Variational Quantum Eigensolver on 1D transverse-field Ising model

Alessandro Sinibaldi
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Outline

1. Hybrid Variational Quantum Algorithms (HVQAs)
2. Variational Quantum Eigensolver (VQE)
3. VQE on 1D transverse-field (TF) Ising model
   - without noise
   - with a real noise model and with noisy channels
4. References

HVQAs

Hybrid Algorithms

Hybrid algorithm:

quantum computing + **classical** computation

- The quantum part is restricted to subroutines that need **quantum advantage**.
- The quantum circuits are **shallow**, thus the errors are reduced and they can be implemented on current **NISQ hardware**.
- Fault-tolerant conventional quantum algorithms $\longrightarrow$ **not feasible** on NISQ devices.

Variational Quantum Algorithms

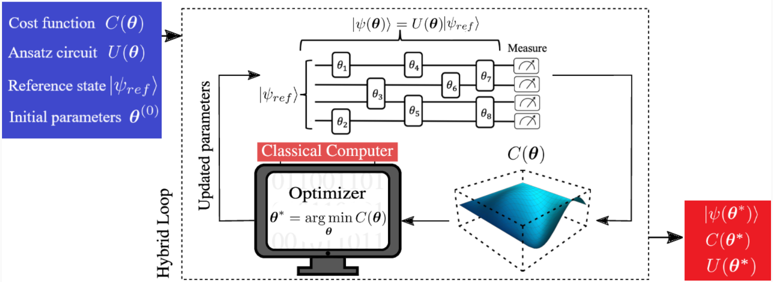
- Hybrid algorithms based on a **variational approach**.
- Key elements:
  - The problem is encoded in a **cost function** $C(\boldsymbol{\theta})$, whose global minimum identifies the solution.
  - $C(\boldsymbol{\theta})$ [1] is computed with a QC on an **ansatz state** $|\psi(\boldsymbol{\theta})\rangle$ obtained with an **ansatz circuit** $U(\boldsymbol{\theta})$ acting on a reference state $|\psi_{ref}\rangle$.
  - A **classical optimizer** (SGD, ADAM, . . .) variationally optimizes the parameters to find:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} C(\boldsymbol{\theta}). \tag{1}$$

[1] and/or its gradients

Variational Quantum Algorithms

- The algorithm is a **hybrid loop**:
  1) At each iteration t, $C(\boldsymbol{\theta}^{(t)})$ [2] **is evaluated** measuring observables on $|\psi(\boldsymbol{\theta}^{(t)})\rangle = U(\boldsymbol{\theta}^{(t)})\,|\psi_{ref}\rangle$.
  2) The optimizer receives $C(\boldsymbol{\theta}^{(t)})$ and **updates** $\boldsymbol{\theta}^{(t)} \to \boldsymbol{\theta}^{(t+1)}$.
  3) The steps 1) and 2) are **iterated** until a final condition is met.



[2] and/or its gradients

ANSATZ CIRCUIT

- $U(\theta)$ defines **how we sample the Hilbert space**, thus it must be enough representative to well approximate the solution.
- There is **no systematic way** to choose the ansatz.
- Two main families:

Physically inspired	**Hardware-efficient**
▸ specific domain knowledge for a particular problem.	▸ heuristic designs with layers of 1-qubit rotations and 2-qubit entangling gates.
▸ very accurate.	▸ initialization dependent.
▸ can address large systems.	▸ not suitable for large systems (“barren plateaus”).
▸ heavy to implement.	▸ efficient to implement.

Examples of VQAs

- There is a variety of VQAs devised for **many applications** (quantum chemistry, machine learning, mathematics ...).
- Two remarkable examples:
  - Quantum Approximate Optimization Algorithm (QAOA). Goal: finding an approximate solution of a combinatorial optimization problem.
  - **Variational Quantum Eigensolver (VQE)**.

