Surrogate-based optimization for variational quantum algorithms

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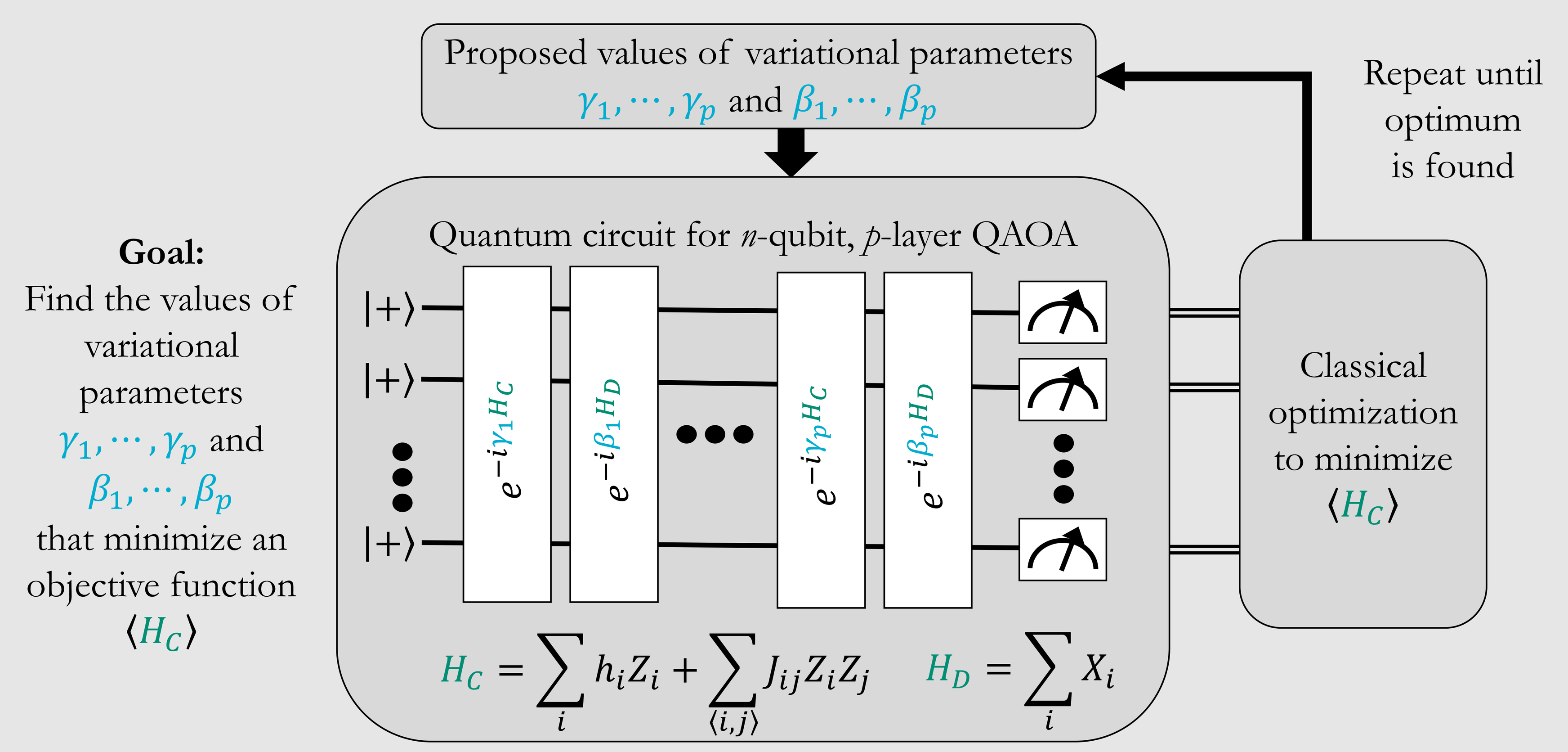
We propose a **surrogate-based optimization technique** for optimizing variational quantum algorithms with noisy samples.
We demonstrate an **improvement over SPSA** on common problems such as QAOA and VQE, using a Gaussian kernel approximation as the surrogate.
We observe **potential advantages over SPSA** in convergence and experimental runtime, particularly for higher-dimensional problems.

