Quantum Search Algorithm and Discrete Schrödinger Dynamics

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Overview

1. Grover's quantum search algorithm
2. Discrete Schrödinger Dynamics on graphs
3. Grover's algorithm as discrete Schrödinger dynamics
4. Appendix: Calculating generators of W and U_f

Search algorithm

Search Problem. There is a connected finite graph $G = (V, E)$. Among all vertices in V, only one vertex v^* is marked. How to find v^*?
We are allowed to query a function (black box) $f : V \to \{0, 1\}$ such that $f(v^*) = 1$ and $f(v) = 0$ if $v \neq v^*$.

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Query complexity: The strategy is to query f on different vertices until we get 1. Each time we can only check 1 vertex. In the worst case, we have to query the black box $n - 1$ times before get v^*.
$\implies$ query complexity $= O(n)$.

Basics of quantum computing

Dirac Notation. In quantum mechanics, a column vector (quantum state) is written as a 'ket',e.g., $|\psi\rangle$. Its conjugate (a row vector) is a 'bra', e.g., $\langle\psi|$. The inner product of $|\psi\rangle$ and $|\phi\rangle$ is a 'braket': $\langle\psi|\phi\rangle$.

Classical Computer	Quantum Computer
bit	qubit (a **unit** vector in a 2-dim Hilbert space)
gate	quantum gate (a unitary matrix)
tape reader	measurement (an orthonormal basis)

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Measurement of a quantum system: we can use an orthonormal basis $\{|0\rangle, ..., |n-1\rangle\}$ to 'measure' a quantum system, and any element in this basis can be an output.
By **Born rule**, the probability of getting result $|j\rangle$ is $|\langle\Psi|j\rangle|^2$. Since $\|\Psi\|_2 = 1$, all probabilities adds up to 1.

More on Dirac notation

Dirac notation can be used to express matrix.

Example

Let $|e_0\rangle = \frac{1}{\sqrt{n}} \begin{pmatrix} 1 \\ 1 \\ .. \\ 1 \end{pmatrix} = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} |j\rangle$. What is $|e_0\rangle \langle e_0|$?

$$|e_0\rangle \langle e_0| = \frac{1}{\sqrt{n}} \begin{pmatrix} 1 \\ 1 \\ .. \\ 1 \end{pmatrix} \frac{1}{\sqrt{n}} (1, 1, ..., 1) = \frac{1}{n} \begin{bmatrix} 1 & 1 & ... & 1 \\ 1 & 1 & ... & 1 \\ ... & ... & ... & ... \\ 1 & 1 & ... & 1 \end{bmatrix} := \frac{1}{n} J_n,$$

where J_n is a n-by-n all-ones matrix.

Back to the search problem

On a quantum computer, we can use orthonormal basis $|j\rangle$ $(j = 0, 1, ..., n-1)$ to enumerate vertices. This basis is called *computational basis*.
The function f can be implemented as a *quantum oracle* U_f (a unitary matrix).

$$U_f |j\rangle = (-1)^{f(j)} |j\rangle = \begin{cases} -|j\rangle & (j \text{ is marked}) \\ |j\rangle & (j \text{ is not marked}) \end{cases}$$

The most crazy thing of quantum computer is that it allows linear combinations of orthonormal basis! This means, we can have a 'superposition' of all vertices at a time!

Grover's algorithm

- Prepare a state $|e_0\rangle = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} |j\rangle$. It is a uniform superposition of all possible 'vertices'.
- Apply the quantum oracle U_f.
- Apply gate (unitary matrix) $W := 2|e_0\rangle\langle e_0| - \mathbb{I}_n$. ($\mathbb{I}_n$ is identity matrix.)
- Repeat step 2 and 3 for K times, where K is the closest integer to $\frac{\pi}{4}\sqrt{n} - \frac{1}{2}$.
- Measure the resulting state in computational basis. With probability at least $1 - \frac{1}{n}$, the measurement outcome is v^*.

