CAFQA: A Classical Simulation Bootstrap for Variational Quantum Algorithms

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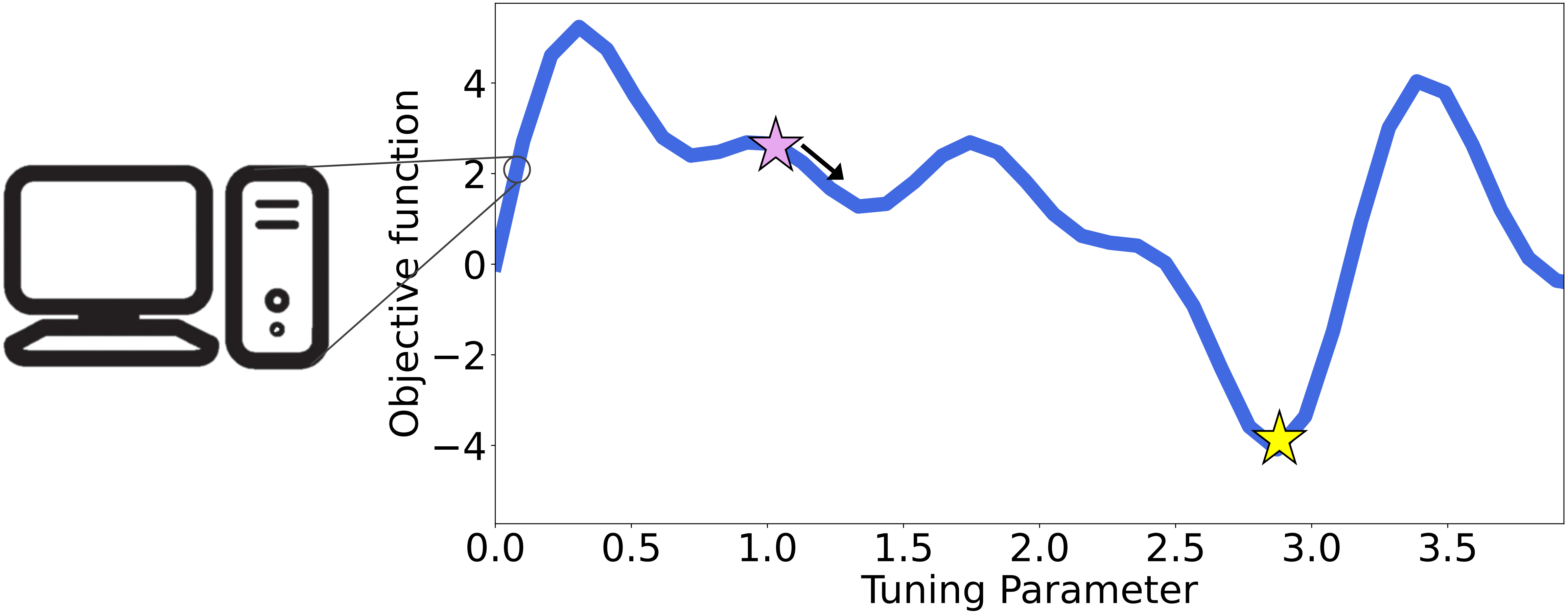
1: UChicago, 2: Super.tech, 3: MIT, 4: Tufts, 5: Duke

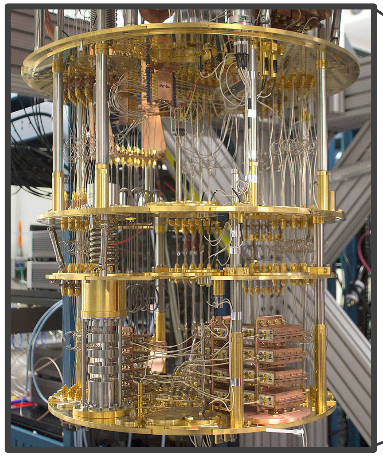
Observed to recover 99+% of the initialization accuracy lost in ~100-year old method!!

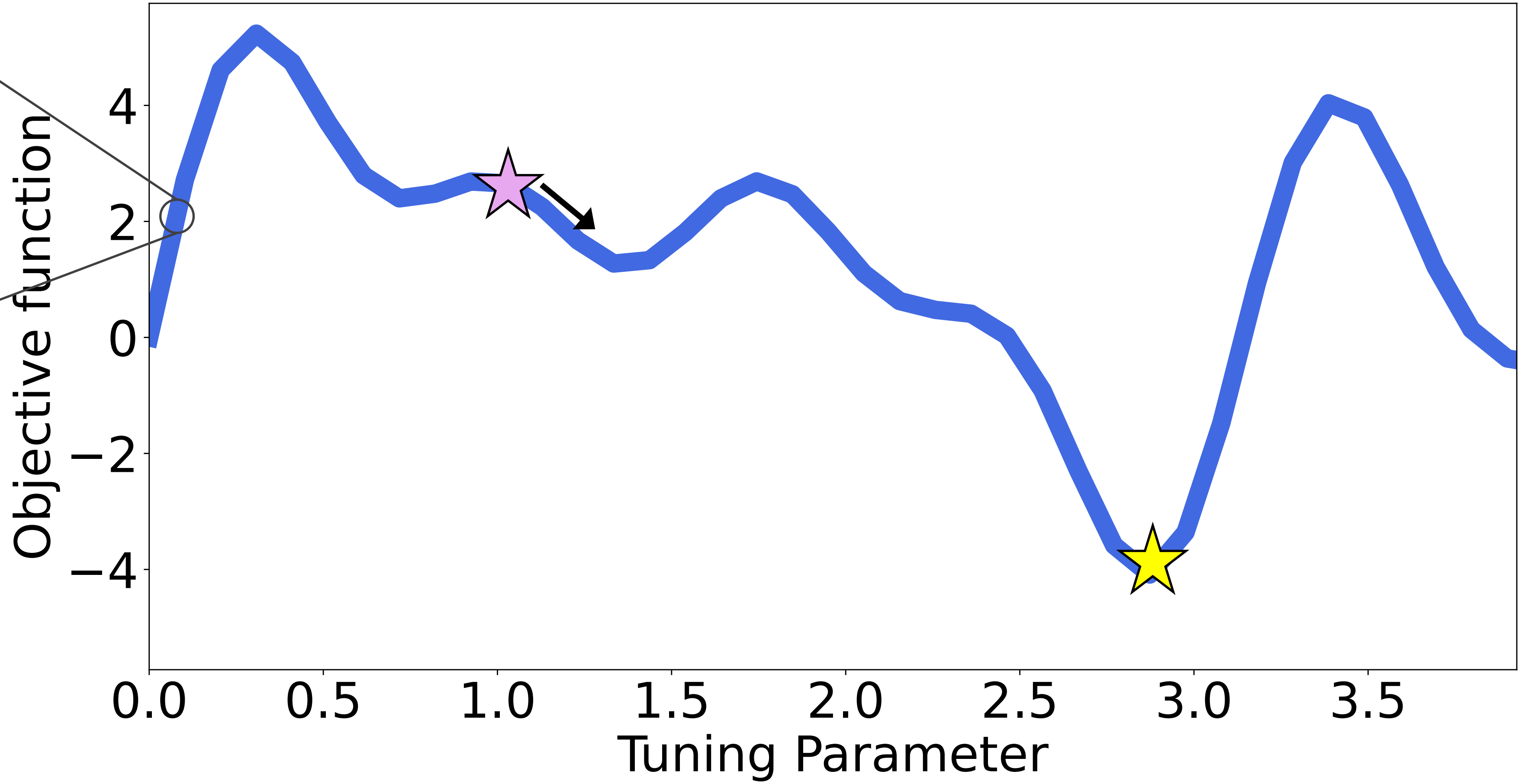
arXiv:2202.12924

Navigating a classical optimization contour

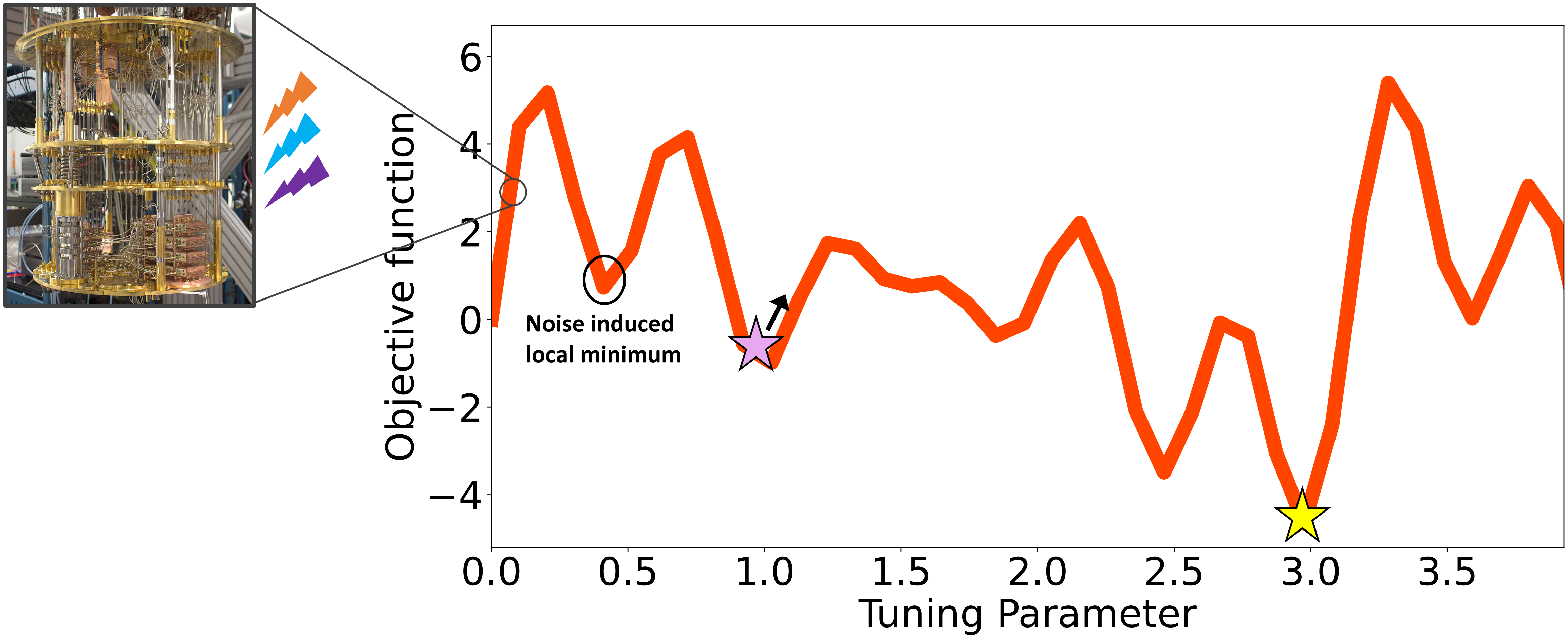


Navigating an ideal Variational Quantum Algorithm contour



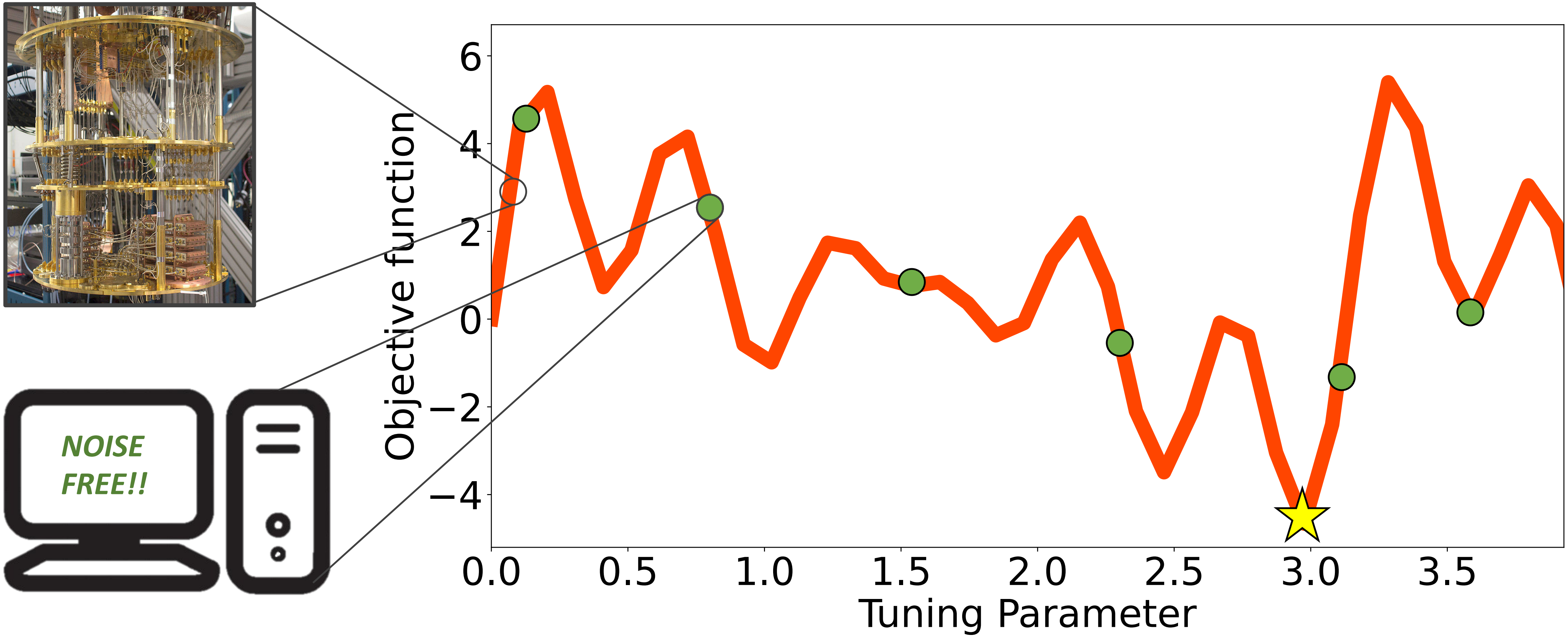


Navigating a noisy Variational Quantum Algorithm contour



CAFQA: Clifford Ansatz For Quantum Accuracy

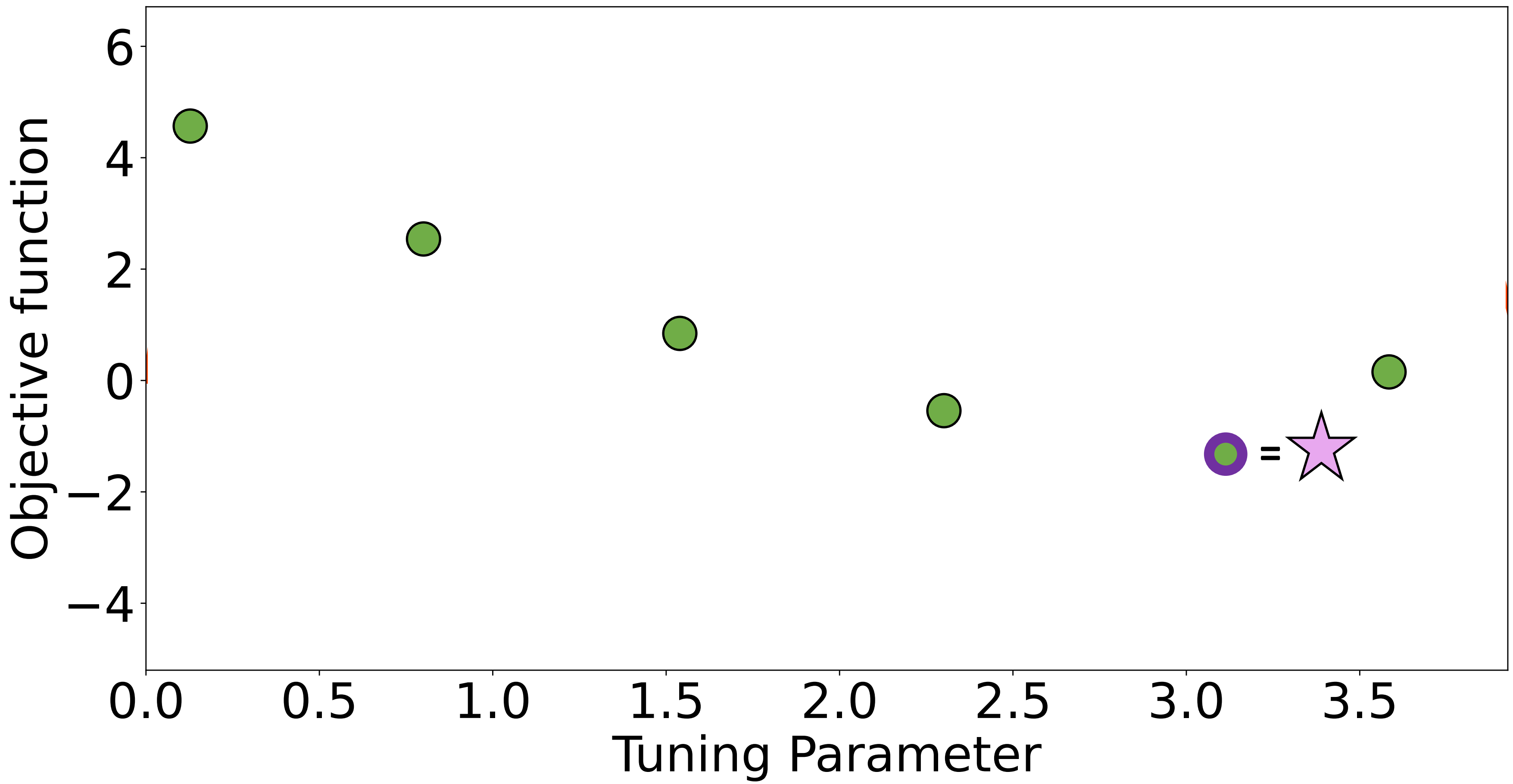
CAFQA Insight #1: Portion of the quantum space is classically simulable (Clifford space).



