End-to-end Integration of Hyperparameter Tuning into Variational Quantum Algorithms

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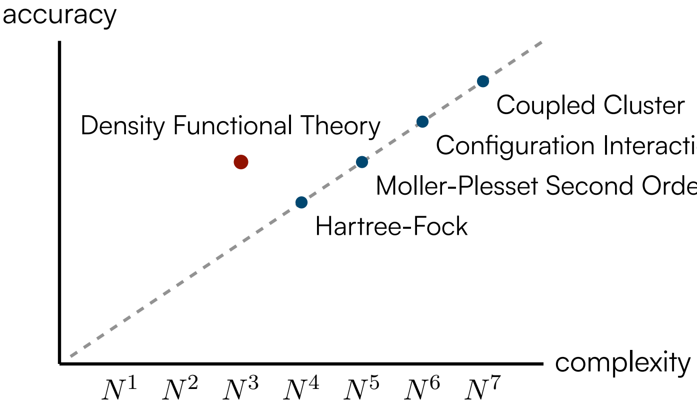
Quantum Computing as a New Paradigm for Computation

Quantum computing uses specialized quantum technology to solve complex problems that classical computers cannot solve quickly enough.

Credit: PSNC

Examples of Complex Problems

Quantum Chemistry, Electronic Structure of Molecular Systems.



Credit: Janosh Riebesell

Examples of Complex Problems

Discrete logarithm, Prime factorization in cryptography.

Easy to compute forward

$$x = g^a$$

$\uparrow$ Given a and g

$$G = \{1, g, g^2, \ldots, g^{N-1}\}, \quad g^N = 1$$

$\downarrow$ Given p, x and g

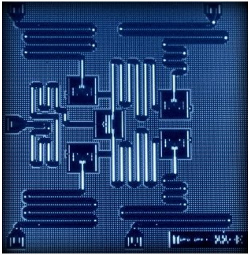
$$a = \log_g(x \mod p)$$

Hard to compute backward

Credit: Anthropic's Claude Sonnet 3.5 LLM

Quantum Computing Hardware Since 2016

- The first generally available cloud-based quantum processor had 5 quantum bits, or qubits:



Credit: IBM

- Use cases limited to proof-of-concept demonstrations:

arXiv > quant-ph > arXiv:2103.13855

Quantum Physics

[Submitted on 25 Mar 2021 (v1), last revised 19 Sep 2022 (this version, v3)]

Demonstration of Shor's factoring algorithm for N=21 on IBM quantum processors

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Scaling Up Quantum Computing Hardware

Generally available state-of-the-art devices can have as many as 433 noisy qubits.

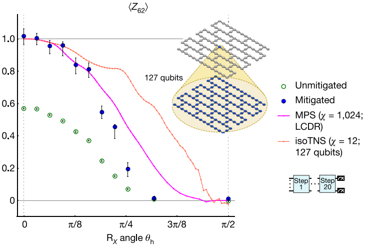
	2022	2023	2024	2025
IBM	433 Qubit	1121 Qubit	1386 Qubit	4158+ Qubit
IONQ	25 Qubit	29 Qubit	35 Qubit	64 Qubit
Ψ PsiQuantum	0 Qubit	0 Qubit	0 Qubit	1000000+ Qubit

Credit: Tobias Osborne

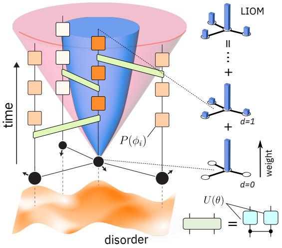
Despite increasing qubit numbers, Quantum Advantage is yet to be realized.

Variational Quantum Algorithms (VQAs) in the Wild

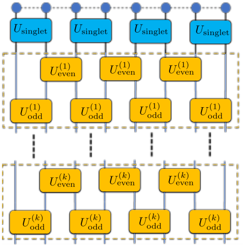
Utility Before Fault Tolerance
(Nature 618, 500—505)



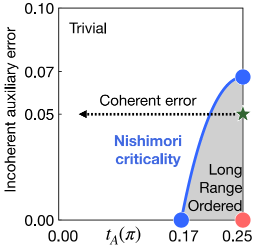
Quantum Many-body Dynamics
(arXiv:2307.07552)