Query complexity: We use the quantum oracle U_f $K \sim \sqrt{n}$ times.
$\Longrightarrow$ query complexity $= O(\sqrt{n})$. Quantum Speedup

Geometric visualization: amplitude amplification

Decompose the input state into two parts:

$$|e_0\rangle = \frac{1}{\sqrt{n}}|v^*\rangle + \frac{1}{\sqrt{n}}\sum_{j\neq v^*}|j\rangle = \sin\theta\,|v^*\rangle + \cos\theta\,|\phi\rangle\,,$$

where $\sin\theta = \frac{1}{\sqrt{n}}$, $|\phi\rangle = \frac{1}{\sqrt{n-1}}\sum_{j\neq v^*}|j\rangle$ is a unit vector.
We can prove $WU_f|e_0\rangle = \sin 3\theta\,|v^*\rangle + \cos 3\theta\,|\phi\rangle$, and inductively, $(WU_f)^k|e_0\rangle = \sin(2k+1)\theta\,|v^*\rangle + \cos(2k+1)\theta\,|\phi\rangle$. By Born rule, the probability we get $|v^*\rangle$ is

$$p = |\sin(2k+1)\theta|^2.$$

When $(2k+1)\theta = \frac{\pi}{2}$, the probability of getting v^* is 1. At this time, $k \approx \frac{\pi}{4}\sqrt{n} - \frac{1}{2}$.

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Schrödinger equation

The dynamics of quantum systems are described by Schrödinger equation:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle ,$$

where $\hbar$ is the Planck constant, $|\Psi(t)\rangle : \mathbb{R}^3 \times [0, \infty) \to \mathbb{C}$ is the *wave function*, $\hat{H}$ is the *Hamiltonian*.

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For a single non-relativistic particle, the Hamiltonian is a linear partial differential operator

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(x, t).$$

Copenhagen interpretation of $|\Psi(t)\rangle$: $|\Psi(t)|^2$ is the probability density of the particle in $\mathbb{R}^3$ at time t.

Wave functions on graph

Let $G = (V, E)$ be a connected finite graph, $V = \{v_1, v_2, ..., v_n\}$.
We can cook up a definition of wave functions on graph G analogous to its counterpart on Euclidean space.

$$|\Psi\rangle : V \to \mathbb{C} \text{ s.t. } |\Psi|^2 = 1.$$

In other words, $|\Psi\rangle$ is a $n-$dimensional complex-valued unit vector in the Hilbert space $H_G = \mathbb{C}^n$.

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$$|\Psi\rangle = (\Psi_1, ..., \Psi_n)^T \in H_G.$$

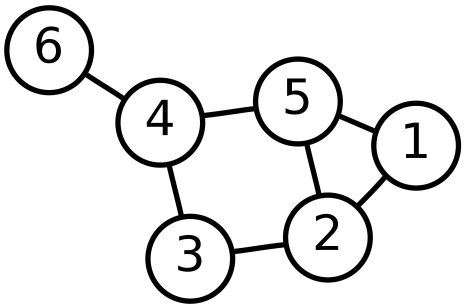
Copenhagen interpretation of $|\Psi\rangle$: $p = (|\Psi_1|^2, |\Psi_2|^2, ..., |\Psi_n|^2)$ is the probability mass function of the 'particle' on the graph G.

Graph Laplacian

The Laplacian operator on the (undirected) graph $G = (V, E)$ is a $n-$by$-n$ symmetric matrix

$$L_{ij} = \begin{cases} -deg(v_i) & (i = j) \\ 1 & ((i,j) \in E) \\ 0 & elsewhere \end{cases}$$

For example, the Laplacian of the graph on the left is



$$L = \begin{bmatrix} -2 & 1 & & & 1 & \\ 1 & -3 & 1 & & 1 & \\ & 1 & -2 & 1 & & \\ & & 1 & -3 & 1 & 1 \\ 1 & 1 & & 1 & -3 & \\ & & & & 1 & -1 \end{bmatrix}$$

Laplacian of N-complete graph

A graph with N vertices is called a *N-complete* graph if any vertex is connected to all the other vertices.

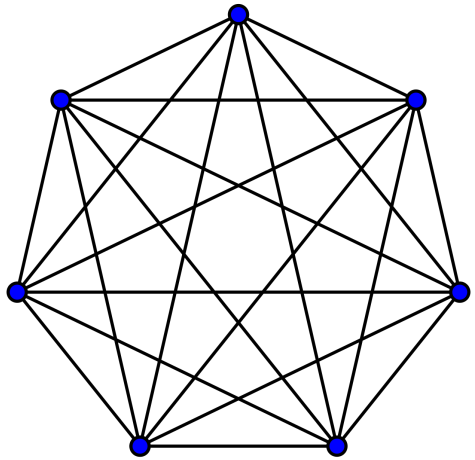


Figure: A 7-complete graph

Laplacian of $N-$complete graph is of a neat form:

$$L = J_N - N\mathbb{I}_N,$$

where J_N is a $N-$by$-N$ all-ones matrix, and $\mathbb{I}_N$ is the $N-$by$-N$ identity matrix.