CAFQA: Clifford Ansatz For Quantum Accuracy

CAFQA Insight #2: Efficiently search the discrete space classically to find the lowest objective (w/ Bayesian Optimization).

Bayesian Optimization



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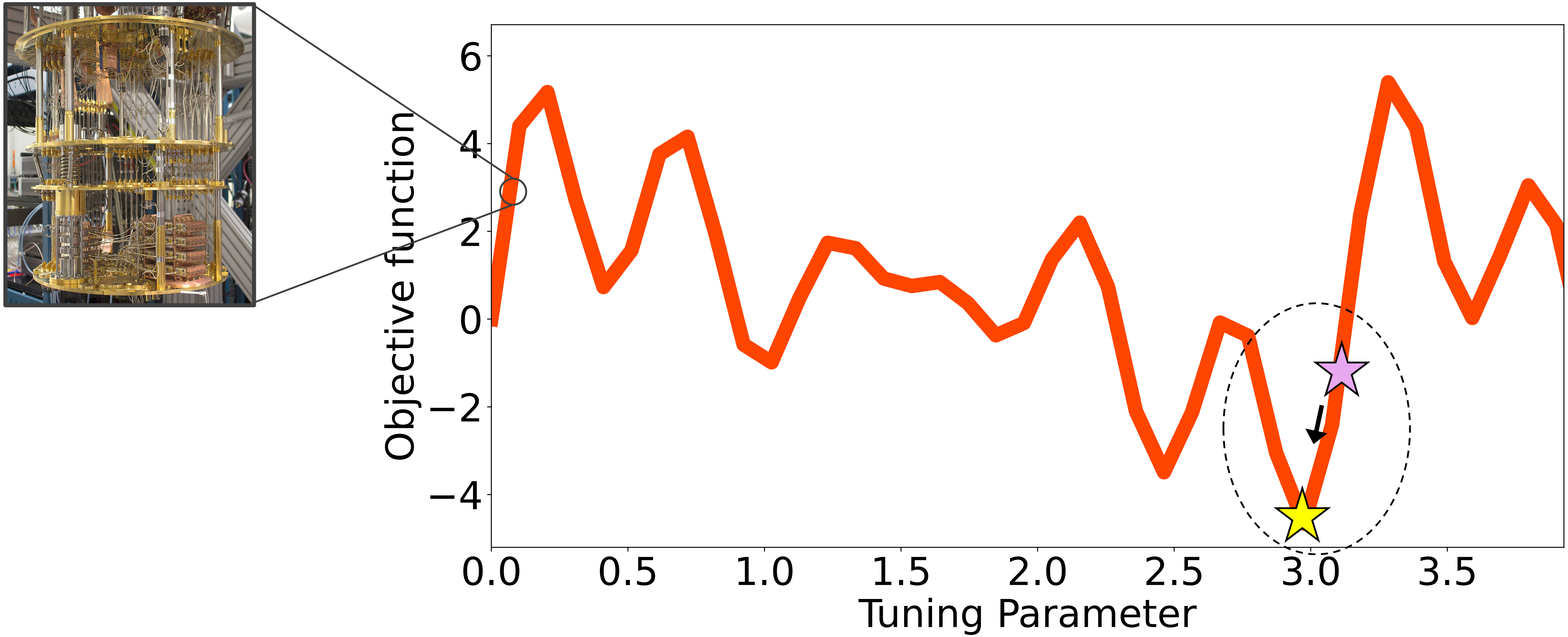
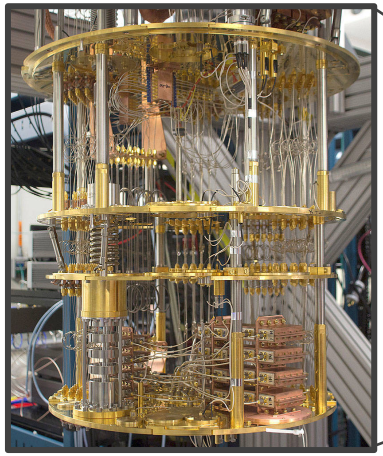
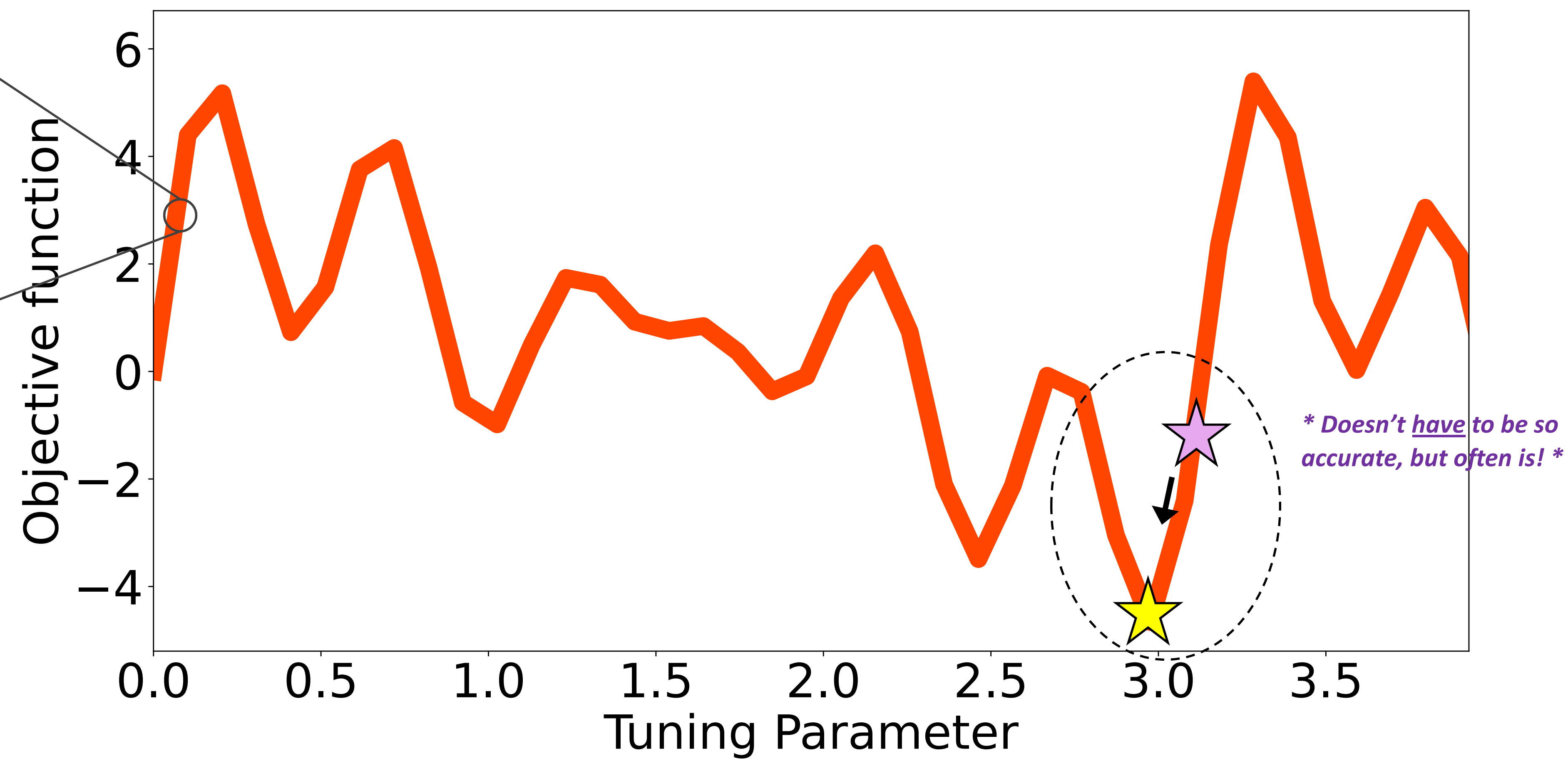
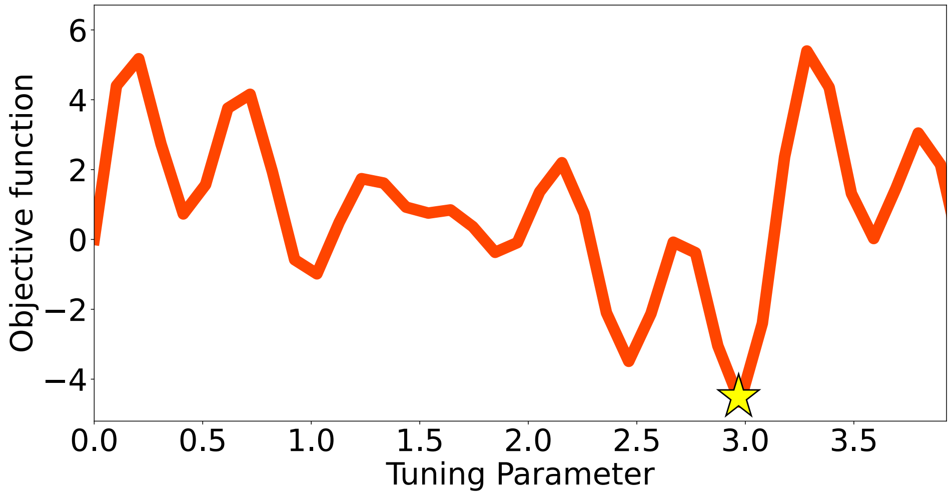


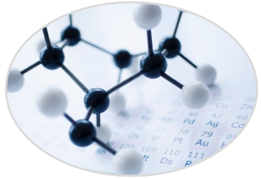
CAFQA: Clifford Ansatz For Quantum Accuracy





How VQA works





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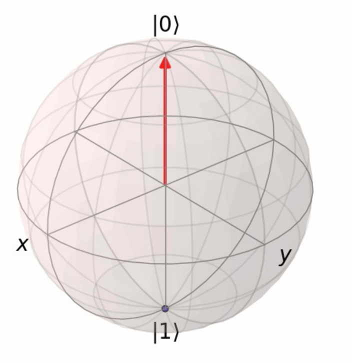
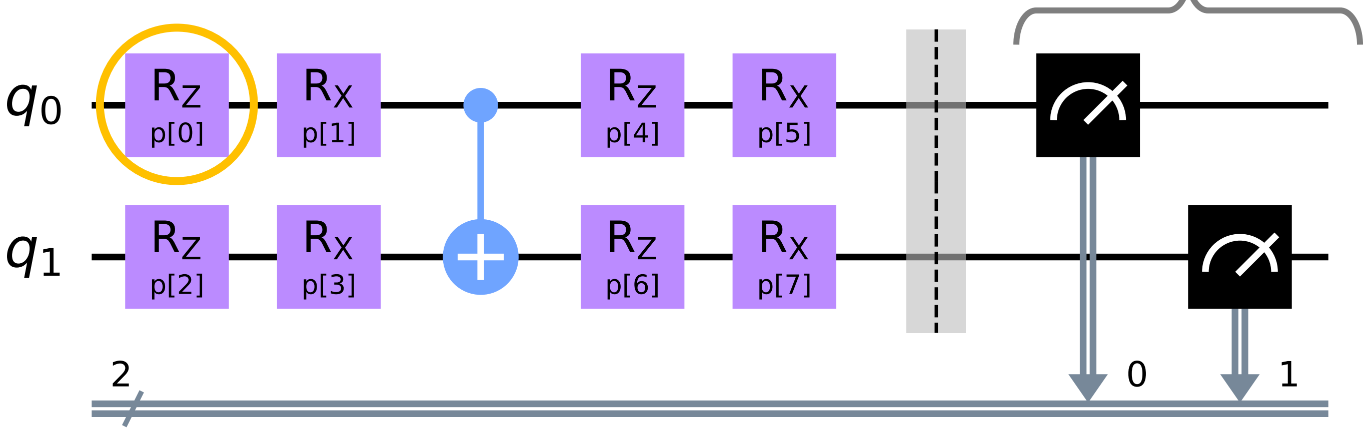
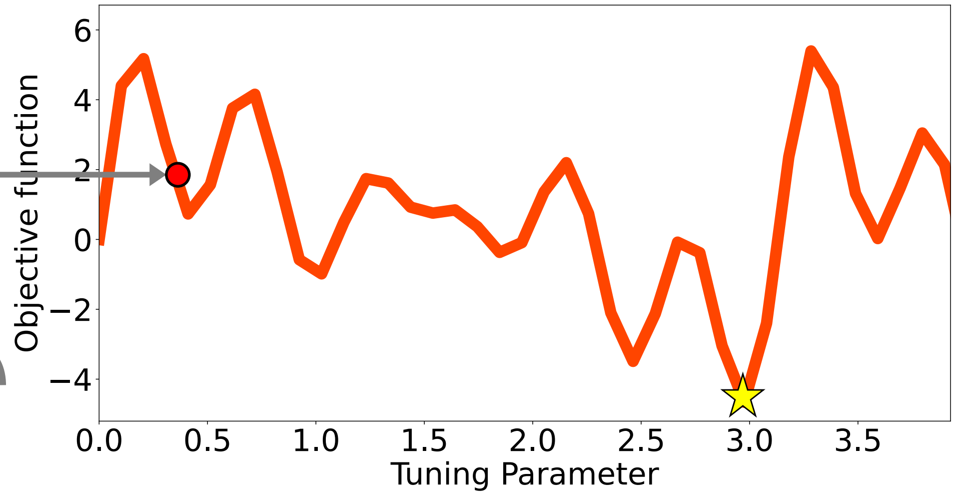




