Variational quantum Ansatz tree approach for the heat equation

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INTRODUCTION

Abstract

Variational quantum algorithms are a promising tool for solving partial differential equations. In this paper, we study variational algorithms for solving systems of linear equations generated by a finite difference scheme of the heat equation at a single time step. We focus on a fundamental possibility to achieve quantum superiority within the quantum variational approach. We analyze the optimal choice of the time evolution partition and have found that the time grid parameter controls the computational speed-up with respect to the classical algorithms. We also found that there are two main problems in the efficient implementation of variational algorithms for solving a linear system: i) the measurement of the loss function and ii) the construction of the variational Ansatz. The direct variational approach is based on the minimization of the expectation value of some auxiliary Hamiltonian [1,2]. This approach demonstrates the fundamental possibility of solving systems of linear equations on a quantum computer, but suffers from both above problems. The Hadamard test based approach [1] solves the first problem of the loss function measurement by using a specific measurement basis. The Ansatz tree approach [3] makes use of a given form of the linear system for constructing the Ansatz. This approach combines both the efficient measurement of the loss function by exploiting the Hadamard test and the efficient construction of the Ansatz by exploiting the special hierarchical optimization technique. This allows us to achieve a fundamental superiority over the classical algorithm. The performance of discussed algorithms is demonstrated by the numerical simulation with the linear system matrix size up to $\mathbf{256} \times \mathbf{256}$ ($2^8 \times 2^8$).

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[3] Huang H. Y., Bharti K., Rebentrost P. //New Journal of Physics. – 2021. – . 23. – №. 11. – . 113021.
[4] Morton K., Mayers D. – Cambridge university press, 2005.

Heat equation

Let us consider the heat equation with constant coefficients, a given initial time constraint, and periodic spatial boundary condition,

$$a^2 \Delta U(\vec{r},t) - \frac{\partial U(\vec{r},t)}{\partial t} = f(\vec{r},t);$$
$$U(\vec{r},0) = \chi(\vec{r}); \qquad U(\vec{r},t) = U(\vec{r}+\vec{R},t),$$

where $f(\vec{r},t)$ and $\chi(\vec{r})$ are the heat sources and initial distribution function, respectively. For the numerical solution of such equations, a grid of values of the arguments of U is introduced. For simplicity we investigate one-dimensional case. Next we introduced the finite difference scheme

$$(-2-c)U_i^{\tau+1} + U_{i+1}^{\tau+1} + U_{i-1}^{\tau+1} = b_i^{\tau},$$
$$U_i^0 = \chi_i, \qquad U_0^{\tau} = U_{N_z}^{\tau},$$

where

$$c = \frac{(\delta z)^2}{a^2 \delta t}, \qquad b_i^{\tau} = (f_i^{\tau} + \frac{U_i^{\tau}}{\delta t})\frac{(\delta z)^2}{a^2}.$$

We use an implicit difference scheme that yields the stability of the solution for arbitrary parameters of the equation and the grid size. The single time step evolution from $t = \tau$ to $t = \tau + 1$ is carried out by solving the linear system

$$Ax = b,$$

where

$$A(c) = \begin{pmatrix} -2-c & 1 & 0 & \cdots & 0 & 1 \\ 1 & -2-c & 1 & \cdots & 0 & 0 \\ 0 & 1 & -2-c & \cdots & 0 & 0 \\ \vdots & & \ddots & \ddots & & \vdots \\ 0 & 0 & \cdots & -2-c & 1 & 0 \\ 0 & 0 & \cdots & 1 & -2-c & 1 \\ 1 & 0 & \cdots & 0 & 1 & -2-c \end{pmatrix},$$

$$x = \begin{pmatrix} U_0^{\tau+1} \\ U_1^{\tau+1} \\ \vdots \\ U_{N-1}^{\tau+1} \end{pmatrix}, \qquad b = \begin{pmatrix} b_0^{\tau} \\ b_1^{\tau} \\ \vdots \\ b_{N-1}^{\tau} \end{pmatrix}.$$

