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Surrogate-based optimization for variational quantum algorithms

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OVER-QC

NSF

QISE-NET

QUANTUM INFORMATION SCIENCE AND ENGINEERING NETWORK

U.S. DEPARTMENT OF ENERGY NNSA

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Agenda

Variational quantum algorithms (VQA)

- Overview
- Existing optimization techniques

Surrogate-based optimization for VQA

- Overview
- Comparison to existing techniques

Summary

Variational quantum algorithms (VQA)

Variational quantum algorithms (VQA)

Near-term quantum computers are **noisy** and have **limited coherence times**

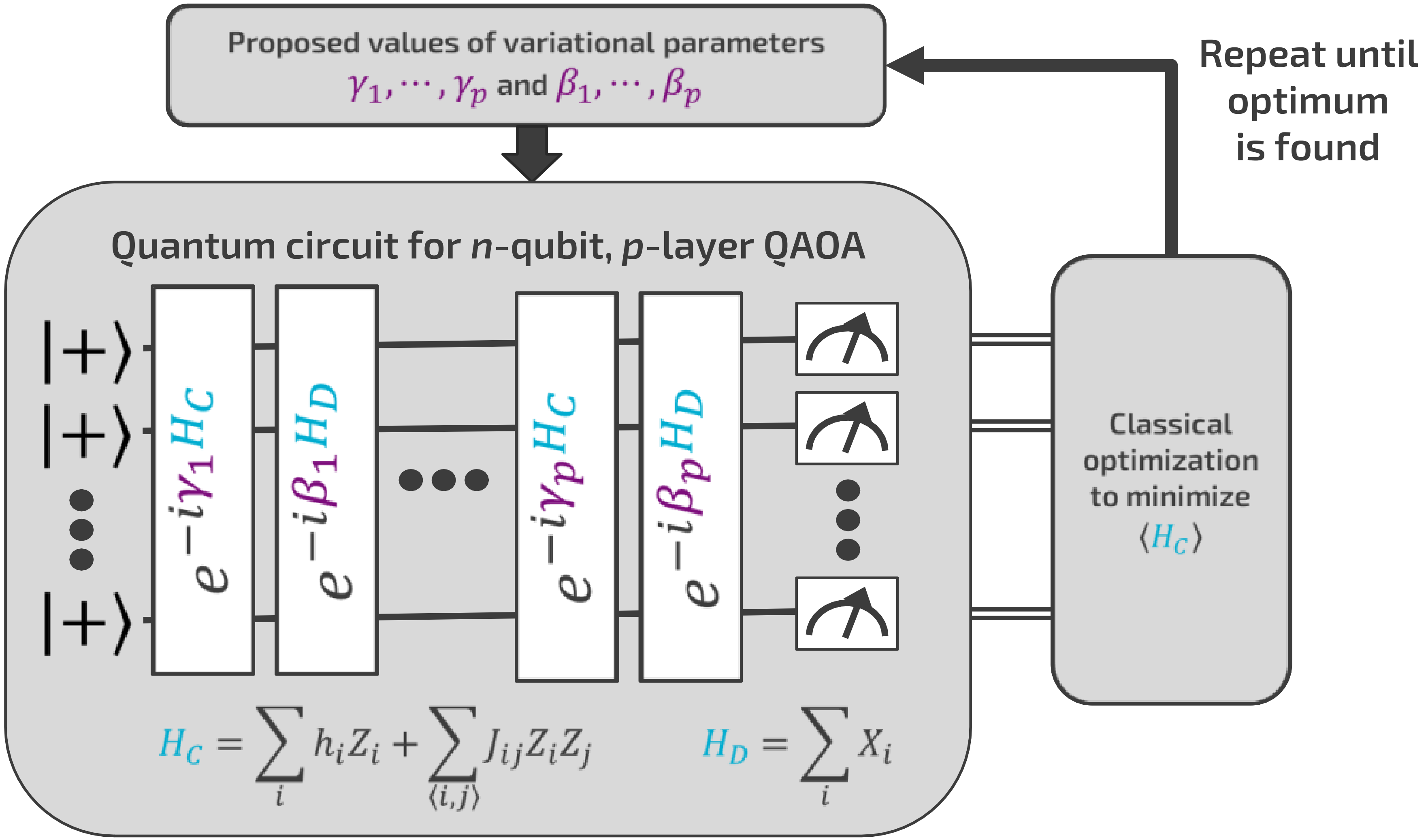
It will be years before we can run large-scale computations on a QC

For now, much research is focused on **variational quantum algorithms**

- Hybrid of quantum + classical computation
- Run many small-scale quantum programs, supplemented by classical optimization

Quantum Approximate Optimization Algorithm (QAOA)

