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Statistical Learning Techniques for Variational Quantum Algorithms

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A key part of variational quantum algorithms is the **classical optimization loop**, which converges on an optimal solution by **updating the variational parameters** on each iteration.

If we can improve the efficiency of this classical optimization loop by making **better parameter estimates** for a given number of quantum circuit evaluations, we can hope to **improve the overall performance** of these near-term algorithms.

Background and Motivation

Variational quantum algorithms are a class of techniques intended to be used on near-term quantum computers. The goal of these algorithms is to perform large quantum computations by breaking the problem down into a large number of shallow quantum circuits, complemented by classical optimization and feedback between each circuit execution.

One path for improving the performance of these algorithms is to enhance the classical optimization technique. Given the relative ease and abundance of classical computing resources, there is ample opportunity to do so.

In this work, we aim to adapt recently-developed approaches to the problem of statistical learning for optimization under uncertainties in order to formulate improved statistical estimates of variational cost functions from noisy quantum circuit results.

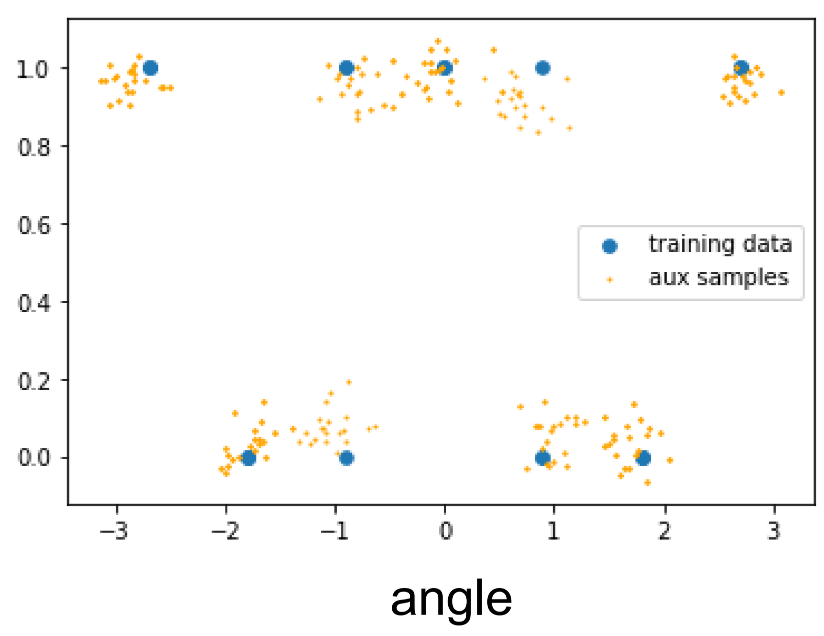
Statistical Learning via PLoM

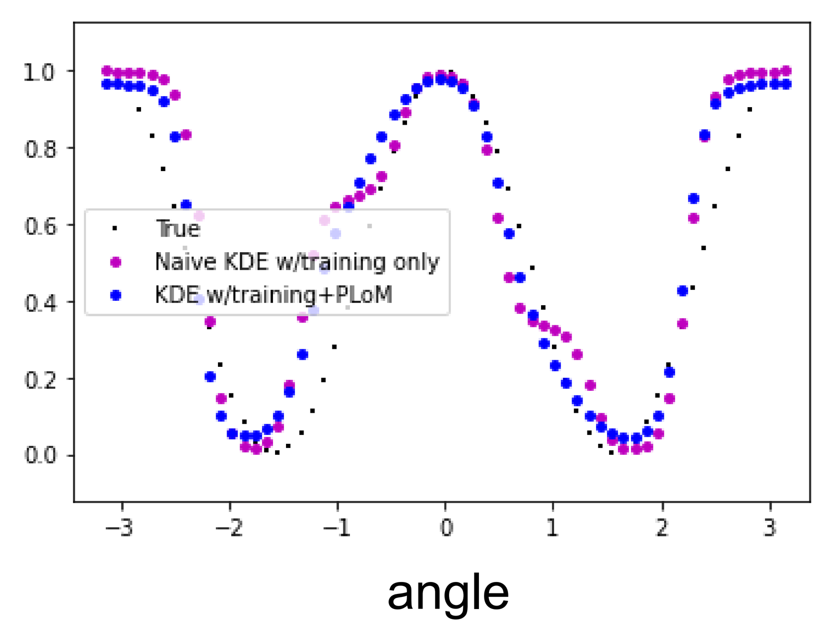
Probabilistic learning on manifolds (PLoM) is a technique for characterizing a process with uncertainty, particularly in the case where the process is "expensive" and we want to minimize the number of samples we need to take.
[Ghanem and Soize, Int. J. Numer. Meth. Engng. 113, 2018]

