OptTrot

Optimized Trotter Circuit Library

Memebers
Hyunseong Kim
Hanseo Kim
Gaya Yun

Mentor
Sayomeo Ray

Abstract

OptTrot is a library of generating optimized Trotter circuit for a given hamiltonian. Trotterization is a standard way to accomplish time evolution circuit on gate model computer, however, their long depth circuit has significantly contributed to the hurdle of practical application. In the library, we combined commuting partition method and Pauli Frame search method. If the given Pauli term mutually commuted with Pauli Frame axis, then the Clifford gate combination was reduced to combinations of CNOT gate. Moreoever their specific decomposition is easily derived from Gauss elimination of matrix over module 2 field.

1 Introduction

OptTrot is a library for generating optimized Trotter circuits, for practical use in various applications.

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 with quadratic, $O(t^2)$, error.

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

However, standard Trotterization method increases circuit depth with linear order by number of Pauli terms. That is, a hamiltonian whose number of local terms are N has, at least, N time deeper circuit than single Pauli term evolution circuit. 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 taskes. 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[1], Qubitization[2], Taylorization[3], and Fractional query[4]. 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[5]. Only problem is a high cost of the Trotterization circuit. However, it is not a problem of Trotterization. It is a problem of circuit synthesis process of standard method[6].

How can we optimize the circuit synthesis for trotter evolution circuit? There have been various studies of circuit optimization, but for specificialy for trotter circuit. Schmitz et al would be a milestone paper[7]. They analyzed what term would be rotated when we

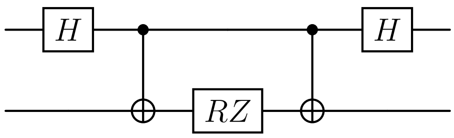

Figure 1: Example of trotter evolution circuit. Where $H = X \otimes Z$

apply entanglement gates on quantum circuit and suggested a practical method to find a better depth evolution circuit of given Hamiltonian.

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

We will focus on attemption that author Kim's study, and combine them with Schmitz et al. The application of commuting partition to optimize the trotter circuit.

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[5].

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

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 $H = c_i P_i + c_j P_j$.

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

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,

$$H = H_1 + H_2 + H_3 \tag{4}$$
$$H = c_1 P_1 + c_2 P_2 + c_3 P_3 + c_4 P_4 + c_5 P_5 \tag{5}$$
$$H_1 = c_1 P_1 + c_3 P_3 \tag{6}$$
$$H_2 = c_2 P_2 \tag{7}$$
$$H_3 = c_4 P_4 + c_5 P_5 \tag{8}$$

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

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

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

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

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

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

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

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 Optimizing a circuit with commuting pairs

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

2.1 Pauli Frame method

One method to optimize the Trotter circuit is using *Pauli Frame*[7]. Pauli Frame is a collection of Pauli terms indicating axes on each quantum circuit wires when we apply Rotation Z gate on the circuit.

Using the method, we can chase the what Pauli elements were applied, and what elements we can rotate on the circuit.

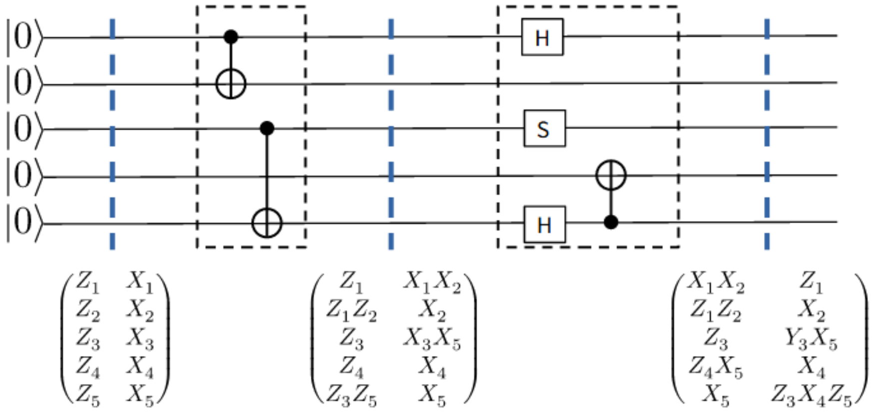

Figure 2: Example of Pauli Frame analysis of a quantum circuit. The dashed blue lines are corresponded to the below Pauli Frame. If we apply RZ gate on 5th qubit after we applied two CNOT gates, then the rotation gate is corresponding to $\exp(-itZ_3Z_5)$.

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.

The original paper formulated the problem as Traversal purchaser problem(TPP)[7]. However, they did not solve the TPP problem and used a dynamic programming method to find a proper frame. The reason is that, two calculate a distance between two frames, B_i, B_j, we have to know all Frame information before we calculate. However, what frame would be sufficient to represent a trotter path for the hamiltonian composites with entanglement gates?. We cannot know the solution of such problem when arbitrary hamiltonian was given. Moreover, when two frames were given, what Clifford gates would yields the transformation from B_i to B_j?. There is no solid frameworks to make the transformation. The questions are remained from Schmitz et al paper.

2.2 Path search over commuting cliques

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.

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

The answer is shotly applying a CX gate on line 1 and 2. The CNOT combination of i, j-th wires are identical to XOR of $w_i \oplus w_j$.

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

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

The solution could be derived with simple linear algebra on specific field, $\mathbb{Z}/2\mathbb{Z}$. Logical *XOR* and *AND* operators form commuting field, $(\mathbb{Z}/2\mathbb{Z}, \wedge, \&)$. See the proof in Appendix A. The Gauss elimination process yields an solution of the above problem.