Goal:
Find the values of variational parameters $\gamma_1, \cdots, \gamma_p$ and $\beta_1, \cdots, \beta_p$ that minimize an objective function $\langle H_C \rangle$

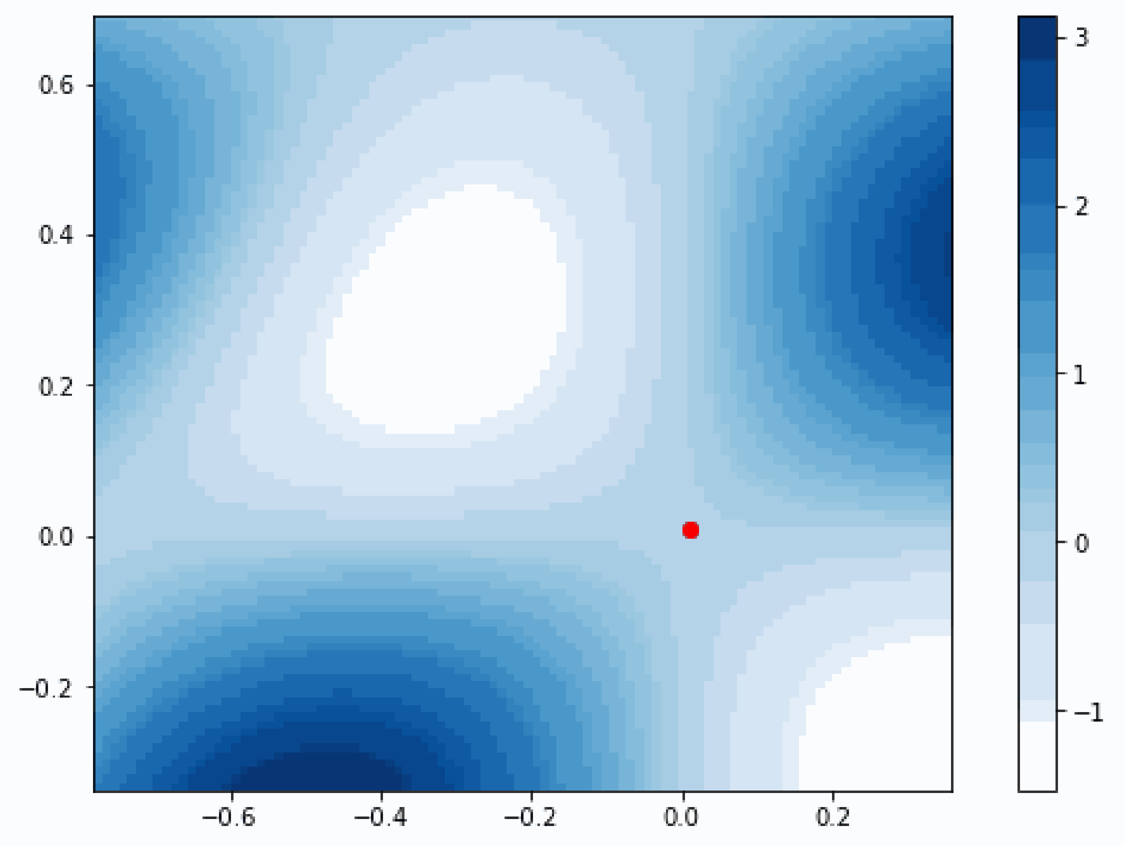


Classical optimization: SPSA

SPSA (Simultaneous Perturbation Stochastic Approximation) is the most commonly-used technique for optimizing variational quantum algorithms with noisy samples.

1. Attempt to **follow the gradient** in the objective function landscape
   - Take two (noisy) samples near an initial point
   - Approximate the gradient based on these samples
   - Move in the direction of the gradient for the next iteration
2. Repeat until convergence

SPSA example (animation)



