Error Mitigating Quantum Computations of Molecular Ground States

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Abstract

Quantum Computers have the potential to solve chemistry problems of great industrial importance but near term devices are susceptible to errors. Thus, error mitigation techniques like Richardson Extrapolation are being explored to reduce the effect of errors. **In this project, we compare the Richardson method with a simpler polynomial-fitting method to extrapolate the zero noise ground state energy of the hydrogen molecule.**

Background

- Quantum Computers use quantum mechanical properties such as superposition and entanglement to perform computations.
- Recently, a hybrid quantum-classical algorithm – Variational Quantum Eigensolver (VQE) – has been devised which optimizes electrons in molecular orbitals to minimize the energy of molecular systems.
- However quantum computers are plagued with errors due to hardware deficiencies like imperfect qubits and quantum gates.

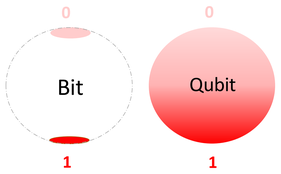

Fig 1: *Comparing the space of states of classical bits with that of qubits.*

- Constrained by the number of qubits, error mitigation techniques are being explored to reduce the effects of errors.

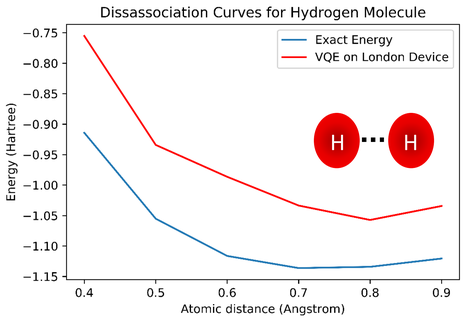

Fig 2: *As we stretch 2 hydrogen atoms apart, we compute the minimum energy of the molecule using VQE on IBM's noisy quantum computer at London and compare it with the exact energy .*

Error Mitigation Techniques

Richardson Extrapolation

- Noisy expectation value of any observable can be expressed as
  $$E(\lambda) = E^* + a_1\lambda + a_2\lambda^2 + a_3\lambda^3 + \ldots$$
  where λ is the noise rate and E^* is the noise free expectation value.
- By cancelling out terms from the expansion, we can better our approximation.

Polynomial Extrapolation

- Given energies at various noise scaling factors, we can fit polynomial function using nonlinear least squares as shown in Fig 4b.
- Evaluating these functions at zero noise, we can extrapolate noise free energy.

Results

Fig 4: *Using noise model simulation of IBM's quantum computer at London, we compare Richardson technique with polynomial fitting technique in improving the VQE-computed ground state energy of the Hydrogen molecule. Noise was amplified while optimizing in the VQE process.*

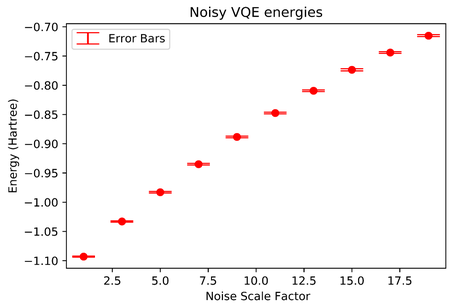

Fig 4a : *As noise gets worse, the energies get worse as well. Exact energy here is -1.13 Hartree.*

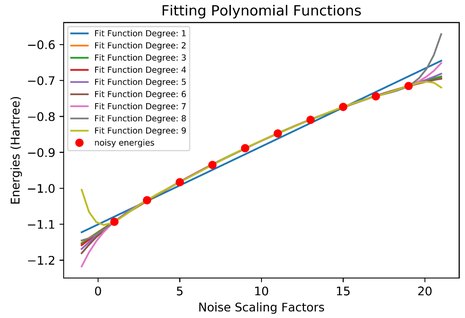

Fig 4b : *Using Least Squares to fit polynomial functions through the noise energies.*

