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Automating quantum circuits design via large language models

Designing effective quantum circuits is a central challenge in quantum computing, covering a wide range of tasks including constructing feature maps for quantum machine learning, designing ansätze for variational algorithms, and tailoring circuits to specific problem instances. Over the years, a variety of quantum circuits have been proposed through manual design and exploration. However, due to their inherent theoretical complexity and the vastness of the design space, systematically exploring such circuits still requires substantial time and effort. In this work, we propose an agentic system that autonomously generates, evaluates, and refines quantum circuits using large language models. The system is composed of five components: Generation, Storage, Validation, Evaluation, and Review. Through iterative interaction of these components, the system continuously improves quantum circuit designs without human intervention. We demonstrate its capability on the automatic discovery of quantum feature maps for image classification tasks, where the best feature map generated outperforms existing quantum baselines and achieves competitive accuracy compared to classical kernels across MNIST, Fashion-MNIST, and CIFAR-10. Beyond feature maps, our framework naturally extends to variational quantum eigensolver, error mitigation strategies, and other algorithms, enabling LLM-driven automation in quantum algorithm design and highlighting a pathway toward problem adaptive quantum circuits. Such an automated design system not only supports experts but also lowers the barrier for researchers from other disciplines, facilitating broader participation in the quantum computing field.

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