VQE

Variational Quantum Eigensolver

- Task: find the **ground state** $|\psi_0\rangle$ and the **ground energy** E_0 of an Hamiltonian H:
- The problem must be mapped on qubits $\longrightarrow$ **canonical transformations** such as Jordan-Wigner or Bravyi-Kitaev.
- We consider the **cost function**:

$$C(\boldsymbol{\theta}) = \frac{\langle\psi(\boldsymbol{\theta})|\, H \,|\psi(\boldsymbol{\theta})\rangle}{\langle\psi(\boldsymbol{\theta})|\psi(\boldsymbol{\theta})\rangle}. \tag{2}$$

- Indeed, the **variational principle** guarantees that:

$$\frac{\langle\psi|\, H \,|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0 \;\; \forall\, |\psi\rangle \in \mathcal{H}, \tag{3}$$

therefore $C(\boldsymbol{\theta}^*) \approx E_0$.

Variational Quantum Eigensolver

- How to compute $C(\boldsymbol{\theta})$? H is a linear combination of **Pauli strings**:

$$H = \sum_{\alpha} h_\alpha Q_\alpha, \tag{4}$$

where $h_\alpha \in \mathbb{C}$ and $Q_\alpha \in \{I, X, Y, Z\}^{\otimes n}$. Thus, we measure $\langle \psi(\boldsymbol{\theta}) | Q_\alpha | \psi(\boldsymbol{\theta}) \rangle$.

- In general, Hamiltonians are **sparse** with $O(\text{poly}(n))$ terms.

- How to compute $\nabla C(\boldsymbol{\theta})$? Using the **parameter-shift rule**:

$$\frac{\partial}{\partial \theta_i} C(\boldsymbol{\theta}) = \frac{C(\boldsymbol{\theta} + \boldsymbol{e}_i s) - C(\boldsymbol{\theta} - \boldsymbol{e}_i s)}{2\sin(s)}, \quad s \in \mathbb{R}, \tag{5}$$

where for Pauli strings we can take $s = \pi/2$.

Overlap-based method

- How can we obtain **excited states and energies**? Using **orthogonality** between eigenstates.

- The modified Hamiltonian:

$$H' = H + \alpha \left|\psi_0\right\rangle \left\langle\psi_0\right| \tag{6}$$

has $|\psi_1\rangle$ and E_1 as ground state and ground energy.

- We can iterate the procedure:

$$\boxed{H} \xrightarrow{\text{VQE}} \boxed{|\tilde{\psi}_0\rangle,\, \tilde{E}_0} \longrightarrow \boxed{H' = H + \alpha|\tilde{\psi}_0\rangle\langle\tilde{\psi}_0|} \xrightarrow{\text{VQE}} \boxed{|\tilde{\psi}_1\rangle,\, \tilde{E}_1} \longrightarrow$$

$$\longrightarrow \boxed{H'' = H + \beta(|\tilde{\psi}_0\rangle\langle\tilde{\psi}_0| + |\tilde{\psi}_1\rangle\langle\tilde{\psi}_1|)} \xrightarrow{\text{VQE}} \boxed{|\tilde{\psi}_2\rangle,\, \tilde{E}_2} \longrightarrow \cdots$$

NB: the **error accumulates** through the chain.

VQE on 1D TF Ising model

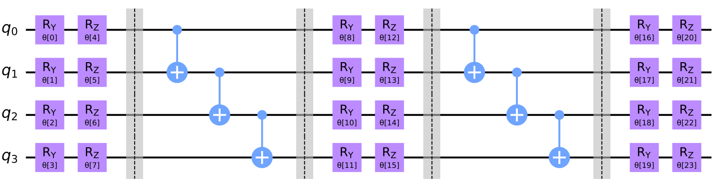
VQE on 1D transverse-field Ising model

- The **Hamiltonian** for n qubits:

$$H = J\sum_{i=1}^{n} Z_i Z_{i+1} + h\sum_{i=1}^{n} X_i, \tag{7}$$

with **periodic boundary conditions**.

- The **ansatz** $U(\boldsymbol{\theta})$: hardware efficient SU2 circuit with RyRz.



