

MATH 217A. Introduction to Quantum Algorithms

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Lecture 2. Random walks and PDEs

In the previous lecture we discussed Feynman's argument that it is possible to simulate classical and probabilistic physical systems, but not quantum systems, efficiently on a classical computer [1]. With this as motivation, let us consider a very simple quantum system, a quantum particle evolving on \mathbb{Z}_N , the integers modulo N , which we may think of as the cycle graph C_N . In considering this system we are taking seriously Feynman's starting assumption that space be discrete; a more familiar physical setting, however, is an electron moving in a (one-dimensional) crystal, where it hops from the neighborhood of one crystal atom to another [2, §13.1].

Postulate 0 of quantum mechanics says that the state of this system is represented by a vector ψ in some (projective) Hilbert space \mathcal{H} . To understand which we introduce:

POSTULATE 1. A (complete) *measurement* of a quantum system is represented by an orthonormal basis $\{e_i\}$ of \mathcal{H} . The *result* of this measurement is probabilistic: the state becomes e_i with probability $|\langle e_i|\psi\rangle|^2$.

Here $\langle e_i|\psi\rangle$ is the inner product $\bar{e}_i \cdot \psi$. In *Dirac notation* $|\psi\rangle = \psi \in \mathcal{H}$, while $\langle e_i| = e_i^\dagger \in \mathcal{H}^\dagger$ is the dual (adjoint) of e_i .

Notice that this implies that the state of the quantum system should be a unit vector, *i.e.*, $\sum_i |\langle e_i|\psi\rangle|^2 = 1 = \langle \psi|\psi\rangle = \psi^\dagger \psi$, so that the result probabilities sum to 1. It also explains why it is only the element in $P(\mathcal{H})$ that matters: we can choose any norm 1 representative of the equivalence class of scalar multiples of $\psi \in \mathcal{H}$ since multiplying ψ by a unit complex number, a phase, does not change the results of measurements, nor their probabilities.

For the system of a particle evolving quantum mechanically on \mathbb{Z}_N , it is reasonable to take $\{e_x \mid x \in \mathbb{Z}_N\}$ to be a measurement, *i.e.*, to imagine that there is an experiment that would measure the location (position) of the particle.* Thus the Hilbert space in which the state of this system lies is \mathbb{C}^N . Writing the state $\psi \in \mathbb{C}^N$ in the position basis, we have:

$$\psi = \begin{pmatrix} \langle e_0|\psi\rangle \\ \langle e_1|\psi\rangle \\ \vdots \\ \langle e_{N-1}|\psi\rangle \end{pmatrix} =: \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{N-1} \end{pmatrix}.$$

What should be the dynamics of this system? We assume that the evolution is *local* (the change in ψ_x depends only on the values of ψ_y for $y \in \mathcal{N}(x) \subset \mathbb{Z}_N$, some neighborhood of

* There are, however, situations in which this is not a reasonable assumption and in which it would be more appropriate to take the distinct locations to be *indistinguishable*. We may discuss this later.

x), homogeneous (translation invariant), and symmetric (invariant under $x \mapsto -x$). The simplest model is linear:

$$\begin{aligned} \frac{d\psi_0}{dt} &= a\psi_0 + b\psi_1 && + b\psi_{N-1} \\ \frac{d\psi_1}{dt} &= b\psi_0 + a\psi_1 + b\psi_2 && \\ &\vdots && \ddots \\ \frac{d\psi_{N-1}}{dt} &= b\psi_0 && + b\psi_{N-2} + a\psi_{N-1} \end{aligned}, \quad (1)$$

using the smallest nontrivial, symmetric neighborhood, $\mathcal{N}(x) = \{x-1, x, x+1\}$.

More generally, such linear dynamics take the form

$$\dot{\psi} = A\psi. \quad (2)$$

The condition that ψ always has norm 1 imposes constraints on A :

$$1 = \psi^\dagger \psi \implies 0 = \frac{d}{dt}(\psi^\dagger \psi) = \dot{\psi}^\dagger \psi + \psi^\dagger \dot{\psi} = \psi^\dagger A^\dagger \psi + \psi^\dagger A \psi = \psi^\dagger (A^\dagger + A) \psi,$$

which implies $A^\dagger = -A$, *i.e.*, A is skew-Hermitian, or $A \in \mathfrak{u}(N)$, the Lie algebra of $U(N)$ (which is the Lie group of transformations of \mathbb{C}^N preserving the ℓ^2 -norm). Thus we can write $A = -iH$, where H is real and symmetric, and (2) becomes

$$i\dot{\psi} = H\psi. \quad (3)$$

H is called the *Hamiltonian* of the system, and (3) is the Schrödinger equation.

In principle, it is easy to solve (3): Since H is symmetric, we can diagonalize it to be $H = O\Lambda O^\top$, where O is orthogonal and $\Lambda = \text{diag}(\lambda_0, \dots, \lambda_{N-1})$ is the diagonal matrix with the eigenvalues of H along its diagonal. Then (3) becomes $iO^\top \dot{\psi} = \Lambda O^\top \psi$, or $i\dot{\phi} = \Lambda\phi$ if we set $\phi = O^\top \psi$. This system is uncoupled, so we can solve for each component $\phi_k(t) = \phi_k(0)e^{-i\lambda_k t}$; then $\psi(t) = O\phi(t)$.