Parameterized ansatz circuit



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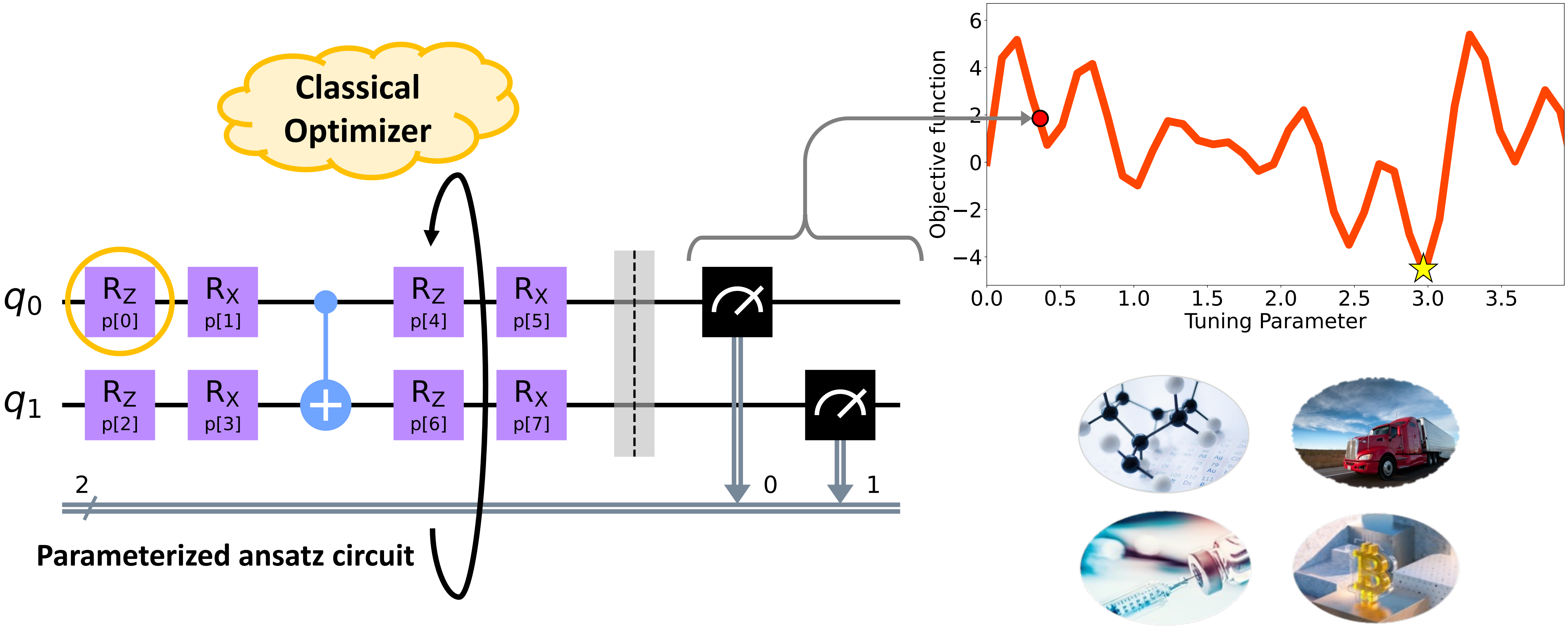
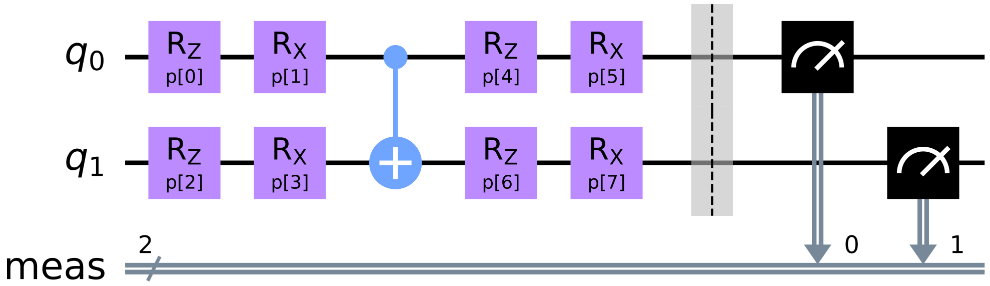


Classical simulability of Clifford quantum circuits

Parameterized ansatz circuit



Classical simulability of Clifford quantum circuits

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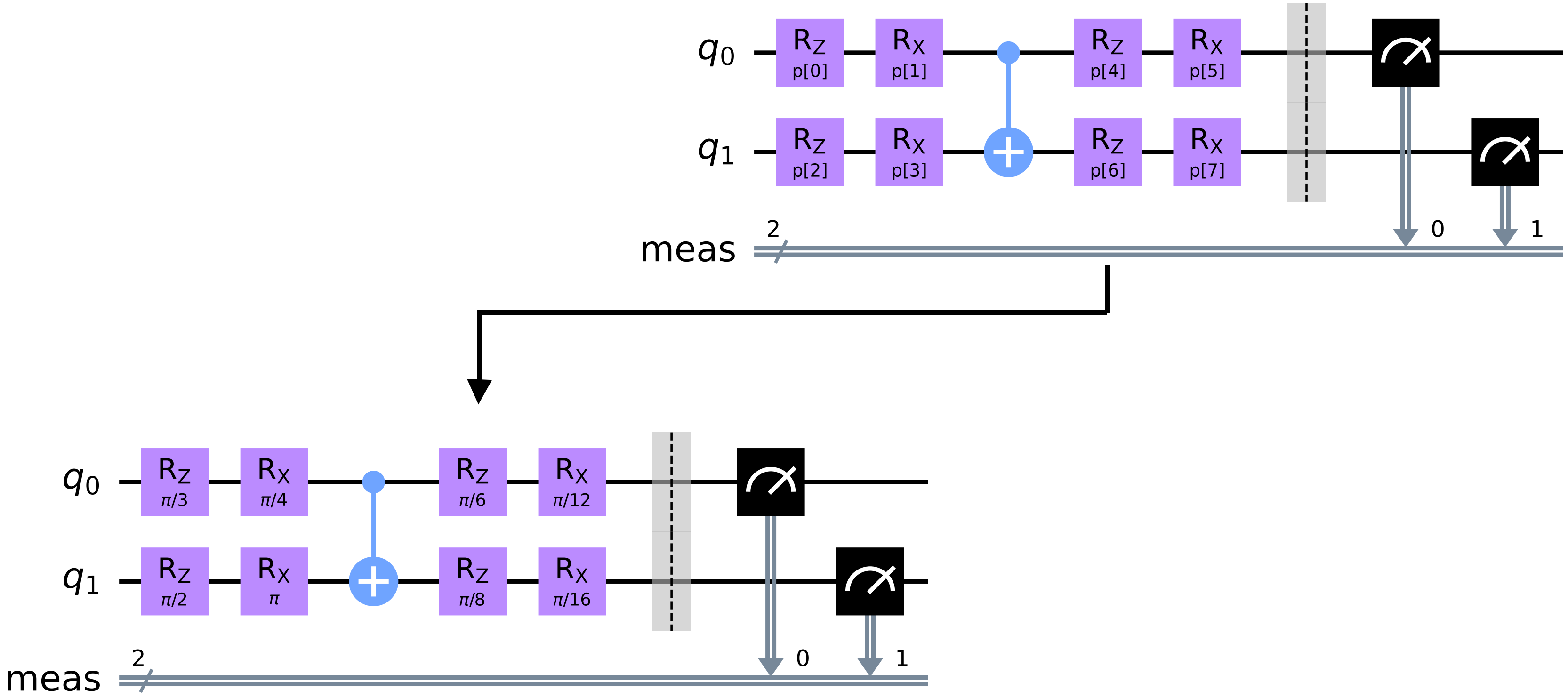


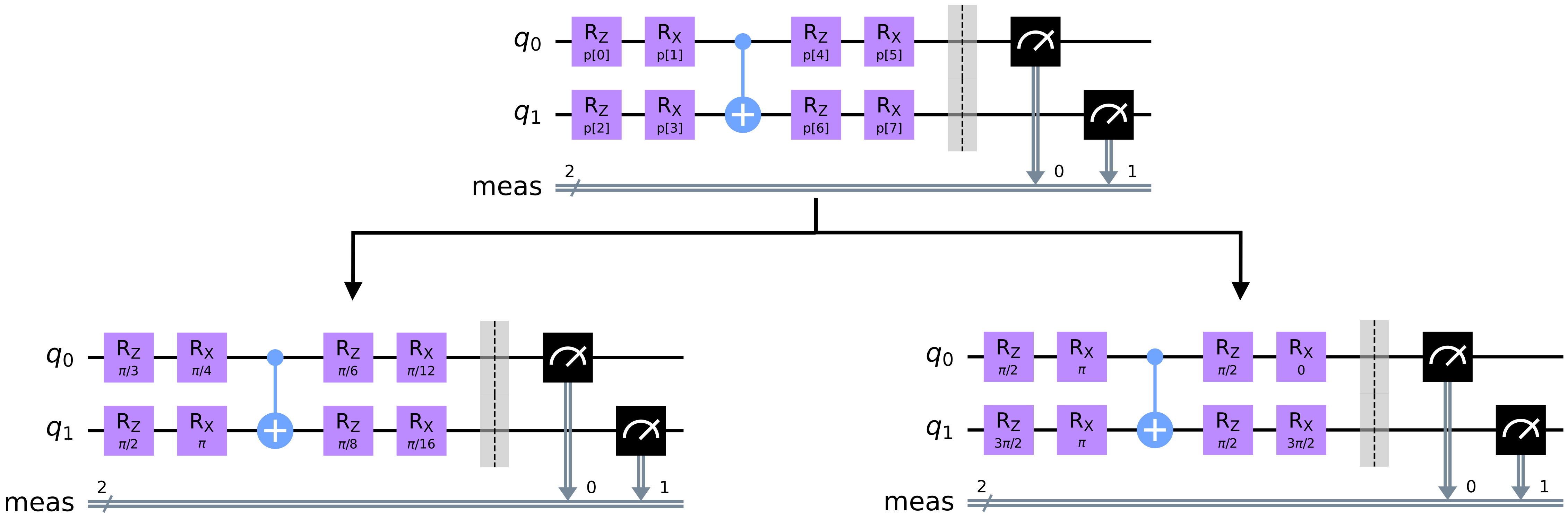
A classically <u>intractable general</u> circuit

Continuous angles = [0, 2*pi]

Classical simulability of Clifford quantum circuits

Gottesman–Knill theorem [‘98] - A QC circuit can be classically simulated efficiently if: (a) it has only Clifford gates, (b) classical qubit prep and measurement.

Parameterized ansatz circuit



A classically <u>intractable general</u> circuit

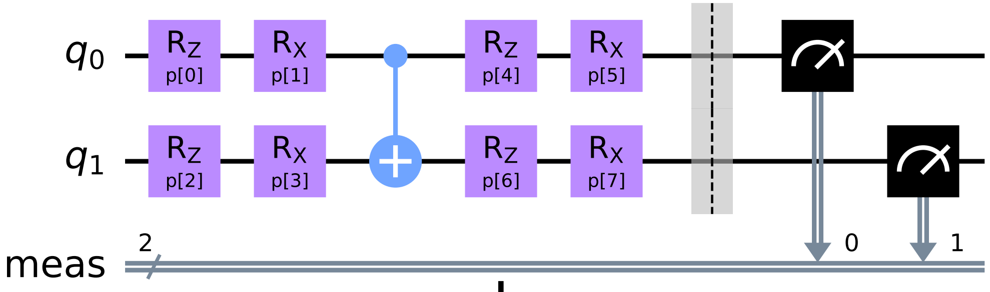
Continuous angles = [0, 2*pi]

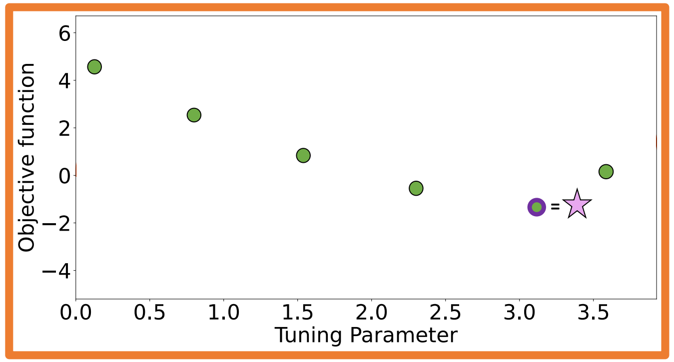
A classically <u>simulable Clifford</u> circuit

Discrete angles = {0, pi/2, pi, 3*pi/2}

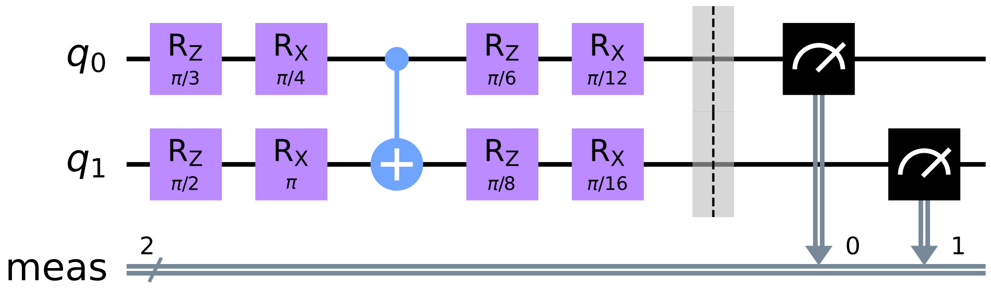
Classical simulability of Clifford quantum circuits

Parameterized ansatz circuit





CAFQA



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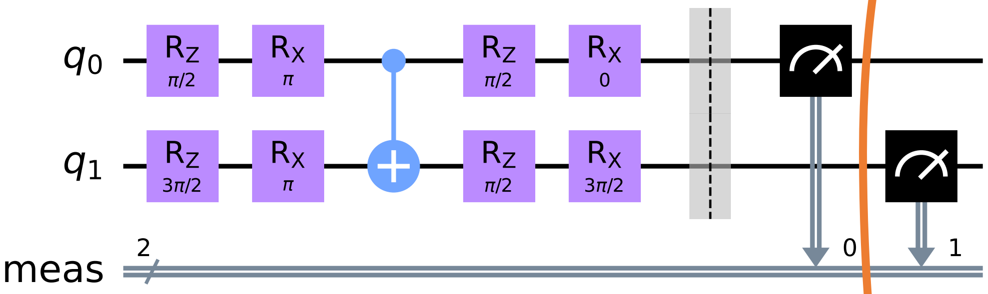

