Quantum Circuit Ansatz Structures for Ising Model & A Comparative Analysis of Classical and Quantum Optimization Methods

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Quantum Variational Eigensolver

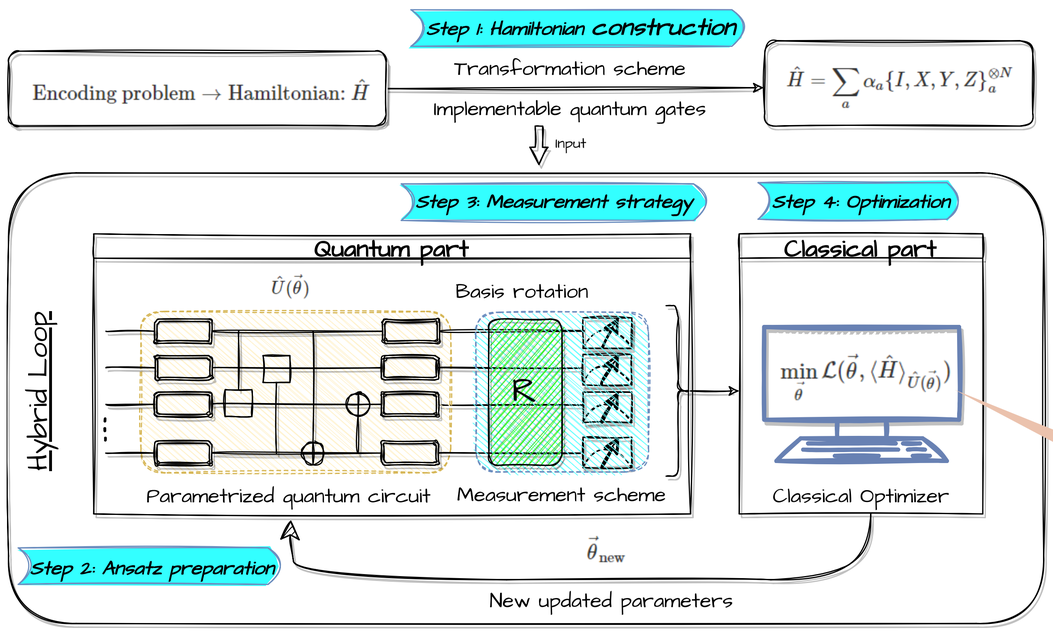

Figure 1: VQE Architecture

Parametrized Quantum Circuit (PQC) structure

The Ansatz structure is studied based on the symmetries of TIM Hamiltonian to heuristically guess the ansatz achitecture

- Real representation → Real rotaion gate
- Local interaction → Linear entanglement scheme
- Spin-flip symmetry → reducing $\#\theta_i$

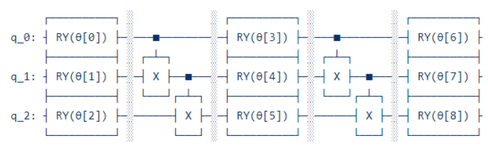

Figure 2: A RealAmplitudes circuit with 2 repetitions on 3 qubits with 'linear' entanglement scheme

Notice !

Keep in mind that the ansatz structure here we obtained from intuitive choice inspired by system symmetries, people also had ideas about more rigorous ways to achieve ansatz structure using chemical dynamics, Hamilton information, and adaptive manners, etc., such as UCC-UCCSD, HVA, ADAPT-VQE, respectively.

Numerical study

Derivative-based method efficiency			
$\nabla f(\theta)$	PSR	FD	SPSA
Comp. cost	2p	2p	2
$g(\theta)$	HES-PSR	QN-BDA	QNSPSA
Comp. cost	3p.p	L	4

Table 1: Computational cost from different methods of computing gradient $\nabla f(\theta_k)$ and Geometry metric $g(\theta)$. Where p is the number of parameters, L is the number of PQC layers of the same rotation generator. HES-PSR is, where we use PSR to estimate HES, for reference, nevertheless, it is obviously impractical.

