

Adiabatic quantum computing with parameterized quantum circuits

arXiv:2206.04373

I. Kolotouros

University of Edinburgh

April 14, 2023

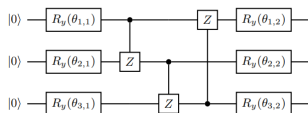
Outline

- 1 Motivation
- 2 Variational Quantum Algorithms
 - Ascending CVaR
- 3 Adiabatic Quantum Computing
- 4 Main Results
 - Parameterized Perturbation Theory
 - Adiabatic Quantum Computing with parameterized quantum circuits
 - Simulated Experiments
- 5 Conclusions/Discussion

Motivation

We are currently in the **NISQ** era:

- Small Scale Quantum Computers.
- Noisy Quantum Circuits.
- Limited Connectivity.



Hybrid Quantum/Classical Algorithms (VQE/QAOA):

- Small Quantum Computer with fixed Architecture.
- Postprocessing of measurements in a classical computer.

Can this framework offer any *practical quantum advantage*?

Variational Quantum Algorithms

- **Step 1.** Problem at hand $\rightarrow H$ where H is an interacting qubit Hamiltonian.

$$H = \sum_{l=1}^L c_l P_l \quad (1)$$

where $c_l \in \mathbb{R}$, P_l a Pauli string, $L = \mathcal{O}(\text{poly}(n))$ and n is the system size.

- **Step 2.** Choose ansatz family $U(\boldsymbol{\theta}) = V(\theta_M) \dots V(\theta_1)$ where $M = \mathcal{O}(\text{poly}(n))$ and initial parameters $\boldsymbol{\theta}_0$.
- **Step 3.** Execute the quantum circuit and measure the parameterized state $|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta}) |0\rangle^{\otimes n}$.
- **Step 4.** Choose an *objective function* whose global minimum will correspond to the solution of the problem (usually the expectation value $E(\boldsymbol{\theta}) = \langle \psi(\boldsymbol{\theta}) | H | \psi(\boldsymbol{\theta}) \rangle$).

Variational Quantum Algorithms

Variational Quantum Algorithm Framework

Input

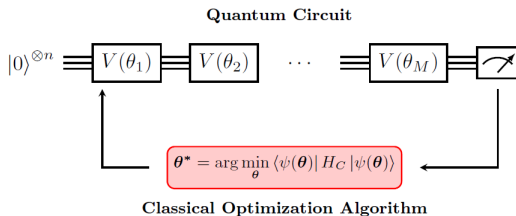
Ansatz Family $U(\theta) = V(\theta_M) \cdots V(\theta_1)$

Initial Parameters θ_0

Output

Optimal Parameters θ^*

Ground State Approximation $|\psi(\theta^*)\rangle$



- **Step 5.** Choose a classical optimization algorithm and update the parameters following the direction that minimizes the objective function. For example:

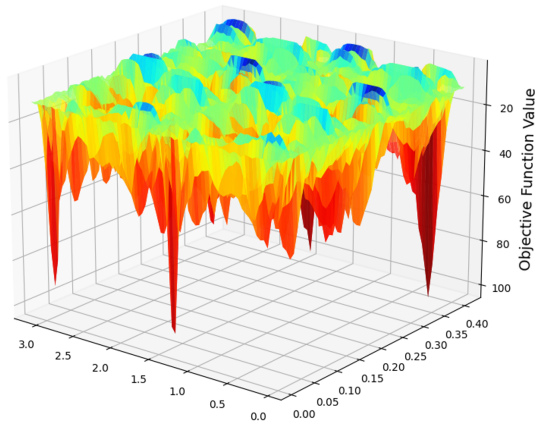
$$\theta_{t+1} = \theta_t - \eta \nabla E(\theta_t) \quad (2)$$

- **Step 6.** When convergence occurs at $\theta^* = \arg \min_{\theta} E(\theta)$ return the ground state approximation $|\psi(\theta^*)\rangle$.

