Poster title:

Enhancing Convergence in Variational Quantum Eigensolver Using CoolMomentum

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Poster abstract:

The current state of quantum processing units (QPU) is characterized by Noisy Intermediate-Scale Quantum (NISQ) devices. Among the methods to utilize NISQ devices, the Variational Quantum Eigensolver (VQE) is prominent for finding ground state energies of quantum systems. However, VQE parameter optimization is NP-Hard, posing significant challenges. To address this, we introduce the CoolMomentum method, a global optimization approach based on Langevin dynamics with simulated annealing. We compare CoolMomentum with ADAM, SPSA, and NFT in VQE using a random weighted Max-Cut problem for up to 20 qubits. Our results confirm that CoolMomentum consistently outperforms the other methods. ADAM and SPSA tend to get trapped in local minima or exhibit infeasible optimization durations, whereas NFT, despite its fast convergence, also suffers from local minima. In contrast, CoolMomentum demonstrates higher accuracy and robustness across various numbers of qubits, highlighting its potential as a superior optimization strategy for VQE.

Poster relevance:

This study has significant implications for advancements in the fields of quantum computing and engineering. It employs the CoolMomentum method, based on Langevin dynamics and simulated annealing, as an optimizer for the Variational Quantum Eigensolver (VQE). The novelty of this research lies in the use of a physics-inspired optimization technique, such as CoolMomentum, to address the challenges of classical optimization in VQE. We numerically analyzed the performance of the conventional optimization methods and confirmed that CoolMomentum consistently outperforms them. CoolMomentum demonstrates substantial potential as an effective optimization strategy for VQE on NISQ devices.

Enhancing Convergence in Variational Quantum Eigensolver Using CoolMomentum

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*Abstract*—The current state of quantum processing units (QPU) is characterized by Noisy Intermediate-Scale Quantum (NISQ) devices. Among the methods to utilize NISQ devices, the Variational Quantum Eigensolver (VQE) is prominent for finding ground state energies of quantum systems. However, VQE parameter optimization is NP-Hard, posing significant challenges. To address this, we introduce the CoolMomentum method, a global optimization approach based on Langevin dynamics with simulated annealing. We compare CoolMomentum with ADAM, SPSA, and NFT in VQE using a random weighted Max-Cut problem for up to 20 qubits. Our results confirm that CoolMomentum consistently outperforms the other methods. ADAM and SPSA tend to get trapped in local minima or exhibit infeasible optimization durations, while NFT, despite its fast convergence, also suffers from local minima. In contrast, CoolMomentum demonstrates higher accuracy and robustness across various numbers of qubits, highlighting its potential as a superior optimization strategy for VQE.

Keywords—Gate-Based Quantum Computer, Noisy Intermediate-Scale Quantum Devices, Quantum-Classical Hybrid Algorithms, Variational Quantum Eigensolver, CoolMomentum

# Introduction

The current state of quantum processing units (QPU) is characterized by Noisy Intermediate-Scale Quantum (NISQ) devices [1]. These devices are improving in scale and error rates but lack full quantum error correction and have limited quantum gate operations. Quantum-classical hybrid algorithms combine QPUs with CPUs are well-known methods for utilizing NISQ devices. Among these, the Variational Quantum Eigensolver (VQE) [2] is a prominent algorithm for finding the ground state energy of quantum systems described by Hamiltonians. VQE is executable on NISQ devices and leverages quantum computing advantages, even without fully error-corrected QPUs. However, parameter optimization in VQE is NP-Hard [3], which makes the search for optimal solutions challenging.

To address this, we introduced the CoolMomentum method [4], a global optimization method based on Langevin dynamics with simulated annealing, to enhance the VQE. We compare CoolMomentum with adaptive moment estimation (ADAM), simultaneous perturbation stochastic approximation (SPSA), and the Nakanishi–Fujii–Todo method (NFT) in VQE. Using a random weighted Max-Cut problem for up to 20 qubits, we numerically analyzed these methods and confirmed that CoolMomentum consistently outperforms the others.

# Experimental Details

## Variational Quantum Eigensolver

VQE is a ground-state calculation method that uses quantum circuits, and its fundamental concept is rooted in the variational principle. Specifically, the energy expectation value obtained from a trial wave function , parameterized by ***θ***, satisfies the principle given by Eq. (1)

where *H* is a given Hamiltonian and *Emin* is the minimum eigenvalue. Since this equality holds only when the trial function is the exact eigenstate of the Hamiltonian, energy and wavefunction of the ground state can be found by minimizing the energy expectation value concerning ***θ***.

## VQE Using CoolMomentum Method

In VQE, the parameter optimization methods are called optimizers. Most optimizers do not guarantee convergence to a global minimum, and computational accuracy suffers due to many local solutions. To address this, we focused on CoolMomentum, a physics-inspired global optimization method likeSimulated Annealing [5]. Borysenko et al. showed that gradually decreasing the momentum coefficient from practically unity to zero is equivalent to Simulated Annealing or slow cooling [4]. In CoolMomentum, Simulated Annealing is applied by gradually reducing the temperature to a minimum value, typically by decreasing the learning rate according to a specific schedule. Alternatively, CoolMomentum achieves this by gradually decreasing the momentum coefficient of the Momentum optimizer.