Schrödinger equation on graph

Suppose the particle is of unit mass $m = 1$, and the Planck constant is normalized as 1, we can formulate the Schrödinger equation on a graph $G = (V, E)$ as

$$i\frac{\mathrm{d}}{\mathrm{d}t}\left|\Psi(t)\right\rangle = \hat{H}\left|\Psi(t)\right\rangle,$$

where $\left|\Psi(t)\right\rangle : [0, T] \to H_G = \mathbb{C}^n$, $\hat{H} = -L + V$.

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V is the *potential operator*. It is a $n-$by$-n$ diagonal matrix:

$$V = Diag(f(v_1), f(v_2), ..., f(v_n)),$$

where $f(v)$ is the potential function on the graph

$$f : V \to \mathbb{R}.$$

Solutions to discrete Schrödinger equation, time evolution operator

We will call Schrödinger equation on graph as *discrete Schrödinger equation:*

$$i\frac{\mathrm{d}}{\mathrm{d}t}\left|\Psi(t)\right\rangle = \hat{H}\left|\Psi(t)\right\rangle, \ \hat{H} \text{ is a Hermitian matrix.}$$

Unlike the Schrödinger equation in $\mathbb{R}^3$ (a linear PDE), Schrödinger equation on graph is a $n-$dimensional system of ODEs.

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Unlike the Schrödinger equation in $\mathbb{R}^3$ (a linear PDE), Schrödinger equation on graph is a $n-$dimensional system of ODEs.
Given an initial condition $\left|\Psi(0)\right\rangle$, the solution can be written as

$$\left|\Psi(t)\right\rangle = e^{-i\hat{H}t}\left|\Psi(0)\right\rangle.$$

In physics, we call $U(t) := e^{-i\hat{H}t}$ the *time evolution operator* of the system, and $\hat{H}$ is the *generator* of $U(t)$.

Overview

Motivating example: Nesterov's accelerated gradient method

$$\min f(x).$$

Fix x_0, set $y_0 = x_0$. In the $k-$th iteration, compute

$$x_k = y_{k-1} - s\nabla f(y_{k-1}), y_k = x_k + \frac{k-1}{k+2}(x_k - x_{k-1}).$$

This method is known to have quadratic convergence rate, which is optimal among all first-order methods.

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This method is known to have quadratic convergence rate, which is optimal among all first-order methods.
Su, Boyd and Candes (2014) showed this method is a discretization of a second-order initial value problem:

$$\ddot{X} + \frac{3}{t}\dot{X} = -\nabla f(X), X(0) = x_0.$$

They gained better understanding and analysis of Nesterov's method, and as a biproduct, they are able to design a family of schemes with similar convergence rate.

Trotter product formula

In our formulation, $\hat{H} = -L + V$. It is tempted to ask if

$$U(t) := e^{-i(-L+V)t} = e^{-i(-L)t} e^{-iVt}?$$

In general, it is not true. (We can prove $e^{A+B} = e^A e^B$ if and only if $[A, B] := AB - BA = 0$.) But for small time $t = \epsilon << O(1)$, the product is a good approximation:

$$U(\epsilon) \approx e^{iL\epsilon} e^{-iV\epsilon}.$$

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Theorem (Trotter Product Formula)

$$e^{(A+B)} = \lim_{N\to\infty} \left(e^{\frac{A}{N}} e^{\frac{B}{N}} \right)^N$$

$$U(t) \approx (e^{i\frac{L}{N}t} e^{-i\frac{V}{N}t})^N$$

Revisit Grover's algorithm

In Grover's algorithm, we want to iterate the unitary transformation WU_f K times, i.e., $(WU_f)^K$.
If we can find some large N and write $W = e^{iH_1/N}$, $U_f = e^{iH_2/N}$, then by Trotter formula:

$$(WU_f)^N = (e^{iH_1/N} e^{iH_2/N})^N \approx e^{i(H_1+H_2)}.$$

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It turns out that

$$H_1 = \frac{\pi}{n}L, \ L \text{ is the Laplacian of } n-\text{complete graph},$$

$$H_2 = -\frac{\pi}{n}V,$$

V has $-n$ at the v^*-th diagonal entry, with all other entries being 0. It can be interpreted as a potential operator. The potential at the vertex v^* is $-n$, while being 0 at all other vertices.

