Adaptive Quantum Natural Gradient Descent with Efficient Backtracking Line Search

QOSF Cohort 6

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Motivation

- **Definition: Gradient Descent (GD)**
  - Optimization method over parameter space based on stochastic exploration of local gradients. (fig 1)

- **Challenge:**
  - Near minimum, **step size may not fit the landscape** and will blow up after too many iterations. (fig 2)

- **Solution:**
  - Efficiently **adapt step size** as gradient nears zero **allowing for optimal fit** in least computation steps required.

- **Value:** Saves time and quantum resources during hybrid computation.

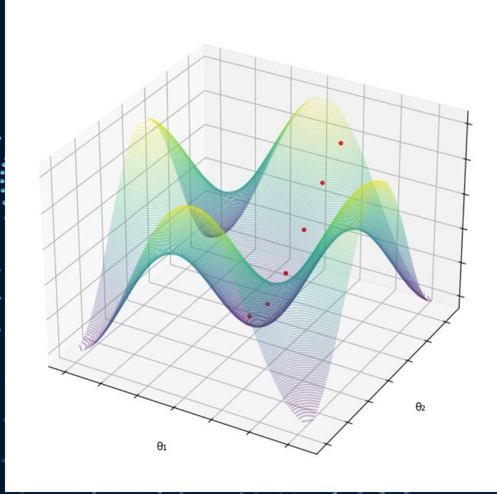
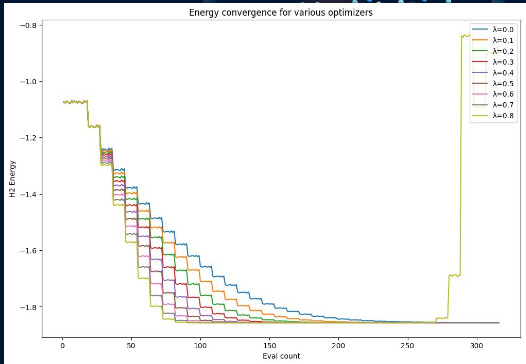
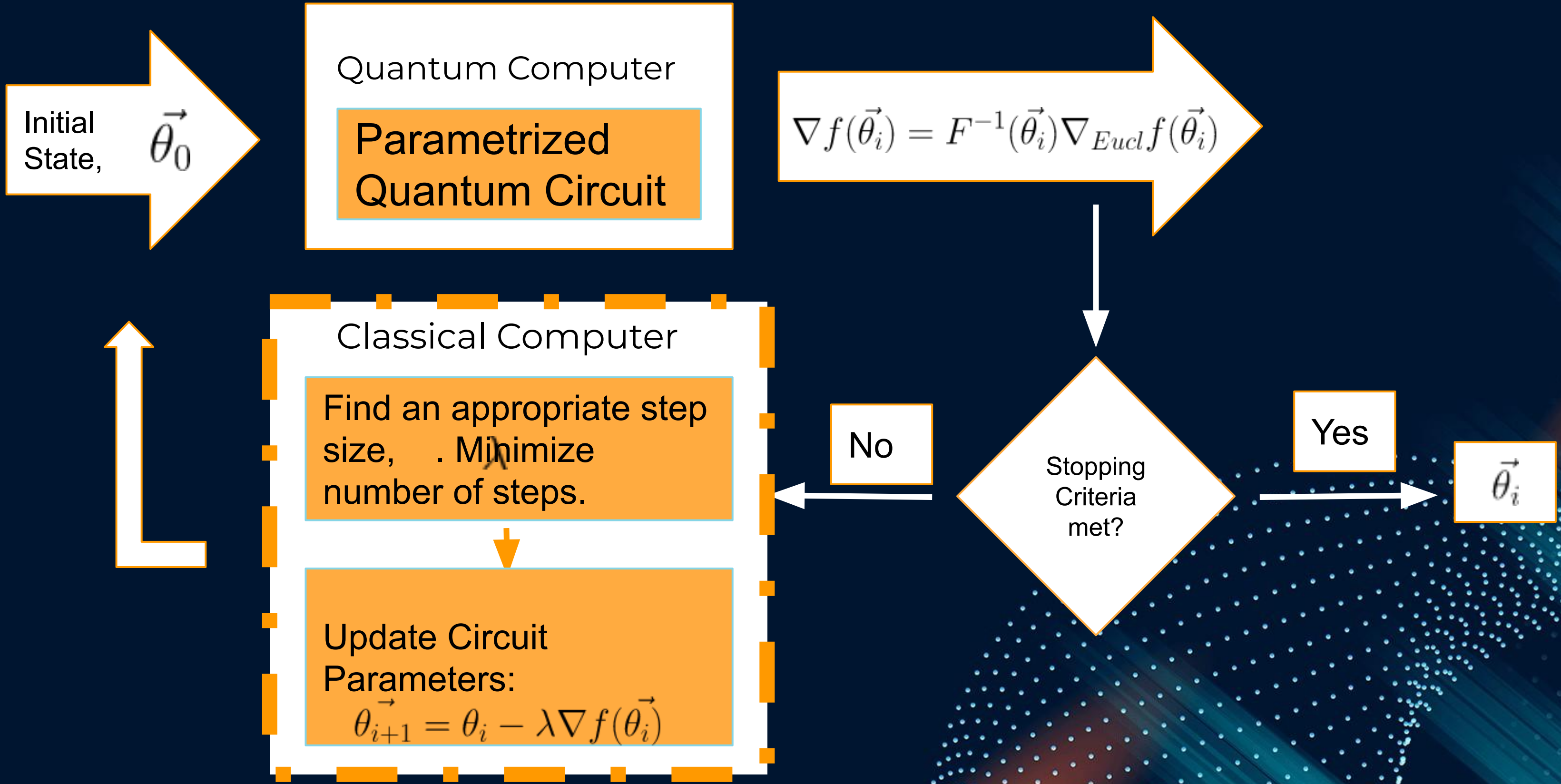