Bottlenecks

Biggest obstacles in VQAs:

- Local minima.
- Performance is sensitive to initial parameters.
- Barren Plateaux.
- No complexity-theoretic arguments about their scaling.



Ascending CVaR (Phys. Rev. Research 4, 023225)

Classical Optimization problems have diagonal Hamiltonians.

- Prepare $|\psi(\boldsymbol{\theta})\rangle \rightarrow$ Measure \rightarrow Sort energy samples.
- Keep only α percentage of lowest energies and minimize it $\rightarrow CVaR_\alpha$

Motivation.

- Choice of α is random.
- We need $1/\alpha$ measurements to achieve the same accuracy.
- We will not achieve the largest overlap with the optimal solution.
- $CVaR_\alpha$ with different α agree on the ground state but the rest of the landscape is different!

We can allow α to vary slowly! Significant improvement in performance in MaxCut, Number Partitioning, and Portfolio Optimization.

Adiabatic Quantum Computing

Conventional algorithms with proven theoretical guarantees *implies* Adiabatic Quantum Computing (AQC).

- Initialize system in an easy-to-prepare ground state of a Hamiltonian H_0 .
- Allow the system of qubits to interact under the Hamiltonian:

$$H(t) = \left(1 - \frac{t}{t_f}\right) H_0 + \frac{t}{t_f} H_1, t \in [0, t_f] \quad (3)$$

- If certain conditions are met, the system will find itself in the ground state of H_1 at $t = t_f$.

To ensure **adiabaticity**:

- The system must be evolved sufficiently slowly so that it never jumps to the instantaneous excited state at any time throughout the evolution.
- The total time t_f is inversely correlated to the *spectral gap*, i.e. the energy difference between the ground state and the first excited state.

Adiabatic Quantum Computing

Bottlenecks:

- Some problems have exponentially (to the system size) small spectral gaps.
- In order to approximate adiabatic evolution in the quantum circuit model large quantum circuits are needed. \implies Inapplicable for NISQ devices.

Parameterized Perturbation Theory

Consider a Hamiltonian H_0 , an ansatz family $U(\theta)$ and initial angles θ^* that produce the ground state of H_0 , i.e.,

$$\theta^* = \arg \min_{\theta} \langle \psi(\theta) | H_0 | \psi(\theta) \rangle \quad (4)$$

Question 1. Suppose that we perturb the Hamiltonian H_0 by a small amount λH_2 with $\lambda \ll 1$. What is the shift vector ϵ that will translate the system from the ground state $|\psi(\theta^*)\rangle$ of H_0 at the ground state $|\psi(\theta^* + \epsilon)\rangle$ of $H_0 + \lambda H_2$?

Parameterized Perturbation Theory

Theorem 1 (Informal). Consider a family of parameterized quantum states $|\psi(\theta)\rangle$ and initial angles θ^* that minimize a Hamiltonian H_0 , i.e., $\theta^* = \arg \min_{\theta} \langle \psi(\theta) | H_0 | \psi(\theta) \rangle$. If we perturb the Hamiltonian H_0 by a small amount λH_2 with $\lambda \ll 1$, then the shift parameters ϵ that will translate the system onto the perturbed ground state $|\psi(\theta^* + \epsilon)\rangle$ (at the point $\theta^* + \epsilon$) of $H_{\lambda} = H_0 + \lambda H_2$ can be found by solving the following mathematical problem:

$$\begin{aligned} & \min \|\epsilon\| \\ & \text{s.t. } A\epsilon + Q = 0 \\ & \mathbf{H}_{\theta^* + \epsilon}^{\lambda} \succcurlyeq 0 \end{aligned} \tag{5}$$

The matrix elements A_{ij} , Q_j , and the Hessian, correspond to observables that are calculated at the ground state of H_0 !

