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Lecture 16

Continuous-time Quantum Walk

- Traverse the glued trees graph

1 Glued tree

Consider a graph obtained by starting from two complete binary trees of depth n, and joining them by a random cycle of length $2 \cdot 2^n$ that alternated between the leaves of the two trees. An example when $n = 4$:

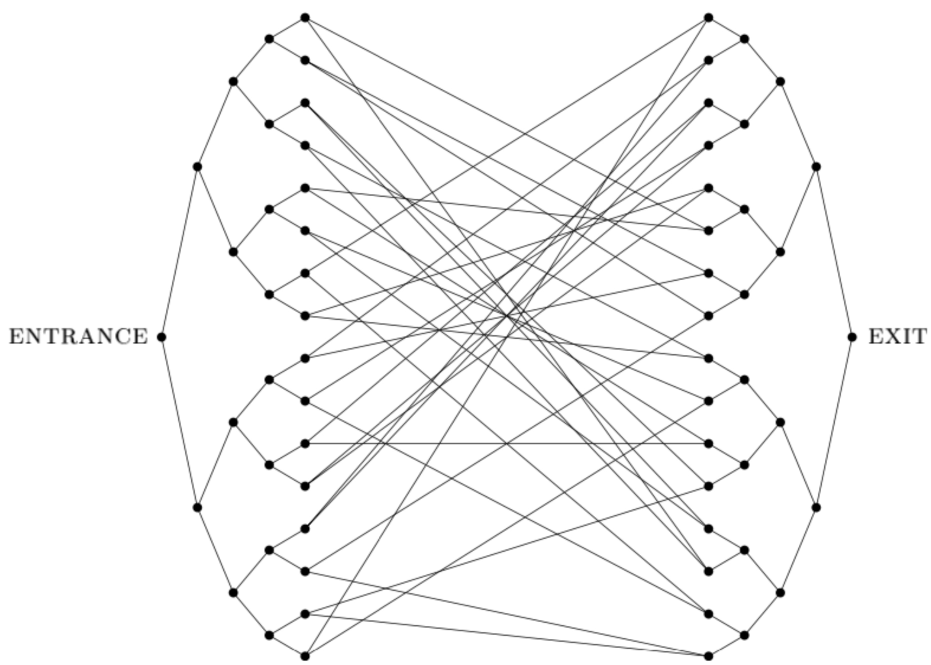


Figure 1: glued tree

This is called a "glued tree".

# of vertices: $2\left(1+2+\cdots+2^n\right) = 2\left(2^{n+1}-1\right) < 2^{n+2} \Rightarrow$ Each vertex can be represented by $(n+2)$-bit binary digits.

Assumption: Entrance: $\underbrace{0\cdots 0}_{n+2}$ (known)

Oracle: Input x, output the neighbors of x. (Classically)

Input a superposition of x

Goal: Output the binary string at the exit.

Note: Any $v \neq$ entrance/exit has 3 neighbors.

Therefore, if x has 2 neighbors and $x \neq 0^{n+2} \Rightarrow x =$ exit.

Classically, it is very easy to get stuck in the middle: a vertex in the right side has two edges going backward, one edge going forward.

In fact: Can prove classical $2^{\Omega(n)}$ lower bound.

2 Quantum walk algorithm to traverse the glued trees graph

We consider continuous-time quantum walk using the adjacent matrix A of the glued tree.

A is 3-sparse $\Rightarrow$ A can be efficiently simulated.

Intuition: Quantum walk on the glued tree G is dramatically simplified due to symmetry.

Define $|\text{col } j\rangle$ to be the uniform superposition over vertices at distance j from the entrance:

$$|\text{col } j\rangle := \frac{1}{\sqrt{N_j}} \sum_{d(a,\text{entrance})=j} |a\rangle$$

N_j: the number of vertices that has distance j to entrance.

$$N_j = \begin{cases} 2^j & 0 \leq j \leq n \\ 2^{2n+1-j} & n+1 \leq j \leq 2n+1 \end{cases}$$

Fact. The subspace $\text{span}\{|\text{col } j\rangle : 0 \leq j \leq 2n+1\}$ is invariant under A.

