AQAlg: Advanced Quantum Algorithms **2022 - 2023**

Lecture 7: Random walks and quantum walks

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1 Random walks: mixing time and hitting time

We consider a simple (undirected, unweighted) and d-regular graph $G = (V, E)$ with $|V| = n$ vertices. A random walk on G starts from some initial vertex (sampled from a distribution p_0 over V), and at every timestep hops uniformly at random to one of its d neighboring vertices. We can describe the probability distribution after t steps using a stochastic transition matrix P where $P_{x,y} = 1/d$ if $(x, y) \in E$ and $P_{x,y} = 0$ otherwise. After t steps the random walk distribution is

$$p_t = P^t p_0.$$

If the graph G is connected then P has a unique stationary distribution π such that $P\pi = \pi$, and moreover this is the unique eigenvalue-1 eigenvector of P. If in addition G is not bipartite, then p_t converges to π as $t \to \infty$, irrespective of the initial distribution p_0. The time it takes to get close to π is quantified by the *mixing time*.

Definition 1 (Mixing time)**.** *The ϵ-mixing time of a random walk with transition matrix P is*

$$\mathrm{MT}(\epsilon) = \min\{t \mid \|P^t p_0 - \pi\|_1 \leq \epsilon, \, \forall p_0\}.$$

On its turn, the mixing time can be related to the *spectral gap* δ of the transition matrix P. If we order the (real) eigenvalues of P as $1 = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq -1$, then the spectral gap is defined as

$$\delta = 1 - \max\{|\lambda_2|, |\lambda_n|\}.$$

The graph is connected and nonbipartite (i.e., has a finite mixing time) if and only if $\delta > 0$. In the exercises you will prove that

$$\mathrm{MT}(\epsilon) \in O\left(\frac{1}{\delta} \log \frac{n}{\epsilon}\right).$$

A different quantity of interest is the random walk *hitting time* $\mathrm{HT}(M)$, defined with respect to some subset of "marked" elements $M \subseteq V$ (e.g., solutions to some search problem). We define it as the expected number of steps of a random walk, starting from the stationary distribution $p_0 = \pi$, until it hits an element of M. The hitting time can also be bounded in terms of the spectral gap:

$$\mathrm{HT}(M) \in O\left(\frac{1}{\delta} \frac{1}{\pi(M)}\right).$$

You will prove this in the exercises (up to a logarithmic factor).

2 Quantum walks

It is clear from the bounds on the random walk mixing time and hitting times that critical roles are played by (i) the stationary distribution of the random walk, which corresponds to the unique eigenvalue-1 eigenvector of P, and (ii) the spectral gap surrounding this eigenvalue. In the following, we show how to construct a *quantum walk* operator $W(P)$ whose stationary state and surrounding gap are closely related to those of P. In the next lecture we will show how this quantum walk can be used to speed up the hitting time of a random walk.

2.1 Quantum walk operator

While a random walk is defined over the vertices of a graph, a quantum walk is defined over its edges. Specifically, the state space of a quantum walk is spanned by states of the form $|x, y\rangle$ for $(x, y) \in E$. You can think about the first register as containing the "current" state x, while the second register contains the "next" state y. In that sense, we could implement a "step" of the quantum walk through the shift operator S defined by

$$S |x, y\rangle = |y, x\rangle .$$

Instead of trivially repeating this, we alternate a step with a "coin toss" that mixes up the next state. We define it using so-called *star states* $|\psi_x\rangle$ for $x \in V$, defined as

$$|\psi_x\rangle = \frac{1}{\sqrt{d}} \sum_{(x,y)\in E} |x, y\rangle .$$

Notice that if we measure this state, then the second register contains a uniformly random neighbor of x. We can define a unitary coin toss operator $C(P)$ based on these star states. Specifically, the coin toss implements a reflection around the star states:

