QFold: Quantum Walks and Deep Learning to Solve Protein Folding

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We develop quantum computational tools to predict the 3D structure of proteins, one of the most important problems in current biochemical research. We explain how to combine recent deep learning advances with the well known technique of quantum walks applied to a Metropolis algorithm. The result, QFold, is a fully scalable hybrid quantum algorithm that, in contrast to previous quantum approaches, does not require a lattice model simplification and instead relies on the much more realistic assumption of parameterization in terms of torsion angles of the amino acids. We compare it with its classical analog for different annealing schedules and find a polynomial quantum advantage, and validate a proof-of-concept realization of the quantum Metropolis in IBMQ Casablanca quantum system.