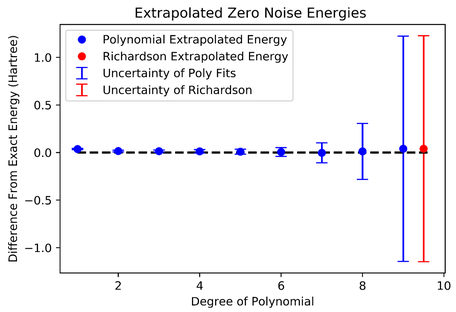

Fig 4c : *Uncertainty of zero noise energy extrapolated by Richardson is worse than that by lower degree polynomials.*

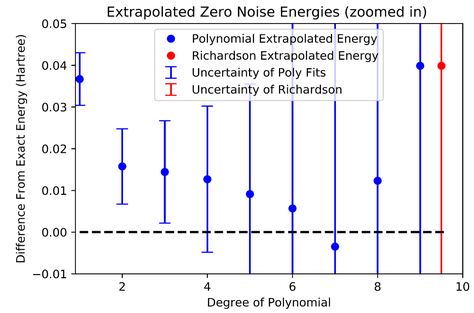

Fig 4d : *Zero energy extrapolated by Richardson is worse than that of lower degree polynomials.*

Fig 5: *Using IBM's quantum computer at London, we compare Richardson technique with polynomial fitting technique in improving the VQE-computed ground state energy of the Hydrogen molecule. Noise was amplified after optimizing parameters in VQE.*

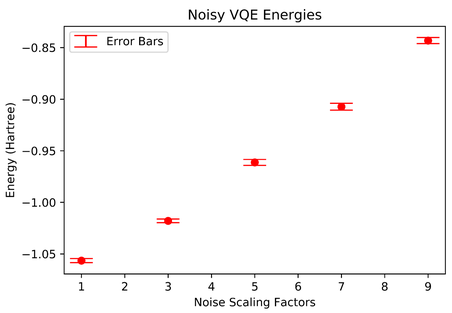

Fig 5b: *As we amplify noise in the optimized circuit, the energies diverge more and more from the exact energy (1.137 Hartree).*

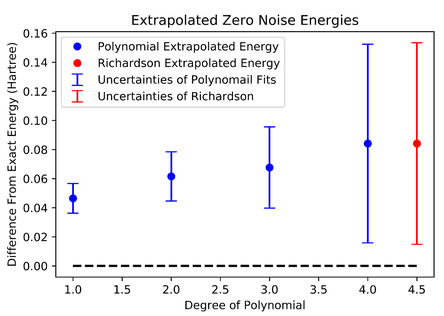

Fig 5c: *Zero Noise energy extrapolated by Richardson is both worse in precision and accuracy than that extrapolated by lower degree polynomial fits.*

Noise Amplification

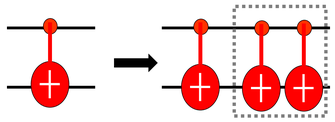

Fig 3: *Since the dominant source of noise on IBM's quantum computers are 2 qubit gates, we can add redundant CNOT gates to amplify noise.*

Methods

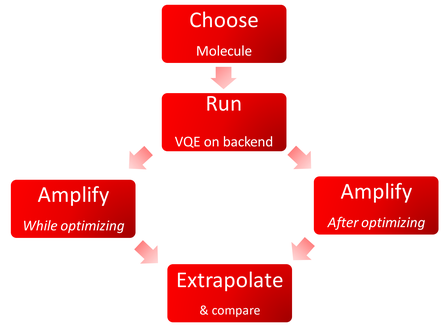

Fig 6 : *Procedure for comparing the two extrapolation techniques*

Conclusion & Future Work

- Zero noise extrapolated energy obtained via polynomial fitting is more precise than that obtained via Richardson technique.
- Since large noise scaling factors can induce unwanted errors on a real device, we hope to devise techniques to amplify noise by smaller noise factors (~1-4) through the "CNOT-ing" approach.
- Also, zero noise extrapolated energies we obtained are not within chemical accuracy.
- This calls for use of other error mitigation strategies such as probabilistic error cancellation and quantum subspace expansion to improve these results.

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