Parameterized Perturbation Theory

The matrix elements A_{ij} , Q_j are given by:

$$\begin{aligned} Q_i &= \lambda \frac{\partial}{\partial \theta_i} (\langle \psi(\boldsymbol{\theta}) | H_2 | \psi(\boldsymbol{\theta}) \rangle) \Big|_{\boldsymbol{\theta}^*} \\ A_{ij} &= \frac{\partial^2}{\partial \theta_i \partial \theta_j} (\langle \psi(\boldsymbol{\theta}) | H_\lambda | \psi(\boldsymbol{\theta}) \rangle) \Big|_{\boldsymbol{\theta}^*}. \end{aligned} \quad (6)$$

The derivatives and the Hessian can be calculated easily using *parameter-shift rules*.

Adiabatic Quantum Computing with parameterized quantum circuits

Algorithm (AQC-PQC). If the perturbation is chosen to be $\lambda(H_1 - H_0)$, the total perturbed Hamiltonian is:

$$H_\lambda = (1 - \lambda)H_0 + \lambda H_1 \implies \text{Adiabatic Quantum Computing Hamiltonian} \quad (7)$$

We can iteratively add perturbation of the form $\lambda(H_1 - H_0)$, with $\lambda \equiv \frac{1}{K}$ where K is the choice of discretization steps.

After K steps we will have approximated the ground state of the target Hamiltonian H_1 .

Adiabatic Quantum Computing with parameterized quantum circuits

Adiabatic Quantum Computing with PQC

Input

Ansatz Family $U(\boldsymbol{\theta}) = V(\theta_M) \cdots V(\theta_1)$

Initial Hamiltonian H_0 , Target Hamiltonian H_1

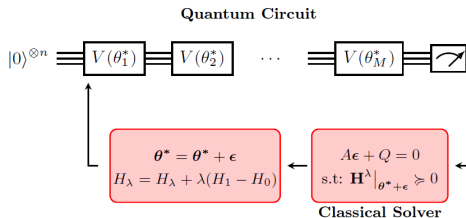
Initial Parameters $\boldsymbol{\theta}^* = \arg \min_{\boldsymbol{\theta}} \langle \psi(\boldsymbol{\theta}) | H_0 | \psi(\boldsymbol{\theta}) \rangle$

$$H_\lambda = (1 - \lambda)H_0 + \lambda H_1$$

Output

Optimal Parameters $\boldsymbol{\theta}^* = \arg \min_{\boldsymbol{\theta}} \langle \psi(\boldsymbol{\theta}) | H_1 | \psi(\boldsymbol{\theta}) \rangle$

Ground State Approximation $|\psi(\boldsymbol{\theta}^*)\rangle$



Adiabatic Quantum Computing with parameterized quantum circuits

Question 2. How many steps K do we need so that we reach the ground state with certainty, provided that the ansatz family can reach all intermediate ground states?

Theorem 2. Consider a time-dependent Hamiltonian $H(\tau) = (1 - \tau)H_0 + \tau H_1$, $\tau \equiv \frac{t}{t_f} \in [0, 1]$. Let $\Delta(\tau) \equiv E_1(\tau) - E_0(\tau)$ be the instantaneous spectral gap and $\delta_\tau(\lambda) \equiv E_0(\tau + \lambda) - E_0(\tau)$ be the energy difference between the ground states at time $\tau + \lambda$ and τ respectively. Moreover, assume that the parameterized family of states contains the ground state for each $\tau \in [0, 1]$ and $|\delta_\tau(\lambda)| \ll \Delta(\tau + \lambda)$. Then AQC-PQC will always return the ground state of the target Hamiltonian H_1 as long as we discretize the time-dependent Hamiltonian into $K > K_0$ where:

$$K_0 \in \mathcal{O} \left(\frac{\text{poly}(n)}{\min_\tau \Delta(\tau)} \right) \quad (8)$$

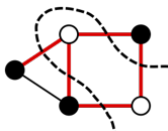
Adiabatic Quantum Computing with parameterized quantum circuits

Advantages over VQAs

- Insensitive to initialization parameters which may lead to bad convergence.
- Requires no energy minimization.
- No Barren Plateaux.
- Only K quantum states preparations (although K may scale exponentially).
- Accuracy of the result depending on the choice of discretization steps.
- $\mathcal{O}(KM^3)$ expectation value calculations.