Surrogate-based optimization for VQA

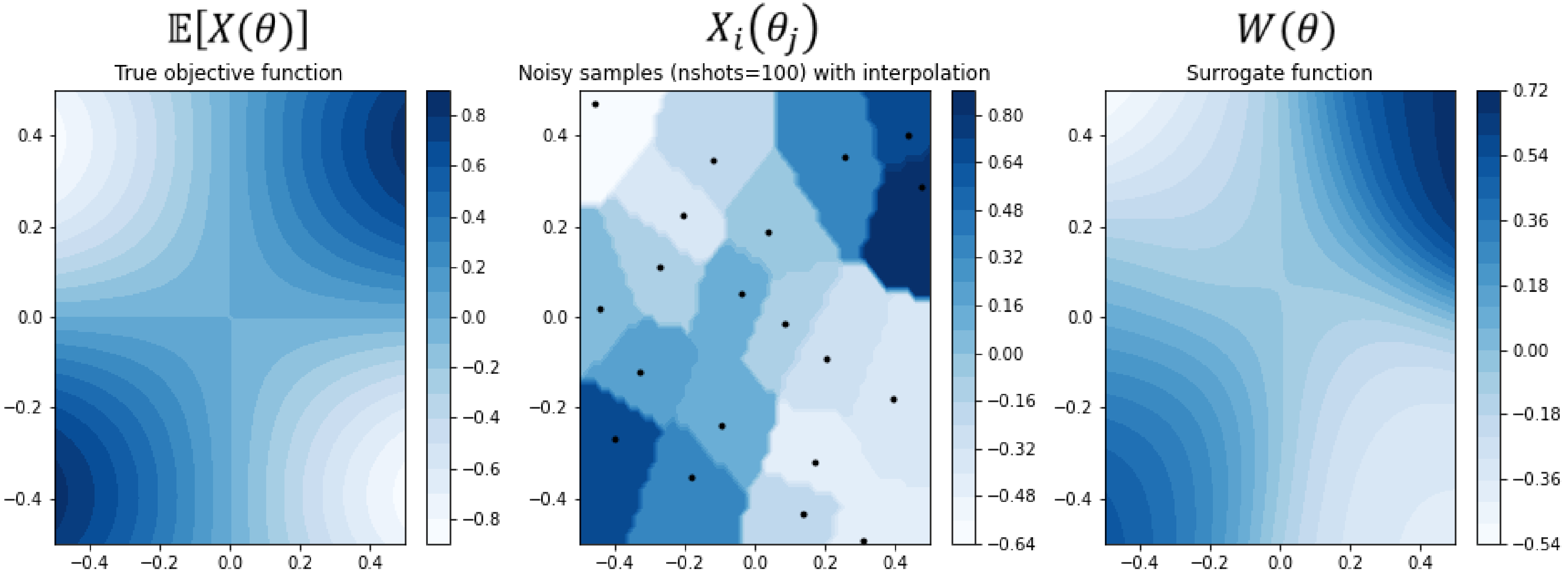
Surrogate-based optimization for VQA

We propose a surrogate-based technique for optimizing variational quantum algorithms with noisy samples.

1. Construct a **surrogate** of the objective function landscape
   - Take many (noisy) samples in a local “patch”
   - Construct the function surrogate in this patch, e.g., using a kernel approximation

Example surrogate: Gaussian kernel approximation

Construct surrogate as a sum of Gaussians centered on each sample point.



θ_j = coordinates of j^{th} sample point
k_j = number of shots taken at j^{th} sample point
$X_i(\theta_j)$ = i^{th} measurement result at coordinate θ_j

Kernel:

$$K(\theta,\theta_j) = e^{-\frac{\|\theta-\theta_j\|^2}{2\sigma}}$$

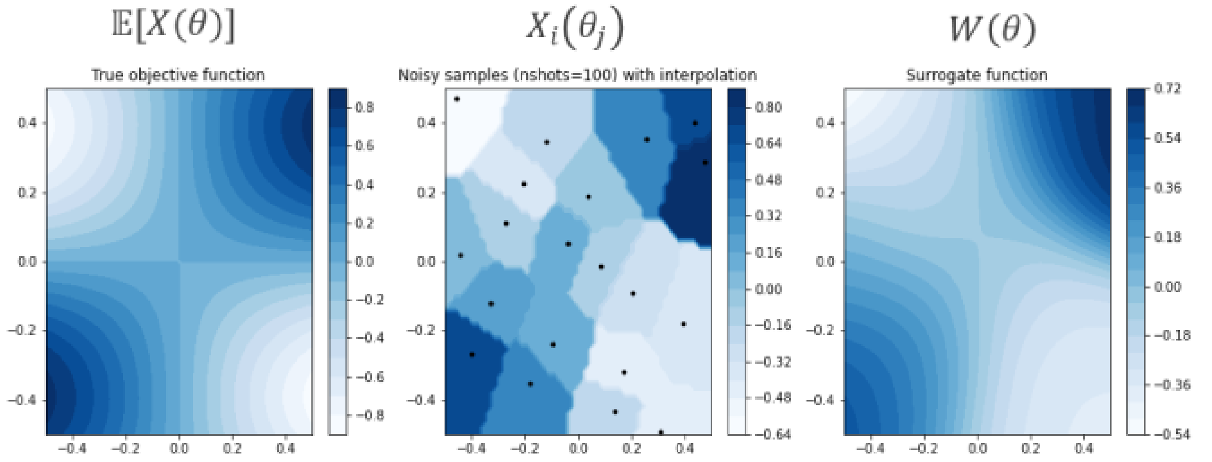
Surrogate:

$$W(\theta) = \sum_j \left(\frac{1}{k_j} \sum_{i=1}^{k_j} X_i(\theta_j) \right) K(\theta,\theta_j)$$