At a high level, PLoM involves the following steps:

1. Take several samples of the uncertain, expensive process. These samples serve as the **training data**.
2. Identify a diffusion manifold for the training data and **compute the associated basis**.
3. Construct an Ito stochastic differential equation and evolve the system, which will **generate additional samples** fluctuating around the diffusion manifold.
4. Combine the training data and the additional samples and use **kernel density estimation (KDE)** to reconstruct the full landscape of the original process.

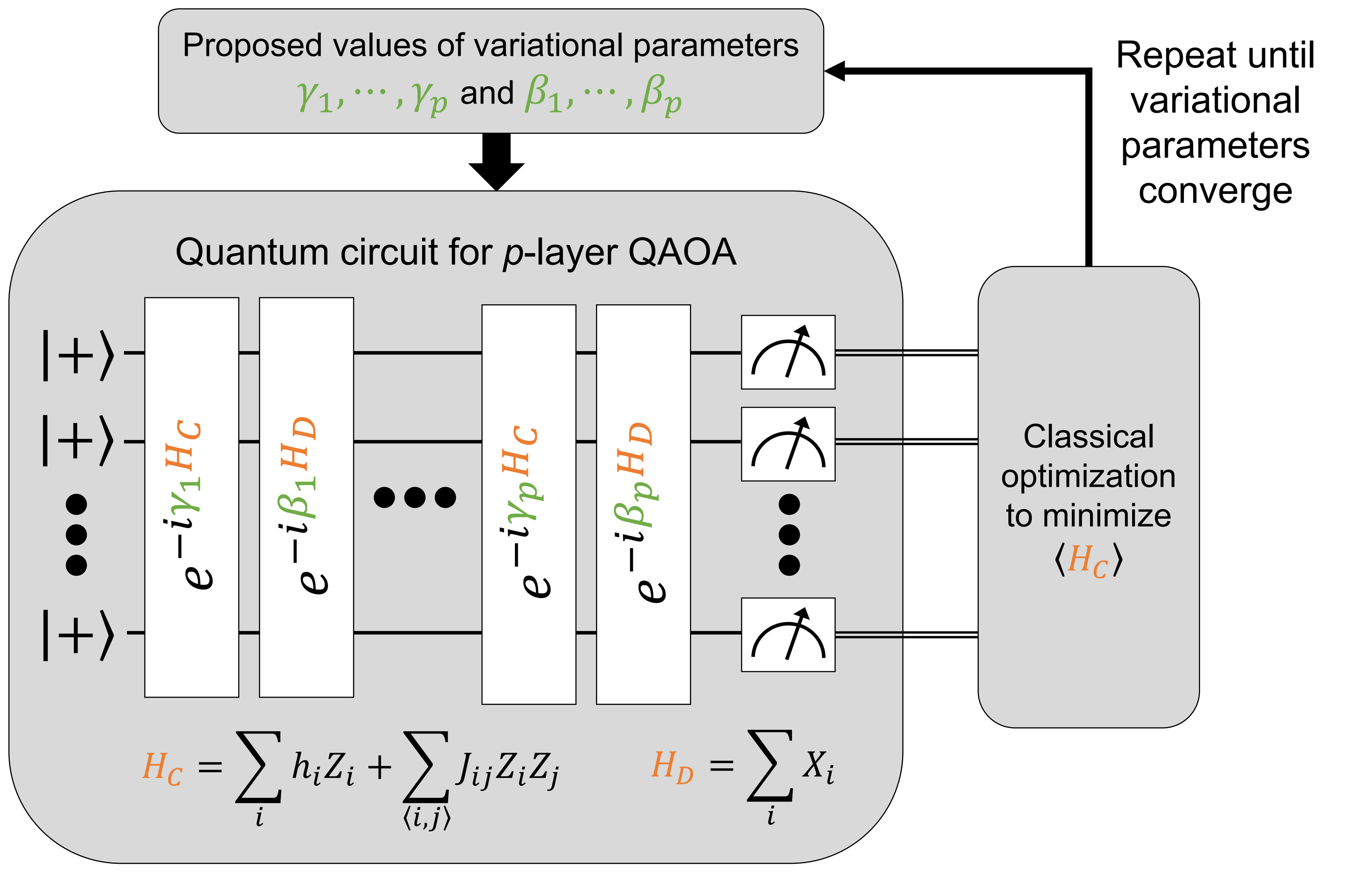
The idea is that the additional samples will cause the KDE reconstruction to be a **more faithful representation** of the original process than using the training data alone.