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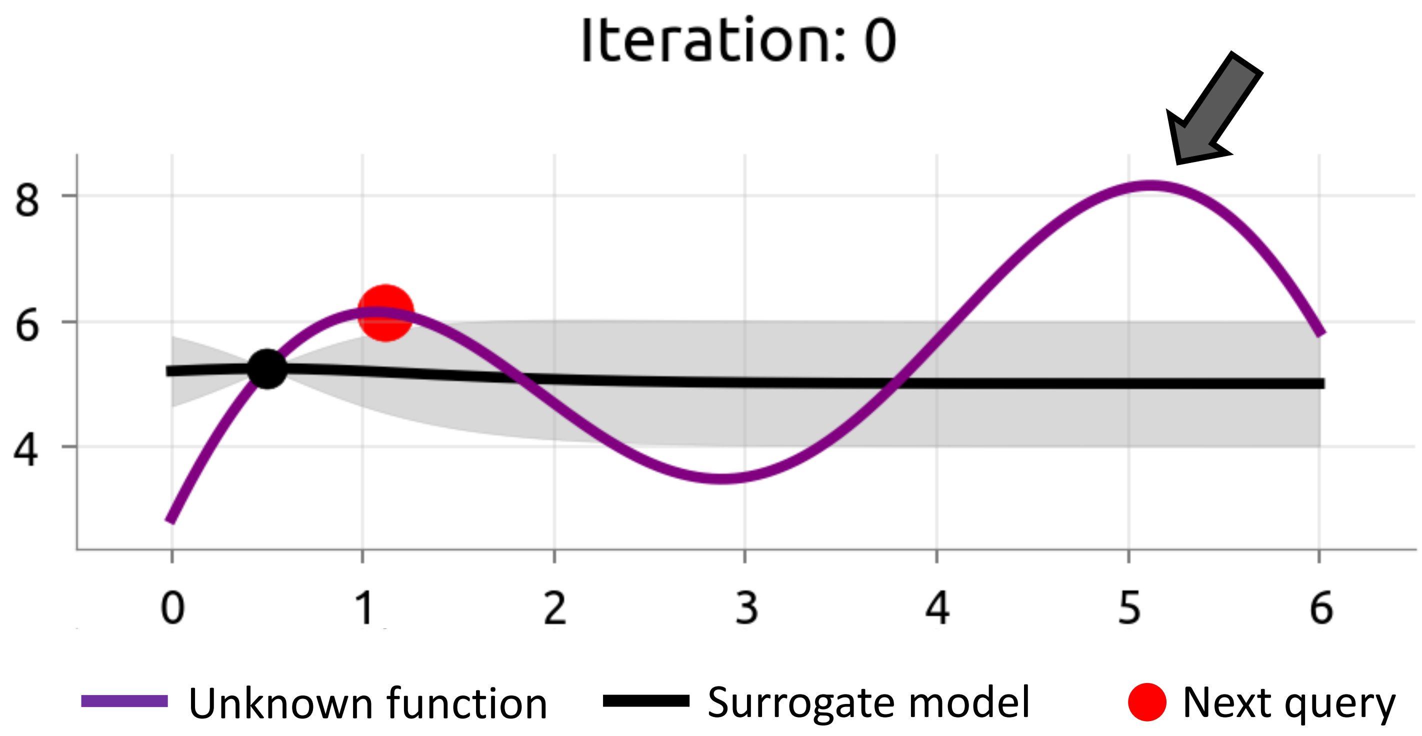
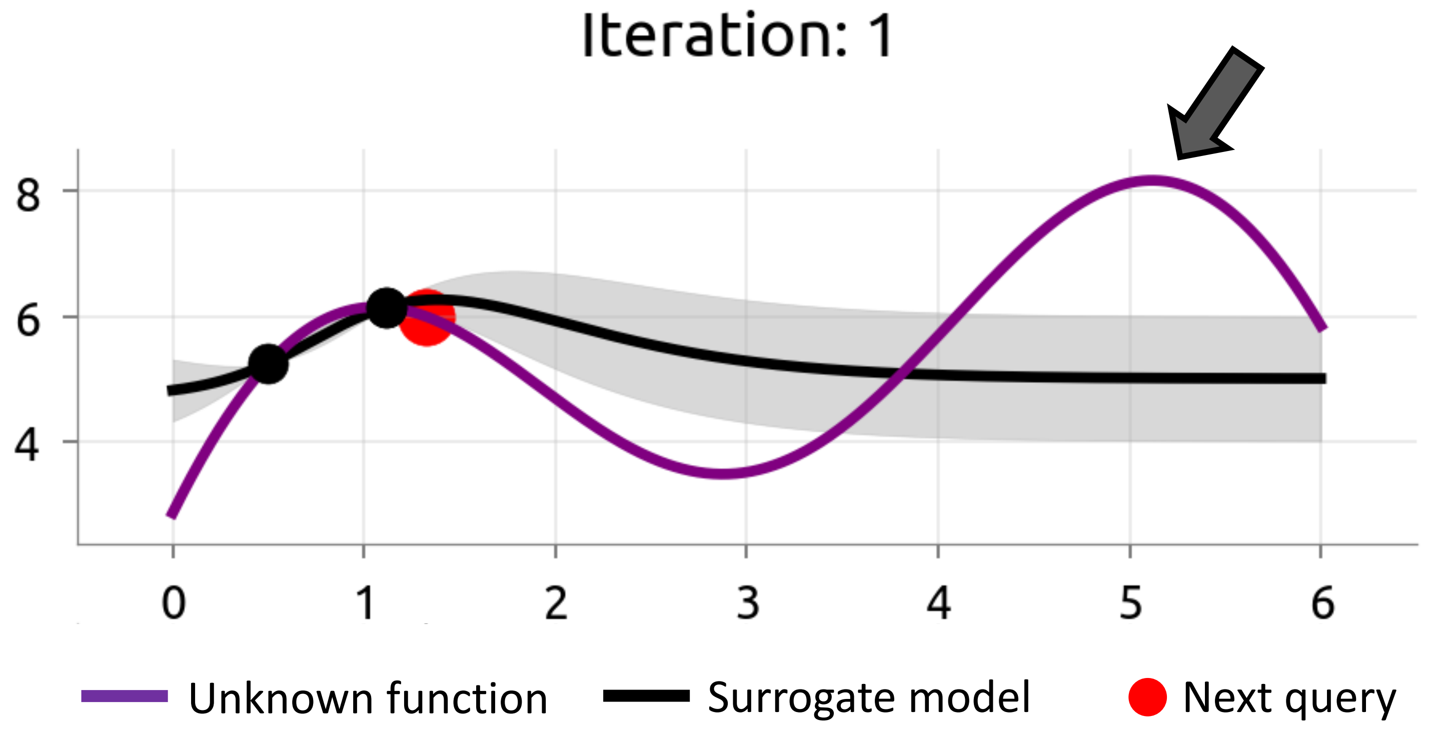
Finding the optimal Clifford point: Bayesian Optimization



https://distill.pub/2020/bayesian-optimization/

Finding the optimal Clifford point: Bayesian Optimization



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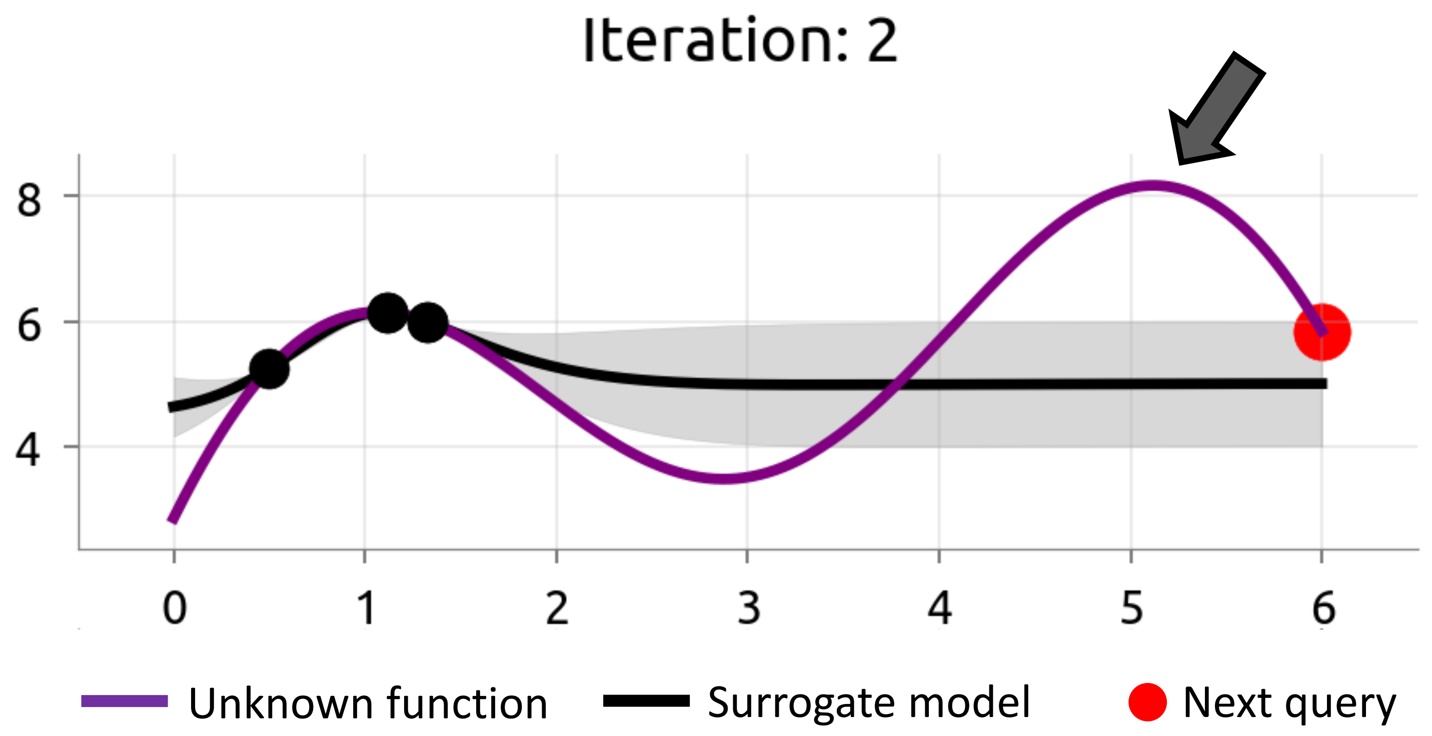

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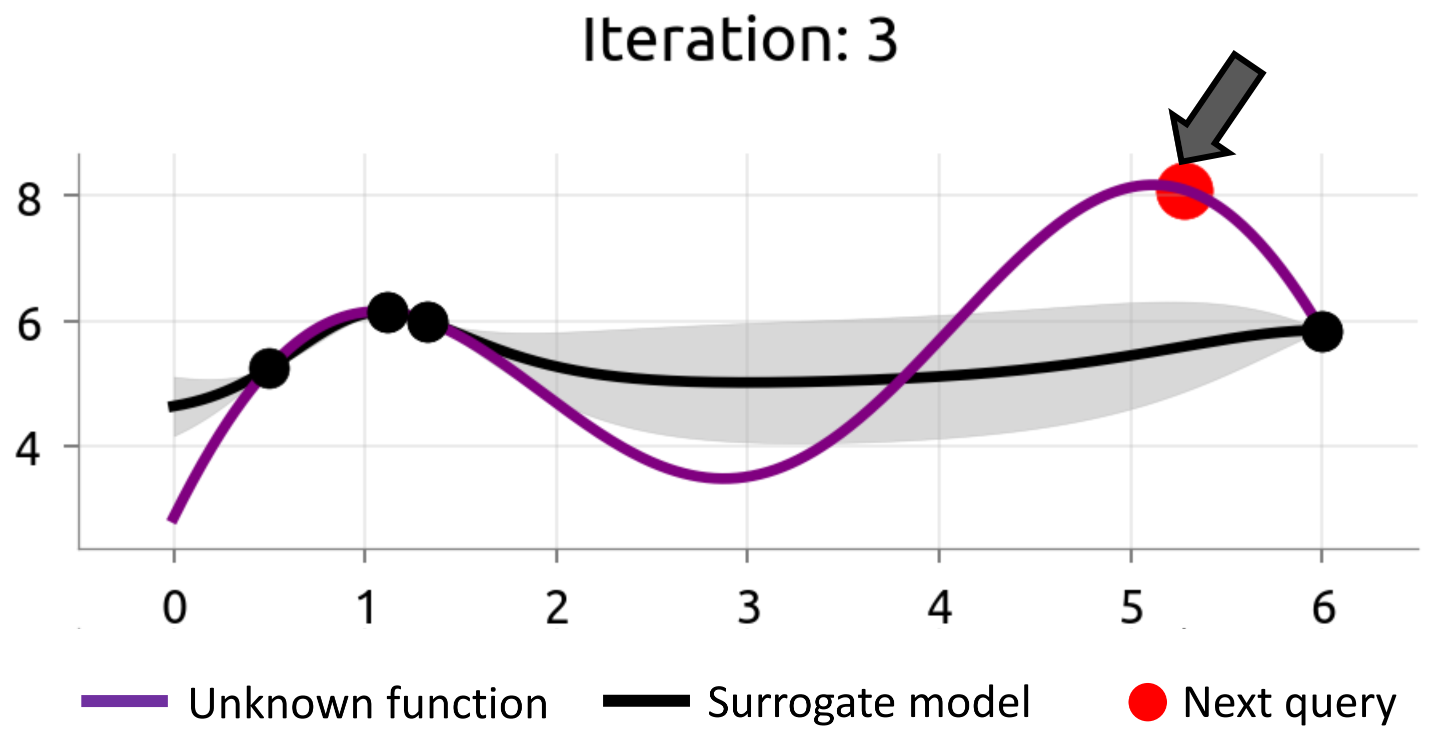

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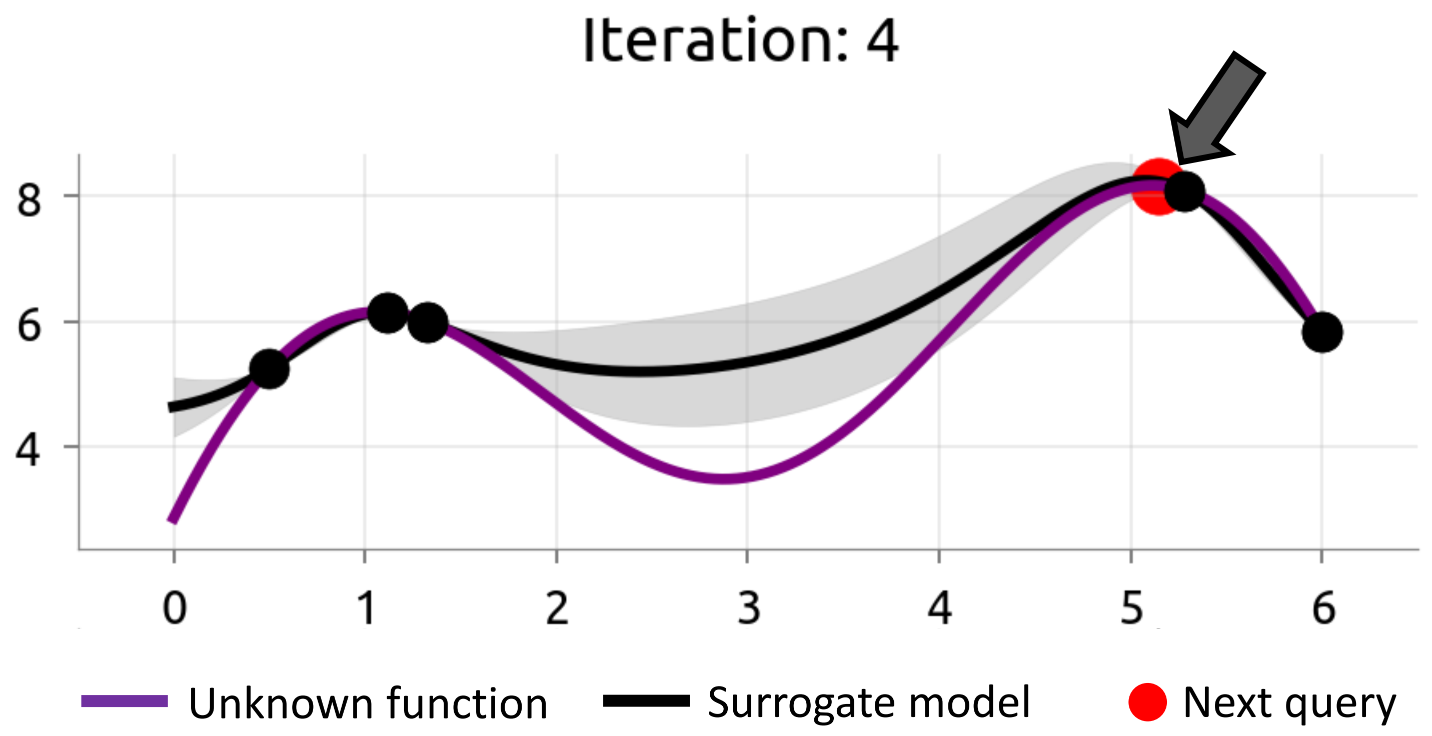

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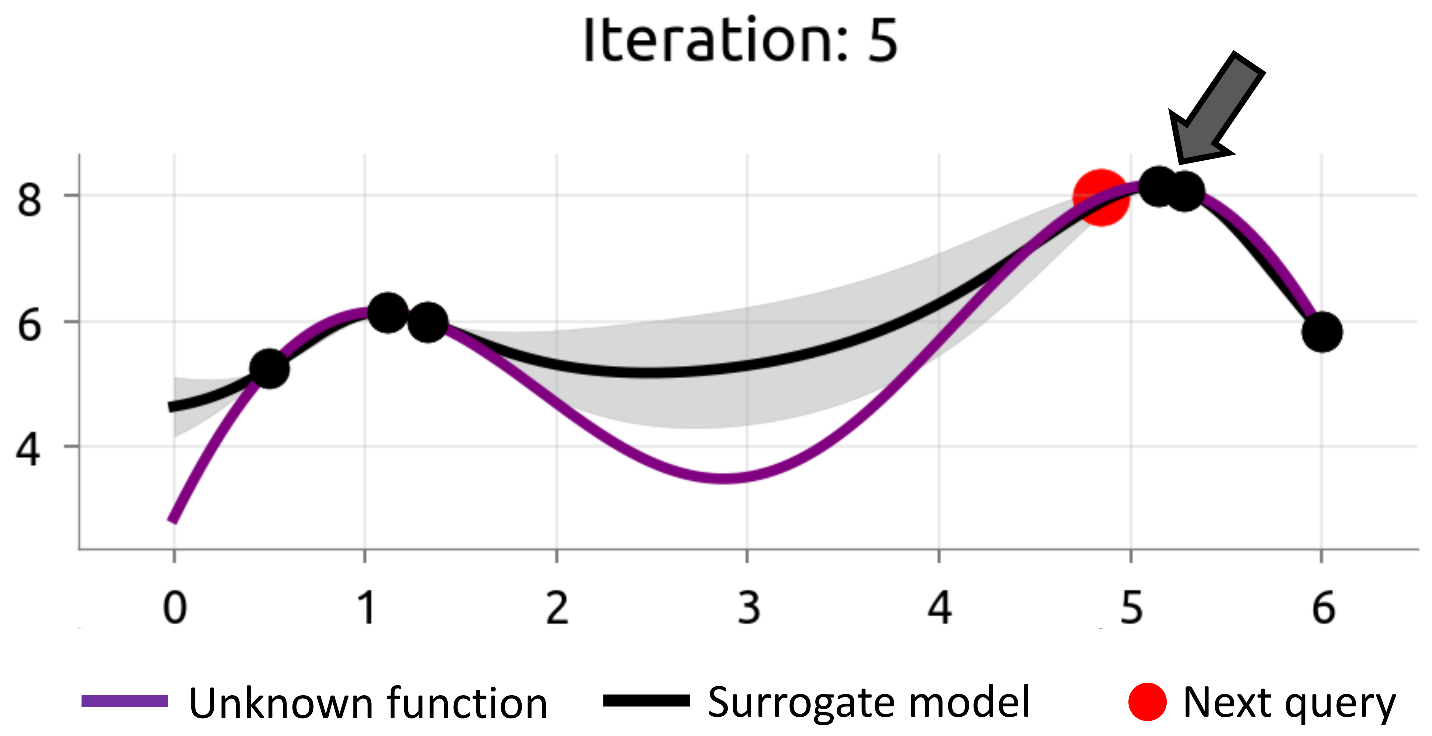

