis, and the z-axis.

We now explain one way to find the quantum state $|\,\phi_p\rangle$ corresponding to a point p on the Bloch sphere. There are other ways to do this, which lead to simpler expressions; we may revisit this question later in the term and explain them.

Suppose we have a point $p = (p_x, p_y, p_z)$ on the Bloch sphere $p_i \in \mathbb{R}$. Since it's on a unit sphere, we must have $p_x^2 + p_y^2 + p_z^2 = 1$. Let us consider the 2×2 matrix

$$M_p = p_x\sigma_x + p_y\sigma_y + p_z\sigma_z,$$

Since $\sigma_x, \sigma_y, \sigma_z$ are Hermitian matrices, M_p must also be Hermitian, that is $M_p = M_p^\dagger$. Now,

$$M_p^2 = (p_x^2 + p_y^2 + p_z^2)I + 2p_xp_y(\sigma_x\sigma_y + \sigma_y\sigma_x) + 2p_yp_z(\sigma_y\sigma_y + \sigma_z\sigma_y) + 2p_xp_z(\sigma_x\sigma_z + \sigma_z\sigma_x) \quad = I.$$

where the last equality follows from the facts that the vector p has length 1 and $\sigma_a\sigma_b = -\sigma_b\sigma_z$ if $a \neq b$.

We can also show that

$$\mathrm{Tr}M_p = p_x\mathrm{Tr}\sigma_x + p_y\mathrm{Tr}\sigma_y + p_z\mathrm{Tr}\sigma_z = 0,$$

since the Pauii matrices all have trace 0. Since $M_p^2 = I$, its eigenvalues have to be ± 1. And since its trace is 0, one of its eigenvalues has to be 1 and the other has to be -1. Now, we will let the eigenvector with eigenvalue $+1$ be the corresponding quantum state $|\,\psi_p\rangle$ to point p on the unit sphere. We already know this holds for the unit vectors on the x, y, and z axes. Note also that since M_p is a Hermitian matrix its two eigenvectors are orthogonal, and since $M_p = -M_{-p}$, the -1 eigenvector of M_p is the point antipodal to $|\,\phi_p\rangle$.

Let's illustrate this by an example. Let $p = \left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right)$. Then

$$M_p = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Now, M_p has eigenvalues 1 and -1, and its eigenvectors are

$$\frac{\sqrt{2+\sqrt{2}}}{2}\,|\,0\rangle + \frac{\sqrt{2-\sqrt{2}}}{2}\,|\,1\rangle \quad \text{and} \quad -\frac{\sqrt{2-\sqrt{2}}}{2}\,|\,0\rangle + \frac{\sqrt{2+\sqrt{2}}}{2}\,|\,1\rangle,$$

where the first eigenvector has eigenvalue $+1$ and the second -1.

These vectors are in fact just

$$\cos\frac{\pi}{8}\,|\,0\rangle + \sin\frac{\pi}{8}\,|\,1\rangle \quad \text{and} \quad -\sin\frac{\pi}{8}\,|\,-\rangle + \cos\frac{\pi}{8}\,|\,1\rangle.$$

This makes sence, because the point $p = \frac{1}{\sqrt{2}}(1,0,1)$ is halfway between $p = (1,0,0)$ and $p = (0,0,1)$, and these points correspond to $\cos\frac{\pi}{4}\,|\,0\rangle + \sin\frac{\pi}{4}\,|\,1\rangle$ and $\cos 0\,|\,0\rangle + \sin 0\,|\,1\rangle$, respectively.