Grover's algorithm as Schrödinger dynamics

$$WU_f = e^{iH_1}e^{-iH_2} = e^{-i\pi(-L/n)}e^{-i\pi V/n},$$

by Trotter product formula,

$$(WU_f)^n = \left(e^{-i\pi(-L/n)}e^{-i\pi V/n}\right)^n \approx e^{-i\hat{H}\pi} = U(\pi),$$

with $\hat{H} = -L + V$, L, V are defined in previous slides. Recall that $K \approx \frac{\pi}{4}\sqrt{n}$, so

$$(WU_f)^K = [(WU_f)^n]^{K/n} \approx U(K\frac{\pi}{n}) = U\left(\frac{\pi^2}{4\sqrt{n}}\right).$$

Physical interpretation of Grover's algorithm

Grover's algorithm can be thought as a discretization of a discrete Schrödinger dynamics on graph as follows:

- Prepare a 'photon' in state $|e_0\rangle$.
- Place it on a $n-$complete graph with the potential field V.

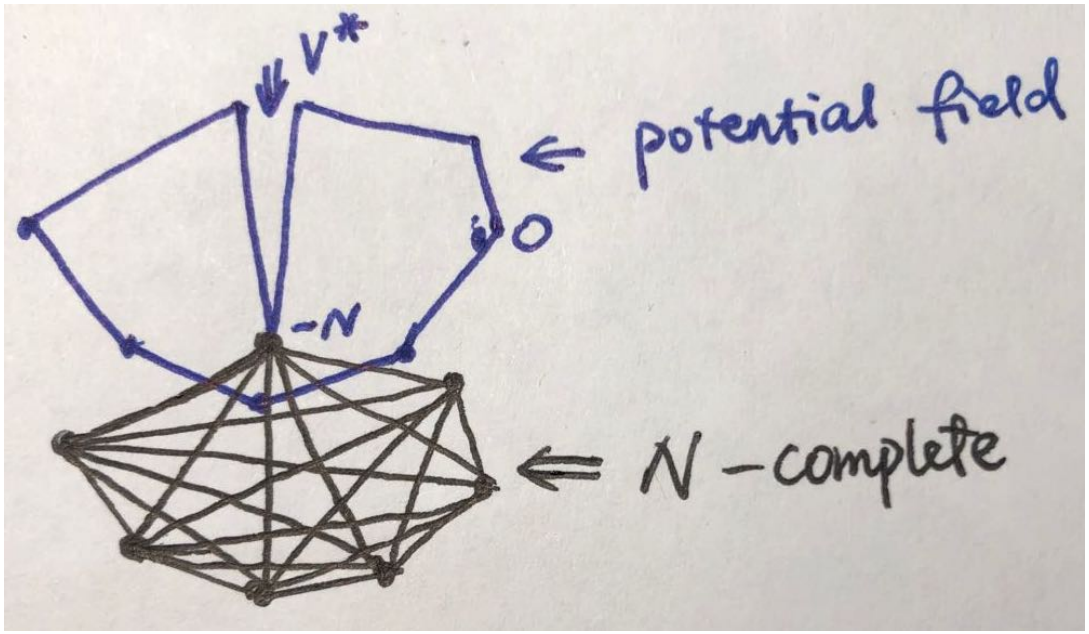

Figure: Physical scenario of Grover's algorithm

Numerical simulation

Set $n = 1000$, and mark vertex # 7. We simulate the Schrödinger equation (on the same L, V as before) on a 1000-complete graph.

