OptTrot
Optimized Trotter Circuit Library

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Abstract

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1 Introduction

Trotterization is a standard method used to implement a time evolution operator by combining several local Hamiltonian evolution operators. By using the method, we can expect the approximated operator closed to the original operator, even the local terms did not commute with each other.

$$\lim_{n \to \infty} (e^{A/2} e^{B/2})^n = e^{A+B} \tag{1}$$

In quantum computing, the method has an advantage of preserving the local structure of the Hamiltonian on a dynamic circuit [1]. However, Trotterization method increases circuit depth with linear order by number of Pauli terms. If the time evolution was an ultimate goal to achieve in quantum circuit, it could be meaningful, but in the most algorithms and applications, time evolution is just a part of the whole process. Thus, reducing techniques are significant to apply the quantum computer to general tasks. In addition, increased circuit depth for reducing Trotter error yields inefficient costs in NISQ era, which makes the algorithm into less practical one.

By the limitation, there are many alternative methods to implement a time evolution operator with shorter depth circit than Trotterization, such as linear combination of unitary(LCU) method[2], Qubitization[3], Taylorization[4], and Fractional query[5]. Such methods make the evolution circuit more practical, however, they loose identity of the given system, especially the cases, when the given hamiltonian is nearly commute or local observable was a dominant feature[1].

Using Trotter error schema with commuting terms, we can analyze the overall error by applying order of local terms.

1.1 Trotter Error by applying order

It is well known that the exponential mapping error is represented with Baker Campbell Hausdorff formula. Usually, the formula is not written with commutator form, Childs et al proved that the error term as a function of sequential commutator of local terms[1].

$$O(\alpha t^2) \tag{2}$$

The results of Childs et al allow us to calculate the error boundary more precisely including a physical structure of the given Hamiltonian.

For example, let a given Hamiltonian was $H = c_i P_i + c_j P_j$.

$$\exp(-it(c_i)P_i)\exp(-it(c_j)P_j) = \exp(-it(c_iP_i + c_jP_j)) + O(\alpha_{com}t^2) \tag{3}$$

then the leading coefficient becomes $\alpha_{com} = \begin{cases} c_i + c_j & \text{if } [P_i, P_j] = 0 \\ c_i - c_j & \text{if } [P_i, P_j] \neq 0 \end{cases}$.

It is affected by coefficients, their size, and sign, and commutation property. In the above example, we cannot observe the commutation and anti-commutation effect, since, if they were commuting to each other, the $O(\alpha_{com}t^2) = 0$. Let us expand the system to more general case. Suppose that the given Hamiltonian has two representations,

$$H = H_1 + H_2 + H_3 \tag{4}$$
$$H = c_1P_1 + c_2P_2 + c_3P_3 + c_4P_4 + c_5P_5 \tag{5}$$
$$H_1 = c_1P_1 + c_3P_3 \tag{6}$$
$$H_2 = c_2P_2 \tag{7}$$
$$H_3 = c_4P_4 + c_5P_5 \tag{8}$$

where, $[H_i, H_j] \neq 0$, and $[P_k, P_l] \neq 0$ if $P_k \in H_i, P_l \in H_j, i \neq j$.

$$\Pi_{l=1}^5 \exp(-it(c_lP_l)) = \exp(-itH) + O(\alpha_{com1}t^2) \tag{9}$$
$$\Pi_{k=1}^3 \exp(-it(H_k)) = \exp(-itH) + O(\alpha_{com2}t^2) \tag{10}$$

Following the $q = 1$ order expansion, then in the first order, the bound error coefficients are reduced to

$$\alpha_{com1} = 2(||c_1c_2[P_1, P_2]|| + ||c_1c_4[P_1, P_4]|| + ||c_1c_5[P_1, P_5]|| \tag{11}$$
$$+ ||c_2c_3[P_2, P_3]|| + ||c_2c_4[P_2, P_4]|| + ||c_2c_5[P_2, P_5]|| \tag{12}$$
$$+ ||c_3c_4[P_3, P_4]|| + ||c_3c_5[P_3, P_5]||) \tag{13}$$
$$\alpha_{com2} = 2(||[H_1, H_2]|| + ||[H_1, H_3]|| + ||[H_2, H_3]||) \tag{14}$$
$$\tag{15}$$

$$0.5\alpha_{com1} = ||c_1c_2|| + ||c_3c_2|| + ||c_1c_4|| + ||c_2c_4|| + ||c_1c_5|| + ||c_2c_5|| + ||c_2c_4|| + ||c_2c_5|| \tag{16}$$
$$0.5\alpha_{com2} = ||c_1c_2 + c_3c_2|| + ||c_1c_4 + c_2c_4 + c_1c_5 + c_2c_5|| + ||c_2c_4 + c_2c_5|| \tag{17}$$