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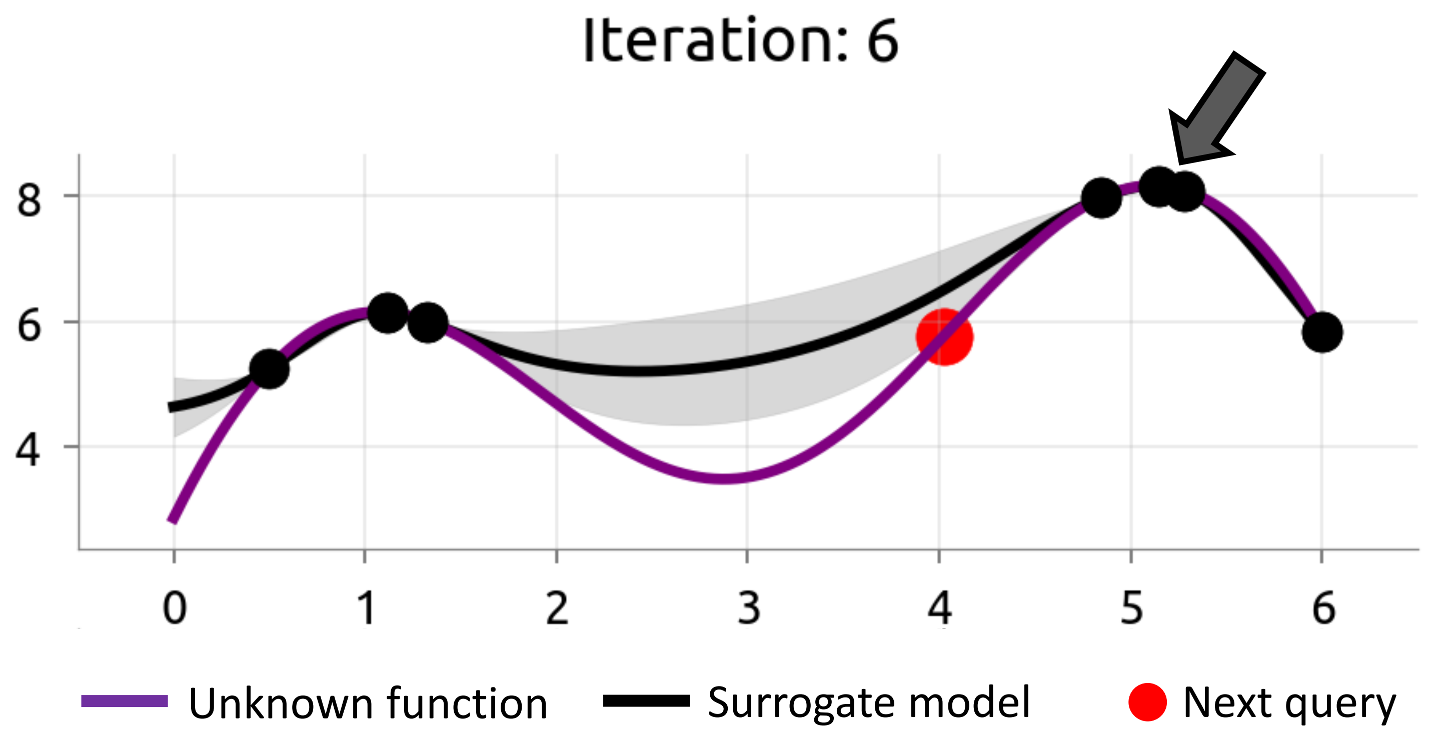

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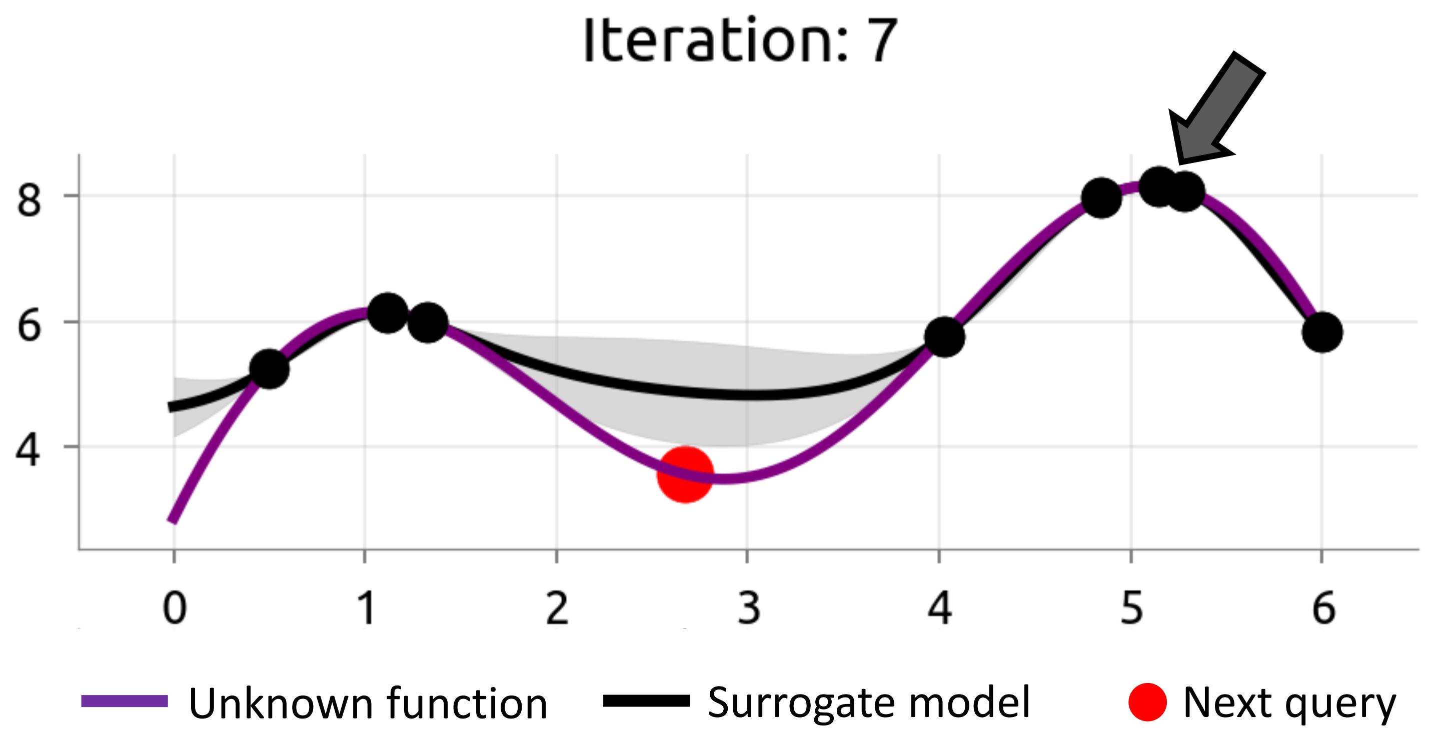

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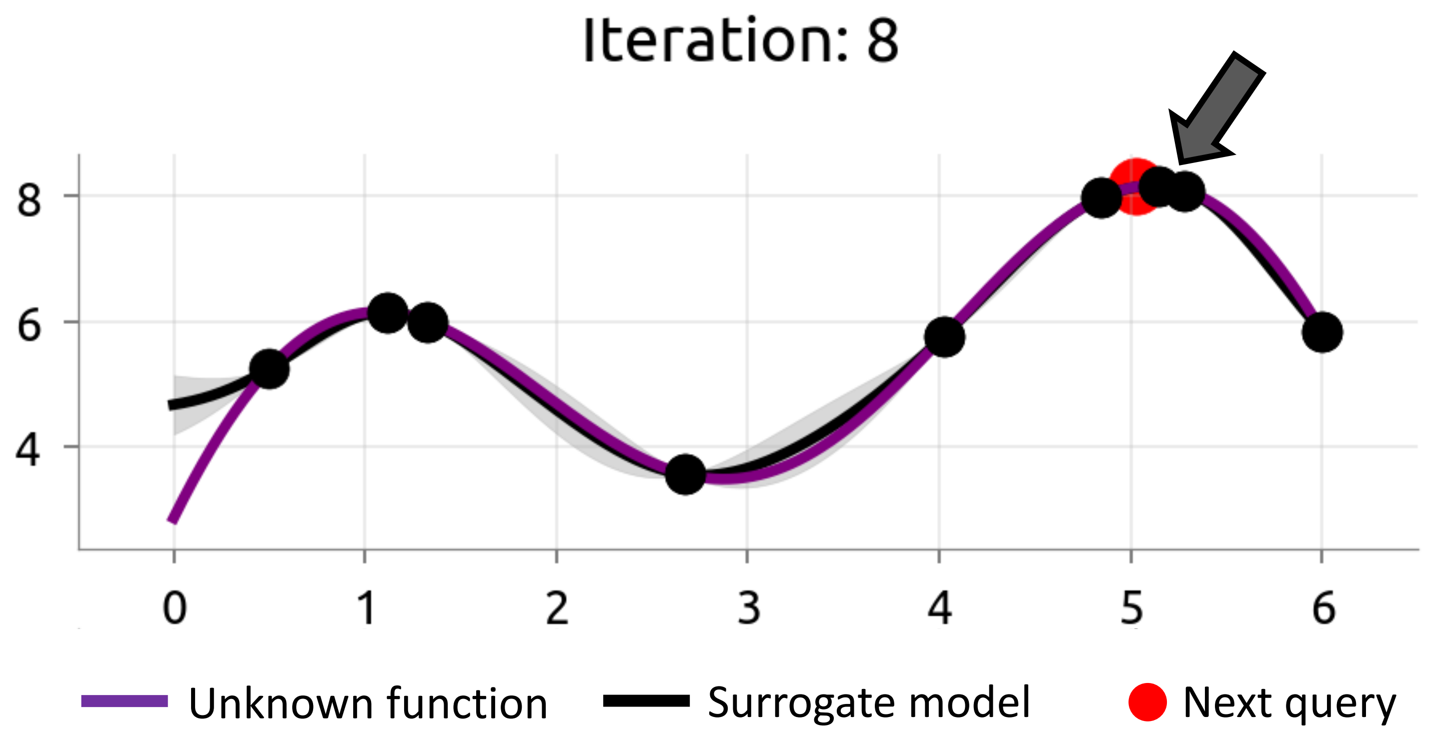

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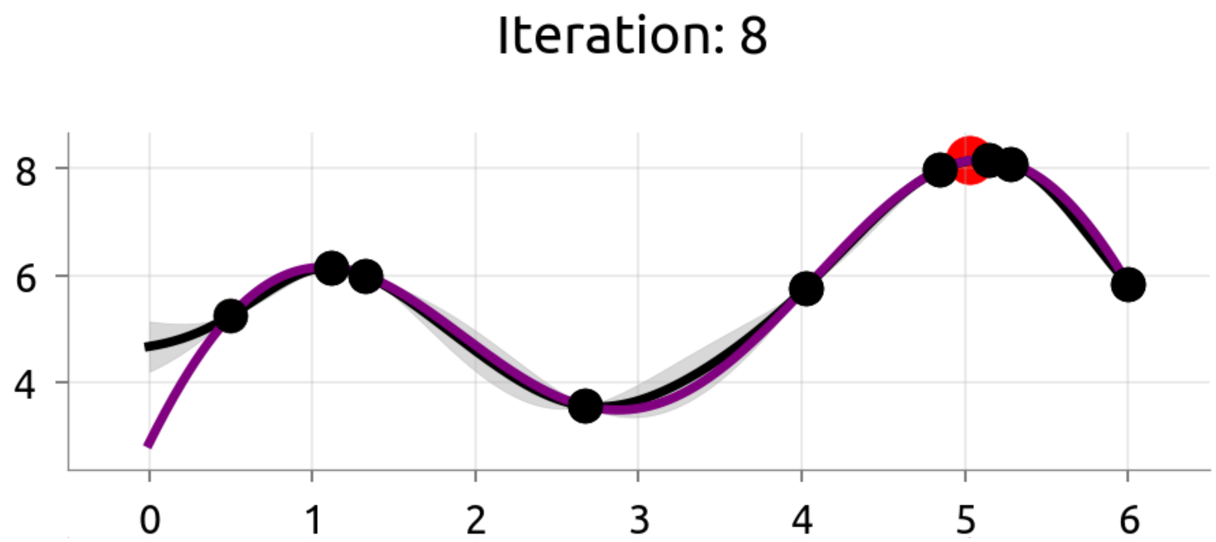
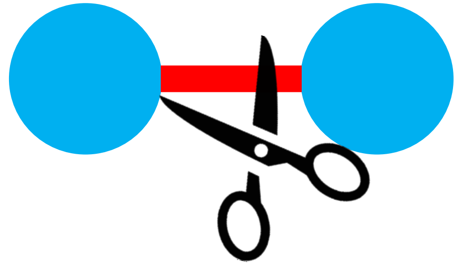


<u>HyperMapper</u> [Nardi 2019]: A Practical Design Space Exploration Framework.

(1) Random forests surrogate model (discrete search space).

(2) Semi-greedy acquisition function.

