Quantum Algorithm for Simulating Time Evolution of a Quantum System.

Note Title 5/11/2012

We saw earlier that the Hermitian operator for the energy of a quantum system plays an important role in quantum mechanics since it governs the time evolution of a quantum system according to Schödinger's equation:

$$i\hbar \frac{d\,\psi(t)}{dt} = H\,\psi(t)$$

Hamiltonian – energy operator.

For time independent systems in which the energy of the system does not change over time, we have that.

$$U(t) = e^{iHt}$$ where $U(t)$ is the unitary operator defining how the system changes over time t.

If $\psi(0)$ is the state at time 0, $\psi(t)$ is the state at time t $\Rightarrow$ $\psi(t) = U(t)\,\psi(0)$

What does it mean to have an operator in the exponent?

One way to see what this means is to diagonalize the matrix representation of H: $H = \sum_j \lambda_j |\phi_j\rangle\langle\phi_j|$

then $f(H) = \sum_j f(\lambda_j)\, |\phi_j\rangle\langle\phi_j|$

specifically $e^{iHt} = \sum_j e^{i\lambda_j t}\, |\phi_j\rangle\langle\phi_j|$

Another way is to look at the Taylor expansion of e^x:

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

this is just composition, so this is a basis-independent way to express H.

$$e^{iHt} = I + H + H^2/2! + H^3/3! + \cdots$$

Our goal will be to take input quantum state $|\psi(0)\rangle$ and Hamiltonian H and calculate $|\psi(t)\rangle = e^{iHt}|\psi(0)\rangle$ within some error ϵ. The system on which H operates will be a system with n qubits. Complexity goal: poly$(n, t, 1/\epsilon)$

First we need some limitations on H. We assume that H is k-local:

$$H = \sum_a H_a$$

each term acts non-trivially on only k qubits.

This is a natural assumption since H describes the energy interactions within the system, a single particle (qubit or set of qubits) can only interact with other particles that are nearby.

Note that a k-local Hamiltonian only has at most $\binom{n}{k}$ $O(n^k)$ terms. Each term can be expressed using a $2^k \times 2^k$ matrix. If k is a constant, a k-local Hamiltonian can be described by a polynomial number of complex numbers.

We could take this a step further and assume that the particles are embedded in d-dimensional space with a bounded number of bits per unit volume. Each H_a acts non-trivially only on qubits within a ball of constant radius. In this case, there can by only $O(n)$ terms.

We will also assume that each term H_a has bounded norm:

$$\max_{\substack{|\psi\rangle \\ \||\psi\rangle\|=1}} \| H_a |\psi\rangle \| \leq h.$$

efficiency + accuracy will be a function of h.

We will want some $|\phi(t)\rangle$ such that $\| |\phi(t)\rangle - |\psi(t)\rangle \| < \delta$, where δ is a constant.

As stated, our problem doesn't have a well-defined output that can be expressed classically. We would like to be able to talk about the classical as well as quantum complexity of this problem.

Typically we have some observable O computable by a quantum circuit. We would like to measure this observable. That is, we would like to generate the eigenvalues of O according to $\langle \psi(t) | \Pi_o | \psi(t) \rangle$

Π_o ↳ projection onto eigenspace for eigenvalue o.

It is believed that this problem is hard classically but we will show that it can be done efficiently using a quantum circuit.

Time is continuous, so we select a small step size Δ. Simulate a sequence of t/Δ time steps. We will handle the case of a time independent H, but if H changes over time, you need to select a small enough Δ so that the change in H over time Δ can be neglected.

In order to achieve $\| \tilde{\psi}(t) - \psi(t) \| < \delta$
we need error to be $\leq \frac{\delta \Delta}{t}$ per time step because
error accumulates additively in the worst case.

Suppose $H = \sum_{a=1}^{M} H_a$ $M = \#$ of terms

We will simulate a time step with $O(M)$ "gates"
with error $O(M^2 \Delta^2 h^2)$ $O(M \Delta^2 h^2)$ per gate.

these are unitary operations on k qubits which then need to be simulated using a Universal gate set.