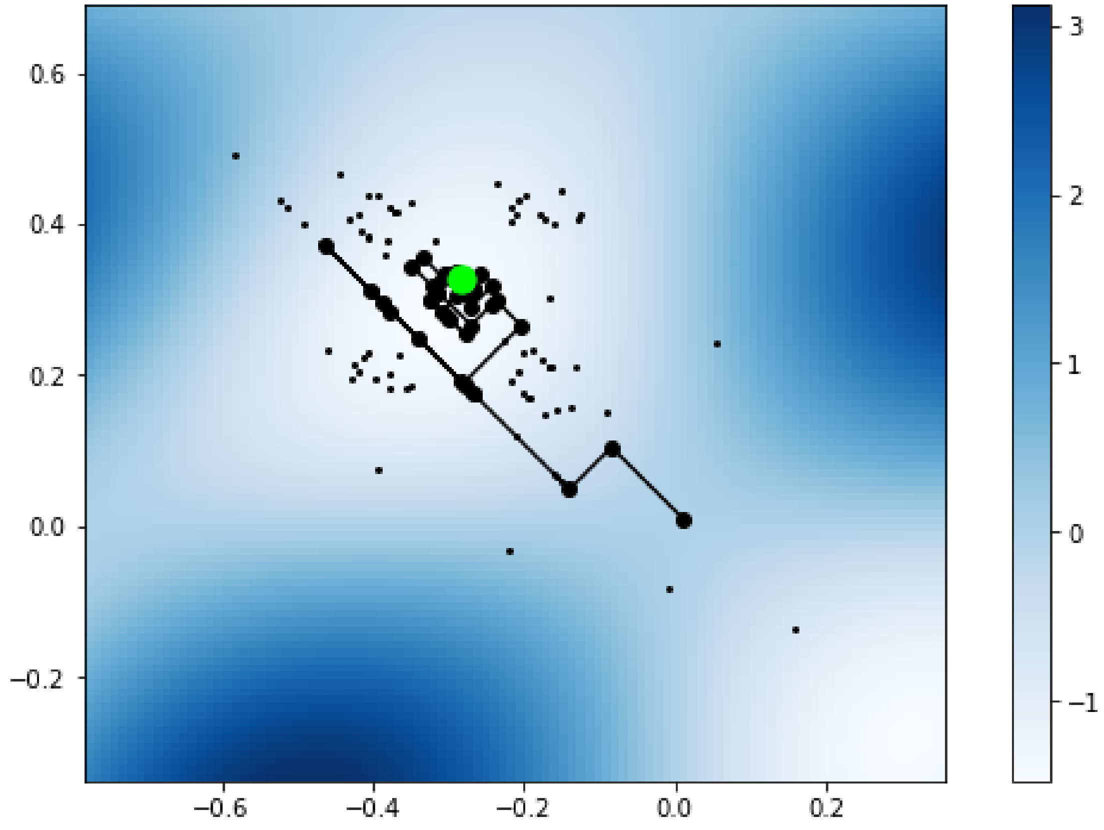
Surrogate-based optimization for VQA

We propose a surrogate-based technique for optimizing variational quantum algorithms with noisy samples.