Quantitative benefits for chemistry applications



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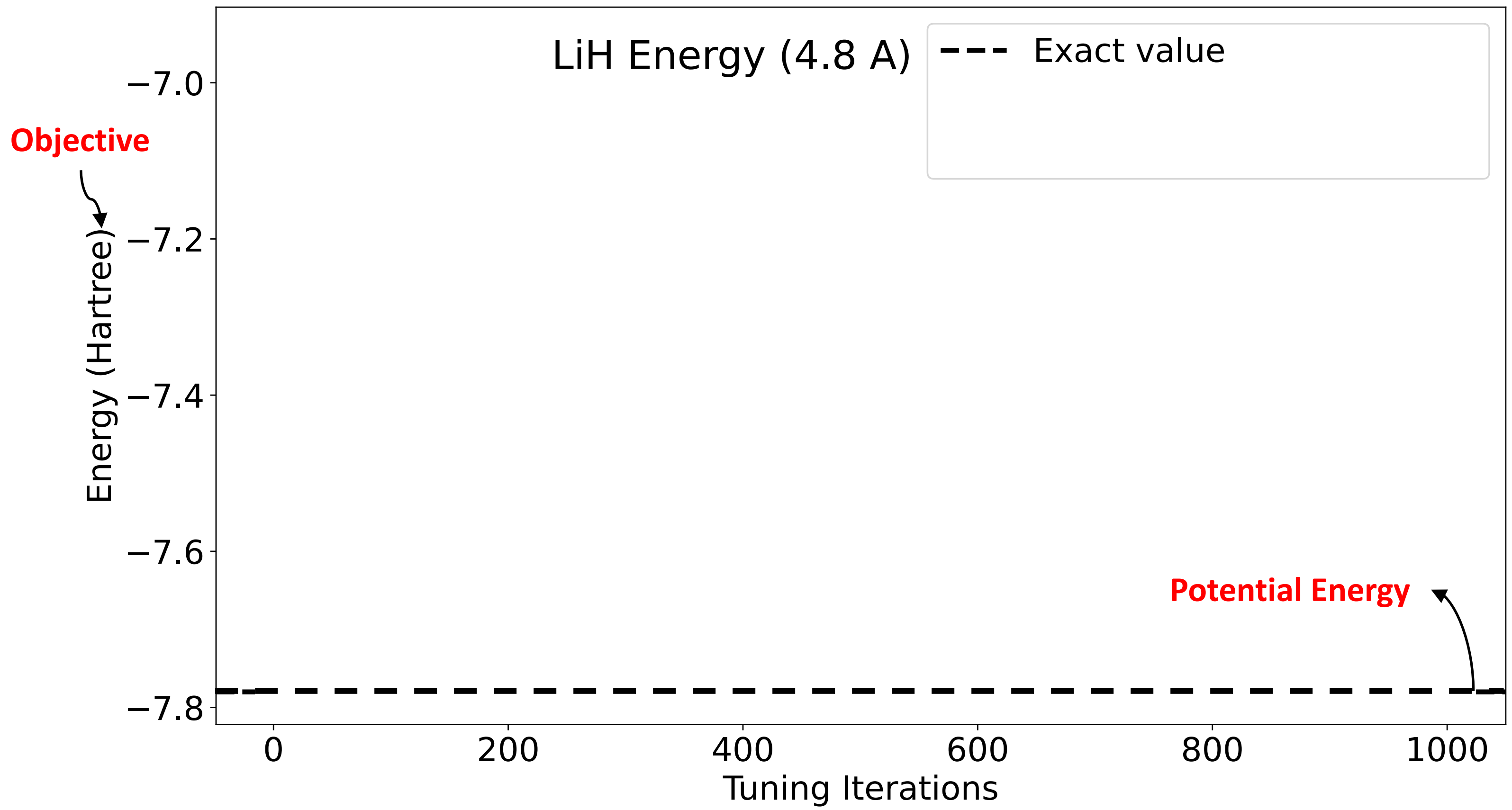

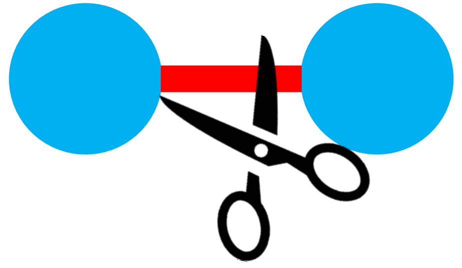

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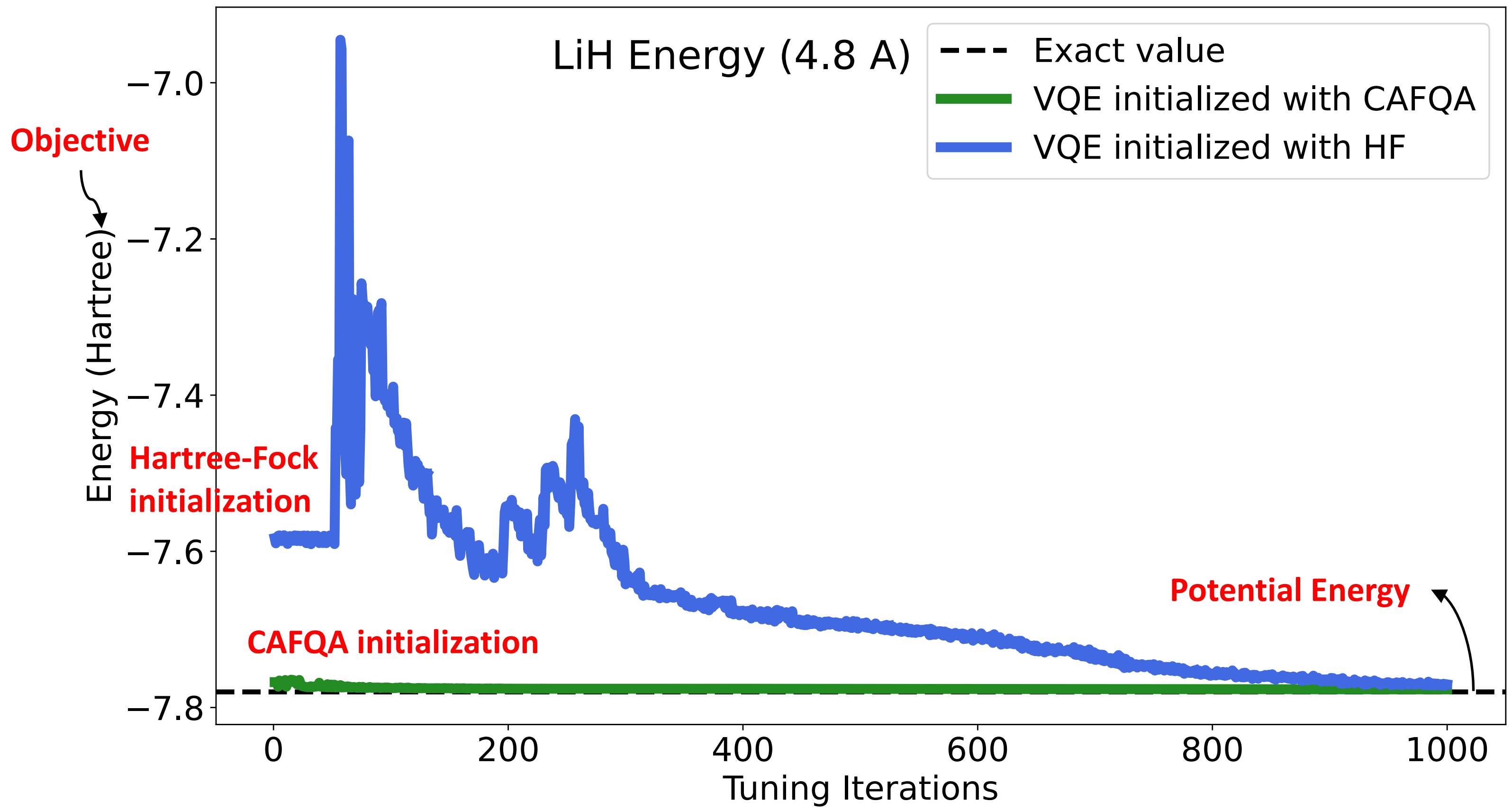

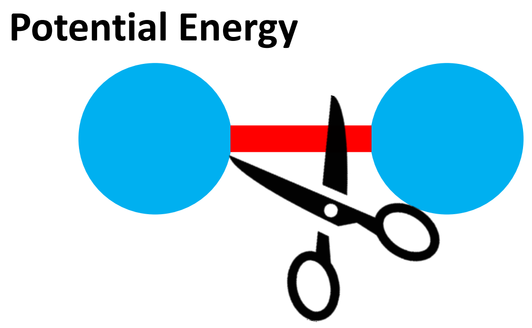

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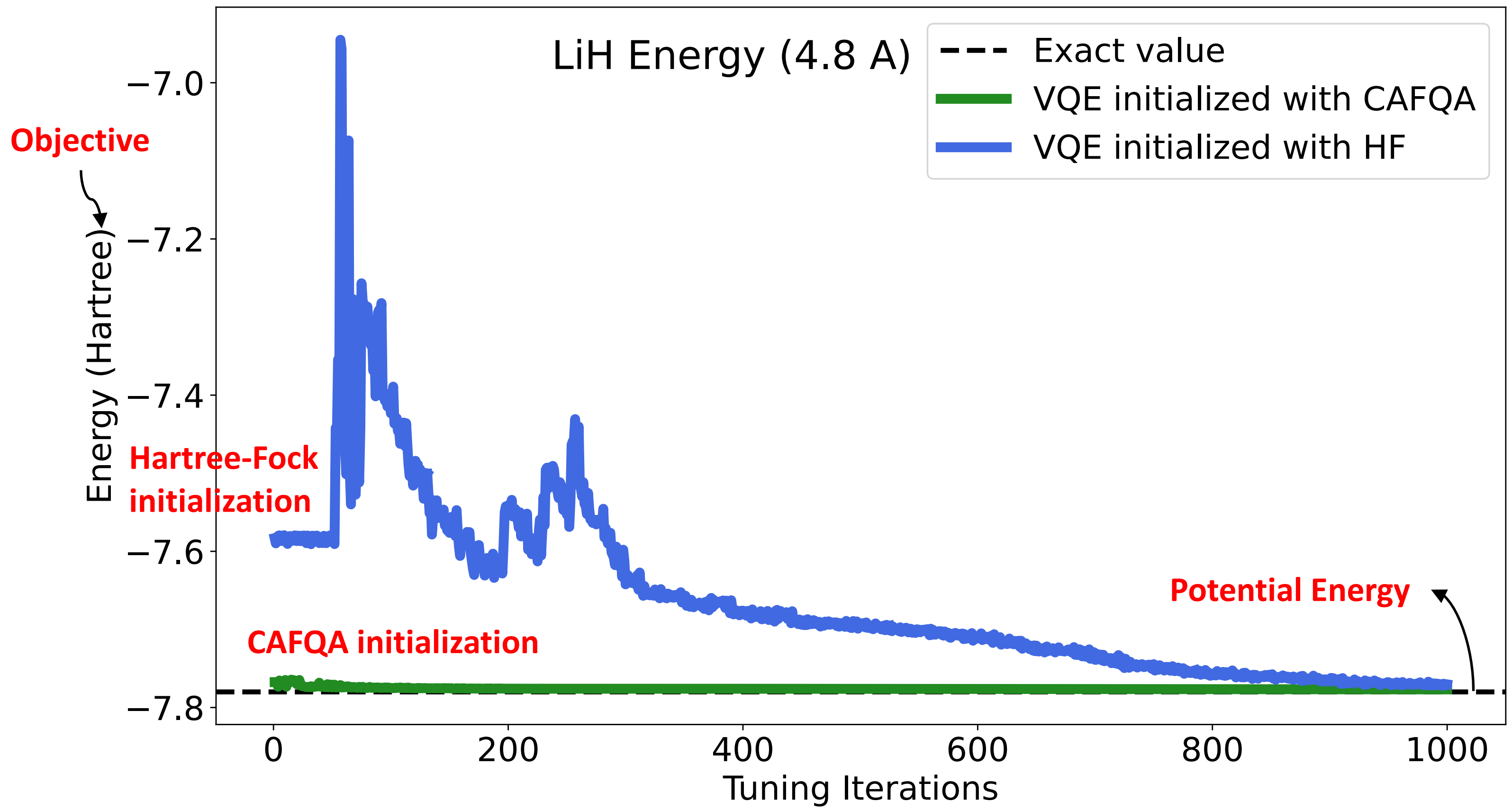
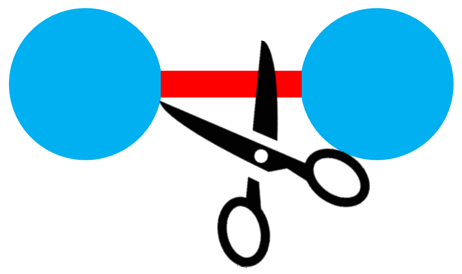
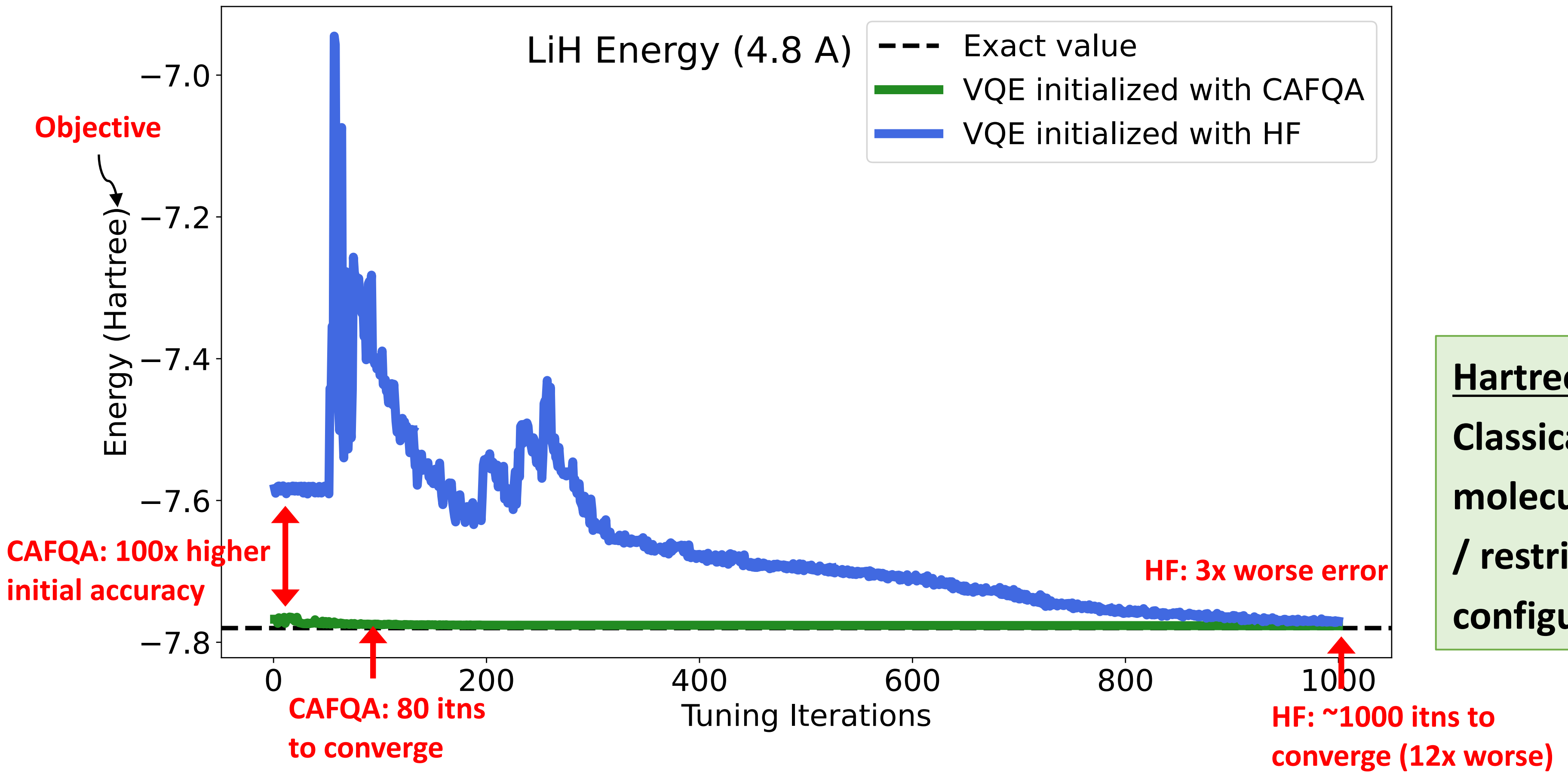


Potential Energy



<u>**Hartree-Fock initialization**</u> **[~1930]: Classically-solvable algorithm in molecular chemistry that approximates / restricts the problem's electronic configuration.**

Quantitative benefits for chemistry applications



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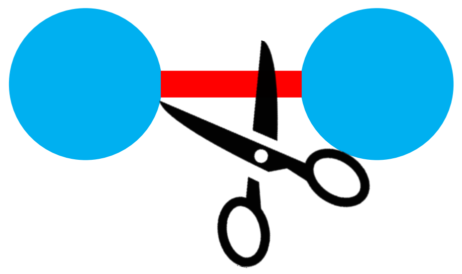