Simulated Experiments

MaxCut. Consider a graph $G(V, E)$ where V is the set of vertices, E is the set of edges and let W be a weight matrix describing the weights of the graph.



Goal. Our target is to find a partition of the vertices into two disjoint sets that “cuts” the maximum number of edges. The MaxCut can be mapped to an Ising Hamiltonian:

$$H_{\text{MC}} = - \sum_{\langle i,j \rangle \in E} \frac{w_{ij}}{2} (1 - \sigma_i^z \sigma_j^z). \quad (9)$$

Simulated Experiments

Number Partitioning. Consider a list of integers $\{n_1, n_2, \dots, n_N\}$.

Goal. Our target is to decide whether there exists a partition of the set into two disjoint subsets S, \bar{S} so that the sums of the elements on each subset are equal. The Number Partitioning problem can be mapped to an Ising Hamiltonian:

$$H_{\text{NP}} = \sum_{i \neq j} (n_i n_j) \sigma_i \sigma_j + \sum_{i=1}^N n_i^2 \quad (10)$$

Simulated Experiments

Transverse-Field Ising Chain. The Hamiltonian describing the TFI chain model (with periodic boundary conditions) is:

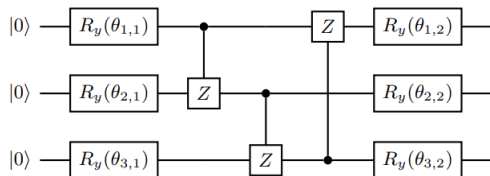
$$H_{\text{TFI}} = - \sum_{k=1}^n J_k \sigma_k^z \sigma_{k+1}^z - h \sum_{k=1}^n \sigma_k^x \quad (11)$$

where (J_k, h) are coupling coefficients.

Technical Details

Initial Hamiltonian for all problems examined: $H_0 = -\sum_{i=1}^n \sigma_i^x$ with ground state $|+\rangle^{\otimes n}$.

Ansatz family used for experiments:



All simulations were performed using **QuEST** and **Qiskit** allowing exact noiseless calculations of expectation values.

Choice of discretization steps.

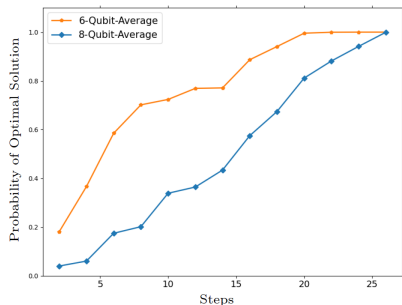


Figure: MaxCut performance.

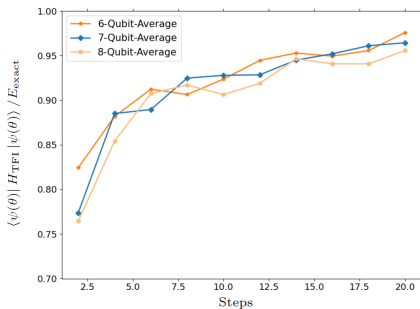
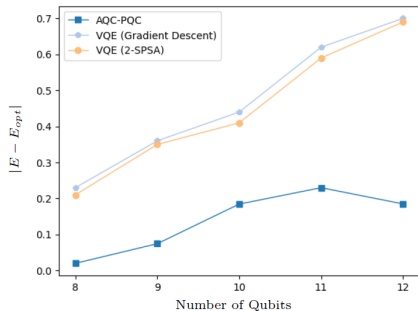


Figure: TFI performance.