Variational Feedback Loop for QAOA

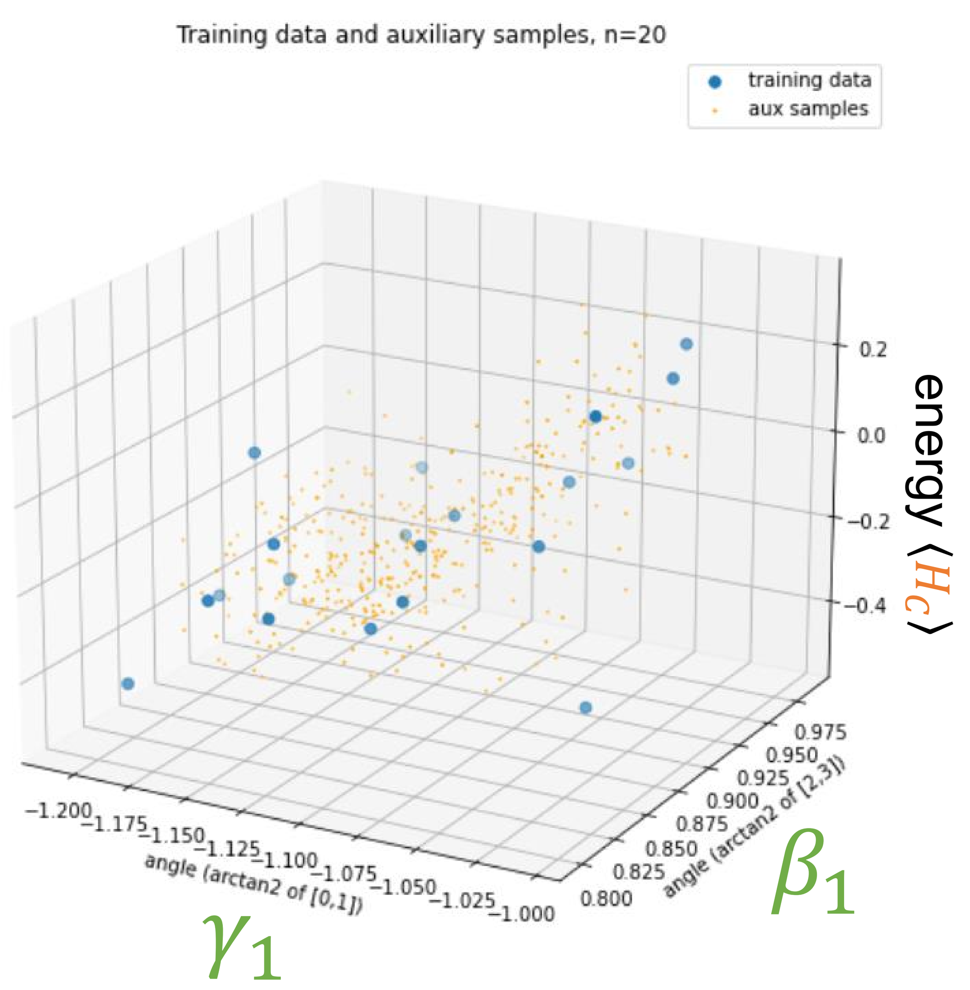
Quantum Approximate Optimization Algorithm (QAOA)

