Quantum (Random) Walks

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Plan

1. Background on classical random walks
2. Quantum walks (coined, Szegedy's model,...)
3. Quantum walks for search and distributed computing

Discrete-time Markov Processes

Formal definition:

Let $S = \{1, ..., |S|\}$ be a finite set.

A sequence of random variables $\{X_n\}_{n \geq 0}$ with values in S, i.e., $X_n \in S$, is a discrete-time Markov process or Markov chain if

$$P(X_{n+1} = j | X_n = i, ..., X_0 = i_0) = P(X_{n+1} = j | X_n = i) \quad (1)$$

In addition, if the right hand side of the above equation does not depend on n, the Markov chain is called homogeneous.

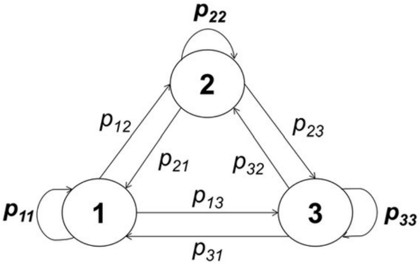
Discrete-time Markov Processes

Let us explain the definition with some simple examples.

Example 1: Nice weather model. The weather in Nice can be in one of the following three states:
S_1 = 'Sunny';
S_2 = 'Cloudy';
S_3 = 'Rainy'.

Discrete-time Markov Processes

There are possible 9 types of transitions between states described by matrix P.



$$\left\{\begin{matrix} \boldsymbol{p_{11}} & p_{12} & p_{13} \\ p_{21} & \boldsymbol{p_{22}} & p_{23} \\ p_{31} & p_{32} & \boldsymbol{p_{33}} \end{matrix}\right\}$$

$$\begin{aligned} P(X_{n+1} = S_3) &= P(X_{n+1} = S_3 | X_n = S_1) P(X_n = S_1) + \\ &\quad P(X_{n+1} = S_3 | X_n = S_2) P(X_n = S_2) + \\ &\quad P(X_{n+1} = S_3 | X_n = S_3) P(X_n = S_3) \end{aligned}$$

Discrete-time Markov Processes

Thus, we can write

$$\pi_{n+1} = \pi_n P,$$

where

$$\pi_{n+1,i} = P[X_{n+1} = i],$$

and

$$\pi_{n,i} = P[X_n = i].$$

Example 2: Symmetric Random Walk on integers.

Let $S = \mathbb{Z}$, $X_0 = 0$ and "toss a coin"

$$\begin{array}{lll} k \to k+1 & \text{w.p.} & \frac{1}{2} \\ k \to k-1 & \text{w.p.} & \frac{1}{2} \end{array}$$

$$P = \begin{bmatrix} \ddots & \ddots & \ddots & & & & \\ & \frac{1}{2} & 0 & \frac{1}{2} & 0 & & \\ & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & \\ & & 0 & \frac{1}{2} & 0 & \frac{1}{2} & \\ & & & & \ddots & \ddots & \ddots \end{bmatrix}$$

Discrete-time Markov Processes

For the infinite lattice it is possible to calculate

$$P[X_t = k] = 2^{-t} \binom{t}{\frac{t+k}{2}},$$

and then using Stirling's approximation $t! \approx \sqrt{2\pi t} e^{-t} t^t$,

$$P[X_t = k] \approx \frac{2}{\sqrt{2\pi t}} e^{-\frac{k^2}{2t}}.$$

Discrete-time Markov Processes

For ergodic Markov chains, the following limit exists:

$$\lim_{n \to \infty} p^{(0)} P^n =: \pi,$$

where the raw vector π is called stationary distribution.

