Hamiltonian Simulation

Quantum Computing

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Motivation

Overview

1. Introduction

Introduction: Hamiltonian Simulation

Hamiltonian

Hermitian operator acting on n qubits which corresponds physically to a system made up of n 2-level subsystems.

Schrödinger's equation

Time evolution of the state $|\psi\rangle$ of a quantum system:

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

Introduction: Hamiltonian Simulation

Solution of the Schrödinger's equation (*time-independent*):

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

Goal

To approximate the unitary operator:

$$U(t) = e^{-iHt}$$

Approximation in the operator (spectral) norm:

$$||A|| := \max_{|\psi\rangle \neq 0} \frac{||A|\psi\rangle||}{|||\psi\rangle||}.$$

$\tilde{U}$ approximates U within ϵ if

$$||\tilde{U} - U|| < \epsilon$$

Proportional Case

Hamiltonian is proportional to Pauli Tensor Product

We consider the simple case where H is proportional to a Pauli matrix on n qubits:

$$H = \alpha s_1 \otimes s_2 \otimes \cdots \otimes s_n$$

Time Evolution Operator (What we are trying to compute)

$$e^{-itH} = e^{-it\alpha s_1 \otimes s_2 \otimes \cdots \otimes s_n}.$$

Matrix Exponential

For any square matrix $A \in \mathbb{C}^{n \times n}$, the matrix exponential is defined by:

$$e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!} = I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \cdots$$

Diagonalizing H

Walkthrough of how to make H diagonal

$$H = \alpha s_1 \otimes s_2 \otimes \cdots \otimes s_n.$$

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- **Identity**:

$$III^\dagger = I$$

- **Pauli-Z**:

$$IZI^\dagger = Z$$

- **Pauli-X**:

$$HXH^\dagger = Z$$

- **Pauli-Y**:

$$U_Y Y U_Y^\dagger = Z \quad \text{where} \quad U_Y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$$

Diagonalization of H

Lemma (Product of Diagonal Matrices)

Let $D = \mathrm{diag}(d_1, \ldots, d_n)$ *and* $E = \mathrm{diag}(e_1, \ldots, e_n)$ *be diagonal matrices. Then their matrix product is diagonal:*

$$DE = \mathrm{diag}(d_1 e_1, \ldots, d_n e_n)$$

Lemma (Tensor Product of Diagonal Matrices)

Let $A = \mathrm{diag}(a_1, \ldots, a_m)$ *and* $B = \mathrm{diag}(b_1, \ldots, b_n)$ *be diagonal matrices. Then their tensor product is diagonal:*

$$A \otimes B = \mathrm{diag}(a_1 b_1, a_1 b_2, \ldots, a_m b_{n-1}, a_m b_n)$$

Diagonalization of H

$$
\begin{aligned}
H &= \alpha(s_1 \otimes \cdots \otimes s_n) \\
&= \alpha(U_1 z_1 U_1^\dagger) \otimes \cdots \otimes (U_n z_n U_n^\dagger) \quad \text{(Diagonalize each } s_i\text{)} \\
&= \alpha(U_1 \otimes \cdots \otimes U_n)(z_1 \otimes \cdots \otimes z_n)(U_1^\dagger \otimes \cdots \otimes U_n^\dagger)
\end{aligned}
$$

And thus,

$$
e^{-itH} = e^{-i\alpha t(U_1 \otimes \cdots \otimes U_n)(z_1 \otimes \cdots \otimes z_n)(U_1^\dagger \otimes \cdots \otimes U_n^\dagger)}
$$

$$e^{-itH} = e^{-i\alpha t(U_1\otimes\cdots\otimes U_n)(z_1\otimes\cdots\otimes z_n)(U_1^\dagger\otimes\cdots\otimes U_n^\dagger)}$$

The conjugation property of the matrix exponential

$$e^{UHU^\dagger} = Ue^H U^\dagger$$

This identity is easily proven using the power series definition for matrix exponential.

we diagonalize e^{-itH} with an appropriate unitary transformation:

$$\begin{aligned} e^{-itH} &= e^{-i\alpha t(U_1\otimes\cdots\otimes U_n)(z_1\otimes\cdots\otimes z_n)(U_1^\dagger\otimes\cdots\otimes U_n^\dagger)} \\ &= (U_1 \otimes U_2 \otimes \cdots \otimes U_n)e^{-i\alpha t z_1\otimes z_2\otimes\cdots\otimes z_n}(U_1^\dagger \otimes U_2^\dagger \otimes \cdots \otimes U_n^\dagger), \end{aligned}$$

where $z_i \in \{I, Z\}$.

Implementation via Quantum Circuits

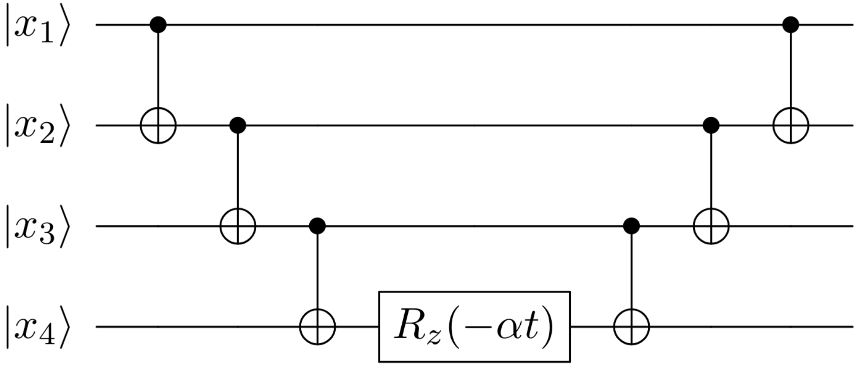
The main challenge reduces to implementing:

$$e^{-i\alpha t Z\otimes Z\otimes\cdots\otimes Z}. \tag{1}$$

The action of the k-qubit Z-interaction unitary on a computational basis state is given by:

$$e^{-i\alpha t Z\otimes\cdots\otimes Z}|x\rangle = \begin{cases} e^{-i\alpha t}|x\rangle & \text{if } \sum_{i=1}^{k} x_i \text{ is even} \\ e^{i\alpha t}|x\rangle & \text{if } \sum_{i=1}^{k} x_i \text{ is odd} \end{cases}$$

Quantum Circuit for $k = 4$



$$R_z(\theta) = \begin{bmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{bmatrix}$$

Generalization to Weighted Sums of Pauli Matrices

For H as a weighted sum of commuting Pauli matrices:

$$H = \sum_{j=1}^{m} \alpha_j \sigma_{s_j}, \tag{2}$$

the evolution follows as:

$$e^{-iHt} = \prod_{j=1}^{m} e^{-i\alpha_j \sigma_{s_j} t}. \tag{3}$$

This requires $O(mn)$ quantum gates.