Want: $M^2 \Delta^2 h^2 \leq \frac{\delta \Delta}{t} \Rightarrow \Delta \leq \frac{\delta}{M^2 h^2 t}$

Total # "gates" $\frac{t}{\Delta} M \Rightarrow O\left(\frac{M^3 h^2 t^2}{\delta} \right)$

First address how to simulate a "gate" (arbitrary unitary operation on k qubits) using a universal gate set.

First go from operation k-qubits to 2-qubits.
This can be done exactly with overhead $O(2^k)$

Then by Solovay-Kitaev any 2-qubit gate can be simulated to within accuracy $O(\epsilon)$ with a universal gate set using polylog $(1/\epsilon)$ gates.

Need $\epsilon = \frac{\Delta^2 h^2 M}{2^k} \Rightarrow \text{polylog}\left(\frac{2^k}{\Delta^2 h^2 M} \right) 2^k$

this ensures error in time step remains $O(M^2 \Delta^2 h^2)$

universal gates per "gate".

plugging in $\frac{1}{\Delta} = O\left(\frac{M^2 t\, h^2}{\delta}\right)$ $\quad$ $\text{polylog}\left[\frac{h^2 M^3 t^2 2^k}{\delta^2}\right] 2^k$

k is considered a constant.

The overall cost of the simulation in # of universal gates:

$$O\left(\frac{h^2 M^3 t^2}{\delta} \text{ polylog}\left(\frac{hMt}{\delta}\right)\right)$$

Note that if the system is geometically local

$M = O(n) = O(V)$ $\quad$ V = spatial volume of the system.

If $\Omega = (Vt)$ $\quad$ $L = O(\Omega^3 \text{ polylog } \Omega)$

Now we return to the question of how to simulate a time step with $O(M)$ gates with error. $O(M\Delta^2 h^2)$ per gate.

The unitary we would like to implement is

$$e^{iHt} = e^{iH\Delta} = e^{i\sum_a H_a \Delta}$$

Let $A_a = iH_a\Delta$

approximate $\exp\left(\sum_a A_a\right)$ by $\prod_a \underbrace{\exp(A_a)}$

$\exp\left(\sum_a A_a\right) - \prod_a \exp(A_a)$

each acts non-trivially on at most k qubits.

First, we examine the case where the A_a commute:

$$\underbrace{\left(I + \sum_a A_a + \frac{1}{2}\sum_{a,b} A_a A_b + \cdots\right)} - \underbrace{\prod_a \left(I + A_a + \frac{1}{2}A_a^2 + \cdots\right)}_{(*)}$$

Terms of order k: $\frac{1}{k!} \sum_{1 \le a_1, \ldots a_k \le M} A_{a_1} A_{a_2} \cdots A_{a_k}$

The signature for a terms is $(n_1, \ldots, n_M)$ $\quad$ n_a = # of A_a

Since the A's commute, a term can be rearranged as:

$$(A_1)^{n_1} (A_2)^{n_2} \cdots (A_M)^{n_M}$$

How many terms have a particular signature $(n_1, \dots, n_M)$?

$$\frac{1}{k!} \binom{k}{n_1} \binom{k-n_1}{n_2} \cdots \binom{k-n_1-\cdots-n_{M-1}}{n_M}$$

coefficient for that term

$$= \frac{1}{(n_1)!} \frac{1}{(n_2)!} \cdots \frac{1}{(n_M)!}$$

this is exactly the coefficient for the term $(A_1)^{n_1} \cdots (A_M)^{n_M}$ in $(*)$

So for commuting terms, the error is 0.

Now for the non-commuting case:

$$\left(\cancel{I} + \cancel{\sum_a A_a} + \frac{1}{2}\sum_{a,b} A_a A_b + \cdots\right) - \underbrace{\prod_a \left(I + A_a + \frac{1}{2}A_a^2 + \cdots\right)}$$

$$- \left(I + \sum_a A_a + \sum_{k=2}^{\infty} (\leq n^k \text{ terms}) |h\Delta|^k\right)$$

$$\leq \sum_{k=2}^{\infty} M^k h^k \Delta^k = O(M^2 h^2 \Delta^2)$$

since $Mh\Delta \ll 1$. $\left(\Delta \leq \frac{1}{hM}\right)$