Ansatz tree approach

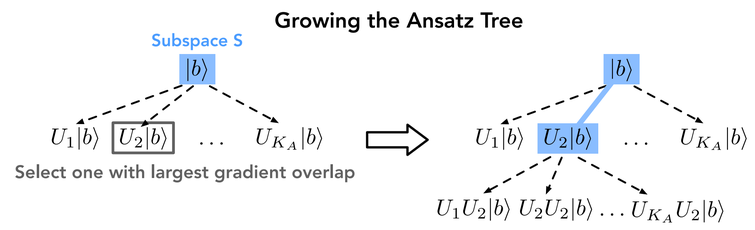
The algorithm has a branched tree structure and is referred to as the Ansatz tree approach (ATA). The ATA is based on an efficient decomposition of the matrix A (1) into a superposition of unitary matrices

$$A = \sum_{i=1}^{K_A} \beta_i U_i.$$

The efficient decomposition means that: (i) the unitary operators of the decomposition can be presented by quantum circuits with a polylogarithmical depth, (ii) the number of U_i also scales polylogarithmically with the size of the matrix A.

$$L_R(x) = ||Ax - |b\rangle||_2^2 = x^\dagger A^\dagger A x - 2Re\{x^\dagger A |b\rangle\} + 1;$$

$$x = \alpha_0 |b\rangle + \alpha_1 U_{v_1} |b\rangle + \alpha_2 U_{v_2} U_{v_1} |b\rangle + \dots,$$



At each next step, we perform the following:

1. Find the optimal $x^s = \sum_{j=0}^{m} \alpha_j |j\rangle$ by optimizing the loss function (1) over the parameters $\alpha_0, \dots, \alpha_m$.
2. Add a new node with the largest gradient overlap to the subspace S: $S \leftarrow S \cup \{|m+1\rangle\}$, $|m+1\rangle = \text{argmax}_{|c\rangle \in C(S)} |g|$.

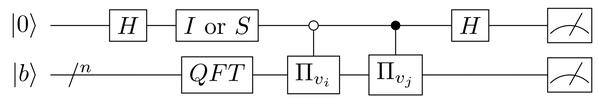
$$A = QFT^\dagger \left(\sum_{i,j} d_{ij} Z_i Z_j + \sum_i s_i Z_i + \zeta I \right) QFT =$$
$$\sum_{i \neq j} d_{ij} QFT^\dagger Z_i Z_j QFT + \sum_i s_i QFT^\dagger Z_i QFT + \zeta I$$

RESULTS

Quantum circuits and measuring

Here we exploit the decomposition of the matrix A into the Pauli products Π_{v_i} in the Fourier representation and denote

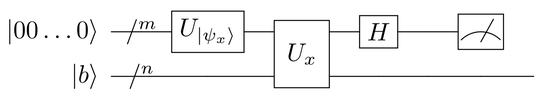
$$|i\rangle = U_{v_i} |b\rangle = QFT^\dagger \Pi_{v_i} QFT |b\rangle .$$



Quantum circuit for measuring real or imaginary part of $\langle i| A |j\rangle$ and $\langle i| A^2 |j\rangle$ depending on the I or S gate.

$$|\psi_x\rangle = \sum_{i=0}^{m-1} \alpha_i |i\rangle .$$

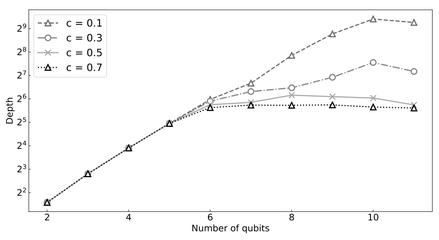
$$U_x = \sum_{j=0} |j\rangle\langle j| \otimes U_{i_j} U_{i_{j-1}} \dots U_{i_1},$$



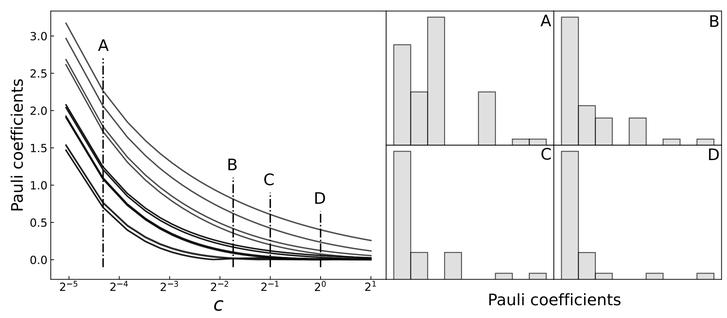
The quantum circuit which generates the normalized solution $|x\rangle$. he solution $|x\rangle$ is generated in the lower qubit register once one measures the state $|\mathbf{00\dots0}\rangle$ in the auxiliary register.

