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Math 217a. Introduction to Quantum Algorithms

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Lecture 3. Continuous and discrete time classical random walks

In the previous lecture we discussed classical and quantum random walks on $\mathbb{Z}_N$, in continuous time, and took continuum limits in space to get the heat and Schrödinger equations.

> Problem 3.1. The classical and quantum random walk evolutions preserve the ℓ^1- and ℓ^2-norms, respectively, of the state vector. Can you construct a system of linear ODEs, local on $\mathbb{Z}_N$, that preserves the ℓ^3-norm? If not, can you prove it is impossible? Or can you construct a nonlocal, or nonlinear system that does so? For context and hints see [1] and [2].

The physical systems Feynman considered in his original paper [3], however, are discrete in time, as well as in space. So we want to consider discrete time random walks, starting with classical ones.

Discrete time integrated random walk

The continuous time dynamics from the last lecture is $\dot{p} = bLp$, which has solution

$$p(t) = e^{bLt}p(0) = M(t)p(0), \tag{1}$$

where $M(t)$ is a one-parameter family of *Markov* matrices, *i.e.*, matrices with non-negative entries summing to 1 in each column, which thus preserve the ℓ^1-norm.

> A Markov matrix P is *embeddable* if there is an *intensity* matrix Q, such that $P = e^Q$ and e^{Qt} is a Markov matrix for $t \geq 0$. Q has non-negative off-diagonal entries, and each column sums to 0. For each t, $M(t)$ defined by (1) is embeddable, since it is embedded in the one-parameter family $M(t) = e^{bLt}$. See Davies [4] for a recent survey of results on this topic.

Integrating the continuous time evolution of (1) for time Δt will give a discrete time evolution matrix $M(\Delta t) = e^{bL\Delta t}$.

Since the dynamics is translation invariant: $L = -2I + X + X^{-1}$, where $X_{ij} = \delta_{i,j+1}$, $i, j \in \mathbb{Z}_N$, we can compute $M(\Delta t)$ by diagonalizing L using the discrete Fourier transform:

$$F_{kx} = \frac{1}{\sqrt{N}} e^{-2\pi i k x/N} = \frac{1}{\sqrt{N}}\omega^{-kx}, \text{ where } \omega^N = 1, \text{ so } (F^{-1})_{yk} = \frac{1}{\sqrt{N}}\omega^{yk}.$$

For practice let's check that this is really F^{-1}:

$$(F^{-1}F)_{yx} = \frac{1}{N}\sum_k \omega^{yk}\omega^{-kx} = \frac{1}{N}\sum_k \omega^{(y-x)k} = \begin{cases} 1 & \text{if } y - x = 0; \\ \frac{1}{N}\frac{1-\omega^{(y-x)N}}{1-\omega^{y-x}} = 0 & \text{otherwise.} \end{cases}$$

The calculation for FF^{-1} is similar. Now let's see that the discrete Fourier transform diagonalizes X:

$$(F^{-1}XF)_{yx} = \frac{1}{N}\sum_{kl}\omega^{yk}\delta_{k,l+1}\omega^{-lx} = \frac{1}{N}\sum_{k}\omega^{yk}\omega^{-(k-1)x} = \omega^x\frac{1}{N}\sum_k\omega^{k(y-x)} = \omega^x\delta_{yx}.$$

Similarly, $(F^{-1}X^{-1}F)_{yx} = \omega^{-x}\delta_{yx}$. Thus

$$(F^{-1}LF)_{yx} = -2 + (\omega^x + \omega^{-x})\delta_{yx} = -|1-\omega^x|^2\delta_{yx} =: D_{yx}.$$

Now $M(\Delta t) = Fe^{bD\Delta t}F^{-1}$. The first column of $e^{bD\Delta t}F^{-1}$ is just the diagonal of $e^{bD\Delta t}$, so the zeroth column of $M(\Delta t)$ is the discrete Fourier transform of this:

$$\big(M(\Delta t)\big)_{y0} = \sum_x F_{yx}e^{-b|1-\omega^x|^2\Delta t} = \frac{1}{\sqrt{N}}\sum_x \omega^{-yx}e^{-b|1-\omega^x|^2\Delta t}. \tag{2}$$

$M(\Delta t)$ is a circulant matrix, so this suffices to determine it completely.

PROBLEM 3.2. The elements of M are real since the x and $-x$ terms in the sum (2) are complex conjugates. Prove from the formula (2) that they are non-negative, and sum to 1 in each column.