Notice that if we change H to $H + EI$, where $E \in \mathbb{R}$ and I is the N -dimensional identity matrix, all the eigenvalues simply shift by E , to $\lambda_k + E$, and $\psi(t)$ is multiplied by a phase, becoming $\psi(t)e^{-iEt}$. As we noted earlier, this phase has no physical meaning (its physical interpretation is a choice for the 0 of energy which, at least in non-general relativistic theories, has no physical consequences). Thus we can add any convenient multiple of the identity to the Hamiltonian.

Writing the model (1) in terms of the Hamiltonian, set $b = i\gamma$ and, taking advantage of this freedom, set $a = -2i\gamma$, so that

$$H = \begin{pmatrix} 2\gamma & -\gamma & & -\gamma \\ -\gamma & 2\gamma & -\gamma & \\ & & \ddots & \\ -\gamma & & -\gamma & 2\gamma \end{pmatrix} = -\gamma \begin{pmatrix} -2 & 1 & & 1 \\ 1 & -2 & 1 & \\ & & \ddots & \\ 1 & & 1 & -2 \end{pmatrix} = -\gamma L,$$

where $L = A - D$ is the *graph Laplacian*. Here A is the *adjacency matrix* of a graph: A_{xy} is 1 if vertices x and y are connected by an edge and 0 otherwise; D is a diagonal matrix with d_{xx} being the *degree* of vertex x , namely the number of other vertices with which it shares an edge. Equation (3) with $H = -\gamma L$ describes continuous time quantum evolution on *any* graph. For the cycle C_N , the system of differential equations is

$$i \frac{d\psi_x}{dt} = -\gamma(\psi_{x+1} - 2\psi_x + \psi_{x-1}), \quad x \in \mathbb{Z}_N. \quad (4)$$

The form of the right hand side on (4) (and the name “graph Laplacian”) suggests taking a continuum limit. Suppose we define a metric on the graph C_N by assigning a length $\epsilon = 1/N$ to each edge. Then it discretizes the unit interval with periodic boundary conditions, and thus ψ discretizes a function $S^1 \rightarrow \mathbb{C}$. Assuming this function is sufficiently smooth, we can write:

$$\psi_{x+1} - 2\psi_x + \psi_{x-1} \mapsto \psi(x + \epsilon) - 2\psi(x) + \psi(x - \epsilon) = \epsilon^2 \frac{\partial^2 \psi}{\partial x^2} + O(\epsilon^3).$$

So if we take the $\epsilon \rightarrow 0$ limit, keeping $\gamma\epsilon^2 = \kappa$ constant, we get the familiar continuum Schrödinger equation:

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

In physical units, $\kappa = \hbar/2m$.

Now consider a classical stochastic particle hopping from vertex to adjacent vertex. Let

$$p = \begin{pmatrix} p_0 \\ p_1 \\ \vdots \\ p_{N-1} \end{pmatrix}$$

be the probability distribution (state) of the system, where p_x denotes the probability that the particle is at position x ; thus $\|p\|_1 = \sum_x p_x = 1$. If the rate for the particle to hop to an adjacent vertex is b , the evolution is described by:

$$\begin{aligned} \frac{dp_0}{dt} &= ap_0 + bp_1 && + bp_{N-1} \\ \frac{dp_1}{dt} &= bp_0 + ap_1 + bp_2 && \\ &\vdots && \ddots \\ \frac{dp_{N-1}}{dt} &= bp_0 && + bp_{N-2} + ap_{N-1} \end{aligned} \quad (5)$$

Since p must always have unit ℓ^1 -norm,

$$0 = \frac{d}{dt}(p_0 + \cdots + p_{N-1}) = (a + 2b)(p_0 + \cdots + p_{N-1}) \implies a = -2b.$$

Thus (5) becomes

$$\frac{dp}{dt} = bLp \tag{6}$$

and, just the case of quantum evolution, this holds for *any* graph. Also, just as in the case of quantum evolution, we can take the continuum limit of (6) by letting the edge length $\epsilon \rightarrow 0$ while keeping $b\epsilon^2 = \kappa$ constant. For sufficiently smooth $p(x)$ this gives

$$\frac{\partial p}{\partial t} = \kappa \frac{\partial^2 p}{\partial x^2} \tag{7}$$

This is the *diffusion* or *heat* equation.

The classical model described by (6) is a *continuous time (classical) random walk*. By analogy, the quantum model described by (4) is a *continuous time quantum random walk*.

References

- [1] R. P. Feynman, “Simulating physics with computers”, *Int. J. Theor. Phys.* **21** (1982) 467–488.
- [2] R. P. Feynman, R. B. Leighton and M. Sands, *Lectures on Physics*, Vol. III. (Menlo Park, CA: Addison-Wesley 1965).