Therefore, by the distribution of $\{c_i\}$ and commutation relationship of the local terms, the constructed error rate vary. However, Eq(10) is just a re-ordering of Eq(9), since

$$\exp(-it(H_1)) = \exp(-it(c_1P_1))\exp(-it(c_3P_3)) \tag{18}$$
$$\exp(-it(H_2)) = \exp(-it(c_2P_2)) \tag{19}$$
$$\exp(-it(H_3)) = \exp(-it(c_4P_4))\exp(-it(c_5P_5)) \tag{20}$$
$$\tag{21}$$

This is not et al, local Hamiltonian consist of mutually commuting Pauli terms provides us a lot of freedom to optimize the circuit. Whatever we switch and reorder the Pauli terms in the applying trotter circuit, if the larger structure, $\exp(-itH_j) = \Pi_k \exp(-itc_jkP_jk)$, was preserved then, the trotter error would be bounded while we reduce the number of gates in the implementation. Thus, we don't have to choose one between trotter error and large gate error to optimize the evolution circuit.

Note: The partitioning the hamiltonian into large local terms does not yields the optimized order in every situation. The term α only indicates upper bound of the error. So, the minimum trotter error could be worse than the arbitrary applying case. In here, the main focus is reducing errors associated with gate operations by using minimum number of gates.

2 Mutually Commuting Parition

3 Optimizing a circuit with commuting pairs

Clique: optimal condition: sum $\Sigma_i c_i \approx 0$.

3.1 Pauli Frame method

The current stage does not treat the routine finding optimal path search in Pauli Frame space. It is because that we have not much tools to deal find the path and weight between the given frames, excepting the dynamics programming approach.

I, Z family would be a good example to see the complxity of the problem. Consider that the local term of the Hamiltonian composite of Z family. Then, for a given frame B and suppose that we have to make next frame to have $P = IIZZ$. Since, we don't have to consider terms containing X, Y, we can simply write the term as single column, and the required entanglement gate is CX gate only.

$$B = \begin{bmatrix} ZZZI \\ ZZIZ \\ ZIZZ \\ IZZZ \end{bmatrix} \rightarrow B' = \begin{bmatrix} IIZZ \\ \cdots \\ \cdots \\ \cdots \end{bmatrix} \tag{22}$$

The answer is shotly applying a CX gate on line 1 and 2. Now, let the representation as binary vector

$$B = \begin{bmatrix} ZZZI \\ ZZIZ \\ ZIZZ \\ IZZZ \end{bmatrix} = \begin{bmatrix} 1110 \\ 1101 \\ 1011 \\ 0111 \end{bmatrix} = \begin{bmatrix} \vec{w}_1 \\ \vec{w}_2 \\ \vec{w}_3 \\ \vec{w}_4 \end{bmatrix} \tag{23}$$

Then the problem becomes the next statement.

Find the minimum size subgroup $\{w_k\} \subset B$ whose XOR products is P where,

$$P = \wedge_k \vec{w}_k \tag{24}$$

More simply, it is equivalent with finding a binary vector $\vec{x} \in \{0, 1\}^N$ of

$$P = \otimes_{i=1}^{N} x_i \& \vec{w}_i \qquad (25)$$

There is no proper polynomial algorithm of the problem [1]. In addition, the general local Hamiltonian terms are harder than the only Z-family cases. Every attempt would be an approximation unless the new frameworks are developed.

Observation 1 *For N qubit system, the maximum size of mutually commuting Pauli subgroup, P, is 2^N. Let $G \subset P$ be a generator of P where, $\forall p \in P, \exists \{g_i\} \subset G$ such that, $p = \wedge_i g_i$.*

4 Conclusion

In the report, we overlook the trotter error affected by order and hamiltonian structure in n-th order Suzukit-Trotter formula.

References

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[1]We might verify this statement!