$$C(P) = 2 \left(\sum_{x\in V} |\psi_x\rangle \langle\psi_x| \right) - I.$$

The quantum walk operator $W(P)$ is now described as

$$W(P) = S \cdot C(P).$$

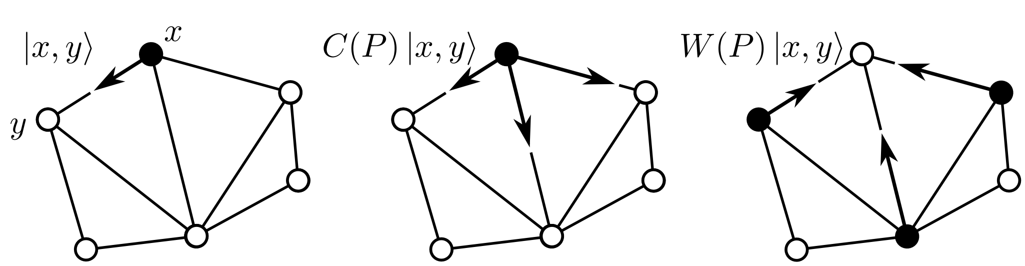

Figure 1: Figure demonstrating a single quantum walk step. (l) A basis state $|x, y\rangle$ is identified with the (directed) edge (x, y). (m) The coin toss $C(P)$ maps an initial state $|x, y\rangle$ to a superposition of outgoing edges. (r) The shift S maps a state $|x, y\rangle$, localized on node x, to a state $|y, x\rangle$, localized on node y.

Exercise 1. *Show that the following quantum state is a stationary state of* $W(P)$*:*

$$|\pi\rangle = \frac{1}{\sqrt{n}} \sum_{x \in V} |\psi_x\rangle = \frac{1}{\sqrt{nd}} \sum_{(x,y) \in E} |x, y\rangle .$$

In fact, we can characterize the full invariant subspace of the quantum walk by first noticing that $W(P)$ is a product of two reflections (around which subspaces?), and then invoking the following lemma. In the exercises we show that the resulting subspace is spanned by $|\pi\rangle$ and the set of "closed flows" on the graph.

Lemma 1. *Consider two projectors* Π_1 *and* Π_2*. The invariant subspace of the product of reflections* $(2\Pi_2 - I)(2\Pi_1 - I)$ *is spanned by the states in* $(\ker(\Pi_1) \cap \ker(\Pi_2)) \cup (\ker(\Pi_1)^\perp \cap \ker(\Pi_2)^\perp)$*.*

Proof. Consider any u such that $(2\Pi_2 - I)(2\Pi_1 - I)u = u$. In particular, this implies that $(2\Pi_1 - I)u = (2\Pi_2 - I)u$ or equivalently $\Pi_1 u = \Pi_2 u$. Hence $\Pi_1 u \in \ker(\Pi_1)^\perp \cap \ker(\Pi_2)^\perp$. Similarly we can prove that $(I - \Pi_1)u \in \ker(\Pi_1) \cap \ker(\Pi_2)$. Finally, since we can expand u as $\Pi_1 u + (I - \Pi_1)u$, we find that $u \in (\ker(\Pi_1) \cap \ker(\Pi_2)) \cup (\ker(\Pi_1)^\perp \cap \ker(\Pi_2)^\perp)$. □

Similarly one can prove that the eigenvalue-(-1) subspace of $W(P)$ corresponds to $(\ker(\Pi_1) \cap \ker(\Pi_2)^\perp) \cup (\ker(\Pi_1)^\perp \cap \ker(\Pi_2))$.

2.2 Szegedy's spectral lemma

In the previous section we characterized the stationary subspace of the quantum walk operator. In this section we give a characterization of the remaining nontrivial ($\neq \pm 1$) eigenvalues, and in particular the spectral gap surrounding the stationary subspace. This key result was first proven by Szegedy in 2004 [Sze04], but it can alternatively be derived from a lemma by Jordan from 1875 [Jor75]. In its most abstract form, it characterizes the spectrum of a product of reflections. For our particular case, we formulate the lemma (without proof) in terms of the eigenvalues λ_j and eigenvectors $|v_j\rangle = \sum_{x \in V} v_j(x) |x\rangle$ of the random walk operator P.