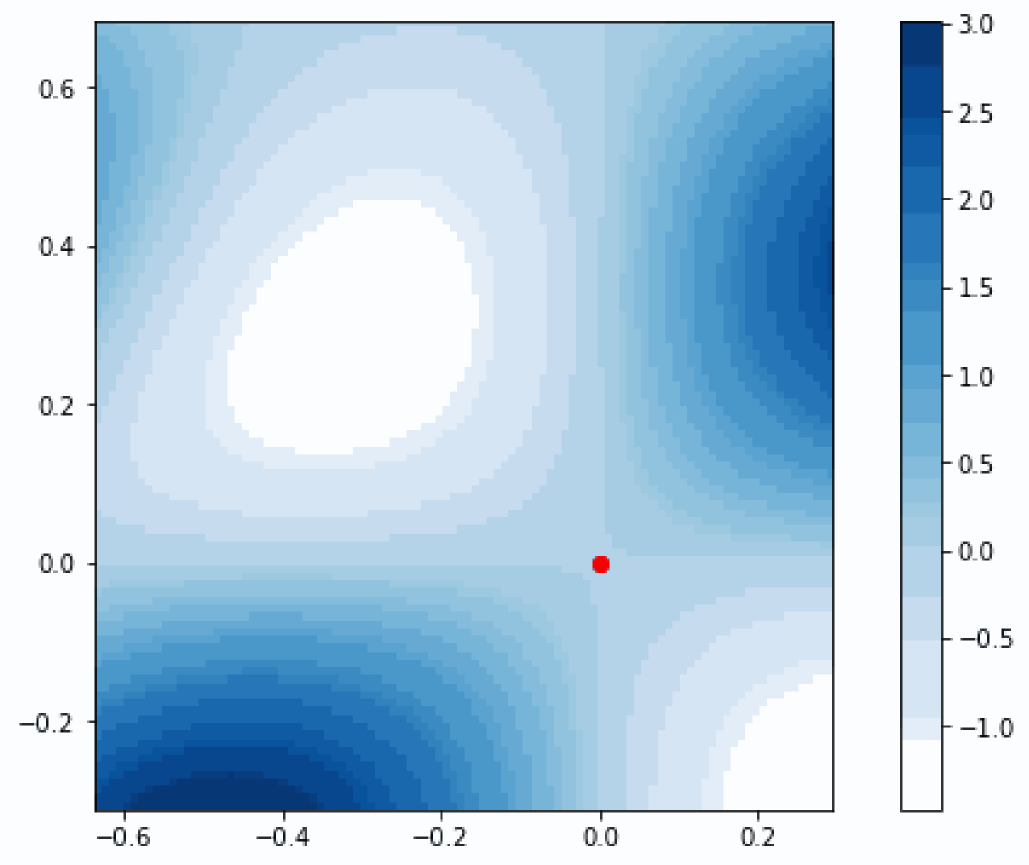
1. Construct a **surrogate** of the objective function landscape
   - Take many (noisy) samples in a local "patch"
   - Construct the function surrogate in this patch, e.g., using a kernel approximation
   - Use the surrogate to estimate the coordinates of the minimum in this patch
   - Use these coordinates as the center of the next patch
2. Repeat until convergence



Comparison to SPSA (animation)



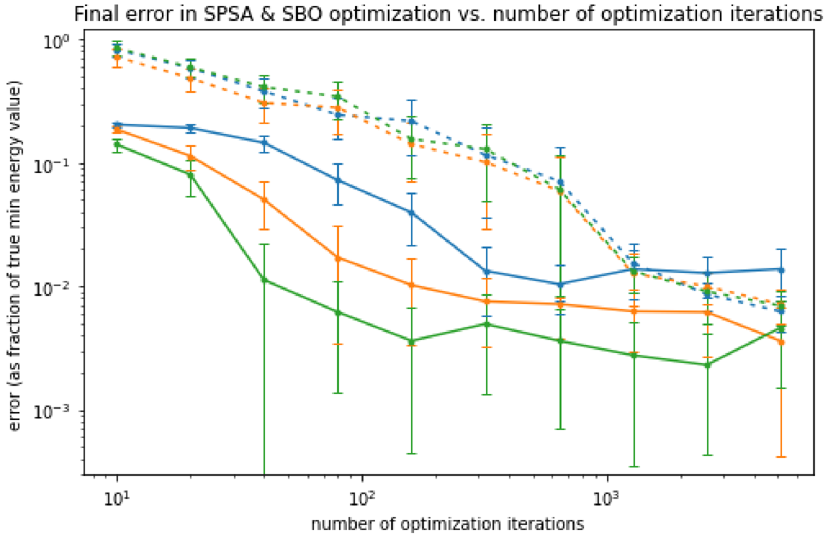
SPSA
40 iterations, 2 points per iteration



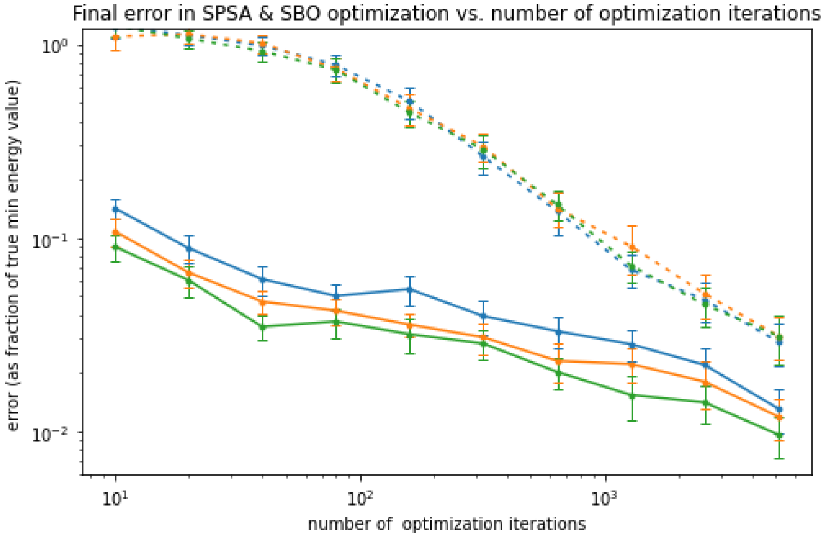
SBO with Gaussian kernel approximation
10 iterations, 8 points per iteration

