Trotterization

Simulating Hamiltonians like zoom zoom

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Quantum Algorithms

April 22, 2022

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Hamiltonian Simulation

"...nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem because it doesn't look so easy"

~ **Richard Feynman**

- The universe is of quantum nature, which means that to simulate particles or any other natural entities you need to simulate its Hamiltonian.
- However, efficient computation of evolution given the Hamiltonian has not been achieved for a general Hamiltonian.
- Simulation of Hamiltonians is a *BQP*-complete problem.

Applications

Ground State Preparation

- Consider Hamiltonian H with spectral decomposition:

$$H = \sum_{i=0}^{n} \lambda_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$$

- The state $|\psi_0\rangle$ is referred to as the ground-state and it's corresponding eigenvalue λ_0 is the ground energy.
- Very important problems in condensed matter physics, quantum chemistry and quantum information.

Applications

Protein Folding

- Simulation of the physical process from which amino acid chain folds into it's native 3-d structure
- Protein folding problem is classically *NP*-Hard
- Since the protein itself is a quantum system, the evolution of the protein into its native state will be described by some hamiltonian H.
- Finding the native structure of the protein is equivalent to the problem of finding the ground state of H
- Potential speed up in the drug discovery pipeline

Dynamics

- Consider a system whose Hamiltonian at time t is $H(t)$ and it's initial state $|\psi_0\rangle$. For time t:

$$|\psi(t)\rangle = U(t)\,|\psi_0\rangle$$

- Using Schrodinger's equation and assuming Hamiltonian is time independent, we get:

$$|\psi(t)\rangle = e^{-\iota t H}\,|\psi_0\rangle$$

- Constructing an operator of evolution U on a set of qubits that is equivalent to applying the above evolution on the given system.
- If the required precision of approximation is ϵ, then U must satisfy:

$$||U - e^{-\iota t H}|| < \epsilon$$

Methods of Simulation

The different methods used for simulating the Hamiltonian evolution include:

1. Taylor Expansion
2. Quantum Walks
3. Trotterization (zoom zoom)

Taylor Expansion

- We can express e^{-iHt} as a Taylor expansion:

$$e^{-iHt} = \sum_{n=0}^{\infty} \frac{(-iHt)^n}{n!} = I - iHt - \frac{H^2t^2}{2} + \frac{iH^3t^3}{6} \ldots$$

- For shorter periods, the latter terms can be truncated to get an efficient quantum algorithm

Trotterization

- The Trotterization method focuses on constructing a circuit with efficient gate complexity for the target system whose Hamiltonian can be decomposed of the following form:

$$H = \Sigma_{i=1}^{\tau} H_i$$

where H_i is a Hermitian that can be exponentiated with $O(1)$ gate complexity.

k-local Hamiltonian

A k-local Hamiltonian is a Hamiltonian that operates non-trivially on only k out of the n-qubits in a system.

This suggests that for a given k-local Hamiltonian, the gate complexity is independent of n, satisfying the required criterion.

Decomposition

- Decomposition of a given Hamiltonian into sum of simpler Hamiltonians can be done in multiple ways.
- One simple approach that can be used is to decompose it into the Extended Pauli Basis.
- An n-qubit Hamiltonian H can be decomposed as follows:

$$H = \sum_{i_1, i_2, \ldots, i_n} \frac{1}{2^n} h_{i_1, i_2, \ldots, i_n} \sigma_{i_1} \otimes \sigma_{i_2} \otimes \ldots \otimes \sigma_{i_n}$$

where, $i_k \in \{0, 1, 2, 3\}$ and

$$h_{i_1, i_2, \ldots, i_n} = \frac{1}{2^n} Tr((\sigma_{i_1} \otimes \sigma_{i_2} \otimes \ldots \otimes \sigma_{i_n}) H)$$

Trotter Order

- There exist different orders of approximation
- With greater order we have a lesser error rate but the gate complexity grows.

First order Trotterisation

- Let's consider a simple system $H = A + B$ such that A, B can be implemented in $O(1)$ gate complexity. The required unitary evolution:

$$U(t) = e^{-\iota t(A+B)}$$

- The first order approximation of the above unitary would be:

$$L_1(t) = e^{-\iota tA} e^{-\iota tB}$$

Trotter Order (Contd.)

