Quantum Speedup for Protein Structure Prediction

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Summary

The paper presents a novel quantum algorithm for Protein Structure Prediction (PSP) in three dimensions, specifically utilizing the hydrophobic-hydrophilic model on a body-centered cubic lattice. This quantum method achieves a quadratic speedup over classical techniques. The algorithm utilizes Grover's optimization for searching the most stable protein conformation. The algorithm's time complexity is $O(2^{n/2})$, and its space complexity is $O(n^2 \log n)$, making it optimal with respect to oracle-related quantum algorithms for NP-complete problems. The study includes experimental validations on IBM's quantum simulator, confirming the algorithm's high probability of finding the desired protein conformation.

Limitations

- **Computational Power**: The smallest instance of the PSP algorithm requires hundreds of logical qubits. This demand far exceeds what's currently available on any quantum device or simulator, making it impossible to test the algorithm in its complete form.
- **Quantum Speedup**: Although the proposed quantum method offers a quadratic advantage over classical methods, a square root improvement over 2^n still makes the problem computationally intractable. This quantum advantage only pushes back the computational limitations but only partially overcomes them.
- **Limited Sequence Length**: The algorithm's experimental validation is conducted on relatively short amino acid sequences (up to $n = 3$), which may not fully represent the complexity of real protein structures.
- **Real-world Application**: The algorithm hasn't been tested on real-world proteins.