CS 294-2 Hamiltonians, Schrodinger's Equation, Uncertainty Relations. 10/26/04
Fall 2004 Lecture 15

Ankur Mehta, mehtank@eecs.berkeley.edu

1 1-D Random Walk

1.1 Classical

Each time step, go one step in a random direction.

If you call the distance travelled in time step i by x_i, then

$$x_i = \begin{cases} +1 & w.p.\ 1/2 \\ -1 & w.p.\ 1/2 \end{cases}$$

and the total distance travelled in n steps is $X = x_1 + \ldots + x_n$. Now, $E(X) = nE(x_i) = 0$ so it is expected that you end up where you started from. However, $var(X) = n(var(x_i)) = nE[(x_i - E(x_i))^2] = nE(x_i^2) = n$, and so in n time steps you have covered a distance of $O(\sqrt{n})$. Alternately, it takes $O(k^2)$ time to go a distance k.

1.2 Probabilistic

We have $X \in \mathbb{Z}$ representing the total distance travelled, and a coin $b \in \{0,1\}$. Every step of the walk we update our position depending on the coin, then flip the coin in preparation for the next step. That is,
WALK : $X \leftarrow X + (-1)^b$; pick new b randomly; repeat.

The (binomial) probability distribution for X is maximum at $X = 0$ and trails off farther away.

1.3 Quantum

Similar to the probabilistic random walk, we have $X \in \mathbb{Z}$ representing the total distance travelled, but now our coin $|b\rangle \in \mathbb{C}^2$ is a quantum bit. The coin flip is implemented as some unitary operator U (e.g. the Hadamard transform H). That is,
WALK : $|X,b\rangle \leftarrow |X + (-1)^b, b\rangle$; $|b\rangle \leftarrow U|b\rangle$; repeat.

The quantum walk takes $O(k)$ time to go a distance k. There are naturally many different ways to reach 0 after k time steps, but each of those ways is likely to carry a different phase, so they interfere destructively. Correspondingly, there are fewer ways to get outside some distance away from the start, so there is more constructive interference. The probability distribution for X after k time steps is small at $X = 0$ with two peaks centered at $\pm ck$ for some constant c.

2 Schrodinger's Equation

This equation gives how a quantum state $|\psi\rangle$ evolves over time. In natural units where $\hbar = c = 1$, Schrodinger's equation is

$$i\frac{d|\psi\rangle}{dt} = H|\psi\rangle$$

where H is the Hamiltonian operator. The Hamiltonian is a hermitian operator, and so corresponds to an observable, namely energy.

Because the Hamiltonian is hermitian, it has an orthonormal set of eigenstates $|v_i\rangle$ with eigenvalues (energies) λ_i. A state in one of these eigenstates evolves as follows:

$$|\psi(t=0)\rangle = |v_i\rangle \implies |\psi(t)\rangle = e^{-i\lambda_i t}|v_i\rangle.$$

Thus in the energy eigenstate basis, the unitary time evolution operator $U(t) : |\psi(t)\rangle = U(t)|\psi(0)\rangle$ is given by

$$U(t) = e^{-iHt} = \begin{bmatrix} e^{-i\lambda_1 t} & & 0 \\ & \ddots & \\ 0 & & e^{-i\lambda_n t} \end{bmatrix}.$$

3 1-D particle

In the case of a 1-D particle, the state $|\psi\rangle = \psi(x,t)$ is the amplitude of the particle at position x at time t. In this case, the Hamiltonian operator $H = \partial^2/\partial x^2$, so Schrodinger's equation reads

$$i\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}.$$

A state with velocity $\sim k$ is given by $\psi(x) = e^{ikx}$, so the amplitude with which an arbitrary state ϕ has velosity k is given by

$$\langle \psi | \phi \rangle = \langle e^{ikx} | \phi \rangle = \int_{-\infty}^{\infty} e^{ikx}\phi(x,t)dx.$$

This is similar to the Fourier transform of the wavefunction, that is, we can describe another wavefunction in velocity space as the F.T. of the position wave function:

$$\hat{\phi}(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx}\phi(x,t)dx.$$

4 Uncertainty Relations

As we saw, the position and velocity of a 1-D particle are Fourier transforms of one another. Thus, localizing one comes at the expense of a wider spread in the other. The minimum standard deviation spread comes when both are of Gaussian form, then $\Delta x \Delta v = \Omega(1)$.

Similarly, consider a finite abelian group G. Starting with a distribution $D = \sum_g \alpha_g |g\rangle$, it's Fourier transform becomes a distribution $\hat{D} = \sum_g \hat{\alpha}_g |g\rangle$. We have the following uncertainty relations about these distributions:

$$\sum_g |\alpha_g| + \sum_g |\hat{\alpha}_g| \geq \sqrt{|G|} \qquad\qquad S(D) + S(\hat{D}) \geq \log|G|$$

where $S(D)$ is the entropy of the distribution D.

5 Dirac Equation

Classically, the energy E of a 1-D particle is given by $E = p^2/2m$, where p is its momentum and m is its mass. The quantum analog of this relationship can be obtained by the translating the observables E and p into their respective operators (again in natural units) $E \to \hat{H} = i\partial/\partial t$ and $p \to \hat{p} = -i\partial/\partial x$, yielding Schrodinger's equation

$$i\frac{\partial \psi}{\partial t} = \frac{1}{2m}\frac{\partial^2 \psi}{\partial x^2}.$$

Relativistically, the energy of a particle is given by $E^2 = p^2 + m^2$, so the quantum analog should satisfy $\hat{H}^2 = \hat{p}^2 + m^2\hat{I}$. Consider instead a tensor product of the particle state with an additional qubit state. Then, in matrix form we could have

$$\hat{H} = \left[\begin{array}{c|c} \hat{p} & m\hat{I} \\ \hline m\hat{I} & -\hat{p} \end{array}\right] = \left[\begin{array}{c|c} \hat{p} & 0 \\ \hline 0 & -\hat{p} \end{array}\right] + m\left[\begin{array}{c|c} \hat{0} & \hat{I} \\ \hline \hat{I} & \hat{0} \end{array}\right]$$

such that

$$\hat{H}^2 = \left[\begin{array}{c|c} \hat{p}^2 + m^2\hat{I} & 0 \\ \hline 0 & \hat{p}^2 + m^2\hat{I} \end{array}\right].$$