Optimising Trotter-Suzuki Decompositions for Quantum Simulation Using Evolutionary Strategies (Appendices)

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ABSTRACT

One of the most promising applications of near-term quantum computing is the simulation of quantum systems, a classically intractable task. Quantum simulation requires computationally expensive matrix exponentiation; Trotter-Suzuki decomposition of this exponentiation enables efficient simulation to a desired accuracy on a quantum computer. We apply the Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES) algorithm to optimise the Trotter-Suzuki decompositions of a canonical quantum system, the Heisenberg Chain; we reduce simulation error by around 60%. We introduce this problem to the computational search community, show that an evolutionary optimisation approach is robust across runs and problem instances, and find that optimisation results generalise to the simulation of larger systems.

KEYWORDS

Quantum Computing, Quantum Simulation, Evolutionary Strategies, CMA-ES.

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This document is an appendix to the main GECCO paper. We present here for reference two methods we employed to further optimise the simulation of our example system. Please see the original paper for full context.

A EFFICIENT EXPONENTIATION

The matrix exponentiation required by the Suzuki decomposition, for example e^{X_1} , is expensive as the matrices involved are of size

2^n . In certain cases, we can invoke the following formula to render this calculation more tractable:

$$e^{A \otimes I + B \otimes I} = e^A \otimes e^B \quad (1)$$

Setting $B = 0$ yields

$$e^{A \otimes I} = e^A \otimes I \quad (2)$$

In our case, this results in identities such as the following

$$e^{\alpha X_1 X_2} = e^{\alpha X \otimes X} \otimes I^{n-2} \quad (3)$$

However this reasoning fails for the ‘wrap around’ case $e^{X_n X_1}$

B TERM PERMUTATIONS

The ordering of the H_j terms in the Hamiltonian sum is arbitrary, as matrix addition is commutative: we may choose alternative orderings of terms in the decomposition, as previously noted [?].

Consider a single permutation of terms that is alternated with its reverse over instances of S_2 . Both the error and gate count depend on the permutation chosen. To see this, observe that in the total decomposition similar terms will appear multiple times, but perhaps with different phases. If these terms can be brought next to each other via commutativity, then the order of decomposition may remain unchanged but we can collapse multiple terms into a single term by combining their phases. For example,

$$e^{\alpha X_1} e^{\beta X_1} = e^{(\alpha+\beta)X_1} \quad (4)$$

Thus in choosing a permutation we must take into account both error and gate count.

One way to reduce the number of terms is to group together all X terms (such as $e^{\alpha X_1 X_2}$), Y terms and Z terms, as they commute within these groups. Denoting X as the product of all X terms (order of which does not matter, as all X terms commute with one another), and similarly for Y and Z , we see that repeating S_2 M times gives:

$$\overbrace{\left(\begin{matrix} X & Y & Z & Z & Y & X \\ n & n & 2n & n & n & n \end{matrix} \right) \left(\begin{matrix} X & Y & Z & Z & Y & X \\ n & n & 2n & n & n & n \end{matrix} \right) \left(\begin{matrix} X & Y & Z & Z & Y & X \\ n & n & 2n & n & n & n \end{matrix} \right) \dots}^{M \text{ times}} \quad (5)$$

This yields a total of $6n + 5n(M-1) = (5M+1)n$ terms, improving on $8Mn$, the number of gates without considering term cancellations.

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Figure 1: Trade-offs achieved with different permutations. The balance between gate count and error is dependent on the ordering of e^{H_i} terms within the decomposition. Here, grouping like terms is shown to outperform the canonical ordering given in Equation (18) in the main paper, and an average over 20 random permutations.

We demonstrate this trade-off space in Figure 1, where ‘Grouped’ refers to grouping together similar terms (as discussed above), ‘Canonical’ refers to the permutation arising from Equation (18) in the main paper, and ‘Random’ is calculated via averaging the errors and gate counts at a given r and k for 20 random permutations. Whilst grouping together similar terms can increase error

(compared with other permutations) at a given order of decomposition, the gate count reductions pareto-dominate other permutation choices, although we do not prove global optimality.