QuantumDARTS: Differentiable Quantum Architecture Search for Variational Quantum Algorithms

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Problem Formulation

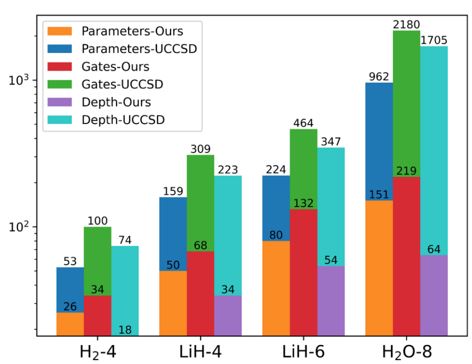
The problem of quantum architecture search (QAS) for variational quantum algorithms (VQA) in this paper can be formulated as follows. Given a candidate quantum gate set $\mathcal{G}$, we find the best composition in the form of PQC and its corresponding unitary $\hat{\mathrm{U}}(\mathcal{A},\theta)$, which minimizes the loss of the original VQA problem. Here $\mathcal{A}$ is the optimal circuit, θ is the best rotation parameters. $\mathbf{U}$ denotes the unitary transformation for the circuit and can be calculated by Eq. 1.

$$\hat{\mathrm{U}} = \prod_{j=1}^{m}\prod_{i=1}^{n}\hat{\mathrm{U}}_{ij} = \prod_{j=1}^{m}\prod_{i=1}^{n}\sigma(\mathbf{M}_{ij}) \tag{1}$$

Ground State Energy Estimation

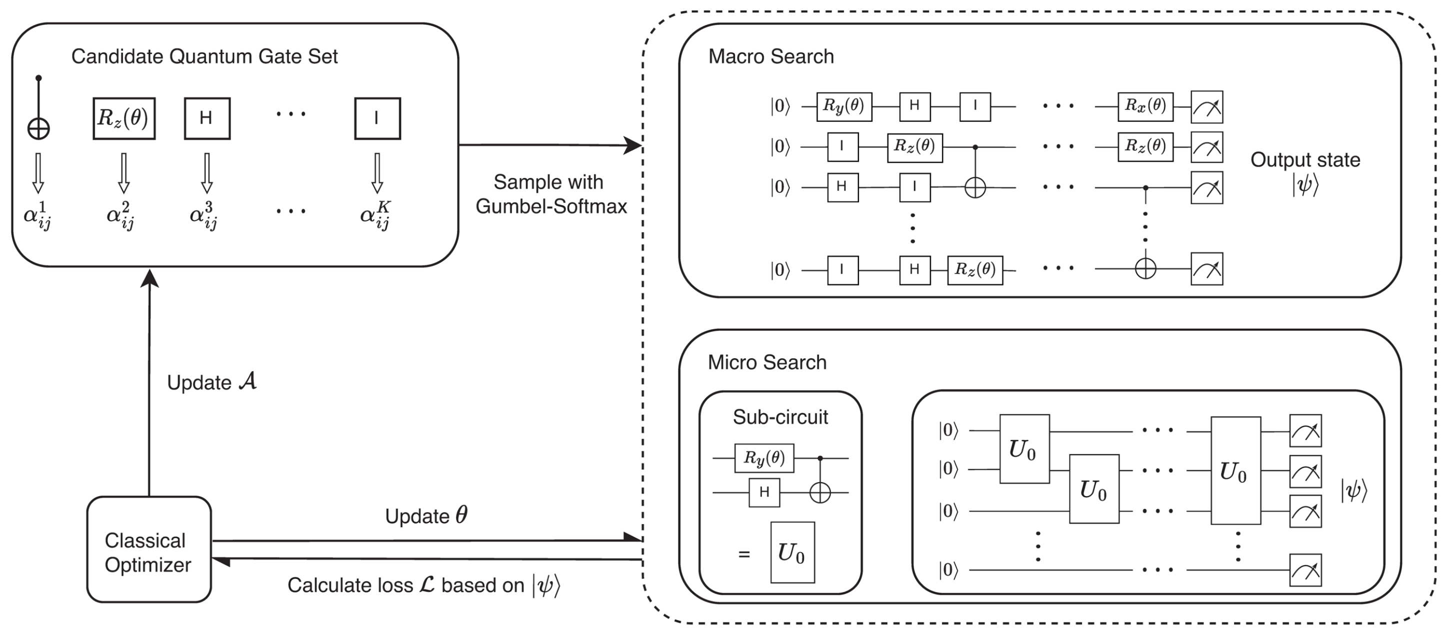
Model	H_2	LiH-4	LiH-6	H_2O-8
UCCSD	5.5×10^{-11}	4.0×10^{-5}	4.0×10^{-5}	4.0×10^{-6}
Ours	4.3×10^{-6}	1.7×10^{-4}	2.9×10^{-4}	3.1×10^{-4}
QCAS	2.2×10^{-2}	8.6×10^{-2}	7.3×10^{-2}	7.0×10^{-1}
DQAS	3.1×10^{-4}	5.3×10^{-4}	1.5×10^{-3}	5.2×10^{-1}
RS	1.9×10^{-2}	1.3×10^{-2}	6.2×10^{-3}	4.0×10^{-1}

Table 1: Comparison of energy errors in Hartree among different models.



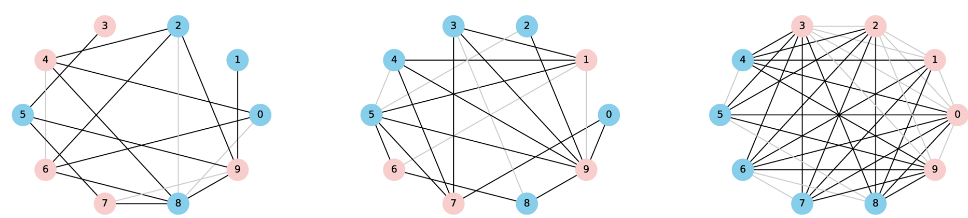
- All the energy errors are lower than chemical accuracy.
- Energy errors are two orders of magnitude lower than other QAS methods in average.
- Circuit depth is about one order of magnitude lower than that of UCCSD.

Methods



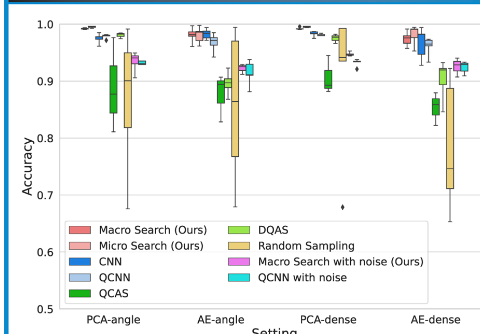
- Macro search: using the sampling results to construct the circuit directly.
- Micro search: sampling a sub-circuit and then constitute the circuit with sub-circuits according to some predefined rules.

Max-Cut



- Macro search can easily find the optimal solutions of 10-node Max-Cut problems with different density.
- Micro search can generate a sub-circuit similar to that in QAOA. Besides, it can find multiple optimal solutions simultaneously.

Image Classification on MNIST



Our macro model and micro model outperform QCNN, CNN and other QAS methods using comparable parameters.