Fast Quantum Algorithm for Protein Structure Prediction in Hydrophobic-Hydrophilic Model

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Summary

The authors present a quantum algorithm based on Grover's search algorithm, leveraging quantum parallelism and interference to achieve a quadratic speedup over classical methods. The algorithm is for the two-dimensional square lattice hydrophobic-hydrophilic (HP) model. The algorithm's space complexity is $O(N^3)$, while its time complexity $O(N^3\sqrt{2^N})$ achieves a quadratic speedup over classical counterparts.

The authors validate the algorithm using the IBM Quantum qasm simulator, considering amino acid sequences of up to length $N = 3$ due to qubit limitations.

Open Problems

1. **Scaling to Real Proteins:** The algorithm's performance is demonstrated on small sequences of amino acids ($N \leq 3$), and it remains to be seen how well it can be scaled to handle larger and more complex protein structures.

2. **Qubit Requirement:** The algorithm's qubit requirement grows with the length of the amino acid sequence. For instance, executing the algorithm for an amino acid sequence of length $N = 3$ requires around 243 qubits, which is beyond the capacity of current quantum devices.

3. **Circuit Depth and Transpilation:** As the algorithm's circuit depth increases with the sequence length, executing the algorithm on real quantum devices requires extensive transpilation, which could lead to cumulative error effects.

4. **Algorithm Validation:** While the paper validates the algorithm on a simulator, achieving experimental validation on real quantum hardware remains a challenge due to the limitations of current devices.