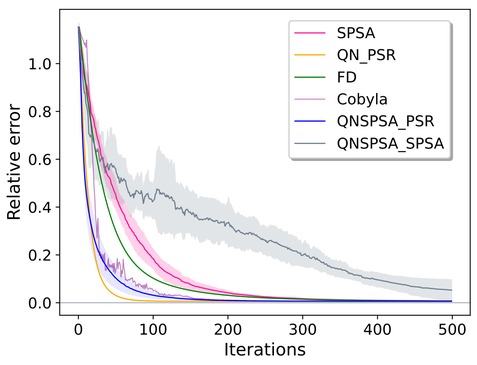

Figure 4: Comparing multiple optimizations of TIM's 12 spins with RealAmplitudes Ansatz

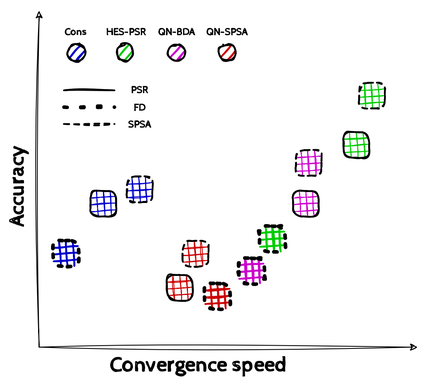

Figure 3: The comparative graphics among combinations of gradient and updating learning rate methods

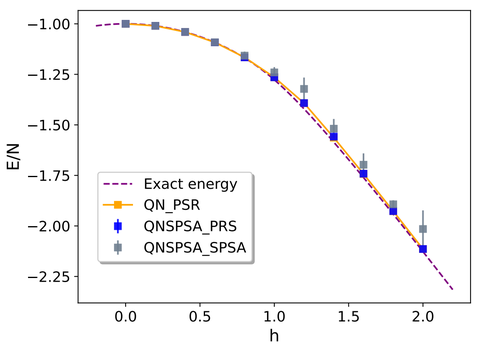

Figure 5: Estimate the average ground state energy for TIM of 12 spins and different external fields with RealAmplitudes ansatz

What's Interesting? The QNSPSA_PSR is proposed as an extension of the usual QNSPSA, which just takes 2p+4 cost according to Tab. 1 while remaining accurate computation from PSR. The combined algorithm QNSPSA_PSR exhibited unexpected theoretical prediction by demonstrating potential not only in reducing computational costs, as it does not scale up significantly with qubits like traditional QN methods, but also in achieving more accurate and faster to optimal solutions, outperforming other methods, even QN_PSR in terms of practical usage.

What we have done so far

In this study, we delved into several **optimization methods**, both classical and quantum, and **analyzed the quantum advantage that each of these methods** offered, and then we proposed a **new combinatorial optimization scheme, deemed as QNSPSA_PSR** which combines calculating approximately Fubini-study metric (QNSPSA) and the exact evaluation of gradient by Parameter-Shift Rule (PSR). The **QNSPSA_PSR method integrates the QNSPSA computational efficiency with the precise gradient computation of the PSR, improving both stability and convergence speed while maintaining low computational consumption**. Our results provide a new potential quantum supremacy in the VQE's optimization subroutine and enhance viable paths toward efficient quantum simulations on Noisy Intermediate Scale Quantum Computing (NISQ) devices. Additionally, we also conducted a **detailed study of quantum circuit ansatz structures** in order to find the one that would work best with the Ising model and NISQ, which we **utilized the symmetry of the investigated model.**

Keyword Ising Model, Variational Quantum Eigensolver, Quantum Optimization, Ansazt Construction

