



QuantumDARTS: Differentiable Quantum Architecture Search for Variational Quantum Algorithms

Wenjie Wu¹ Ge Yan¹ Xudong Lu¹ Kaisen Pan¹ Junchi Yan¹

¹MoE Key Lab of AI, Shanghai Jiao Tong University, Shanghai, China

Background



□ Variational Quantum Algorithms (VQA) use a classical optimizer to train a parameterized quantum circuit (PQC).



Background



□ Variational Quantum Algorithms (VQA) use a classical optimizer to train a parameterized quantum circuit (PQC).



□ Quantum Architecture Search (QAS)

- Search for variational quantum eigensolver (VQE) ---- without input data
- Search for quantum neural network (QNN) ---- with input data and ground truth

Background



□ Variational Quantum Algorithms (VQA) use a classical optimizer to train a parameterized quantum circuit (PQC).



Quantum Architecture Search (QAS)

- Search for variational quantum eigensolver (VQE) ---- without input data
- Search for quantum neural network (QNN) ---- with input data and ground truth

□ Challenges

- The operation of sampling quantum circuits is not differentiable.
- The search space is too large, and comprised of both discrete and continuous space.

Method





□ An end-to-end differentiable quantum architecture search framework prompted by the Gumbel-Softmax trick



Method

□ An example of micro search for the Max-Cut problem.





Method

□ An example of micro search for the Max-Cut problem.



□ An example of micro search for image classification.



□ Performance on Max-Cut (Macro Search and Micro Search)

• Macro Search results









(a) $P_e = 0.25$.

(b) $P_e = 0.50$.

(c) $P_e = 0.75$.

□ Performance on Max-Cut (Macro Search and Micro Search)

• Macro Search results









(a) $P_e = 0.25$.

(b) $P_e = 0.50$.

(c) $P_e = 0.75$.

• Micro Search results





■ Performance on ground state energy estimation (Macro Search)

Model	H_2	LiH-4	LiH-6	H_2O-8
UCCSD OURS QCAS DQAS RS	$\frac{5.5 \times 10^{-11}}{4.3 \times 10^{-6}}$ $\frac{4.3 \times 10^{-6}}{2.2 \times 10^{-2}}$ $\frac{3.1 \times 10^{-4}}{1.9 \times 10^{-2}}$	$\frac{4.0 \times 10^{-5}}{1.7 \times 10^{-4}}$ $\frac{3.6 \times 10^{-2}}{5.3 \times 10^{-4}}$ $\frac{5.3 \times 10^{-4}}{1.3 \times 10^{-2}}$	$\frac{4.0 \times 10^{-5}}{2.9 \times 10^{-4}}$ $\overline{7.3 \times 10^{-2}}$ $\frac{1.5 \times 10^{-3}}{6.2 \times 10^{-3}}$	$\frac{4.0 \times 10^{-6}}{3.1 \times 10^{-4}}$ $\overline{7.0 \times 10^{-1}}$ 5.2×10^{-1} 4.0×10^{-1}

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





□ Performance on image classification (Macro Search and Micro Search)