- The Trotter error for the given example can be obtained by looking at Baker-Campbell-Hausdorff formula

$$e^{-\iota tA}e^{-\iota tB} = e^{-\iota t(A+B)-\frac{t^2}{2}[B,A]+\iota\frac{t^3}{12}[B,[B,A]]+...}$$

- The error bound is as follows

$$||L_1(t) - U(t)|| \leq \frac{t^2}{2}||[B, A]||$$

- For a n qubit Hamiltonian with τ terms in it's decomposition, the $2l$th order Trotterization is described recursively.

$$L_2(t) = e^{\frac{t}{2}H_1}\cdots e^{\frac{t}{2}H_\tau}\cdots e^{\frac{t}{2}H_1}$$

$$L_{2l}(t) = L_{2l-2}(u_l t)^2 L_{2l-2}((1-4u_k)t)L_{2l-2}(u_l t)^2 \quad Here u_l = 1/(4-4^{1/(2l-}$$

Trotter Error

- The error for pth order is given using the α commutator

$$\text{Err}(t) = O(\tilde{\alpha}_{comm} t^{p+1})$$

- Where α_{comm} is given by Nested commutator of all the permutations of Hamiltonians in the decomposed sum.

$$\tilde{\alpha}_{comm} = \Sigma^{\tau}_{\gamma_1,\ldots\gamma_p+1=1} ||[H_{\gamma_{p+1}}, \cdots [H_{\gamma_2}, H_{\gamma_1}]]||$$

- For the given system $H = \Sigma^{\tau}_{i=0} H_i$, the gate complexity required to achieve constant accuracy is mentioned in 13

$$O(\tau \tilde{\alpha}_{comm} t^{p+1} t^{1+1/p})$$

Randomized Trotterization

- The gate complexity has a direct dependency on τ, which means overall gate complexity would be $O(\tau^2)$.
- This dependency is not negligible for dense Hamiltonian.
- The Hamiltonians that are relevant in quantum chemistry have $\tau = O(n^4)$. This create a $O(n^8)$ scaling factor which is unacceptably high.
- The study gives a random algorithm qDRIFT, to construct the circuit.
- We construct $\hat{H}_i$ such that $H_i = h_i \hat{H}_i$ where $|\hat{H}_i| = 1$ and $h_i = |H_i|$. h_i is the strength of $\hat{H}_i$
- We bound the maximum singular value of H by $\lambda = \Sigma_i h_i$. Similar to Trotter number, we pick N and get new strength $\Gamma = t\lambda/N$
- Apply the operation $e^{\iota \Gamma H_j}$.

Randomized Trotterization(Contd.)

- We pick each term from created above with probability $e^{\iota \Gamma H_j}$.

Algorithm qDRIFT ALgorithm

$i \leftarrow 0$
$\lambda \leftarrow \Sigma_j h_j$
$V_{list} \leftarrow \{\}$
while $i < N$ **do**
    $i \leftarrow i + 1$
    $j \leftarrow$ SAMPLE()
    $V_{list} \leftarrow V_{list}.append(e^{\iota \lambda H_j / N})$
end while

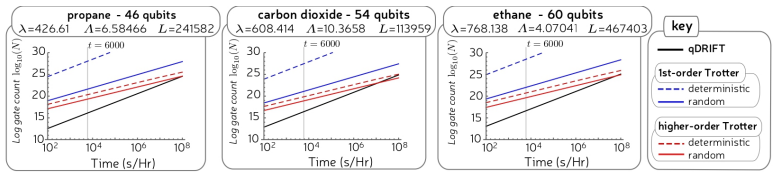

Figure: Gate Complexity for Molecule Simulation

Nearest-Neighbour Lattice Hamiltonian

- Only neighbouring particles interact with each other.

General form of Hamiltonian

$$H = \Sigma_{i=1}^{n-1} H_{j,j+1}$$

Quantum Ising Model

- Model describes the nearest-neighbour interactions determined by spin projections along the z-axis in a lattice.
- It also describes the effect of an external magnetic along the x-axis.

Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - g \sum_i \sigma_i^x$$

Quantum Heisenberg Model

- Model describes nearest-neighbour interactions in a lattice.
- Interactions are determined by spin projections in the x, y and z directions.
- The external magnetic field is described along the z-axis (this axis doesn't matter).

Hamiltonian

$$H = -\sum_{\langle i,j \rangle} (J_x \sigma_i^x \sigma_j^x + J_y \sigma_i^y \sigma_j^y + J_z \sigma_i^z \sigma_j^z) + h \sum_i \sigma_i^z$$

Implementation

Using IBM's Qiskit, we implemented a module that can convert a Hamiltonian or it's decomposition into a circuit for it's simulation using Trotterization.

