Quantum Architecture Search with Neural Predictor Based on ZX-Diagram

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Quantum architecture search (QAS) [1] has attracted significant attention as a strategy to automate the design of parameterized quantum circuits in variational quantum algorithms (VQAs). Yet, it often requires evaluating a large number of candidate circuits, leading to high computational costs. Performance predictors help mitigate this issue by quickly estimating circuit "quality," thereby reducing the number of circuits that must undergo resource-intensive, high-fidelity optimizations. In the noisy intermediate-scale quantum (NISQ) era, VQAs are widely adopted thanks to their error resilience and flexible demands on quantum hardware, though their performance depends strongly on the structure of the underlying quantum circuits. QAS, which systematically explores circuit configurations, naturally complements VQAs by automating the search for high-performance circuit designs.

As illustrated in Fig. 1, First, we convert our quantum circuit search space into a ZX-Calculus-based representation, which serves as the key step in our overall process. We adopt a ZX-Diagram-based approach [2] to effectively capture circuit connectivity and simplify circuit structures. In this representation, Z spiders correspond to linear operators in the Pauli-Z basis, commonly used for phase operations or superpositions and measurements in the Z basis; X spiders correspond to linear operators in the Pauli-X basis, typically used for flip operations or superpositions and measurements in the X basis. Next, within this ZX-Calculus-based search space, we select a smaller subset $\{Z_1, \ldots, Z_m\}$ for full optimization and record their energy labels $\{y_1, \ldots, y_m\}$. These labeled circuits serve as training data for the performance predictor. The trained predictor is then applied to a large pool of new candidate circuits $\{Z_1, \ldots, Z_n\}$, flagging only the most promising ones for deeper evaluation. Ultimately, the best-performing circuit F^* emerges as the final solution.

To demonstrate the effectiveness of our ZX-Diagram-based predictive QAS, we evaluate it on the 6-qubit Transverse Field Ising Model (TFIM). Our method locates the target circuit in just 8 queries on average—surpassing PQAS-GM [3] (58 queries) and TF-QAS [4] (33 queries). This corresponds to an 86% reduction in query overhead compared to PQAS-GM and a 76% reduction compared to TF-QAS. By achieving high predictive accuracy with fewer training samples, our approach significantly accelerates circuit discovery in the NISQ era and lays a strong foundation for scaling up quantum algorithm design in the future.

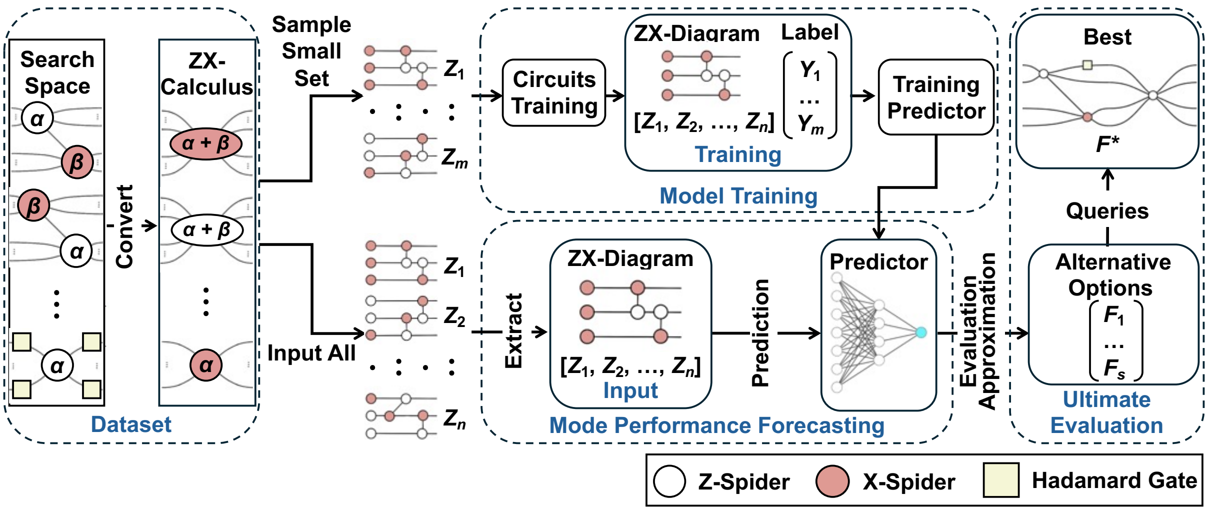

Fig. 1 The workflow of the predictor-based QAS.

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