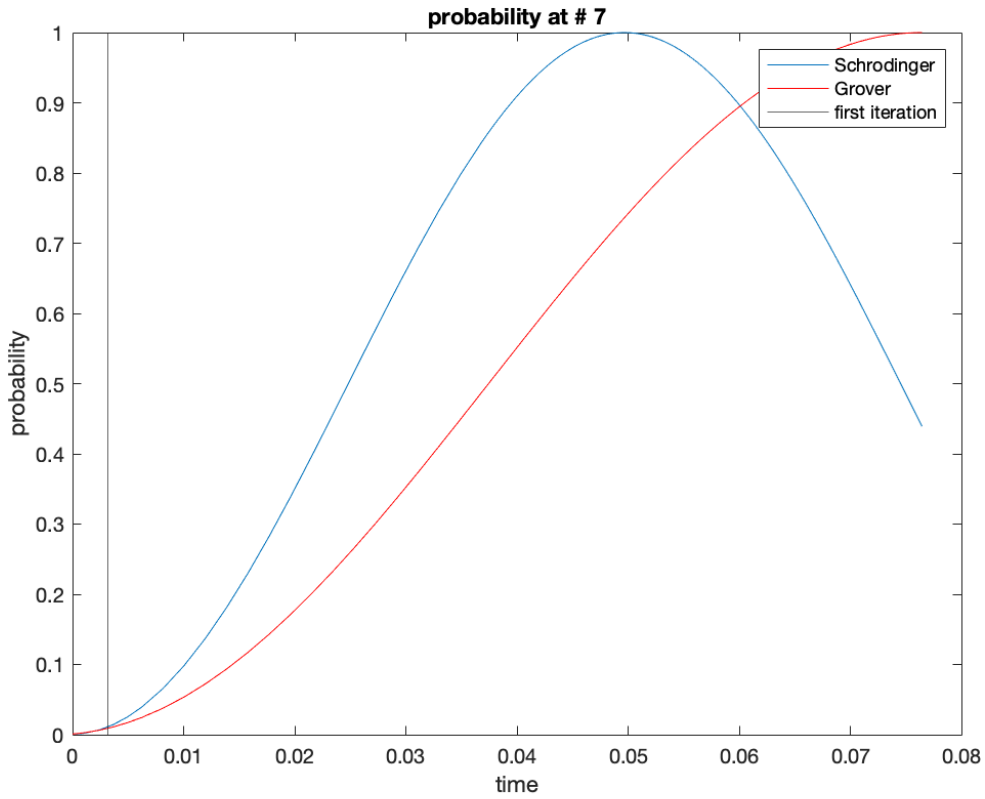

Figure: Comparison between Grover and Schrödinger dynamics

Summary

- We give a 'physical interpretation' of Grover's search algorithm.
- Nielsen and Chuang (they wrote one of the most used references in quantum computation) proposed an alternative approach to Grover's algorithm as a quantum simulation (Section 6.2). Our work is a more detailed exposition of this perspective.
- As what we expect, this 'discrete Schrödinger dynamics' approach **CAN** help us design new quantum algorithms. We are currently working in this direction, and a lot of positive evidence was found.

Overview

W and U_f

Recall that $|e_0\rangle = \frac{1}{\sqrt{n}} \begin{pmatrix} 1 \\ \dots \\ 1 \end{pmatrix}$.

$$W = 2|e_0\rangle\langle e_0| - I = \frac{1}{n} \begin{bmatrix} -(n-2) & 2 & 2 & \dots & 2 \\ 2 & -(n-2) & 2 & \dots & 2 \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & 2 & -(n-2) \end{bmatrix}$$

$$U_f = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & -1 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ & & & & 1 \end{bmatrix}$$

The generator of W

W is a circulant matrix, and we can readily compute its diagonalization:

$$W = FDiag(-1, -1, ..., -1, 1)F^{-1},$$

where F is the Fourier basis. Suppose $W = e^{iH_1}$, we have

$$H_1 = -i \log W = \frac{\pi}{n} \begin{bmatrix} -(n-1) & 1 & 1 & ... & 1 \\ 1 & -(n-1) & 1 & ... & 1 \\ ... & ... & ... & ... & ... \\ ... & ... & ... & 1 & -(n-1) \end{bmatrix}$$

$$= \frac{\pi}{n} L, \ L \text{ is the Laplacian of } n-\text{complete graph.}$$

The generator of U_f

U_f is a diagonal matrix with entries ± 1, suppose $U_f = e^{iH_2}$, we have

$$H_2 = i \log U_f = iDiag(0, 0, ..., i\pi, 0, .., 0) = \frac{\pi}{n} Diag(0, 0, ..., -n, 0, .., 0).$$

Let $V = Diag(0, 0, ..., -n, 0, .., 0)$, it is a potential operator on the graph G, with the only non-trivial potential being $-n$ at the marked vertex. Now, we have $H_2 = \frac{\pi}{n} V$.