Lemma 2. *The nontrivial spectrum of the quantum walk operator* $W(P)$ *can be characterized as follows: for every eigenvalue* $\lambda_j = \cos\theta_j \neq \pm 1$ *of* P *with eigenvector* $|v_j\rangle$*, the quantum walk operator* $W(P)$ *has a pair of eigenvalues and eigenvectors given by*

$$e^{\pm i\theta_j} \text{ with } \theta_j \in (0, \pi), \qquad |\phi_j^\pm\rangle \in \operatorname{span}\left\{ \sum_x v_j(x) |\psi_x\rangle , \sum_x v_j(x) S |\psi_x\rangle \right\}.$$

Moreover, it holds that $\frac{|\phi_j^+\rangle + |\phi_j^-\rangle}{\sqrt{2}} = \sum_x v_j(x) |\psi_x\rangle$*.*

A useful visualization of this lemma is given in Fig. 2. It shows how each nontrivial random walk eigenvalue is mapped to a pair of complex conjugate eigenvalues of the unitary quantum walk operator.

Similarly to random walks, a key property of a quantum walk is the gap around its stationary subspace. We call this the *phase gap* of the quantum walk, and it is defined as $\Delta = \min\{\theta_j \mid \theta_j \neq 0\}$. By Szegedy's lemma we have that $\theta_j = \arccos(\lambda_j)$, and therefore $\Delta = \arccos(\lambda_2)$. Using that $\lambda_2 \leq 1 - \delta$, with δ the spectral gap of the random walk, we can bound this as $\Delta \in \Omega(\sqrt{\delta})$. This shows that a quantum walk has a quadratically larger gap than the corresponding random walk, and this is one of its key features!

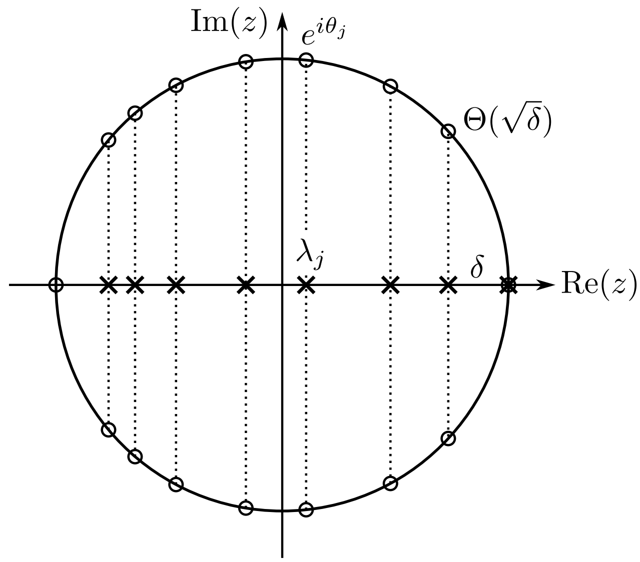

Figure 2: Visualization of the quantum walk spectrum on the complex unit circle. The eigenvalues of P are denoted by crosses ($\times$) and the eigenvalues of $W(P)$ are denoted by circles ($\circ$).

A second useful observation is that a state from the star subspace $\sum_{x\in V} \alpha_x |\psi_x\rangle$ is contained in the subspace spanned by the stationary state $|\pi\rangle$ and the set of nontrivial eigenvectors $|\phi_j^\pm\rangle$. To see this, consider the state $\sum_{x\in V} \alpha_x |x\rangle$ over the *nodes* of the graph, and let its decomposition into eigenvectors of P be given by

$$\sum_{x\in V} \alpha_x |x\rangle = \sum_{j=0}^{n-1} \beta_j |v_j\rangle .$$

Then we can similarly expand

$$\sum_{x\in V} \alpha_x |\psi_x\rangle = \beta_0 |\pi\rangle + \sum_{j=1}^{n-1} \beta_j \frac{|\phi_j^+\rangle + |\phi_j^-\rangle}{\sqrt{2}}.$$

References

[Jor75] Camille Jordan. Essai sur la géométrie à n dimensions. *Bulletin de la Société Mathématique de France*, 3:103–174, 1875.

[Sze04] Mario Szegedy. Quantum speed-up of Markov chain based algorithms. In *Proceedings of the 45th IEEE Symposium on Foundations of Computer Science (FOCS)*, pages 32–41. IEEE, 2004.