Results: QAOA for max-cut

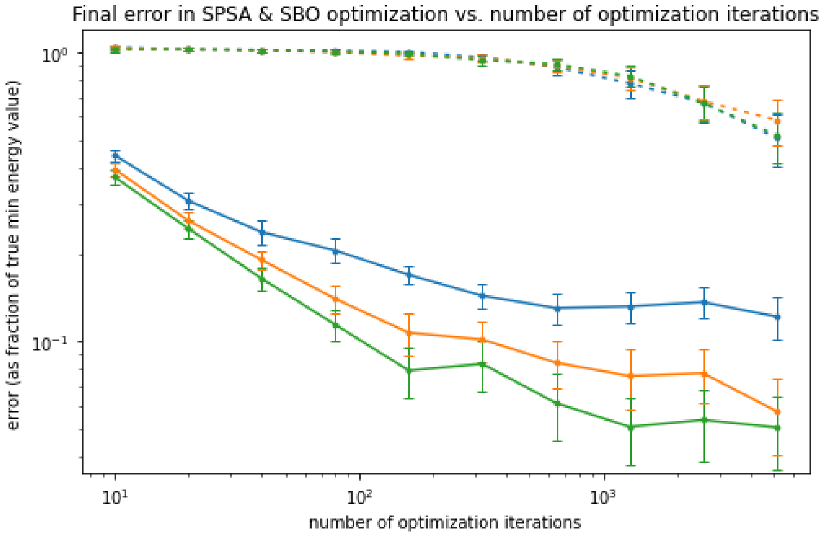
n=4, p=2

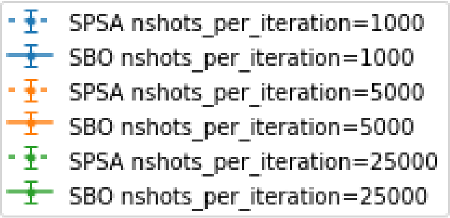


n=6, p=4



n=10, p=7





x-axis: total # of classical optimization iterations
y-axis: relative error in min value found

Potential advantages of SBO vs. SPSA

Often **converges more quickly** in higher-dimensional problems

- Achieves better variational parameter estimates with fewer experimental runs

Allows taking **batches of samples** from many different coordinates within each optimization iteration

- Results in speed and robustness (against drift) advantages in the absence of low-latency circuit loading

Requires **fewer shots** per sample point than SPSA

- Kernel approximation produces a surrogate where shot noise is smoothed out

Summary

Summary

We propose a **surrogate-based optimization technique**, for optimizing variational quantum algorithms with noisy samples.

We demonstrate an **improvement over SPSA** on common problems such as QAOA and VQE, using a Gaussian kernel approximation as the surrogate.

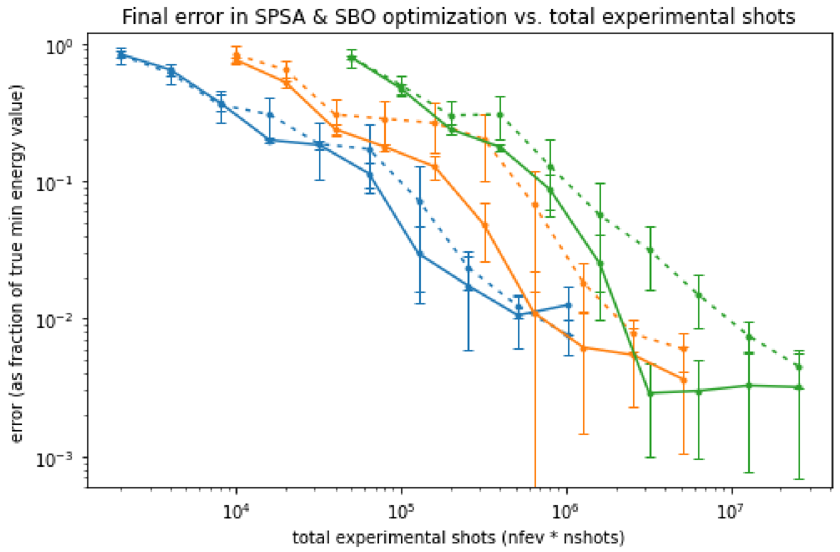
We observe **potential advantages over SPSA** in convergence and experimental runtime, particularly for higher-dimensional problems.

Thank you for listening!

