Quantum-Classical Hybrid Models for Efficient Many-Body Simulations

–Beyond Classical Methods

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1D Transverse Field Ising Model

- One of the most commonly used quantum magnetic system models for studying the ground state properties under **quantum phase transitions**.
- **Hamiltonian**

$$H = -J\sum_i Z_i Z_{i+1} - h\sum_i X_i \tag{1}$$

- **J** controls the coupling strength between spins, while **h** controls the transverse magnetic field strength. When **h/J** changes, the system undergoes a quantum phase transition, transitioning from ferromagnetic to paramagnetic behavior.

Quantum Machine Learning (QML)

- Applying quantum computing capabilities to machine learning tasks such as classification, regression, and optimization.
- Quantum processing models leverage **superposition, entanglement** to achieve more efficient data repressiontation, processing and algorithm acceleration.
- Based on **Variational Quantum Algorithms (VQA):** The computation is variational, with quantum components providing function values and the system iteratively optimizing.

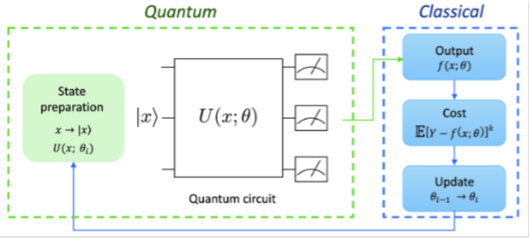

图: VQA

Quantum Neural Networks (QNN)

- A key branch of QML, using **Parameterized Quantum Circuits (PQC)** as neural network components for training and optimization.
- Unlike classical neural networks that require large datasets, QNNs are typically used to optimize quantum system properties, such as ground state energy, to derive the ground state.
- This project employs **Qiskit's EstimatorQNN**, which is equivalent to a QNN built on the VQE framework.

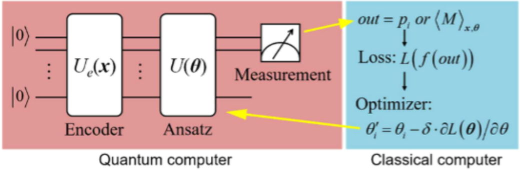

图: QNN

Objective: based on initial proposal obejectives

1. Understand Quantum Many-Body Systems: Study the Ising models and classical solution methods to establish a foundational understanding of the problem domain.
2. Learn QNNs, quantum kernel methods, and Qiskit to implement QML models.
3. Use classical solution like DMRG on 1D quantum many-body data.
4. Construct a QNN to solve for the ground state of the 1D Ising model, i.e., minimize H to obtain the ground state energy E0, and hopefully identify the corresponding ground state.
5. Output physical quantities: mz and mx , to describe the characteristics of the quantum phase transition.
6. Compare QML and classical solution results quantitatively to assess QML's feasibility for quantum many-body problems.
7. Present results and compile a final report summarizing insights and potential future directions.

Implementation

1. **Constructing the Hamiltonian**
   - Use Qiskit's SparsePauliOp to represent each Pauli term, which is concise and efficient.

$$H = -J \sum_i Z_i Z_{i+1} - h \sum_i X_i \tag{2}$$

2. **Constructing the Ansatz**
   - Initially, use **RY-CNOT-RZ** combinations.
   - Later, we will try deeper combinations (multi-layer rotation + entangling layer) and incorporate physically inspired initial states.
3. **QNN Construction Training**
   - Use **EstimatorQNN + TorchConnector** to interface with PyTorch.
   - Perform **VQE optimization:** Adjust the ansatz parameters to minimize H and obtain the ground state.
4. **Validation**
   - Use matrix eigenvalue methods to directly compute the ground state, H , mx , and mz .
   - Compare the parameters obtained by QNN with exact values.

Issues Improvements

Issues

- High accuracy for **E0**, but $< m_x > \approx 0.99$ regardless of changes in h.
- Fails to reflect the characteristics of the quantum phase transition.

Improvements

- Enhance the ansatz by using deeper combinations.
- Modify the initial state based on physical rules to make it easier to converge to the target state's extremum.
- Attempt to incorporate h as an input parameter into the QNN for multi-dimensional optimization.

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Exact Diagonalization Results for N=3
Ground state energy E0: -3.493959
<Z> per site: -0.000000
<X> per site: 0.842363
```

(a) Matrix

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Ground state energy E0 ≈ -3.493222
Magnetization <Z> ≈ 0.009203
Magnetization <X> ≈ 0.999599
```

(b) QNN

图: Program Output

Conclusion

- Successfully built a QNN-based quantum model.
- Energy results are accurate, but physical quantities do not reflect phase transitions, possibly due to convergence to incorrect extrema.
- Future directions: Improve the ansatz, set physically inspired initial states, and increase optimization dimensions.