Suppose that we have circuit of the state where the Pauli Frame representation was,

$$B_i = \begin{pmatrix} w_1 & , \cdot \\ w_2 & , \cdot \\ w_3 & , \cdot \\ w_4 & , \cdot \end{pmatrix}, \begin{aligned} w_1 &= Z_2Z_3Z_4 &&= ZZZI &&= 1110_{sym} \\ w_2 &= Z_1Z_3Z_4 &&= ZZIZ &&= 1101_{sym} \\ w_3 &= Z_1Z_2Z_4 &&= ZIZZ &&= 1011_{sym} \\ w_4 &= Z_1Z_2Z_3 &&= IZZZ &&= 0111_{sym} \end{aligned} \tag{26}$$

and we want to apply $\exp(-itZ1Z2)$ gate on circuit, what CNOT gate combination yieds the quantum circuit state for the unitary operator, by simply applying RZ gate on a wire? Luckily, XOR is commute aslike the CNOT gate becomes a conjugation of itself. Let, $v = [1,1,0,0]^T$, it is a symplectic representation of Z_1Z_2, and $x = [x_1, x_2, x_3, x_4]^T, x_i \in \{0,1\}$.

$$Mx = v \tag{27}$$

$$M = \left[\begin{array}{c|c|c|c} w_1 & w_2 & w_3 & w_4 \end{array}\right] \tag{28}$$

$$\begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \tag{29}$$

With Gauss elimination method, Reduced row echelon form would be obtained.

$$[M \mid v] \rightarrow \left[\begin{array}{cccc|c} 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{array}\right] \tag{30}$$

1. $w_1 \oplus w_2 = 0$
2. $w_2 \oplus w_3 = 1$
3. $w_3 = 0$
4. $w_4 = 0$

Thus, we get $x = [1, 1, 0, 0]$, and

$$[0, 1, 1, 1] \oplus [1, 0, 1, 1] = [1, 1, 0, 0] \tag{31}$$

It means that CNOT over 1st and 2nd yeids $Z1Z2 = IIZZ$ Pauli element on the frame.

$$B_i = \begin{pmatrix} ZZZI & \cdot \\ ZZIZ & \cdot \\ ZIZZ & \cdot \\ IZZZ & \cdot \end{pmatrix} \rightarrow_{CNOT(1,2)} B_{i+1} = \begin{pmatrix} ZZZI & \cdot \\ \mathbf{IIZZ} & \cdot \\ ZIZZ & \cdot \\ IZZZ & \cdot \end{pmatrix} \tag{32}$$

In general case, the local terms are not have the same properties of IZ family terms, of course the same hold for IX, IY families, what about the rest of case?

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, $p = \wedge_i g_i$.*

3 Mutually Commuting Paritition

The remained question is how can we construct mutually commuting partition, from the given hamiltonian and its Pauli polynomial representation. The answer is *we cannot do that efficiently on classical computer*. Suppose that we constructed a graph that indicates commuting relationship of all Pauli terms in the hamiltonian. See Fig

Partitioning the given Pauli elements is equivalent with *Max-clique* problem in computer science and it is a well-known NP-hard problem.

There are practical algorithms in many graph librarieIn addition, many quantum computer companies provide pratical solution for clique problems

Which method is most practical method for the problem? Well, the answer is we don't know yet, sometimes quantum algorithm would show better result with QAOA or anealing system, but by the situation classic method would be better. Choosing an algorithm is a job of researchers or users who want to generate optimized Trotter circuit. In here, providing a convenience interface would be enough.

4 Conclusion

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

A Proof of Modulo field

$(\mathbb{Z}/2\mathbb{Z}, \wedge, \&)$.

Denote, XOR($\wedge$) as $\oplus$ and, AND($\&$) as $\odot$,

$$\begin{aligned} 0 \oplus 0 &= 0 \; 0 \odot 0 &= 0 \\ 0 \oplus 1 &= 1 \; 0 \odot 1 &= 0 \\ 1 \oplus 0 &= 1 \; 1 \odot 0 &= 0 \\ 1 \oplus 1 &= 0 \; 1 \odot 1 &= 1 \end{aligned} \tag{33}$$

Addition

1. a

References

[1] Ronald de Wolf. Quantum computing: Lecture notes, 2023.

[2] Guang Hao Low and Isaac L. Chuang. Hamiltonian simulation by qubitization. *Quantum*, 3:163, July 2019.

[3] Dominic W. Berry, Andrew M. Childs, Richard Cleve, Robin Kothari, and Rolando D. Somma. Simulating hamiltonian dynamics with a truncated taylor series. *Phys. Rev. Lett.*, 114:090502, Mar 2015.

[4] Dominic W. Berry, Andrew M. Childs, Richard Cleve, Robin Kothari, and Rolando D. Somma. Exponential improvement in precision for simulating sparse hamiltonians. In *Proceedings of the forty-sixth annual ACM symposium on Theory of computing*, STOC '14. ACM, May 2014.

[5] Andrew M. Childs, Yuan Su, Minh C. Tran, Nathan Wiebe, and Shuchen Zhu. Theory of Trotter Error with Commutator Scaling. *Physical Review X*, 11(1):011020, February 2021.

[6] M.A. Nielsen and I.L. Chuang. *Quantum Computation and Quantum Information: 10th Anniversary Edition*. Cambridge University Press, 2010.

[7] Albert T. Schmitz, Nicolas P. D. Sawaya, Sonika Johri, and A. Y. Matsuura. Graph Optimization Perspective for Low-Depth Trotter-Suzuki Decomposition, May 2023. arXiv:2103.08602 [cond-mat, physics:math-ph, physics:physics, physics:quant-ph].