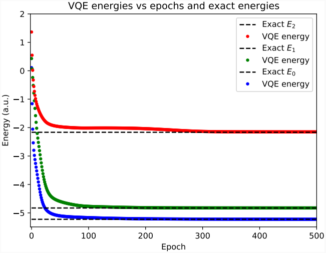
The **number of layers** is changed according to n.

- The classical optimizer: GD with learning rate $\eta = 0.1$.

VQE on 1D transverse-field Ising model

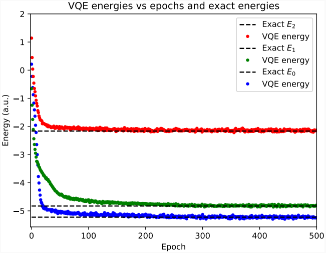
- **Ground energy** and **first two excited energies** for $n = 4$ qubits with 4 layers in $U(\boldsymbol{\theta})$.

(a) State vector simulator



Energy	Error
ground	0.028 %
1^{st} exc.	0.032 %
2^{nd} exc.	0.61 %

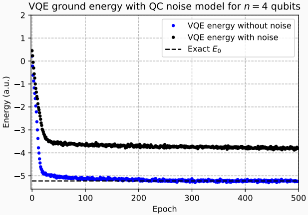
(b) Shot-based simulator (10^4)

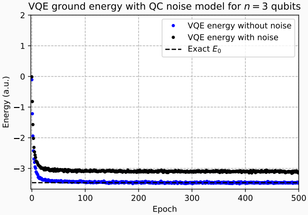


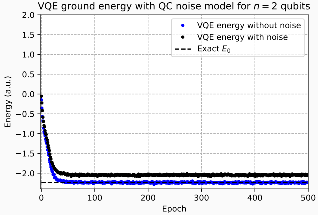
Energy	Error
ground	0.086 %
1^{st} exc.	0.24 %
2^{nd} exc.	0.93 %

Effect of noise model from a real QC

- Let's consider a **noise model from IBM device** (`ibmq_manila`).
- **Ground energy** for different n and layers in $U(\boldsymbol{\theta})$.



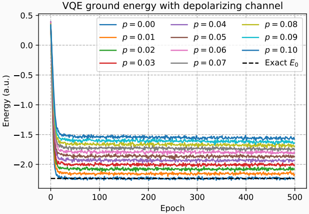


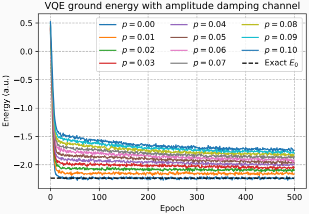


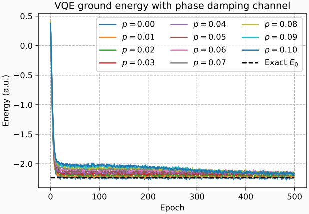
n	Layers	Accuracy
4	4	27.3 %
3	2	10.4 %
2	1	8.54 %

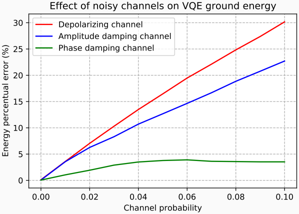
Effect of noisy channels

- Let’s consider **depolarizing, amplitude damping and phase damping** channels with $p \in [0, 0.10]$.
- **Ground energy** for $n = 2$ qubits with 1 layer in $U(\boldsymbol{\theta})$.









References

References

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[2] S. Endo et al. "Hybrid Quantum-Classical Algorithms and Quantum Error Mitigation". In: *Journal of the Physical Society of Japan* 90.3 (Mar. 2021). ISSN: 1347-4073.

[3] S. McArdle et al. "Quantum computational chemistry". In: *Reviews of Modern Physics* 92.1 (Mar. 2020). ISSN: 1539-0756.

[4] M. Schuld et al. "Evaluating analytic gradients on quantum hardware". In: *Physical Review A* 99.3 (Mar. 2019). ISSN: 2469-9934.

[5] A. Sinibaldi. GitHub repository with codes and files. `https://github.com/alleSini99/VQE_on_1D_TF_Ising`. Created: 2022-1-16.