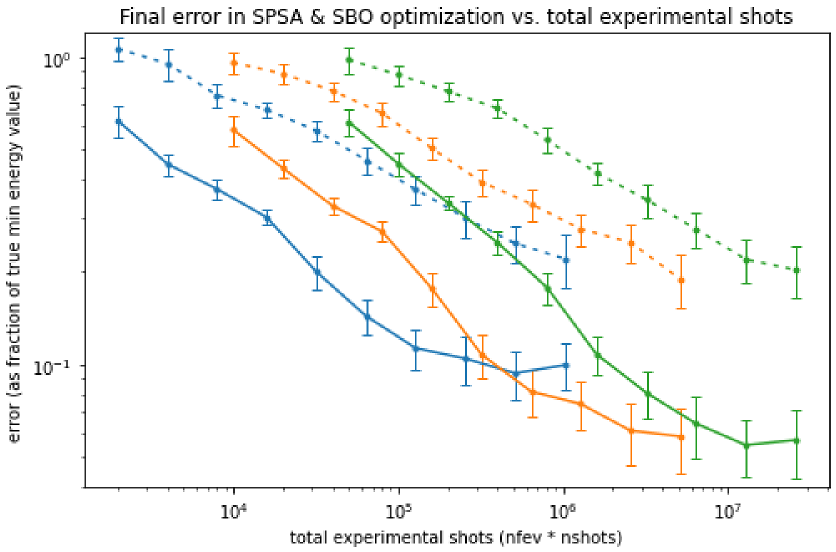
Extra slides

Numerical results: QAOA for max-cut

n=4, p=2



n=6, p=4



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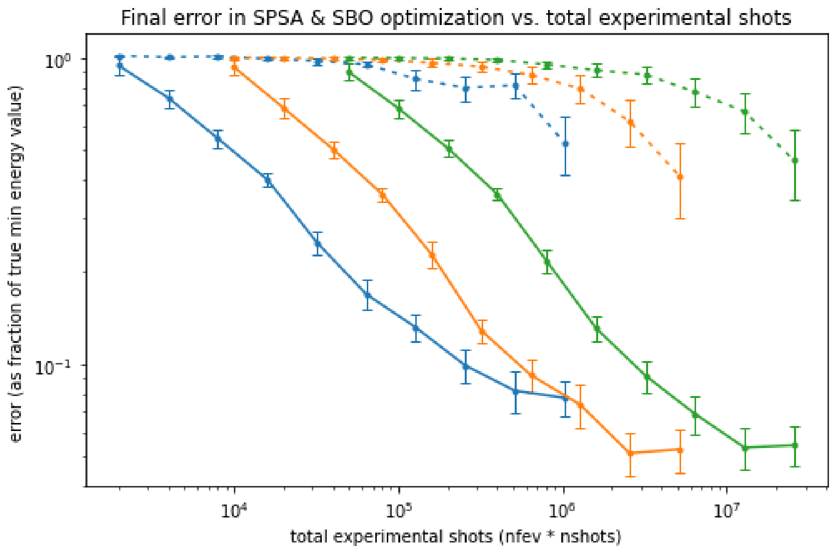
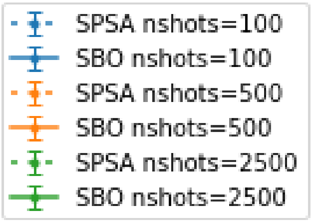