Variational quantum algorithms

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

Example: Quantum Approximate Optimization Algorithm (QAOA)



Surrogate-based optimization for VQA

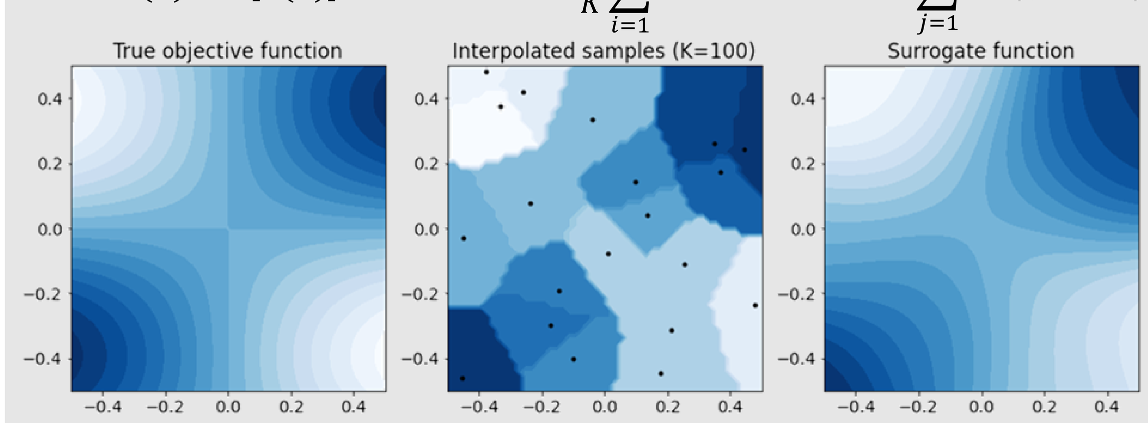
We propose a **surrogate-based optimization (SBO) technique** for optimizing variational quantum algorithms with noisy samples.

- SBO **constructs 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
- Repeat until convergence.

Example surrogate: Gaussian kernel approximation

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

$$V(\boldsymbol{\theta}) = \mathbb{E}[\mathbf{X}(\boldsymbol{\theta})] \qquad \tilde{V}(\boldsymbol{\theta}) = \frac{1}{K}\sum_{i=1}^{K} X_i(\boldsymbol{\theta}) \qquad W(\boldsymbol{\theta}) = \sum_{j=1}^{\tau} \tilde{V}(\boldsymbol{\theta}_j)\,\kappa(\boldsymbol{\theta},\boldsymbol{\theta}_j)$$



Gaussian kernel: $\kappa(\boldsymbol{\theta},\boldsymbol{\theta}_j) = e^{-\frac{\|\boldsymbol{\theta}-\boldsymbol{\theta}_j\|^2}{2\sigma}}$

$\boldsymbol{\theta}$ = coordinates of a sample point

$\mathbf{X}(\boldsymbol{\theta})$ = random variable representing measurement outcomes at coordinate $\boldsymbol{\theta}$

$X_i(\boldsymbol{\theta})$ = single measurement outcome at coordinate $\boldsymbol{\theta}$

K = number of shots taken at a sample point

τ = total number of sample points

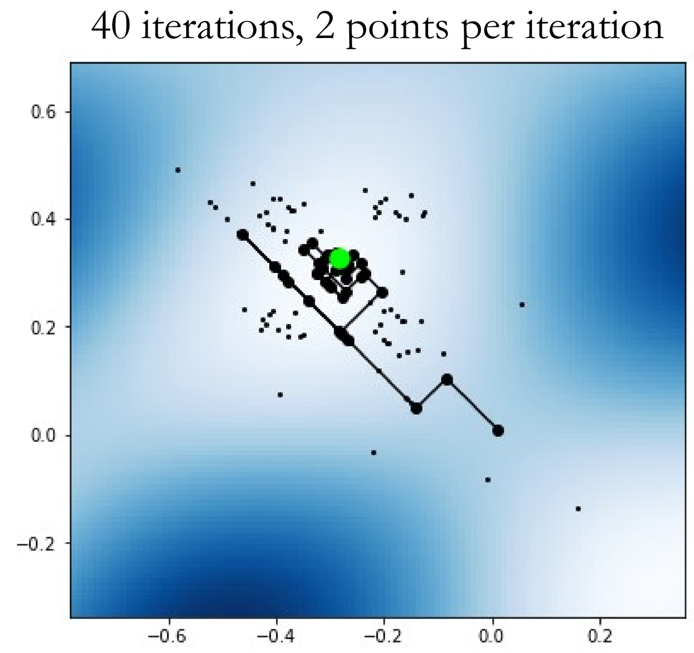
SPSA for VQA

SPSA (Simultaneous Perturbation Stochastic Approximation) is commonly used for optimizing VQAs with noisy samples.