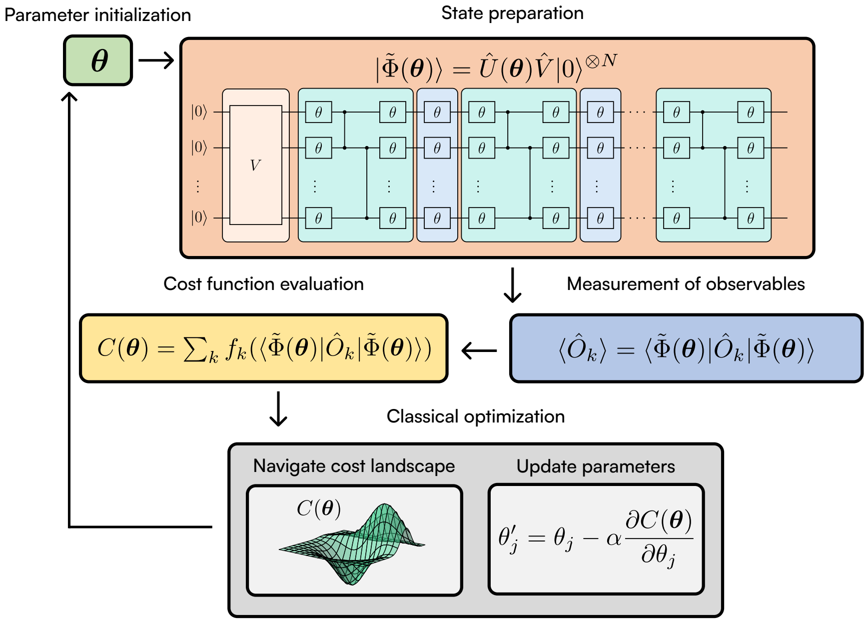
Quantum Spin Chains
(arXiv:2207.0999)



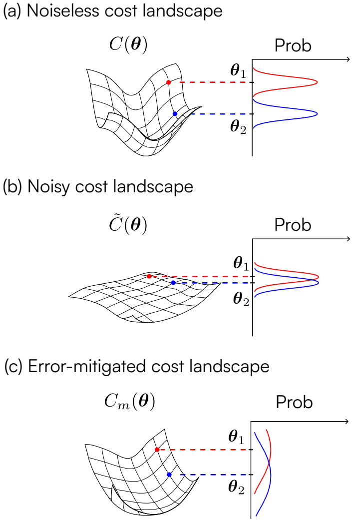
Nishimori transition
(arXiv:2309.02863)



Variational Quantum Algorithms (VQAs)



Cost Landscapes in Variational Quantum Algorithms



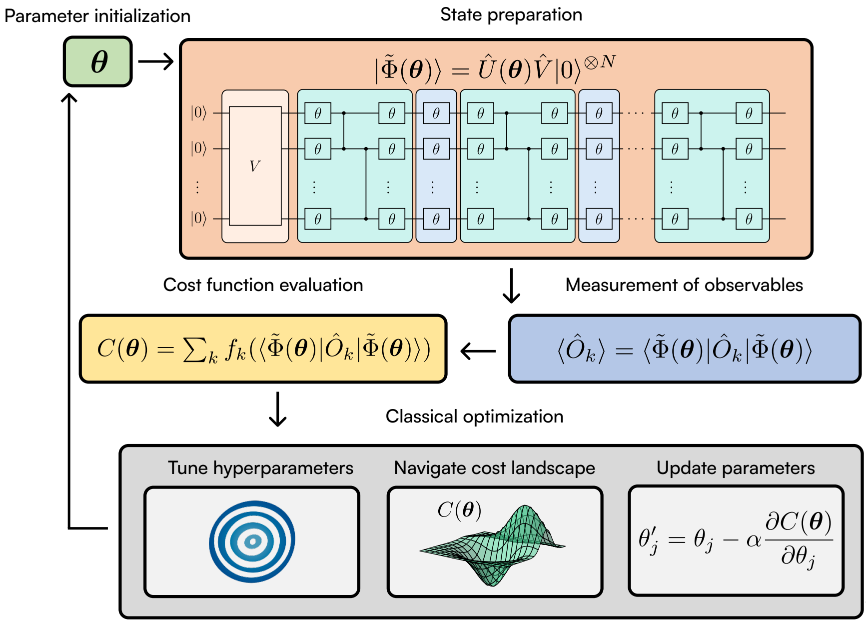
arXiv:2109.0105

(a) Clear separation of cost function values.

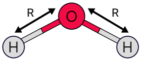
(b) Concentration of cost function values.

(c) Recovery of features keys of noiseless cost function values.