fig (1) - Gradient Descent Steps in 2D parameter space.

fig (2) - QNGD optimizers with varying sensitivity (λ), proportional to step size.



Quantum Natural Gradient Descent: Schematic



Quantum Natural Gradient Descent: State-of-the-art

- ❖ Def. **Quantum Natural Gradient Descent** is an optimization techniques that operates on the complex projective space and utilizes the Quantum Fisher Information or Fubini-Study metric.

Qiskit	Proposed: Adaptive Step Size
Implements regularization techniques (Ridge, Lasso) to find a suitable parameter(s) of quantum circuit.	Dynamically adjust step size. The technique choses a larger step whenever possible, and, as a result, convergence reaches faster.

Backtracking Line Search for Step Size Optimization

- ❖ Given current parameter θ and maximum allowed step-size β, find out k such that

$$k_i \overset{\nabla}{=} \min\left\{k \in [0, k_m] \middle| f(\boldsymbol{\theta}_i) - f(\boldsymbol{\theta}_i - \frac{\beta}{2^k}\nabla f(\boldsymbol{\theta}_i)) \geq \alpha \frac{\beta}{2^k}\|\nabla f(\boldsymbol{\theta}_i)\|_2^2)\right\}$$

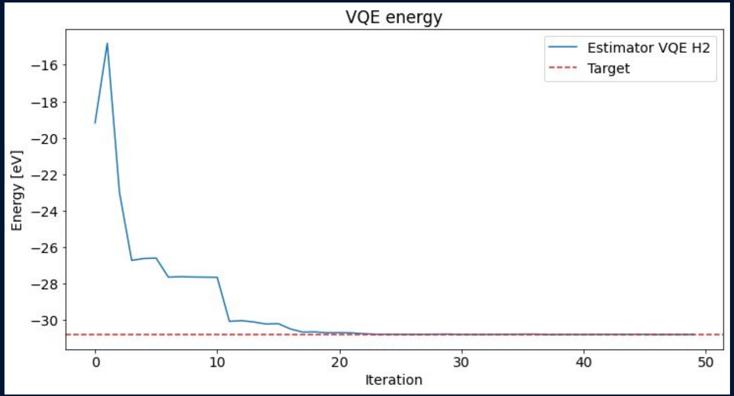
- ❖ Once k is found, adopt λ as the new step-size and update parameters as

$$\boldsymbol{\theta}_{i+1} = \boldsymbol{\theta}_i - \lambda_i \nabla f(\boldsymbol{\theta}_i), \quad \text{where} \quad \lambda_i = \beta / 2^{k_i}$$

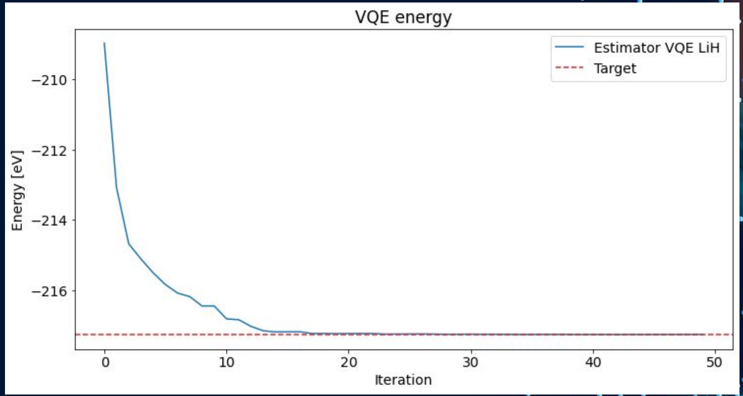
Project Accomplishments

- ❖ We reproduced demonstrated experiments to find the ground state energy of H_2, LiH, and TFI model using modified optimizers.

H_2 molecule



LiH molecule



- ❖ We identified potential implementation vehicles in Qiskit.
  - ➢ We found the **NaturalGradient (NG)** class to be a prime candidate.

Direction & Developments

- **Primary Goal:**
  - Introduce Adaptability to the NaturalGradient class with backtracking line search based on the Armijo condition.
  - **1. Validation:**
    - Comparative study of QNGD and AQNGD in noisy and noiseless environments.
  - **2. Implementation:**
    - We intend to offer a simple integer hyperparameter, **`adaptivity`**, to indicate with what frequency the steps are optimized.
    - I.e. if 1 is passed, this means each step is adapted.
- After writing tests and experiments, we will propose our project to IBM.

References

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Thank you