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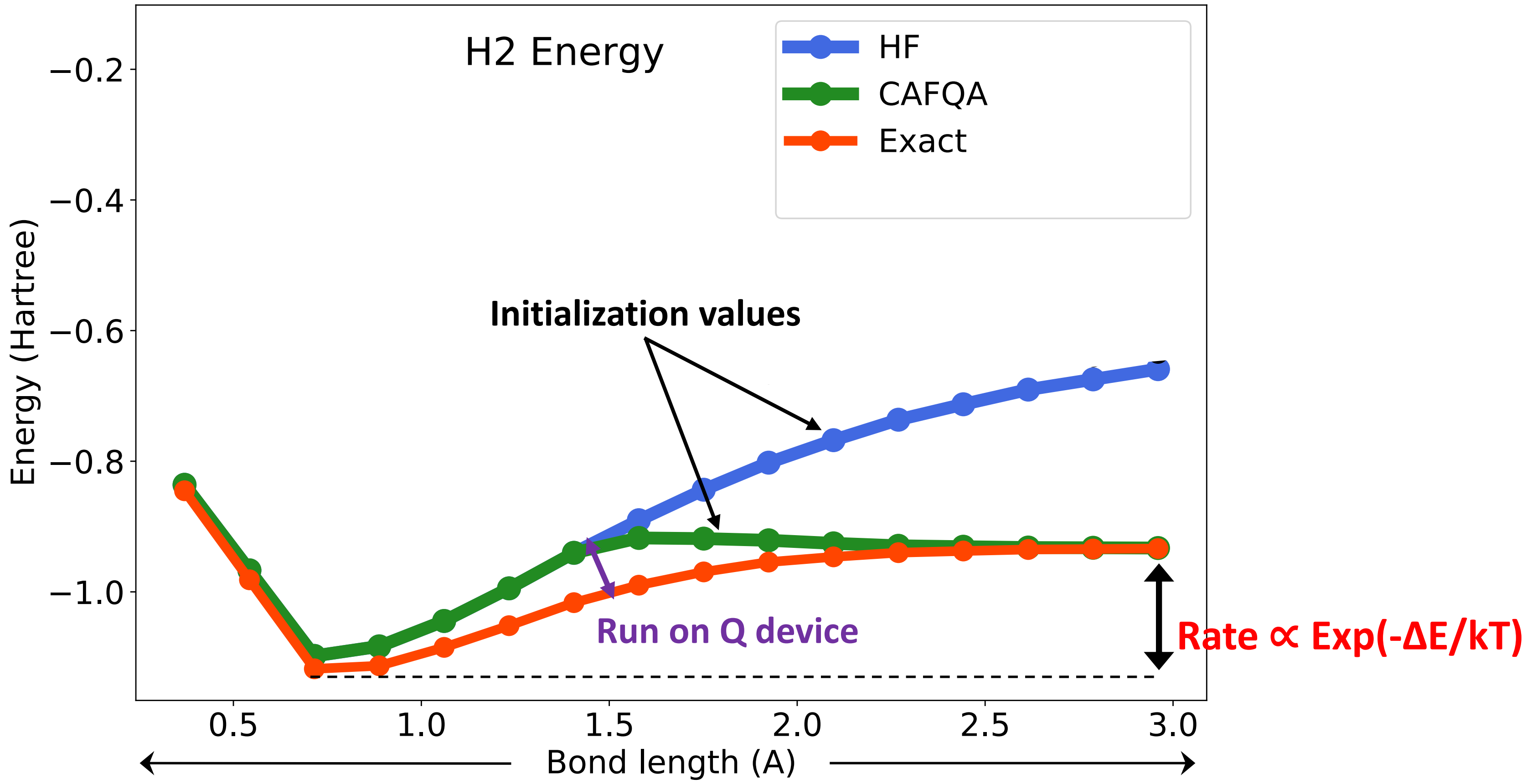

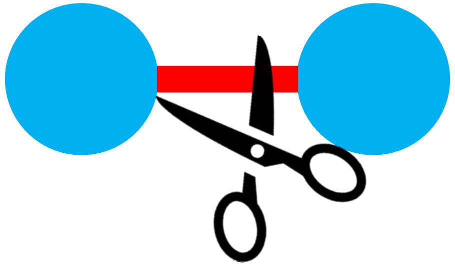

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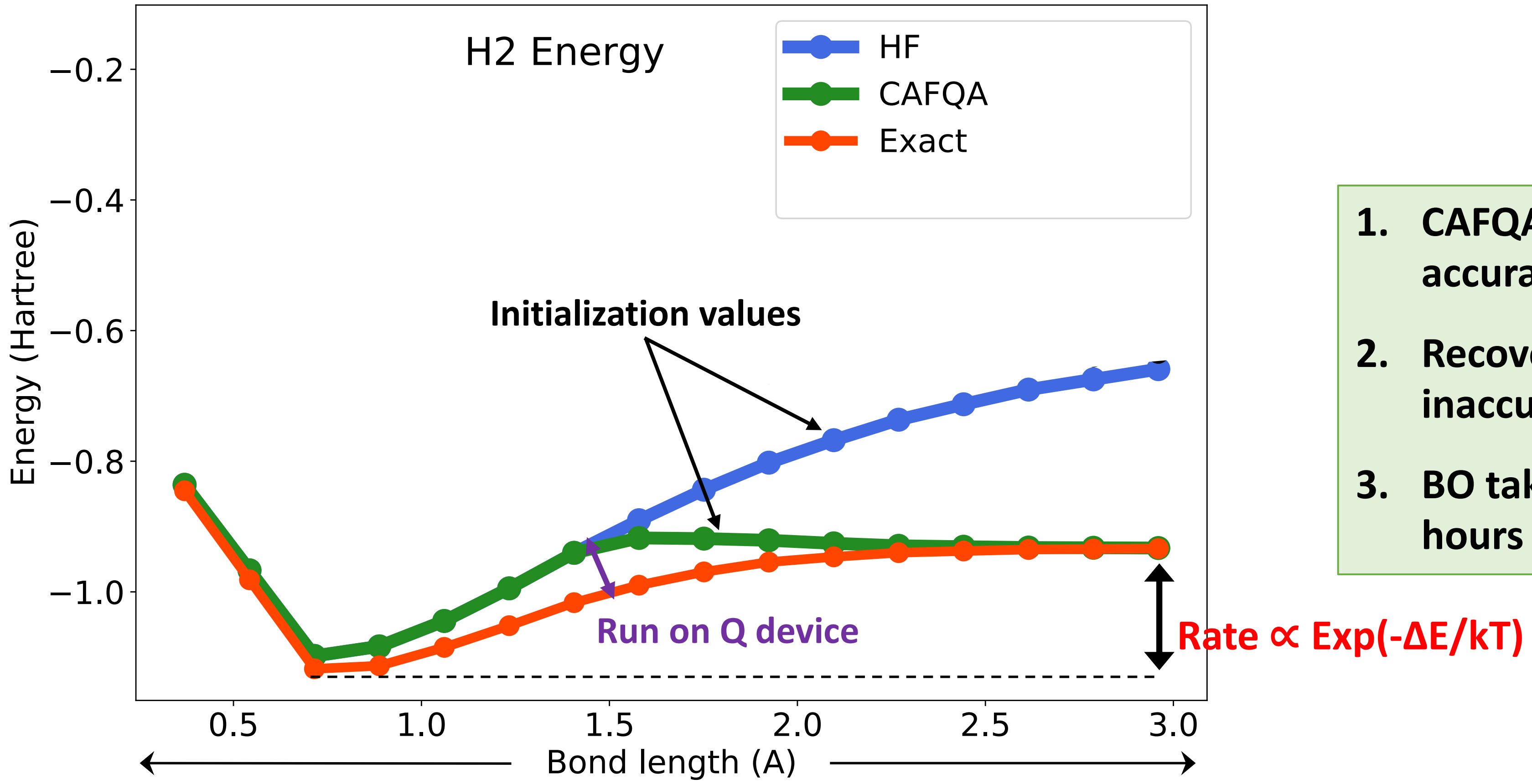

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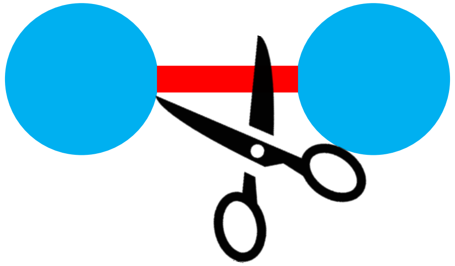
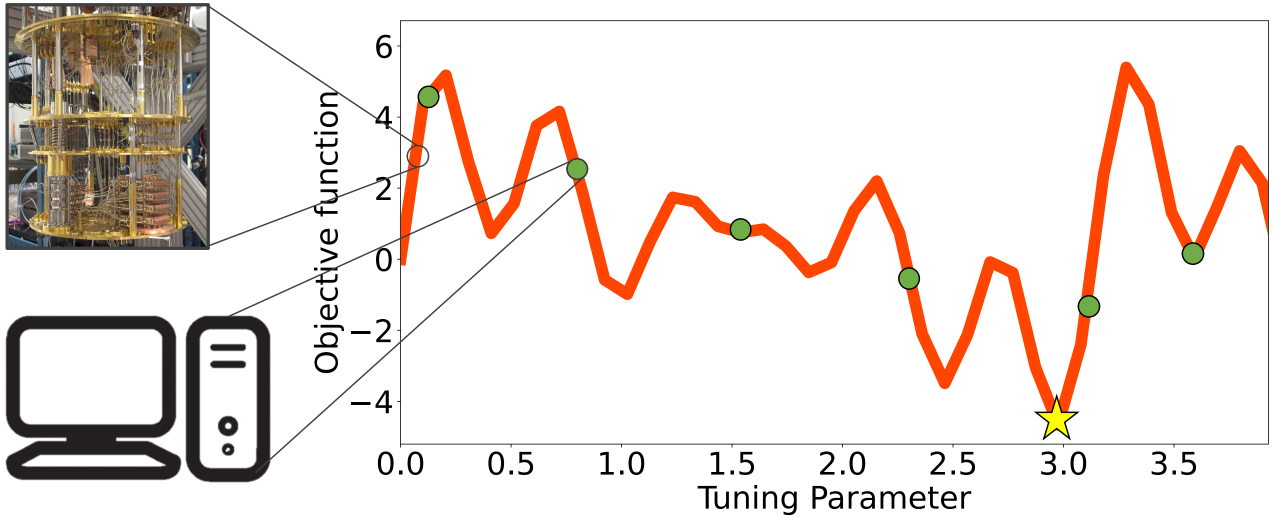


1. **CAFQA achieves 99% mean initialization accuracy (systems up to 34 qubits).**
2. **Recovers up to 99.99% of Hartree-Fock inaccuracy (57x mean).**
3. **BO takes ~2000 iterations (mean), few hours in wall-clock time.**

Key takeaways



1. **Initialization is critical for VQA algorithms to accurately converge on noisy quantum machines.**
2. **CAFQA initializes VQA by classically tuning its ansatz in the Clifford space. CAFQA sim is noise-free.**
3. **CAFQA is classically scalable, it searches the search space efficiently through Bayesian Optimization.**
4. **1-5 orders of magnitude accuracy + performance benefits over prior art.**

Thank you!

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https://github.com/rgokulsm/CAFQA
(Updates with more features and latest Qiskit integration coming soon)

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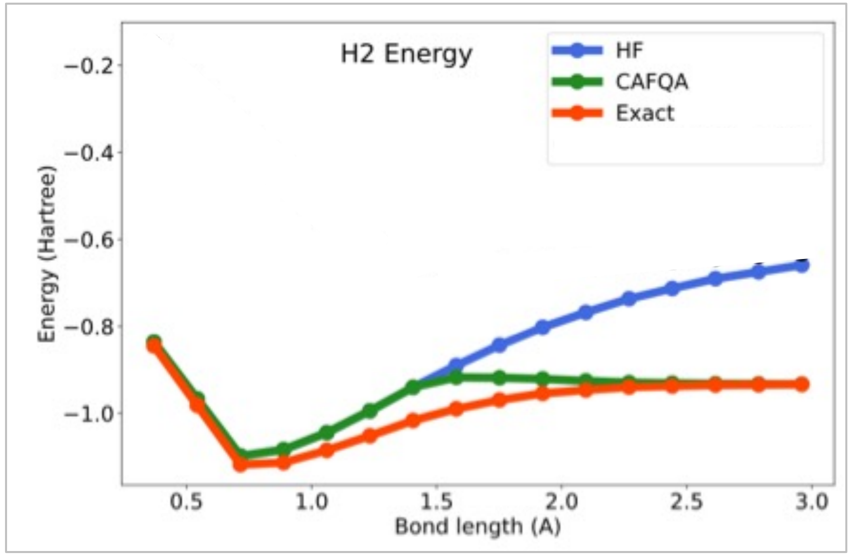
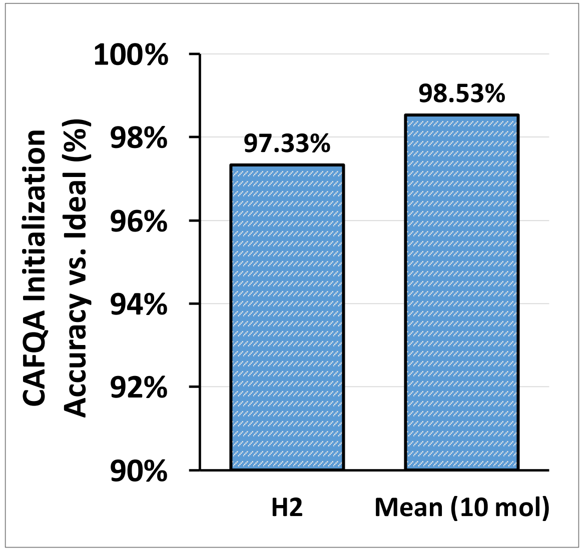
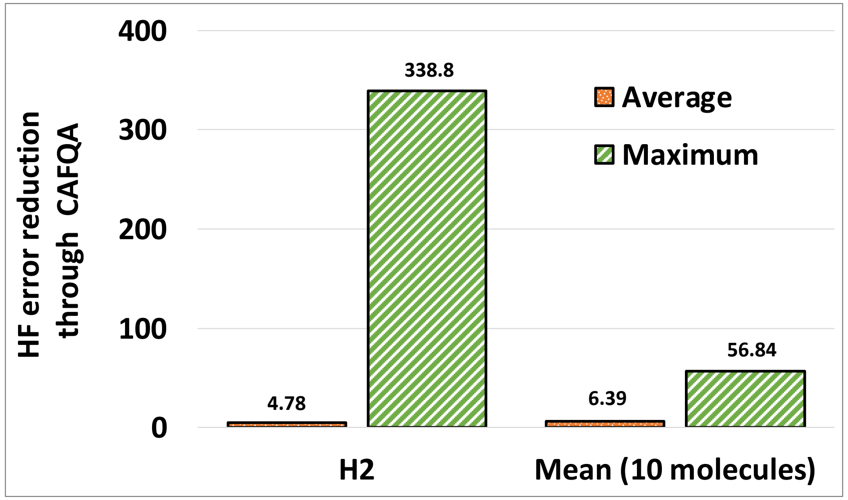
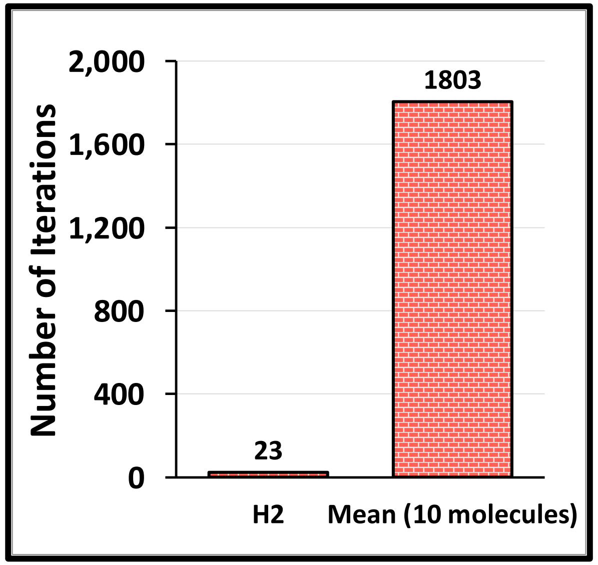
Quantitative benefits for chemistry apps