For large N, $\omega = e^{2\pi i/N} =: e^{2\pi i\epsilon} \approx 1 + 2\pi i\epsilon$, so $1-\omega^x \approx -2\pi i x\epsilon$, for $x \ll N$. In this approximation,

$$M(\Delta t)_{y0} \approx \sum_x e^{-2\pi i yx}e^{-4\pi^2x^2\epsilon^2 b\Delta t}.$$

The zeroth column of $M(\Delta t)$ is thus the discrete Fourier transform of a discretization of a Gaussian; thus it is also a discretization of a Gaussian. In particular, $M(\Delta t)_{y0}$ is not supported only on $y \in \{0, \pm 1\}$, so the Markov matrix for this discrete time integrated random walk is not local in the way that the intensity matrix is.

An alternate (microscopic) perspective

The ODE

$$\dot{p}_x = bp_{x+1} - 2bp_x + bp_{x-1}$$

describes the change in the probability of a particle to be at position x when it is hopping away from x, to $x-1$ or to $x+1$, each with equal probability, at a rate of $2b$ hops per unit time. The adjacent figure shows a typical path, or history, for the particle; the times of the hops constitute a Poisson process. In time Δt any number n of hops is possible, with probability given by

$$\frac{e^{-2b\Delta t}(2b\Delta t)^n}{n!}.$$

Thus

$$\begin{aligned}\Pr(\text{move } y \text{ to right in time } \Delta t) &= \sum_{n=0}^{\infty} \Pr(n \text{ hops}) \Pr(\text{hops right} - \text{hops left} = y) \\ &= \sum_{n=0}^{\infty} \frac{e^{-2b\Delta t}(2b\Delta t)^n}{n!} \binom{n}{(n-y)/2} \frac{1}{2^n}.\end{aligned}$$

The latter term in the sum is approximately a Gaussian around $y = 0$, so the result is a weighted sum of such Gaussians, with the largest weight for $n \approx 2b\Delta t$. Again, we can see that the probability distribution is not supported only on $y \in \{0, \pm 1\}$.

Discrete time local random walk

Can we find a local discrete time random walk? It should be defined by $p_{t+1} = Mp_t$, where M is a Markov matrix with the same sparsity pattern as the intensity bL. If we assign probability q to hopping in each time step, with the probability split equally between left and right, we get:

$$\begin{aligned} p_x(t+1) &= \frac{q}{2} p_{x+1}(t) + (1-q) p_x(t) + \frac{q}{2} p_{x-1}(t) \qquad (3) \\ \implies p_x(t+1) - p_x(t) &= \frac{q}{2}\big(p_{x+1}(t) - 2p_x(t) + p_{x-1}(t)\big).\end{aligned}$$

Assuming $p(t, x)$ is a sufficiently smooth function of t and x, this becomes

$$\begin{aligned} \Delta t \frac{\partial p}{\partial t} &= \frac{q}{2}(\Delta x)^2 \frac{\partial^2 p}{\partial x^2} + \text{ higher order terms} \\ \implies \frac{\partial p}{\partial t} &= \frac{q}{2}\frac{(\Delta x)^2}{\Delta t}\frac{\partial^2 p}{\partial x^2} + \text{ higher order terms.}\end{aligned}$$

Now, taking the $\Delta x, \Delta t \to 0$ limit with $\frac{q}{2}\frac{(\Delta x)^2}{\Delta t} = \kappa$ gives

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

The stochastic process defined by (3) is the usual (discrete time, classical) random walk; we have just shown that despite being local, it has the heat equation as its continuum limit, just as does the nonlocal, discrete time integrated random walk (2).

References

[1] R. D. Sorkin, "Quantum mechanics as quantum measure theory", *Mod. Phys. Lett. A* **9** (1994) 3119–3127; `arXiv:gr-qc/9401003`.

[2] S. Aaronson, "Is quantum mechanics an island in theoryspace?", in A. Khrennikov, ed., *Proceedings of the Växjö Conference Quantum Theory: Reconsideration of Foundations* (2004); `arXiv:quant-ph/0401062`.

[3] R. P. Feynman, "Simulating physics with computers", *Int. J. Theor. Phys.* **21** (1982) 467–488.

[4] E. B. Davies, "Embeddable Markov matrices", *Electronic J. Prob.* **15** Art. 47, `http://www.emis.de/journals/EJP-ECP/article/view/733.html`; `arXiv:1001.1693 [math.PR]`.