Hyperparameter Tuning



Case study: Estimating Ground State Energies



Expand Hamiltonian
in STO-6G basis set

$$\hat{H} = \sum_{ij}^{N_b} \langle i|\hat{T}_e + \hat{V}_{en}|j\rangle \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2}\sum_{ijkl}^{N_b} \langle ik|\hat{V}_{ee}|jl\rangle \hat{a}_i^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_j$$

$$\hat{a}_j \rightarrow \frac{\hat{\sigma}_x + i\hat{\sigma}_y}{2} \otimes \hat{\sigma}_z \otimes \cdots \otimes \hat{\sigma}_z$$

Qubit-mapping
Electronic Hamiltonian

$$\hat{H}_q = \sum_i c_i \prod_k^{Nb} \hat{\sigma}_k^{(i)}$$

$$|\,1 \quad 1 \quad 1 \quad 0 \quad 0\rangle = |\,\Phi_0\rangle$$

Qubit-mapping
Electronic States

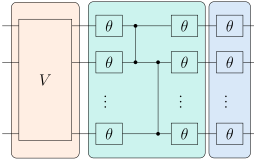
$$C(\boldsymbol{\theta}) = \sum_i c_i \langle \Phi_0|\hat{U}^\dagger(\boldsymbol{\theta}) \prod_k^{N_b} \hat{\sigma}_k^{(i)} \hat{U}(\boldsymbol{\theta})|\Phi_0\rangle$$

VQA

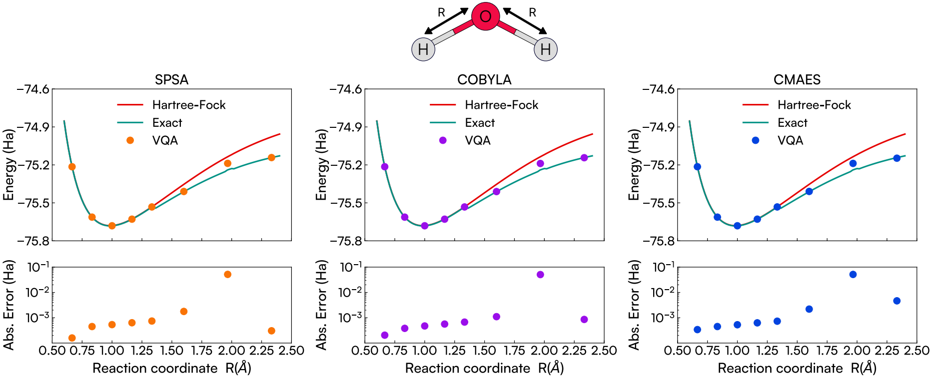
$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, C(\boldsymbol{\theta})$$

Layers of rotation
and entangling gates

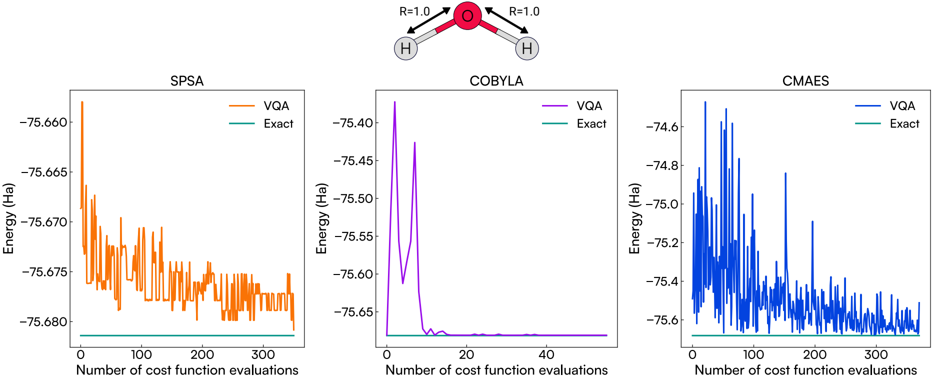
$$U(\boldsymbol{\theta}) =$$



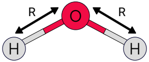
Noiseless Simulation: Potential Energy Surface