Proof. At the entrance:

$$A\,|\text{col } 0\rangle = |v_1\rangle + |v_2\rangle = \sqrt{2}\,|\text{col } 1\rangle$$

At the exit:

$$A\,|\text{col } 2n+1\rangle = |\text{col } 2n\rangle$$

For any $0 < j < n$

$$\begin{aligned} A|\,\text{col}\,j\rangle &= \frac{1}{\sqrt{N_j}} \sum_{d(a,\text{entrance})=j} A|a\rangle \\ &= \frac{1}{\sqrt{N_j}} \left(2 \sum_{d(a,\text{entrance})=j-1} |a\rangle + \sum_{d(a,\text{entrance})=j+1} |a\rangle \right) \\ &= \frac{1}{\sqrt{N_j}} \left(2\sqrt{N_{j-1}}|\,\text{col } \ j-1\rangle + \sqrt{N_{j+1}}|\,\text{col } \ j+1\rangle \right) \\ &= \sqrt{2}(|\,\text{col } \ j-1\rangle + |\,\text{col } \ j+1\rangle). \end{aligned}$$

Similarly, for any $n+1 < j < 2n+1$, we have

$$\begin{aligned} A|\,\text{col } \ j\rangle &= \frac{1}{\sqrt{N_j}} \left(\sqrt{N_{j-1}}|\,\text{col } \ j-1\rangle + 2\sqrt{N_{j+1}}|\,\text{col } \ j+1\rangle \right) \\ &= \sqrt{2}(|\,\text{col } \ j-1\rangle + |\,\text{col } \ j+1\rangle). \end{aligned}$$

The only difference occurs at the middle of the graph, where we have

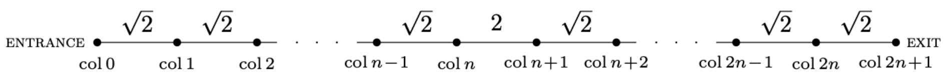
$$
\begin{aligned}
A|\text{col } n\rangle &= \frac{1}{\sqrt{N_n}}\left(2\sqrt{N_{n-1}}|\text{col } n-1\rangle + 2\sqrt{N_{n+1}}|\text{col } n+1\rangle\right) \\
&= \sqrt{2}|\text{col } n-1\rangle + 2|\text{col } n+1\rangle
\end{aligned}
$$

and similarly

$$
\begin{aligned}
A|\text{col } n+1\rangle &= \frac{1}{\sqrt{N_{n+1}}}\left(2\sqrt{N_n}|\text{col } n\rangle + 2\sqrt{N_{n+2}}|\text{col } n+2\rangle\right) \\
&= 2|\text{col } n\rangle + \sqrt{2}|\text{col } n+2\rangle.
\end{aligned}
$$

□

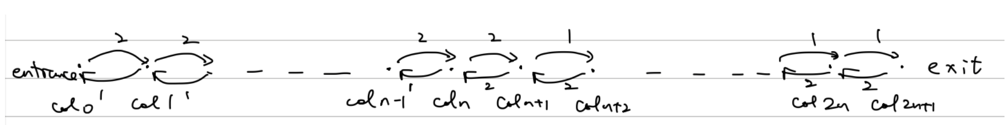
In summary, the matrix elements of A between basis states for this invariant subspace can be depicted as follows:



In classical (l_1-norm) instead of l_2-norm:

$$\frac{1}{N_j}(2N_{j-1}\overrightarrow{\text{col } j-1} + N_{j+1}\overrightarrow{\text{col } j+1}) = \overrightarrow{\text{col } j-1} + 2\cdot\overrightarrow{\text{col } j+1}$$

In contrast, classically it's like: Huge difference between quantum and classical, under l_2-norm and l_1-



norm, respectively!

Equivalence:

- Quantum walk on the glued tree, starting the entrance
- Quantum walk on the weighted path of $2n+2$ vertices(Introduced above).

3 Classical and quantum mixing time

Classically, suppose we start from distribution $p(0) \in \mathbb{R}^{|V|}$ and walk on a graph $G = (V, E)$ with Laplacian $L = \sum_\lambda \lambda v_\lambda v_\lambda^\dagger$, where v_λ is an eigenvector of eigenvalue λ.

$$e^{Lt} = \sum_\lambda e^{\lambda t} v_\lambda v_\lambda^\dagger$$

L is a negative semidefinite matrix, i.e. $\forall\lambda,\ \lambda \leq 0$.

