Quantum Computing for Life Science and Chemistry

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Quantum computing (QC) holds immense promise for revolutionizing life science and chemistry research by offering unprecedented computational power to solve complex problems. This abstract explores the intersection of quantum computing with life sciences and chemistry, delving into its transformative potential and current applications. An emphasis will be to cover various applications in quantum biology, including precision medicine and drug discovery, spatial modelling of tissues, protein folding, and genome assembly in which IBM Quantum has been playing a pivotal research role. Further, we will focus the energy structure problem of quantum chemistry and our proposed quantum simulation techniques for hardware friendly applications. Moreover, the we will discuss the challenges and opportunities in integrating quantum computing with existing computational methods and experimental techniques in life science and chemistry research. By fostering interdisciplinary collaboration we seek to explore new insights and solutions to some of the most pressing challenges in healthcare, pharmaceuticals, and chemistry applications.

QC in Health Care and Life Science

Research into quantum computing for healthcare is currently thriving. Engaging problems include protein folding, genome assembly (see Figure 2), and drug design and discovery. Moreover, it holds promise for medical image/signal analysis, cell classification, and omics dataset analysis. Quantum machine learning techniques are employed to analyze electronic health records, pinpointing and elucidating connections among interventions and outcomes, thereby advancing precision medicine. Recent studies on quantum graph neural network-based breast cancer detection (see Figure 1) indicate potential benefits in the foreseeable future [1].

QC in Chemistry

The current trend in quantum computational chemistry is effective experimentation to achieve high-precision quantum computational advantage. However, high computational gate complexity and fidelity loss are some of the impediments to the realization of this advantage in a real quantum hardware. We seek to address the challenges of building a Hamiltonian operator having exponential functional form, and its implementation in the context of the time evolution problem. Potential energy operators when represented in the first quantization form is an example of such types of operators. Through systematic decomposition and construction, we demonstrate the efficacy of the proposed polynomial encoding method in reducing gate complexity from $\mathcal{O}(2^n)$ to $\mathcal{O}\left(\sum_{i=1}^{r} {}^nC_r\right)$ (for some $r \ll n$). This offers a solution with lower complexity in comparison to the conventional Hadamard basis encoding approach [2].

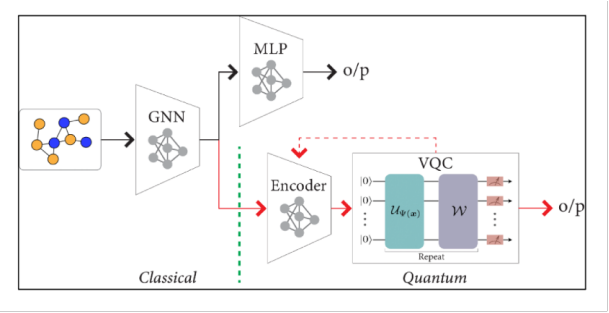

Figure 1: Hybrid quantum classical approach for tumor classification

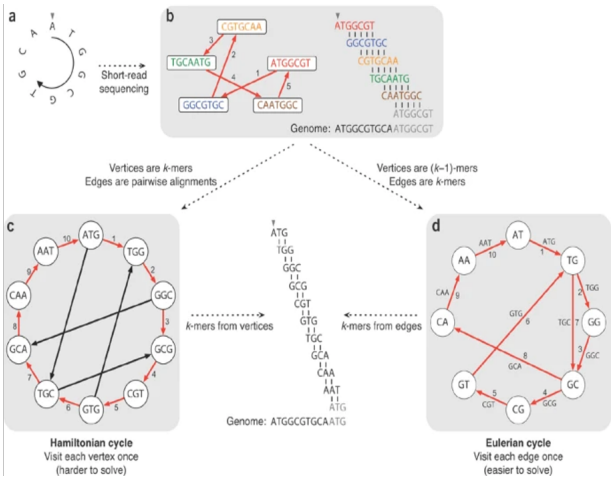

Figure 2: De-novo Genome assembly problem

References

[1] Ray, A., Madan, D., Patil, S., Rapsomaniki, M.A. and Pati, P., 2023. Hybrid quantum-classical graph neural networks for tumor classification in digital pathology. arXiv preprint arXiv:2310.11353.

[2] Laskar, M.R., Dasgupta, K. and Bhattacharya, A., 2023. A Proposed Quantum Hamiltonian Encoding Framework for Time Evolution Operator Design of Potential Energy Function. arXiv preprint arXiv:2308.06491.

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