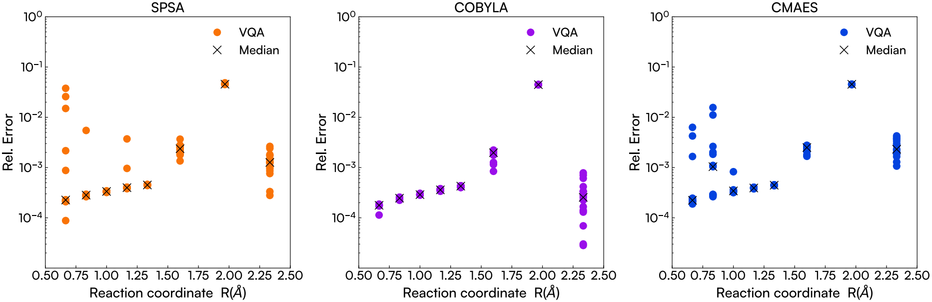


Noiseless Simulation: Cost Function Evaluations

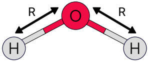


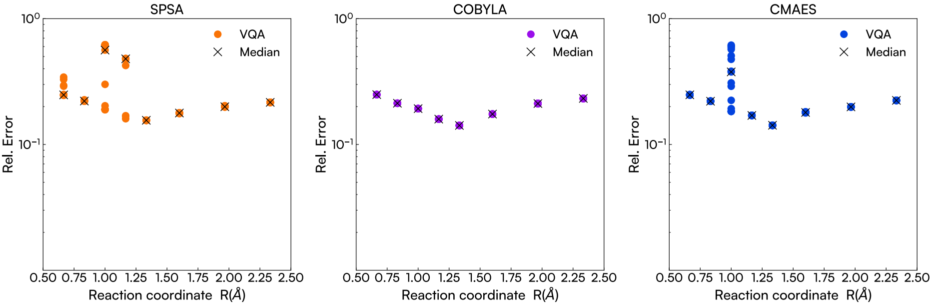
1. Noiseless Simulation: Relative Error



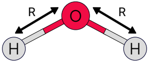


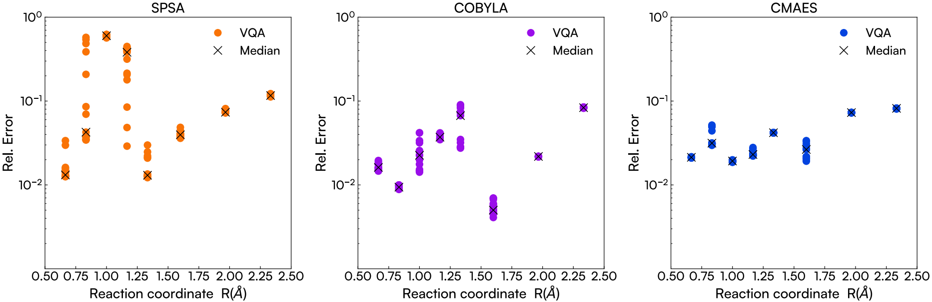
2. Noisy Simulation: Relative Error



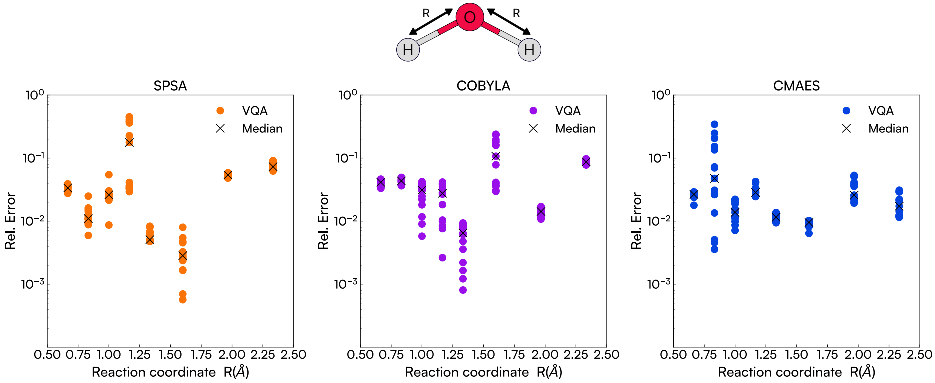


3. Noisy + Readout Error Mitigation Simulation: Relative Error





4. Noisy + Readout Error Mitigation + Zero Noise Extrapolation Simulation: Relative Error



Concluding remarks

- Variational Quantum Algorithms as stepping stones towards Quantum Advantage on start-of-the-art quantum hardware.

- Performance and reliability of Variational Quantum Algorithms is significantly influenced by the behavior of the chosen optimization algorithm.

- Hyperparameter tuning as means to get the best out of classical resources on the way to Quantum Advantage.

Thank You for Listening