Folding lattice proteins with quantum annealing

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Summary

Quantum annealing aims to find the ground state of a Hamiltonian for optimization, and this method is applied to the challenging problem of protein folding using lattice models. The HP model, representing proteins as linear chains of hydrophobic and polar beads on a lattice, is used as a testbed. The authors propose a novel binary encoding approach for lattice proteins inspired by D-Wave applications and a QUBO formulation.

This method outperforms classical simulated annealing, achieving a 100% success rate against exact results for HP chains with up to 30 beads. It also accurately recovers known lowest energies for N = 48 and N = 64 HP chains. The approach combines quantum and classical techniques and demonstrates the successful folding of an N = 14 HP chain using a D-Wave Advantage quantum annealer.

Open Problems

1. **Enhancing Pure Quantum Annealing Performance:** The pure quantum annealing (QA) approach shows less success with larger system sizes. We need to explore ways to improve the performance of pure QA for large protein structures.

2. **Optimizing Penalty Terms:** Penalty terms are needed to ensure the proper chain corresponds to the global energy minimum. We need further optimization of these penalty terms to achieve better results or to handle more complex protein structures.

3. **Noise and Error Mitigation:** Quantum annealers, including the D-Wave system, are susceptible to noise and errors. We need to investigate techniques for mitigating the effects of noise and errors on the quantum annealer's performance for protein folding.