Decomposition

- Given input as a Hamiltonian of size $2^n \times 2^n$, we decompose it into the Extended Pauli Basis

$$H = \sum_j \otimes_k \sigma_a^i$$

Implementation

Trotterization

- We construct the Lie Trotter Expression and other forms of Trotterization

$$e^{-itH} \approx \left(e^{-i(t/r)H_1} e^{-i(t/r)H_1} \ldots e^{-i(t/r)H_L}\right)^r$$

Result

- With this circuit we can take an initial state $|\psi_0\rangle$ that evolves according to the hamiltonian H and obtain:

$$|\psi_t\rangle \approx e^{-itH} |\psi_0\rangle$$

Gate Complexity

- For a simple 2-local Hamiltonian, we plot the experimental gate depth for three methods of Trotterization.

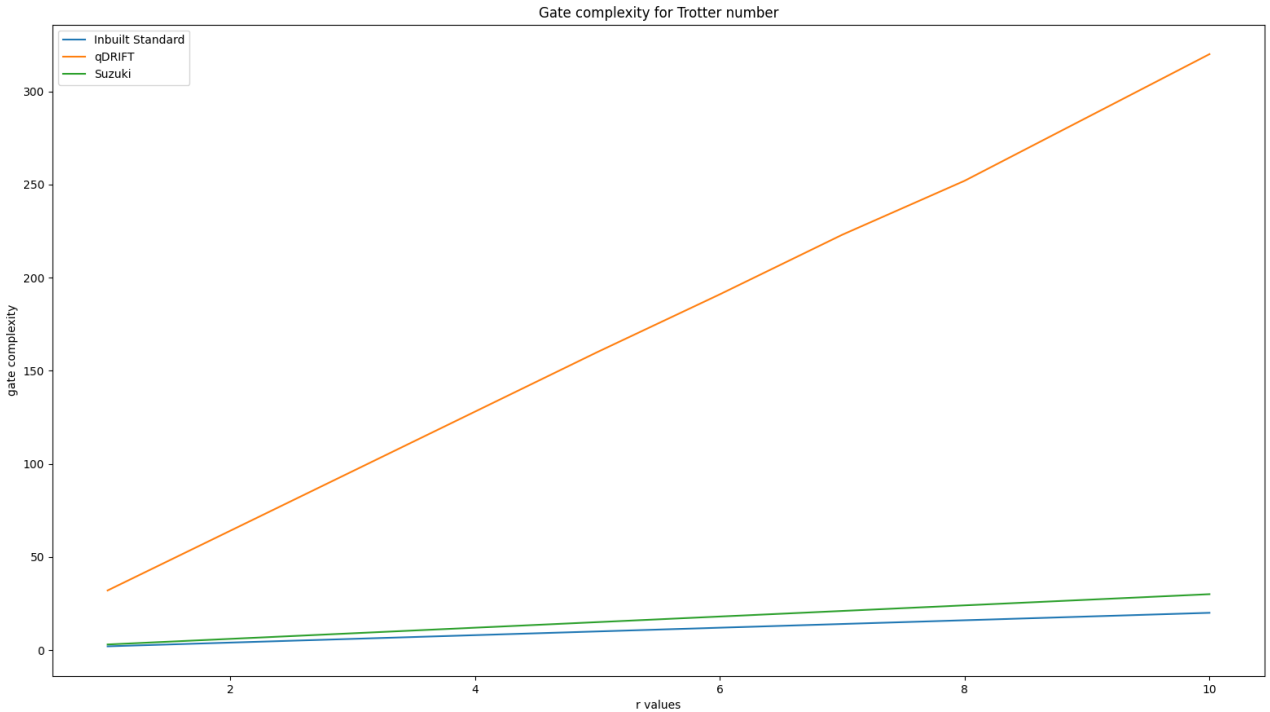

Figure: Gate Complexity of simple Hamiltonian

Future Work

Best Simulation Method

- Plenty of simulation techniques that give advantage in one form or the other based on the system.
- Unclear on what the best Hamiltonian Simulation algorithm would be
- Determining what the best technique would be for a given Hamiltonian is non-trivial

Ideal Decomposition

- Our Hamiltonian can be decomposed as sum of Hermitians that can be exponentiated in O(1) complexity in multiple ways.
- Finding an ideal decomposition is still an open problem

Future Work

Analytical Bounds

- For a simple system and first order, Baker-Campbell-Hausdorff formula presented analytical tight bound.
- It has been achieved for second order Trotterization
- There is no bound of such form for general Trotterization

Future Work

Loose Bounds

- Trotterization is neglected due to high complexity the current bounds.
- Severe gap between the experimental complexity and the complexity provided even by the newest comm bound.