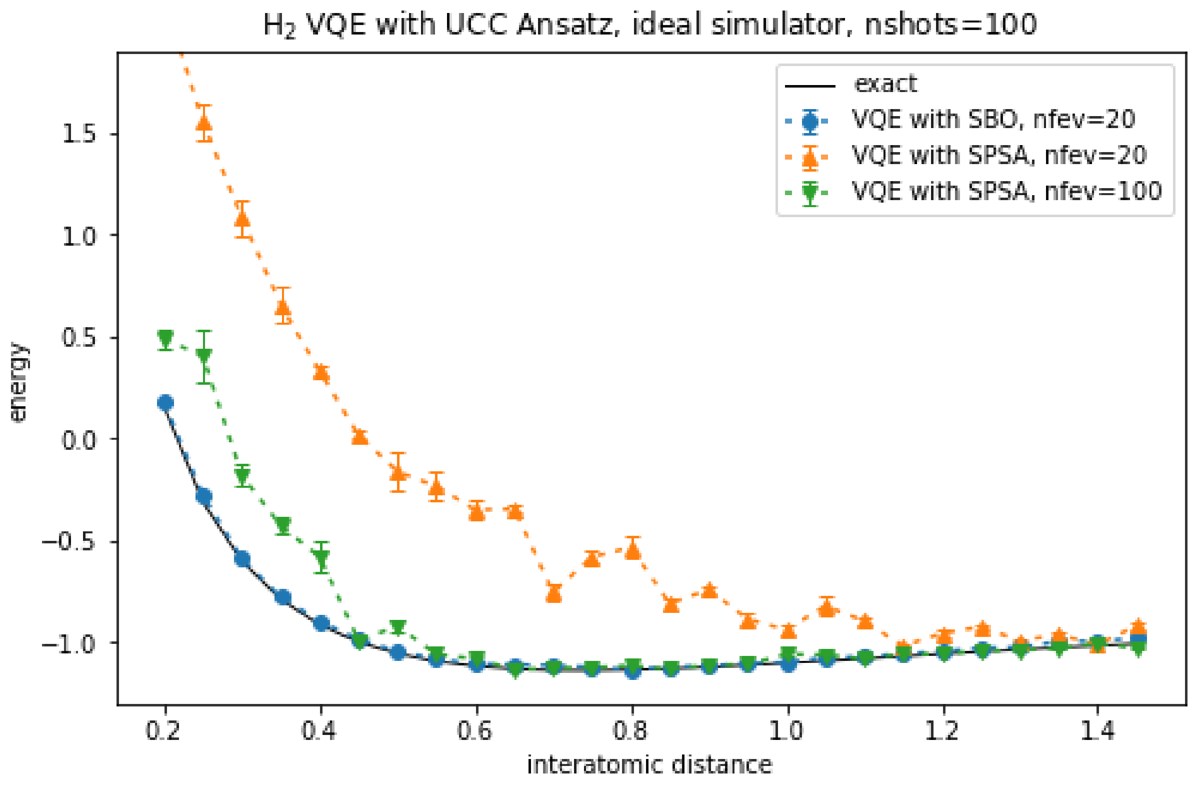
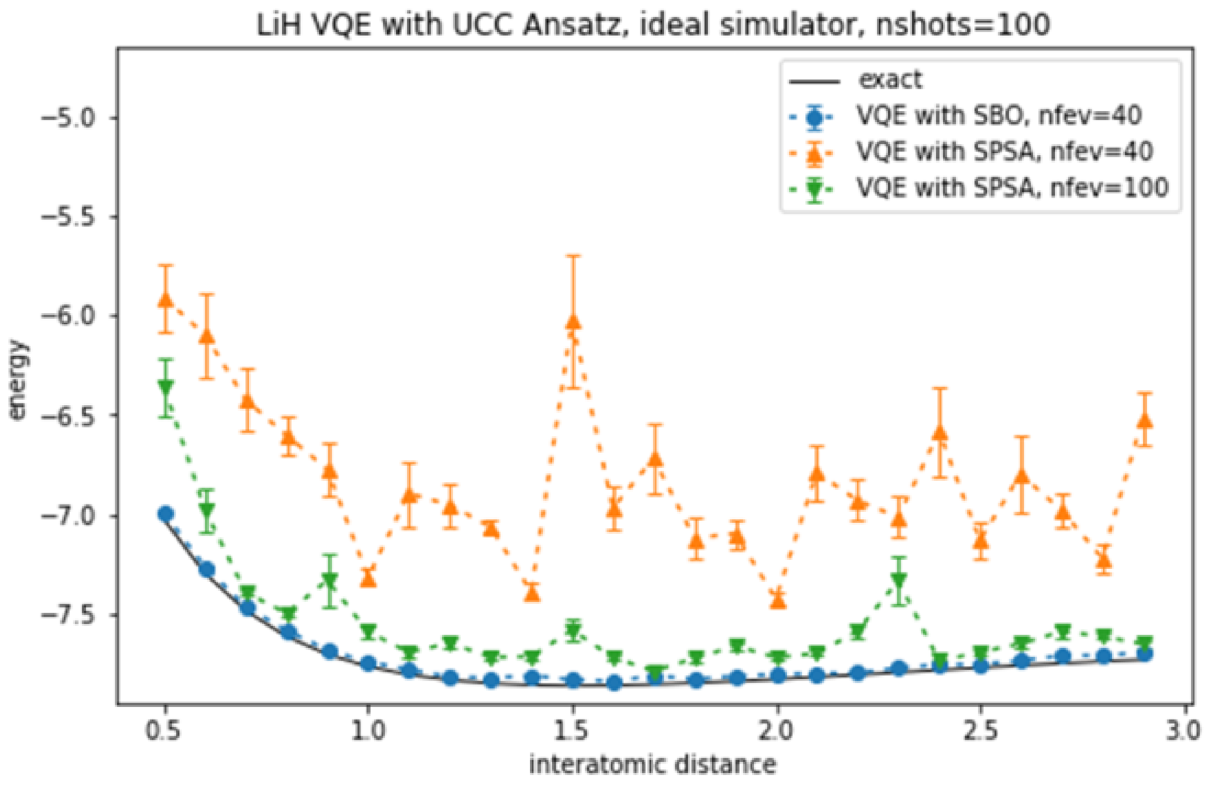




x-axis: total # of experimental shots
y-axis: relative error in min value found

Results: VQE for H_2 and LiH (ideal simulator)





Results: VQE for H_2 and LiH (with hardware noise)