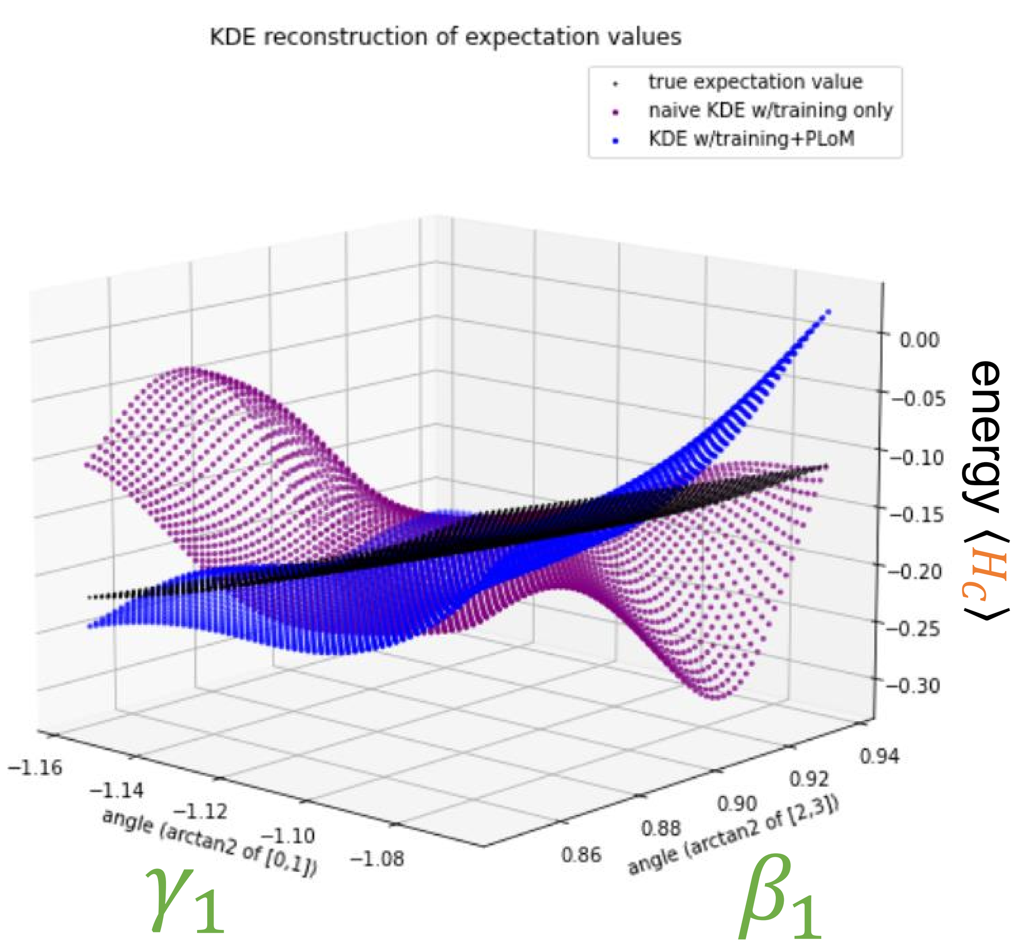


Applying PLoM to QAOA

Idea: a quantum computer is an "expensive" device which has inherent uncertainty in measurement results. This is a scenario where the PLoM technique should be able to provide a more faithful reconstruction of the many-dimensional landscape, which will then provide more accurate information to the classical optimization loop.

For example, if we are searching for the minimum energy value, a more accurate reconstruction may provide new parameter values for each iteration that cause the optimization loop to converge more quickly.





Ongoing Work

Investigate scaling of this approach for QAOA:
- with number of qubits
- with number of QAOA layers (p)

Show whether PLoM maintains an advantage with larger problem sizes.

Show whether a PLoM-based approach can improve overall performance of variational quantum algorithms on near-term devices.

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