QUANTUM MACHINE LEARNING FOR EFFICIENT DRUG DISCOVERY

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Abstract:

The nexus of quantum computing and machine learning—quantum machine learning—offers the potential for significant advancements in chemistry. This review specifically explores the potential of quantum neural networks on gate-based quantum computers within the context of drug discovery. We discuss the theoretical foundations of quantum machine learning, including data encoding, variational quantum circuits, and hybrid quantum-classical approaches. Applications to drug discovery are highlighted,including molecular property prediction and molecular generation. We provide a balanced perspective, emphasizing both the potential benefits and the challenges that must be addressed

KEY WORDS: Quantum Machine Learning, Quantum Neural Networks, Drug Discovery, Variational Quantum Circuits, Molecular Property Prediction