The stationary distribution is given as a solution of the following linear system: (in the matrix form)

$$\pi P = \pi,$$

$$\pi \underline{1} = 1,$$

(and in the element form)

$$\sum_{i=1}^{|S|} \pi_i p_{ij} = \pi_j, \quad j \in S,$$

$$\sum_{i=1}^{|S|} \pi_i = 1.$$

Discrete-time Markov Processes

The rate of convergence to the stationary distribution is determined by the second largest eigenvalue $\lambda_2(P)$, i.e.,

$$||\pi - p^{(0)} P^n|| \leq C|\lambda_2(P)|^n.$$

Discrete-time Markov Processes

We can also consider the first hitting time to set M starting from distribution u:

$$T_M = \min\{n > 0 : \; X_n \in M \;\&\; X_0 \sim u\}.$$

There is a nice formula to compute the expected hitting time:

$$E[T_m] = p_M^{(0)}[I - P_M]^{-1}\underline{1},$$

where P_M is the taboo probability matrix with deleted rows and columns indexed from M and $p_M^{(0)}$ is the respective "pruned" initial distribution $p^{(0)}$.

Continuous-time Markov Process / Walk

Let us present a continuous-time version of Markov chains.

Suppose a random walker on a graph with adjacency matrix A jumps after an exponentially distributed time with rate γd_i from node i, and the next node is chosen with probability a_{ij}/d_i. ($d_i = \sum_j a_{ij}$ is the degree of node i.)

The dynamics of such random walk is described by

$$\dot{\pi}(t) = -\pi(t)\gamma L,$$

where $\pi_i(t) = P[X(t) = i]$ and $L = D - A$ is the graph Laplacian.

Continuous-time quantum walk

Let H be a Hermitian operator associates with the graph.

Some examples: A – adjacency matrix or $L = D - A$ – Laplacian.

Then, a simple way to construct a unitary operator is

$$U(t) = \exp(-iHt)$$

and the evolution of the continuous-time quantum walk is given by

$$|\psi(t)\rangle = U(t)\,|\psi(0)\rangle\,.$$

However,...

Continuous-time quantum walk

There is a *“small” problem*: $U(t)$ is not local.

$$U(t) \approx I - iHt - \frac{1}{2}H^2t^2 \ldots$$

Discrete-time coined quantum walk

Now instead of classical coin let us toss "quantum" coin $|c\rangle$.

"Head" $\leftrightarrow |0\rangle$

"Tail" $\leftrightarrow |1\rangle$

Unlike the case of the classical coin, there is a lot of freedom in the choice of modelling "quantum coin". The most used coin is the Hadamard operator

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

Discrete-time coined quantum walk on integers

In the discrete-time coined quantum walk, the state is $|c\rangle\,|k\rangle$ and its evolution is as follows:

1. Apply the Hadamard operator to the coin state.
2. Apply the shift operator:

$$S\,|0\rangle\,|k\rangle = |0\rangle\,|k+1\rangle\,,$$
$$S\,|1\rangle\,|k\rangle = |1\rangle\,|k-1\rangle\,.$$

3. Repeat or measure.

The evolution can be described by the unitary operator $U = S(H \otimes I)$:

$$|\psi(t+1)\rangle = U\,|\psi(t)\rangle = U^{t+1}\,|\psi(0)\rangle\,.$$

Discrete-time coined quantum walk on integers

Let us start the quantum walk from state $|\psi(0)\rangle = |0\rangle \otimes |0\rangle$. If we apply the unitary operator U once, we get

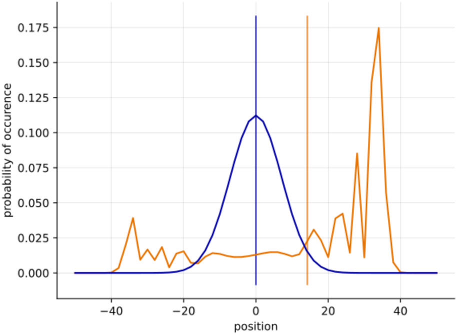
$$|0\rangle \otimes |0\rangle \xrightarrow{H \otimes I} \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |0\rangle$$

$$\xrightarrow{S} \frac{1}{\sqrt{2}}(|0\rangle \otimes |1\rangle + |1\rangle \otimes |-1\rangle).$$

Now if we perform a measurement right after the first step, we find the walker at $k = 1$ w.p. $1/2$ and at $k = -1$ w.p. $1/2$. Same as in the classical case.