The cost function we used here is the expectation value of the Transerve Ising Model (TIM)'s Hamiltonian

$$\min_{\vec{\theta}} \mathcal{L}\left(\vec{\theta}, \langle \hat{H} \rangle_{\vec{\theta}}\right) \equiv \min_{\vec{\theta}} \langle \hat{H}_{\text{TIM}} \rangle_{\vec{\theta}}$$

treated as a toy model to investigate our study method, where

$$\hat{H}_{\text{TIM}} = -J \sum_{n=1}^{N-1} \sigma_{n-1}^z \sigma_n^z - h \sum_{n=0}^{N-1} \sigma_n^x$$

Optimization subroutine in VQE

Derivative-free (sometimes referred to as blackbox optimization) that does not use derivative information in the classical sense to find optimal solutions, interpolates the decrement of the objective function from sets of test points instead. Well-known ones such as **COBYLA, Nelder-Mead, Bayesian optimization**, etc.

The derivative-based methods update parameters through

$$\theta_{k+1} = \theta_k - \eta_k g^+(\theta_k) \nabla f(\theta_k).$$

Essentially, there are two parts when we compute the derivative-based method

Gradient $\nabla f(\theta)$

The numerical technique to calculate the gradient vector $\nabla f(\theta_k)$ widely used is **Finite Difference (FD)** or approximated by the so-called **Simultaneous Perturbation Stochastic Approximation (SPSA)** method

$$\nabla f(\theta_k) \to \nabla \tilde{f}(\theta_k) = \frac{f(\theta_k + \epsilon \vec{\Delta}_k) - f(\theta_k - \epsilon \vec{\Delta}_k)}{2\epsilon} \vec{\Delta}_k, \tag{1}$$

where $\vec{\Delta}_k$ is a random perturbed vector sampled from the zero-mean distribution, usually, the Bernoulli distribution is employed.

The **Parameter-shift Rule (PSR)** allows us to extract the exact derivative from the quantum cost function, herein $f(\theta) \equiv \langle \hat{H}_{\text{TIM}} \rangle_\theta$, which we deem as quantum optimization method

$$\nabla f(\theta_k)_i = s\left[f(\theta_i + \frac{\pi}{4s}) - f(\theta_i - \frac{\pi}{4s})\right]. \tag{2}$$

Pseudo-inverse Geometry metric $g^+(\theta)$

In the second-order derivative-based method entailing the geometric information from space of the cost function, which is embedded in local metric $g(\theta)$ equivalent to **the Hessian matrix (HES)** of the cost function. Another approach that takes into account the quantum space of the quantum circuit ansatz. Namely, Fubini–Study metric is Hessian of PQC space

$$g_{ij}(\theta) = -\frac{1}{2} \partial_{\theta_i} \partial_{\theta_j} |\langle \psi_\theta, \psi_{\tilde{\theta}} \rangle|^2 \Big|_{\tilde{\theta}=\theta}.$$

The optimization method using Fubini-study information is named **Quantum Natural Gradient Descend (QN)**. In practice, we have not yet had the hardware power to compute a full exact QN metric, which leads to two approximations, **Block Diagonal Approximation (QN-BDA)**

$$g_{ij}^{(l)}(\theta) = \langle \psi_\theta^{(l-1)} | K_i K_j | \psi_\theta^{(l-1)} \rangle - \langle \psi_\theta^{(l-1)} | K_i | \psi_\theta^{(l-1)} \rangle \langle \psi_\theta^{(l-1)} | K_j | \psi_\theta^{(l-1)} \rangle, \tag{3}$$

and **employing SPSA to compute the second-order derivative, i.e. QNSPSA**

$$g^k(\theta) \approx \frac{\triangle F}{4\epsilon^2} \left(\vec{\Delta}_k^1 \vec{\Delta}_k^{2\text{T}} + \vec{\Delta}_k^2 \vec{\Delta}_k^{1\text{T}}\right), \tag{4}$$

where l is the layer number in layered PQCs, Hermitian generator K_i of quantum gates at each layer, and $\triangle F$ is the 2-SPSA approximation of second-order derivative.