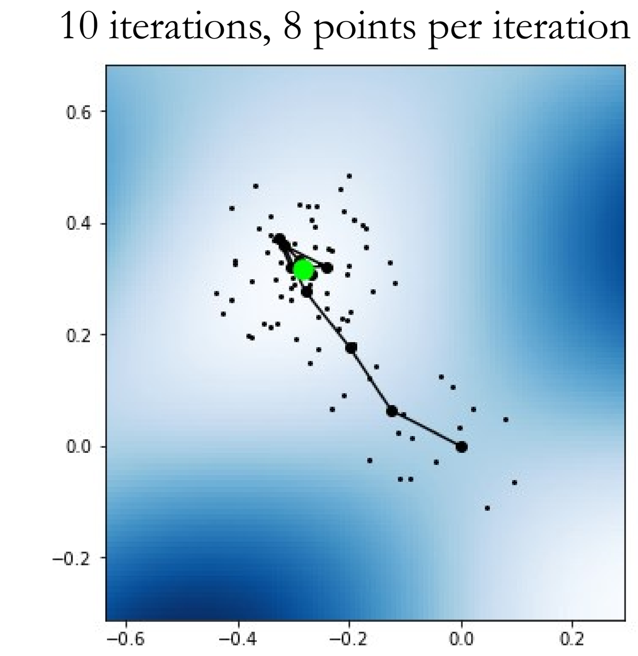
- SPSA attempts to **follow the gradient** in the objective function landscape:
  - Take two (noisy) samples near an initial point
  - Approximate the gradient based on these samples
  - Move in the direction of the gradient for the next iteration
- Repeat until convergence.

Example visualization of SPSA and SBO

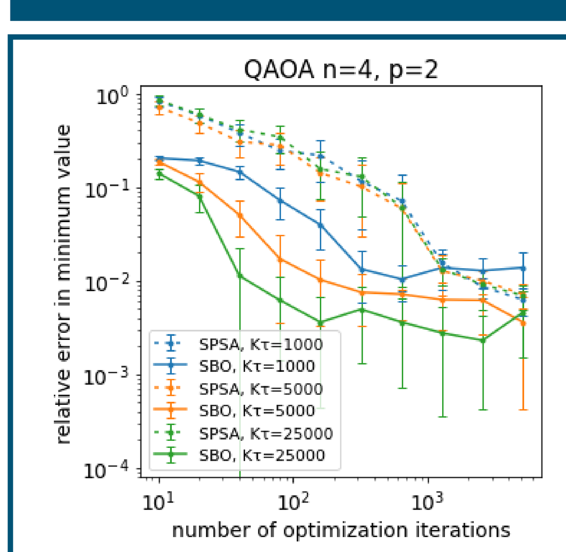
SPSA
40 iterations, 2 points per iteration

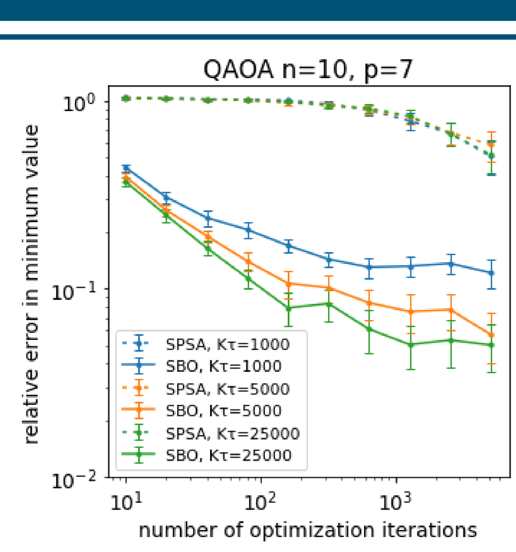


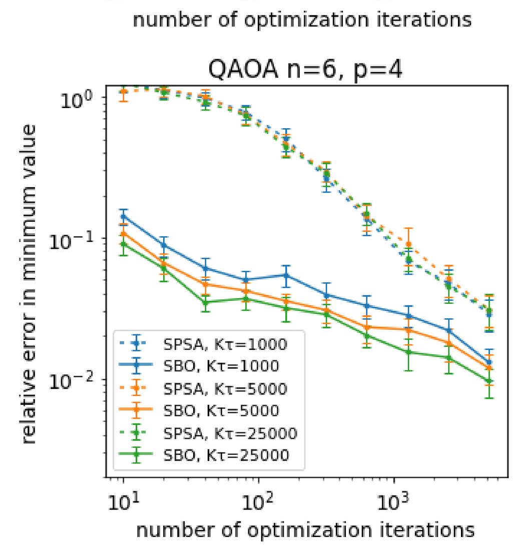
SBO with Gaussian kernel approximation
10 iterations, 8 points per iteration