However, if we delay measurement, things become quite surprising.

Discrete-time coined quantum walk



$P[X_{50} = k]$ after measurement, (the figure is from Wikipedia)
Blue – Classical Random Walk, Orange – Quantum Walk

Discrete-time coined quantum walk

It turns out that

for the quantum walk, after measurement: $\sqrt{E[(X_t)^2]} \sim t$,

whereas for the classical one: $\sqrt{E[(X_t)^2]} \sim \sqrt{t}$.

Other quantum walk models

Some deficiencies of coined quantum walk:

- The coined quantum walk requires auxiliary degrees of freedom;
- The coined quantum walk can only be generalized to regular graphs;
- No natural definition of hitting times.

There have been developed versions of quantum walk that address the two latter points (Szegedy's model, Portugal's staggered model).

Hitting time in Szegedy's model

In Szegedy's model, we can define the quantum hitting time as the smallest number of steps T such that

$$\frac{1}{T+1}\sum_{t=0}^{T} \| \, |\psi'(t)\rangle - |\psi(0)\rangle \, \|^2 \geq 1 - \frac{m}{n},$$

where $m = |M|$ is the size of the target set.

Theorem (Szegedy) The quantum hitting time is quadratically smaller than the classical expected hitting time.

This provides one more theoretical justification of Grover's search algorithm.

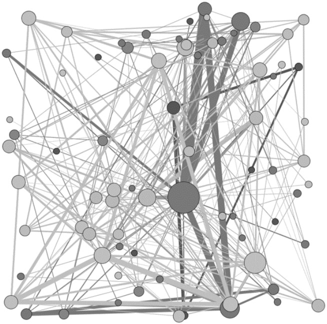
Application to distributed spectrum estimation

- Given symmetric graph matrices such as adjacency matrix A, Laplacian matrix $L = \mathrm{diag}(A\underline{1}) - A$, e.g.,

$$a_{ij} = \begin{cases} 1 & \text{if nodes } i \text{ and } j \text{ are linked,} \\ 0 & \text{otherwise.} \end{cases}$$

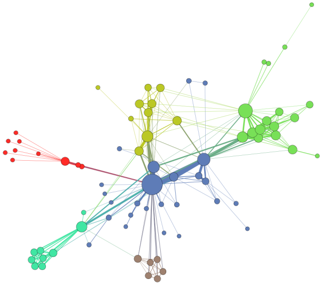
- Find eigenvalues: $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$
  and corresponding eigenvectors: $\mathbf{u}_1, \ldots, \mathbf{u}_n$.

Application to distributed spectrum estimation



Les Misérables network

$\Longrightarrow$



- A classical problem in graph theory,
- More difficult for large, sparse graphs
- An efficient solution is spectral clustering:
  Requires knowledge of top eigenvalues and eigenvectors of graph matrices.

Application to distributed spectrum estimation

- Number of triangles:
  - Total number of triangles in a graph: $\frac{1}{6}\sum_{i=1}^{n}|\lambda_i|^3$.
  - Number of triangles that a node m participated in: $\frac{1}{2}\sum_{i=1}|\lambda_i^3|\,\mathbf{u}_i(m)$
- Dimensionality reduction, spatial embedding and link prediction: Each node is mapped into a point in $\mathbb{R}^k$ space, typically $k << n$.
- Finding near-cliques: Phenomenon of EigenSpokes in eigenvector-eigenvector scatter plot of the adjacency matrix.