$\lambda = 0$ is an eigenvalue with eigenvector $u = \frac{1}{|V|}(1, \cdots, 1)^T$ (for unweighted graph).

When G is connected, $\lambda = 0$ has simple multiplicity.

As a conclusion, we have:

$$\begin{aligned} p(t) &= e^{Lt}p(0) \\ &= \left(|V|uu^T + \sum_{\lambda\neq 0} e^{\lambda t} v_\lambda v_\lambda^T\right) p(0) \\ &= \langle |V|u, p(0)\rangle u + \sum_{\lambda\neq 0} e^{\lambda t} \langle v_\lambda, p(0)\rangle v_\lambda \\ &= u + \sum_{\lambda\neq 0} e^{\lambda t} \langle v_\lambda, p(0)\rangle v_\lambda \end{aligned}$$

Since all other $\lambda < 0$, $\lim_{t\to\infty} p(t) = \frac{1}{|V|}(1, \cdots, 1)^T$.

Quantumly: the quantum walk is unitary: $e^{i\lambda t}$ keeps rotating and doesn't have a limiting state.

Idea: Measure in a uniformly chosen time.

Pick a time t uniformly at random in $[0, T]$, run the quantum walk starting at $a \in V$ for time t, and then measure in the vertex basis. For vertex b:

$$\begin{aligned} p_{a\to b}(T) &= \frac{1}{T}\int_0^T \left|\left\langle b\left|e^{-iHt}\right|a\right\rangle\right|^2 \,\mathrm{d}t \\ &= \sum_{\lambda,\lambda'} \langle b|\lambda\rangle\langle\lambda|a\rangle\,\langle a|\lambda'\rangle\,\langle\lambda'|b\rangle\,\frac{1}{T}\int_0^T e^{-i\left(\lambda-\lambda'\right)t}\,\mathrm{d}t \\ &= \sum_\lambda |\langle a|\lambda\rangle\langle b|\lambda\rangle|^2 + \sum_{\lambda\neq\lambda'} \langle b|\lambda\rangle\langle\lambda|a\rangle\,\langle a|\lambda'\rangle\,\langle\lambda'|b\rangle\,\frac{1-e^{-i\left(\lambda-\lambda'\right)T}}{i\left(\lambda-\lambda'\right)T}. \end{aligned}$$

Suppose H is non-degenerate: no two eigenvalues are the same.

Since $|-e^{-i(\lambda-\lambda')T}| \leq 2$, we have

$$p_{a\to b}(\infty) := \sum_\lambda |\langle a|\lambda\rangle\langle b|\lambda\rangle|^2 \tag{$*$}$$

How about apply $(*)$ to the glued tree?

We can prove A under $\mathrm{span}\{|\mathrm{col}\ j\rangle : 0 \leq j \leq 2n+1\}$ has a non-degenerate spectrum, and the difference between eigenvalues is at least $\Omega(n^{-3})$.

Denote $A = \sum_\lambda \lambda\,|\lambda\rangle\,\langle\lambda|$, and define R as the reflection operator such that

$$R\,|\mathrm{col}\ j\rangle = |\mathrm{col}\ 2n+1-j\rangle \quad \forall\ 0 \leq j \leq 2n+1.$$

Apparently $R^2 = I \Rightarrow R$ only has eigenvalue ± 1. Further observation:

- R and A commute.
- Linearly-independent eigenvectors of R are $\frac{1}{\sqrt{2}}(|\mathrm{col}\ j\rangle \pm |\mathrm{col}\ 2n+1-j\rangle)\ \ 0 \leq j \leq n$.

As a result, for any $|\psi\rangle$ such that $R\,|\psi\rangle = |\psi\rangle$ (resp. $-\,|\psi\rangle$), $|\psi\rangle$ is a linear combination of $\frac{1}{\sqrt{2}}(|\mathrm{col}\ j\rangle + |\mathrm{col}\ 2n+1-j\rangle)$ among all j (resp. $\frac{1}{\sqrt{2}}(|\mathrm{col}\ j\rangle - |\mathrm{col}\ 2n+1-j\rangle)$ among all j).

$$\Rightarrow \langle\mathrm{ent}|\psi\rangle = \langle\mathrm{exit}|\psi\rangle \quad (\text{resp. } \langle\mathrm{ent}|\psi\rangle = -\,\langle\mathrm{exit}|\psi\rangle)$$