Efficient single time transition

$$x = A_{sol}^{ATA} |b\rangle = (\alpha_0 I + \alpha_1 U_{i_1} + \alpha_2 U_{i_2} U_{i_1} + \dots) |b\rangle \sim A^{-1} |b\rangle$$



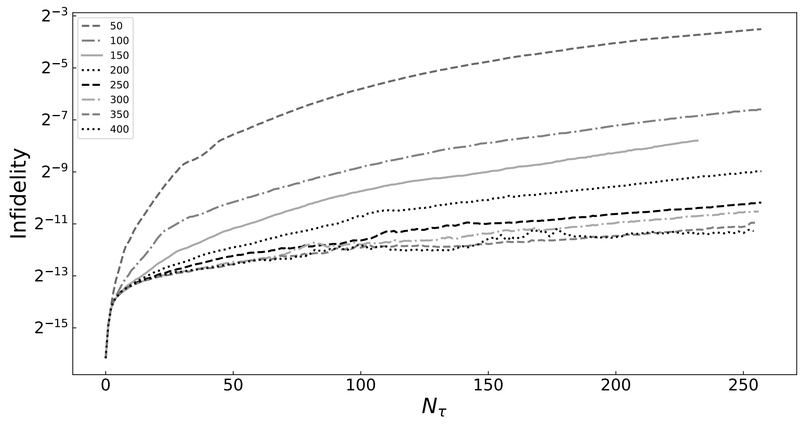
Dependence of the depth of the tree reaching the fidelity of 0.99 on the number of qubits.



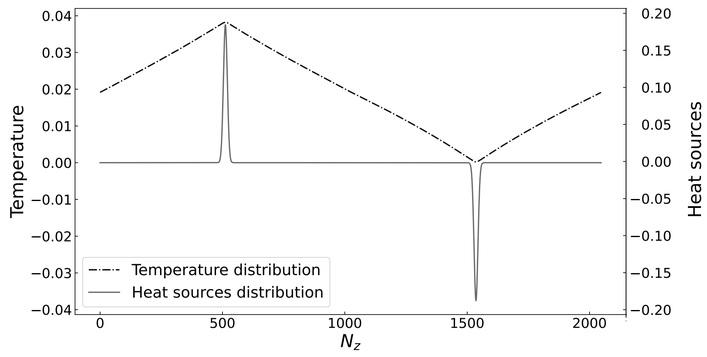
The absolute value of nonzero coefficients of the decomposition into Pauli products of matrix A_F^{-1} as a function of c for 4 qubits.

Time-dependent solution

$$b^\tau = \frac{(\delta z)^2}{a^2} f^\tau + c\, x^\tau = \frac{(\delta z)^2}{a^2} QFT^\dagger \left(\sum_{i=0}^{K_f^t} h_i^\tau \Pi_{hs_i^\tau} \right) \times QFT\, |0\rangle^{\otimes n}$$
$$+ c\, QFT^\dagger \left(\sum_{i=0}^{K_x^t} \kappa_i^{\tau-1} \Pi_{\kappa s_i^{\tau-1}} \right) \times QFT\, b^{\tau-1} = \dots$$
$$= QFT^\dagger \left(\sum_{i=0}^{K_b^0} \kappa_i^0 \Pi_{\kappa s_i^0} \right) QFT\ |0\rangle^{\otimes n}$$



The infidelity of accurate and sequential dropped out solutions depending on the number of time steps (the number of dropout applications) for different D_{cut} and $n = 11$.



Stationary solution for a quasi-singular heater and cooler for $n = 11$. The functions shown are normalised since ATA yields a solution up to a constant.

Summary

- Ansatz tree approach application show that the depth depends polynomially (saturates with the growth of n) on the number of qubits for certain values of the grid parameter c. This reveals the fundamental ability of the Ansatz Tree Approach to demonstrate the quantum superiority for the heat equation. This approach can be considered as the most promising. The reason is that Ansatz Tree Approach makes use of the explicit form of the matrix, unlike the other algorithms discussed, which use the universal entanglers.
- We can conclude that the presented strategy of dropping Pauli products with small coefficients is a promising tool to avoid the problem of the exponential decay of the probability, as well as a preparation an arbitrary quantum state of high dimensions, since the infidelity grows subexponentially (approximately linearly) with the number of time steps.
- The important difference with the HHL approach is that we build up the ansatz tree in a classical manner: once we learned the ansatz tree for the time step t we need not repeat all the proceeding steps while constructing the initial condition for the next time step. This allows us to circumvent the exponentially decay of the probability to get the correct answer.