## Problem Settings

We numerically demonstrated the performance of the methods using a max-cut problem. The Hamiltonian *H* is

where *I* is the identity matrix, *Zi* denotes the Pauli *Z* operator on qubit *i* and *wij* corresponds to integer weights selected uniformly at random in the interval [−10, 10]. In our experiments, we used a quantum circuit where a single *RY* gate was applied to each qubit. The rotation angle for each qubit was determined using one variational parameter per qubit. Thus, the trial state is expressed as:

where *n* is the number of qubits, *θi* is the rotation angle of the *RY* gate applied to the *i*-th qubit, and *Y* represents the Pauli-*Y* matrix. The initial values of the circuit parameters were randomly sampled from a uniform distribution [−*π*, *π*). During the numerical simulation, we sampled the outcome 8192 times to estimate the energy expectation value. We compared CoolMomentum with optimization algorithms such as simultaneous perturbation stochastic approximation (SPSA) [6], adaptive moment estimation (ADAM) [7], and the Nakanishi–Fujii–Todo method (NFT) [8]. The hyperparameters for SPSA and NFT were selected based on Ref. [5]. For ADAM, we used an initial learning rate of *η* = 0.1 with a decay schedule of *β*1 = 0.9 and *β*2 = 0.999. For CoolMomentum, we used an initial learning rate of *η*0 = 0.02 and an initial momentum coefficient of *ρ*0 = 0.999.

(c)

(b)

(a)

# Results

  

Fig. 1 (a) and (b) show the convergence of the expectation values for each optimization process in 10-qubit VQE on an aer simulator and ibm\_kawasaki, respectively. The black dashed line indicates the ground state energy. (c) shows the mean residual energy as a function of the number of qubits, averaged over 20 instances, with error bars representing the standard error on the aer simulator.

## Convergence of the Expectation Values

Fig. 1 (a) and Fig. 1 (b) present the expectation values of each optimizer over 200 iterations for 𝑛 = 10. The instances used in Fig. 1 (a) and (b) are identical, and each optimizer reaches the global energy of -63. Using the real QPU ibm\_kawasaki, which has 127 qubits, we employed the T-REx method [9] for error mitigation. During optimization, energy fluctuations with CoolMomentum were initially larger than those with ADAM, NFT, and SPSA, but gradually decayed after 100 iterations, ultimately converging due to overdamping at the end of the optimization process. This design allows CoolMomentum to explore the global solution space before converging. On the ibm\_kawasaki, error mitigation corrections caused expected values to fall below the ground state energy, but each optimizer converged near the ground state energy within a similar number of iterations as on the simulator. This suggests that the computational characteristics of CoolMomentum are preserved even when using NISQ devices.

## Scaling of Problem Size

Fig. 1 (c) illustrates the residual energy obtained when solving the max-cut problem with *n* ∈ [6, 20] nodes using each optimizer. Residual energy [10] is calculated as

measures the closeness of the final output-state energy to the ground state energy. In Eq. (4), is the expectation value of the Hamiltonian *H* at the parameter ***θ***, *Emin* denotes the ground state energy, and *Emax* is the energy of the highest excited state. Consequently, the residual energy maintains a consistent level of accuracy as the number of qubits increases. Furthermore, CoolMomentum demonstrated a tendency to achieve lower energy than other optimizers, even under the aforementioned conditions.

# Discussion

In this study, we solved a Max-Cut problem using VQE with CoolMomentum and confirmed that this method achieved higher accuracy than other optimizers. Additionally, the use of the T-REx method suggests that the convergence characteristics of CoolMomentum can be maintained, even when using an actual QPU. Therefore, CoolMomentum is expected to mitigate the risk of falling into the local minima in NISQ. The results indicate that the combination of Langevin dynamics and simulated annealing is an efficient approach for VQE.

##### References

1. J. Preskill, “Quantum Computing in the NISQ era and beyond,” Quantum, vol. 2, art. no. 79, August 2018.
2. A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O’Brien, “A variational eigenvalue solver on a photonic quantum processor,” Nat. Commun., vol. 5, art. no. 4213, July 2014.
3. L. Bittel and M. Kliesch, “Training Variational Quantum Algorithms Is NP-Hard,” Phys. Rev. Lett., vol. 127, art. no. 120502 September 2021.
4. O. Borysenko and M. Byshkin, “CoolMomentum: a method for stochastic optimization by Langevin dynamics with simulated annealing,” Sci. Rep., vol. 11, art. no. 10705, May 2021.
5. D. Tsukayama, J. Shirakashi, and H. Imai, “CoolMomentum mitigating local minima in variational quantum eigensolvers,” Jpn. J. Appl. Phys., vol. 62, art. no. 088003, August 2023.
6. J. C. Spall, “Implementation of the simultaneous perturbation algorithm for stochastic optimization,” IEEE Trans. Autom. Control., Vol. 37, pp. 332-341, March 1992.
7. D. P. Kingma and J. L. Ba, “Adam: A Method for Stochastic Optimization,” arXiv:1412.6980v9 [cs.LG], January 2017.
8. K. M. Nakanishi, K. Fujii, and S. Todo, “Sequential minimal optimization for quantum-classical hybrid algorithms,” Phys. Rev. Res., vol. 2, art. no. 043158, October 2020.
9. E. van den Berg, Z. K. Minev, and K. Temme, “Model-free readout-error mitigation for quantum expectation values,” Phys. Rev. A, vol. 105, art. no. 032620, March 2022.
10. G. B. Mbeng, R. Fazio, and G. E. Santoro, “Quantum Annealing: a journey through Digitalization, Control, and hybrid Quantum Variational schemes,” arXiv:1906.08948 [quant-ph] December 2019.