Comparison of SPSA and SBO for typical QAOA and VQE problem instances



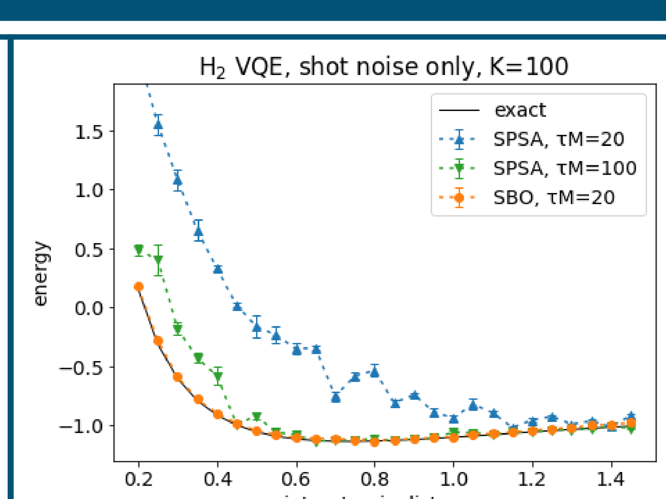


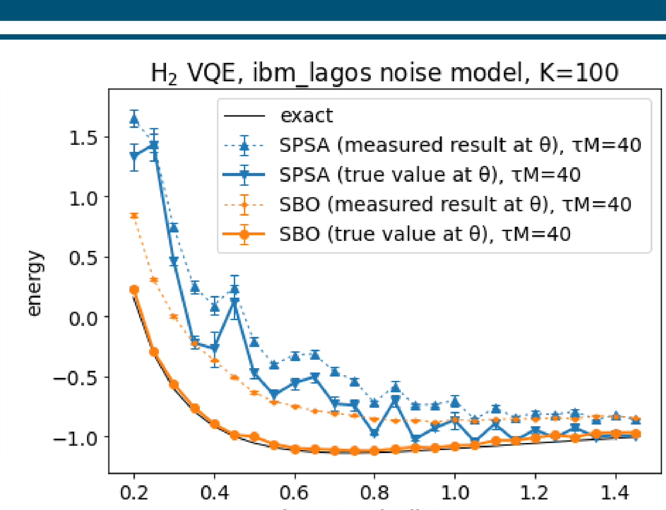


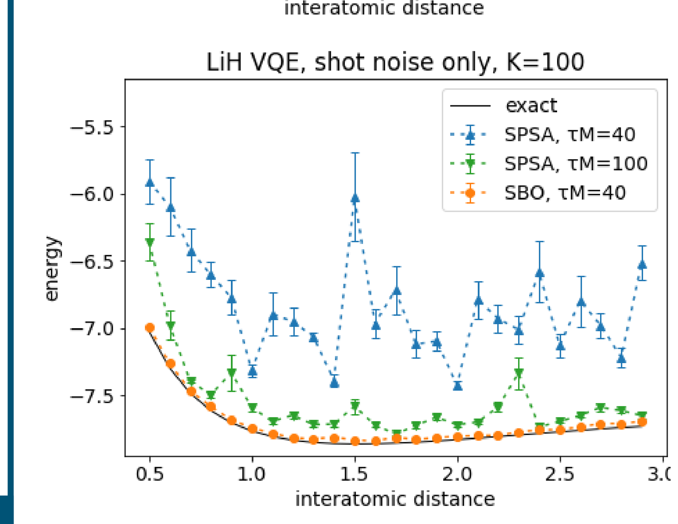
K = number of shots per sample point
τ = number of sample points per iteration
$K\tau$ **= total number of shots per iteration**

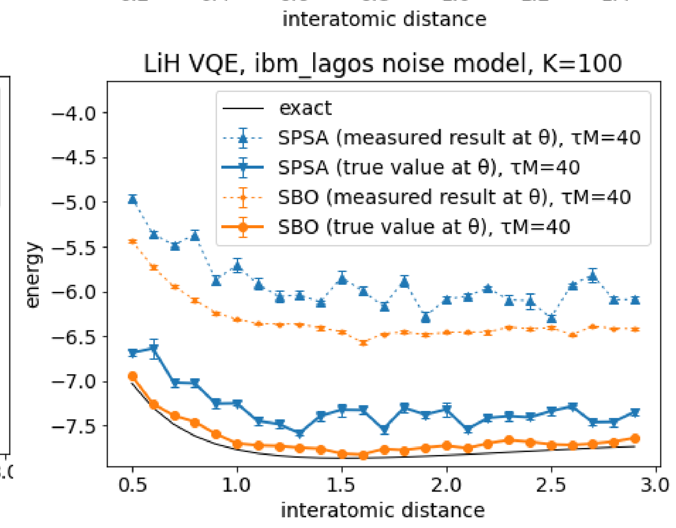
SBO provides an increasing advantage over SPSA as the QAOA problem size increases.

QAOA









K = number of shots per basis per sample point
τ = number of sample points per iteration
M = number of optimization iterations
τM **= total number of energy measurements**

Both with and without hardware noise, SBO produces a better estimate of the ground state energy of H_2 and LiH than SPSA.

VQE

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

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