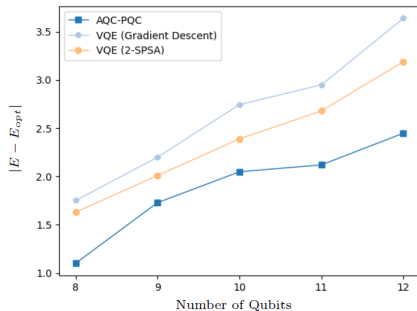
Accuracy improves with the increase of discretization steps!

Classical Optimization Problems:

MaxCut



Number Partitioning



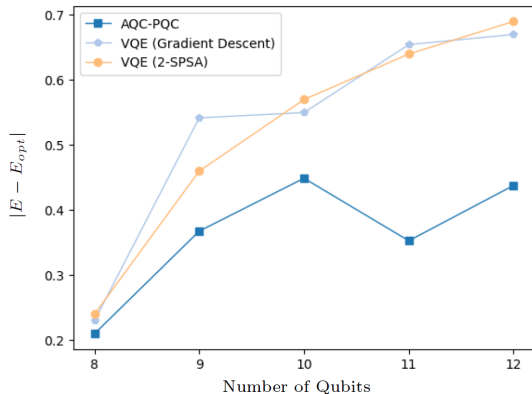
AQC-PQC vs VQE

Classical Optimization Problems:

MaxCut	Optimal Solution Overlap (%)					
	7 Qubits	8 Qubits	9 Qubits	10 Qubits	11 Qubits	12 Qubits
AQC-PQC	82.7	74.3	93.1	50	28.1	56.6
VQE	62.3	54.7	60.8	39.2	22.1	11.1

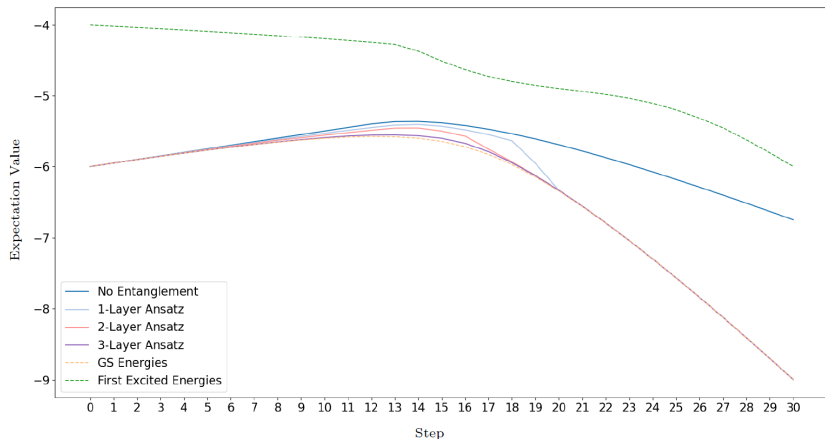
Number Partitioning	Optimal Solution Overlap (%)					
	7 Qubits	8 Qubits	9 Qubits	10 Qubits	11 Qubits	12 Qubits
AQC-PQC	37.5	21.9	24.7	12.6	5	4.6
VQE	28.5	6.2	6.4	1.2	0.8	0.4

Transverse-Field Ising Chain:



Ansatz Expressiveness

$$H_k = \left(1 - \frac{k}{30}\right) H_0 + \frac{k}{30} H_{\text{MC}}, \quad k \in [30] \quad (12)$$



Discussion and Future work.

- Optimal algorithm for solving the classical problem:

$$\begin{aligned} & \min \|\epsilon\| \\ \text{s.t. } & A\epsilon + Q = 0 \\ & \mathbf{H}_{\theta^* + \epsilon}^\lambda \succcurlyeq 0 \end{aligned}$$

- Test performance and compare with VQE on larger instances.
- Limitations?
- Bounds on performance if ansatz cannot reach intermediate ground states?
- Bounds on performance if the quantum device has given accuracy on angles?

Thank you all.

“Adiabatic quantum computing with parameterized quantum circuits”, I. Kolotouros, I. Petrongonas, M. Prokop, P. Wallden. (arXiv:2206.04373)