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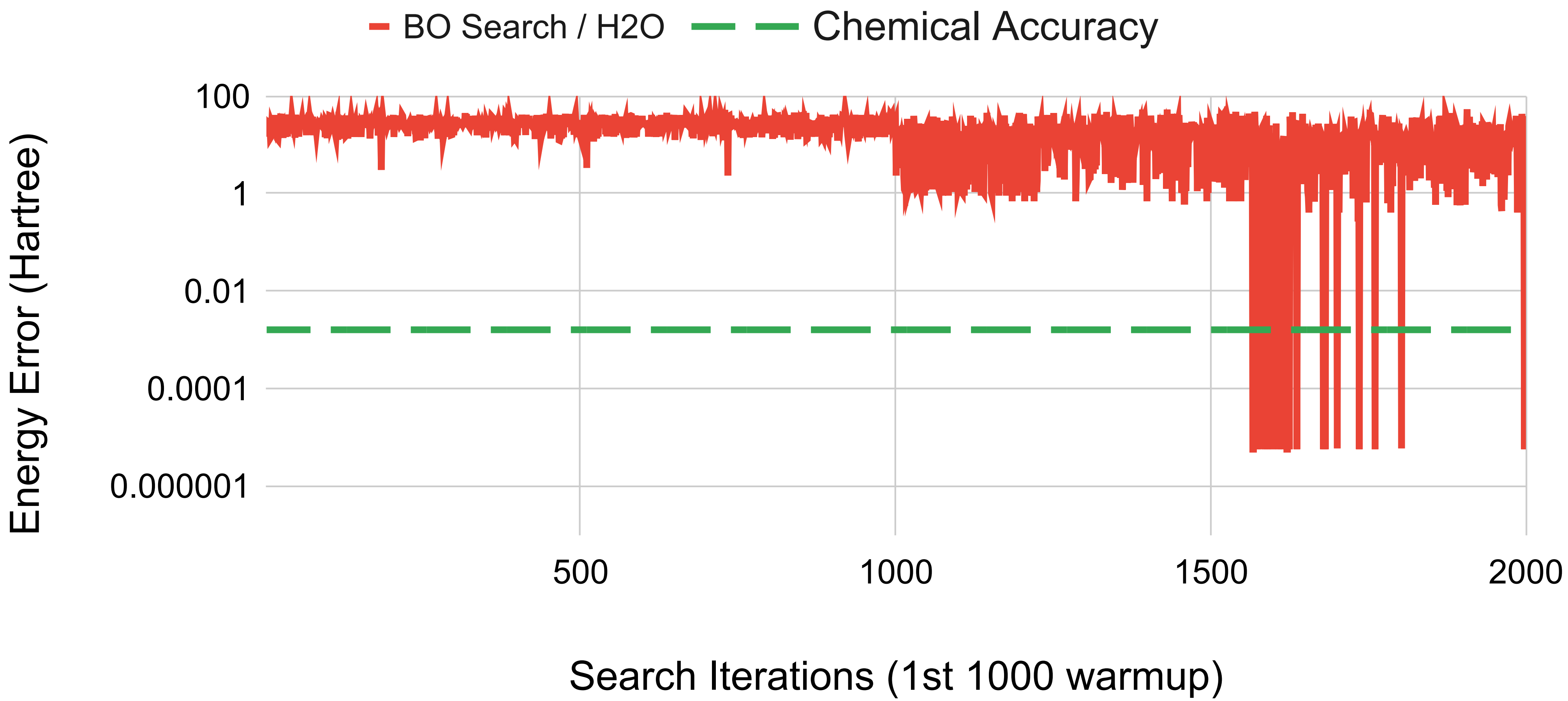
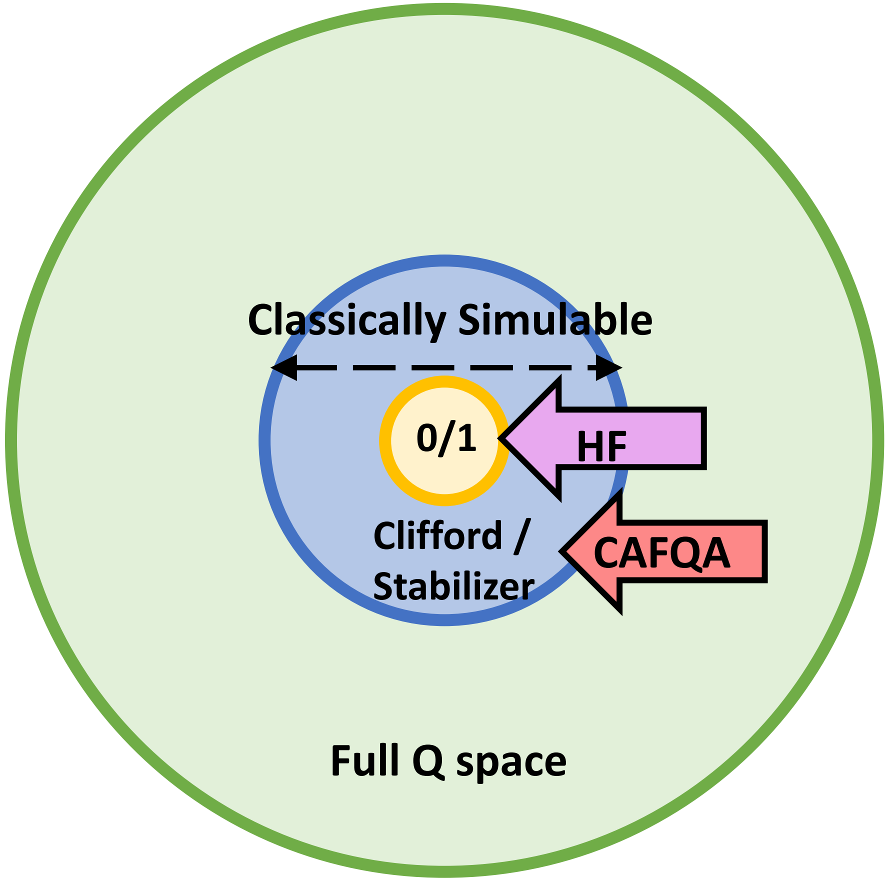


***HyperMapper*: a Practical Design Space Exploration Framework [Nardi, et al., 2019]**
(1) Random forests surrogate model (discrete problem space), (2) Greedy acquisition function

Hartree-Fock (for chemistry) vs CAFQA initialization

- Hartree Fock: (best) bitstring of 1s and 0s
  Example: |1011>
- CAFQA: (best) equal superposition of multiple strings.
  Example: 0.5* (|1011> + |1010> + |0011> + |0010>)



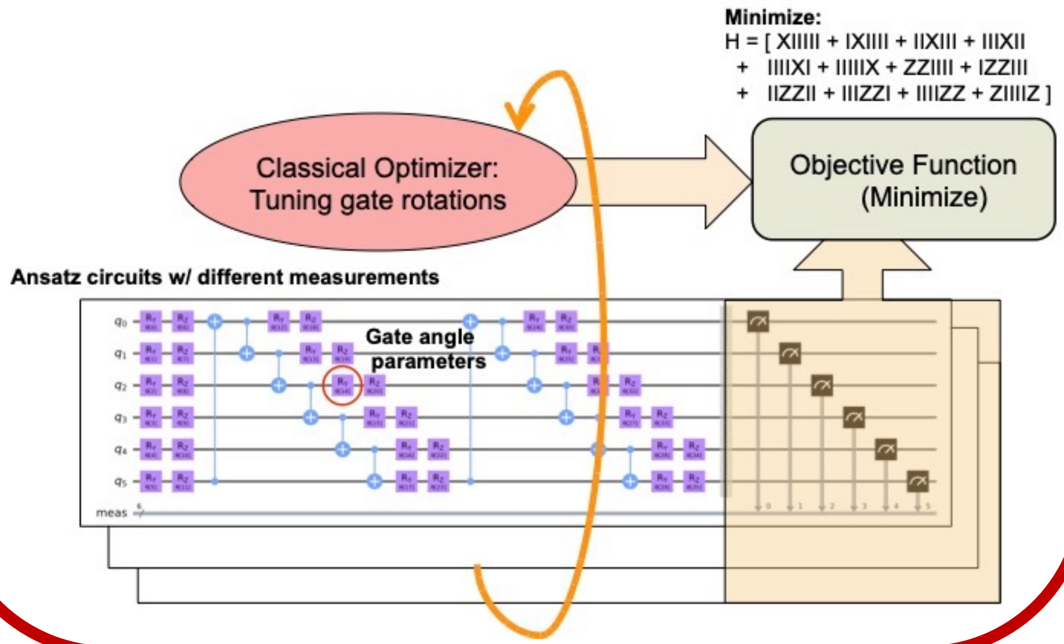
Hartree-Fock computational basis states*   ⊂   CAFQA stabilizer states*   ⊂   Arbitrary quantum states
**** = classical simulable in poly time***

How to find the optimal CAFQA solution?

Classical

Classical discrete search:

- Ideal evaluation
- Tractable only in the Clifford space
- Efficient discrete search (Bayesian Optimization)

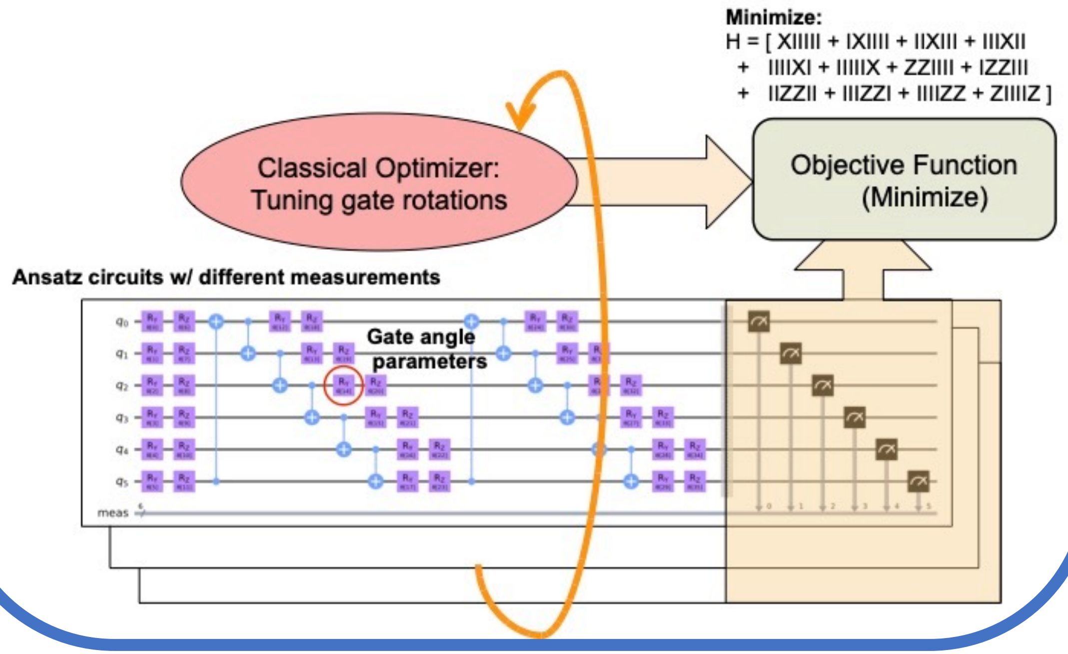


Ansatz w/ CAFQA initialization

Quantum

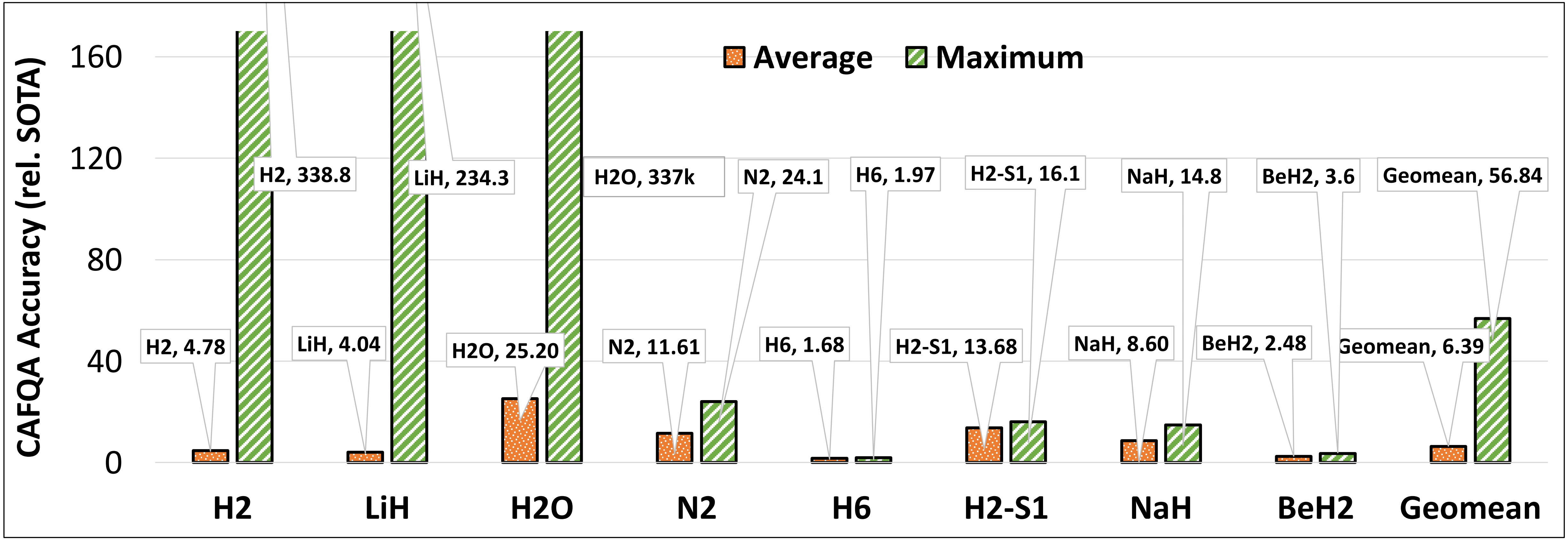
Quantum continuous search:

- Noisy evaluation
- Tractable across the full parameter space
- Efficient continuous search (eg. SPSA, ImFil)

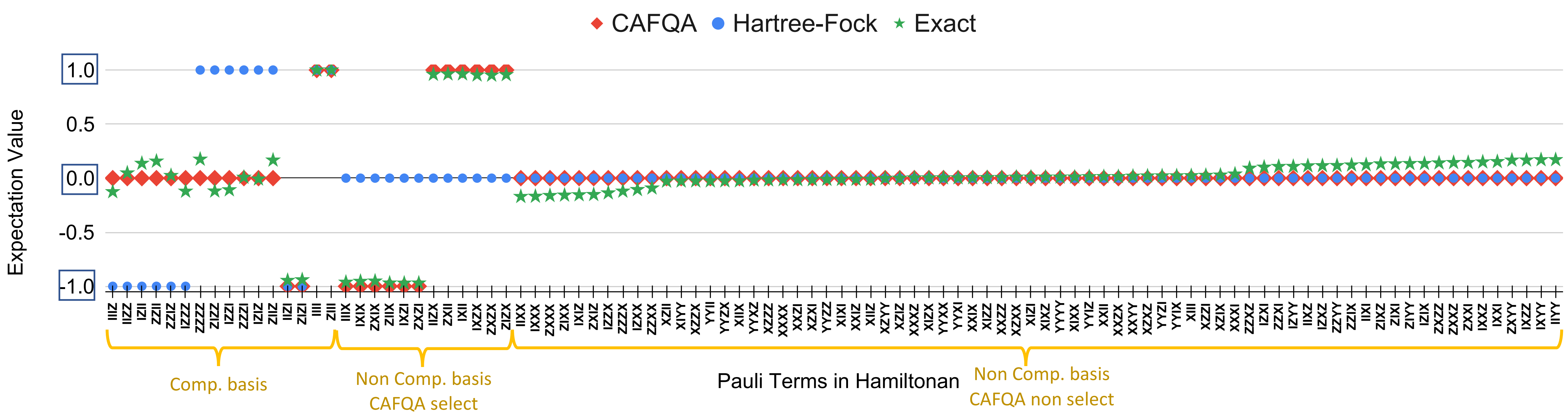


CAFQA initialization is noise-free and classically tractable in the Clifford space, which is searched efficiently via Bayesian Optimization. Post-CAFQA traditional VQA is performed on the quantum device.

Evaluation: CAFQA benefits over HF across molecules



CAFQA analysis: LiH at 4A



Search Iterations