Application to distributed spectrum estimation

Challenges in classical techniques for distributed implementation:

- Power iteration:

$$\mathbf{b}_{\ell+1} = \frac{1}{\|\mathbf{b}_\ell\|}\mathbf{A}\mathbf{b}_\ell \qquad \Longrightarrow \qquad \begin{aligned} \lambda_1 &= \lim_{k\to\infty} \frac{\mathbf{b}_{k+1}\mathbf{b}_k^\mathsf{T}}{\|\mathbf{b}_k\|} \\ \mathbf{u}_1 &= \lim_{k\to\infty} \frac{\mathbf{b}_k}{\|\mathbf{b}_k\|} \end{aligned}$$

  Drawback: Only principal components; orthonormalization is needed.

- Inverse iteration method, Arnoldi-type methods:
  Drawback: Also require orthonormalization.

Application to distributed spectrum estimation

Central idea – Complex Power Iterations

- Approach based on Fourier transform of Quantum Walks.
- Let $\mathbf{b}_t = e^{i\mathbf{A}t}\mathbf{b}_0$ be a solution of $\frac{\partial}{\partial t}\mathbf{b}_t = i\mathbf{A}\mathbf{b}_t$, Schrödinger equation, describing the dynamics of QW.
- From the spectral theorem, we have

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i\mathbf{A}t}e^{-it\theta}dt = \sum_{j=1}^{n}\delta_{\lambda_j}(\theta)\mathbf{u}_j\mathbf{u}_j^{\intercal}$$

Application to distributed spectrum estimation

Idea of smoothing by Gaussian kernel:

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-t^2 v/2} e^{i\mathbf{A}t}\mathbf{b}_0 e^{-it\theta}\,dt$$

$$= \sum_{j=1}^{n} \frac{1}{\sqrt{2\pi v}} \exp\left(-\frac{(\lambda_j-\theta)^2}{2v}\right)\mathbf{u}_j(\mathbf{u}_j^T\mathbf{b}_0)$$

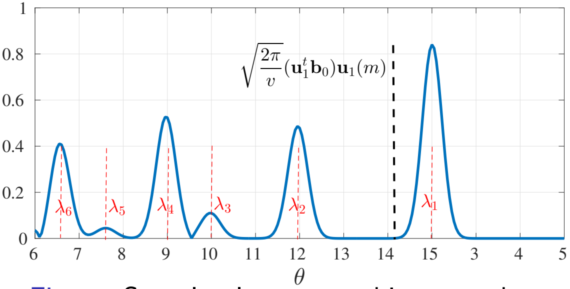


Figure: Sample plot at an arbitrary node m

Application to distributed spectrum estimation

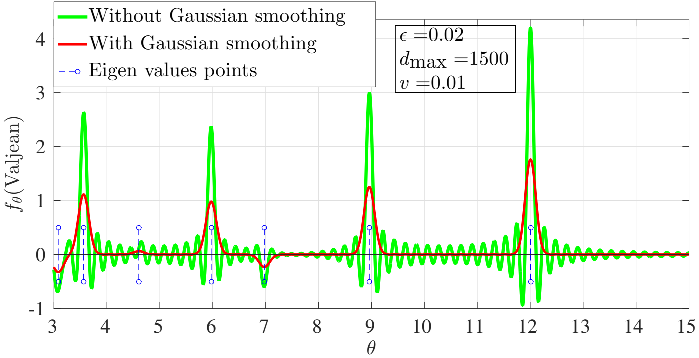


Figure: Effect of Gaussian smoothing

Application to distributed spectrum estimation

With the help of continuous-time QW on a graph: $|\psi(t)\rangle = e^{i\mathbf{A}t}|\psi(0)\rangle$: $|\psi(t)\rangle$ is a complex amplitude vector $\{\langle i|\psi(t)\rangle, 1 \leq i \leq n\}$ with the probability of finding QW in node i at time t is $|\langle i|\psi(t)\rangle|^2$.

Practical implementation can be made with either:

- a combination of a splitting chain of polarized gates and quantum Fourier transform; or
- diffusion of complex fluid.

For more details see e.g.,

J. Wang and K. Manouchehri, *Physical Implementation of Quantum Walks*. Springer, 2013.

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Representative references on quantum walks

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Thank you

Any questions?