Now, for any eigenvalue λ and corresponding eigenvector $|\lambda\rangle$ of A, we have

$$AR\,|\lambda\rangle = RA\,|\lambda\rangle = \lambda\cdot R\,|\lambda\rangle \Rightarrow \langle\mathrm{ent}|\lambda\rangle = \pm\,\langle\mathrm{exit}|\lambda\rangle$$

Therefore,

$$\begin{aligned}
p_{\text{ent}\to\text{exit}}(\infty) &= \sum_\lambda |\langle \text{ent}|\lambda\rangle\langle \text{exit}\,|\lambda\rangle|^2 \\
&= \sum_\lambda |\langle \text{ent}|\lambda\rangle|^4 \qquad \text{(Cauchy-Schwarz inequality)} \\
&\geq \frac{1}{2n+2}\left(\sum_\lambda |\langle \text{ent}|\lambda\rangle|^2\right)^2 \\
&= \frac{1}{2n+2}
\end{aligned}$$

$$\begin{aligned}
|p_{\text{ent}\to\text{exit}}(\infty) - p_{\text{ent}\to\text{exit}}(T)| &= \left|\sum_{\lambda\neq\lambda'} \langle \text{exit}\,|\lambda\rangle\langle\lambda|\,\text{ent}\rangle\,\langle \text{ent}\,|\lambda'\rangle\,\langle\lambda'|\,\text{exit}\rangle\,\frac{1-e^{-i(\lambda-\lambda')T}}{i\,(\lambda-\lambda')\,T}\right| \\
&\leq \frac{2}{\Delta T}\sum_{\lambda,\lambda'} |\langle \text{exit}\,|\lambda\rangle\langle\lambda|\text{ent}\rangle\,\langle \text{ent}|\lambda'\rangle\,\langle\lambda'|\,\text{exit}\rangle\,| \\
&= \frac{2}{\Delta T}\sum_{\lambda,\lambda'} |\,\langle \text{ent}|\lambda\rangle|^2\,|\,\langle \text{ent}|\lambda'\rangle|^2 \\
&= \frac{2}{\Delta T} = O\left(\frac{n^3}{T}\right).
\end{aligned}$$

Final algorithm:

1. Take $T = Cn^4$ for large enough, fixed constant C. Take $t \in [0, T]$ uniformly random.
2. Apply efficient simulation of A, the adjacency matrix of glued tree, which is 3-sparse. For time t. with initial state $|\text{entrance}\rangle$ (known).
3. Measure the outcome. If it hase 2 neighbors and is not entrance, output it's binary string. Otherwise, start over.

Taking $T = Cn^4$, the success probability is $\geq \frac{1}{2n+2} - O\left(\frac{n^3}{T}\right) = \Omega\left(\frac{1}{n}\right)$.
With $O(n)$ attempts, we succeed with probability $\geq \frac{2}{3}$.
The cost in each attempt comes from Hamiltonian simulation of A.
A is 3 -spare $\Rightarrow$ poly(n) cost in simulation.
In all: poly(n) cost (quantum queries + gates) with success probability $\geqslant \frac{2}{3}$.
Exponential quantum-classical separation established.

Remark 1: For the Boolean hypercube, it can also be regarded as an st-connectivity problem: From a vertex, reach its opposite vertex. All vertices labelled with (arbitrary) 0-1 strings.

Fact: Not only quantumly this is easy, so does classically: poly (n) queries suffice. In other words, hypercube is much simpler than the glued tree classically.

Remark 2: To prove the exponential classical lower bond for the glued tree and $\Delta = \Omega(n^{-3})$. check: Chills, Clave, Deotto, Farhi, Gutmann, and Spielman. Exponential algorithmic speedup by quantum walk. STOC 2003. arXiv: quant-ph/0209131.

Remark 3: The state-of-the-art result for glued tree: Jeffery and Eur. Multidimensional quantum walks, with application to k-distinctness. STOC 2023, arXiv: 2208.13492 $O(n)$ quantum query, $O\left(n^2\right)$ quantum gates.

Remark 4: Superpolynouisal quartum-classical separation for more general graphs? Yes: My work with Balasubramanian and Harrow. Random ensembles. arXiv: 2307.15062