Progress Summary

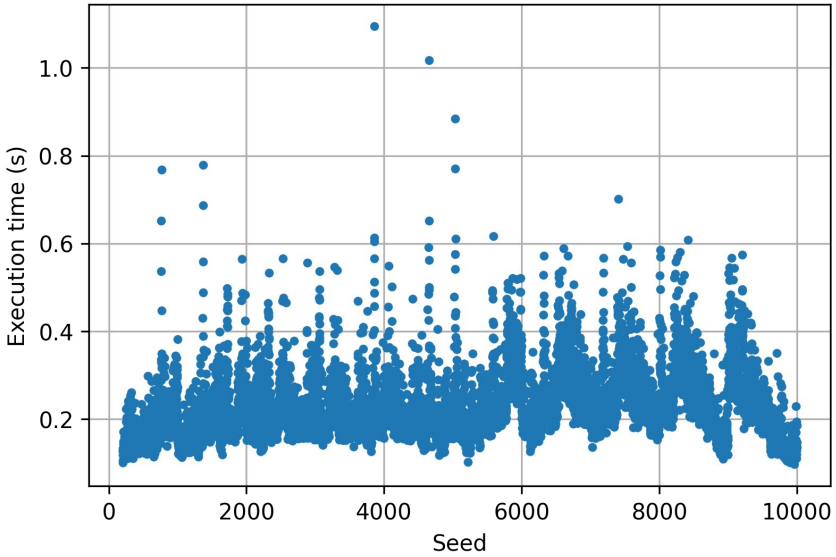
11-18-2022

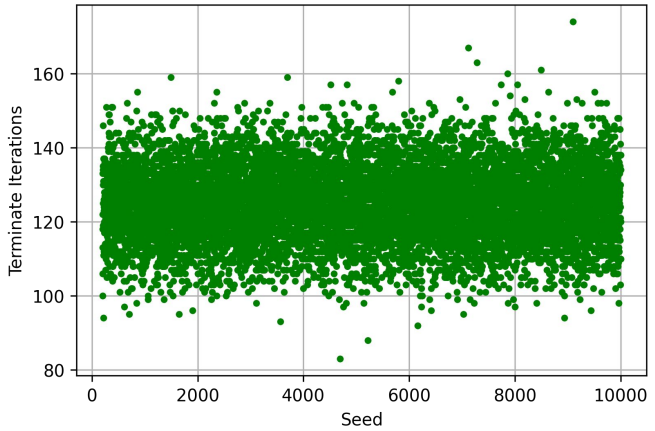
Outline

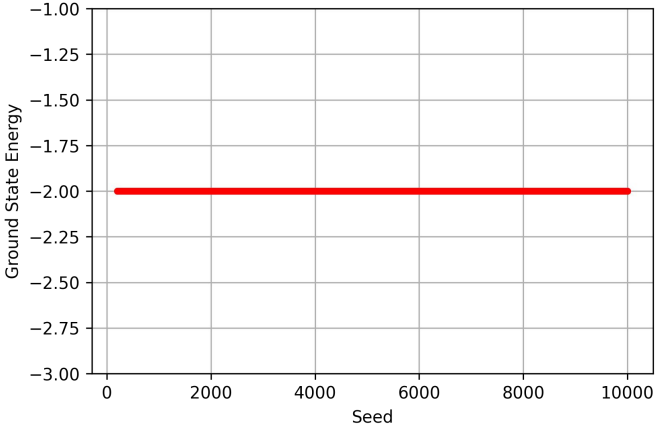
- Benchmarking Results
  - Different Seeds on different optimizers
  - Depth
- Increasing the depth does not solve the convergence problem
- The convergence paper: ansatz dependency
- Writing up a report

Benchmarking: 2x2

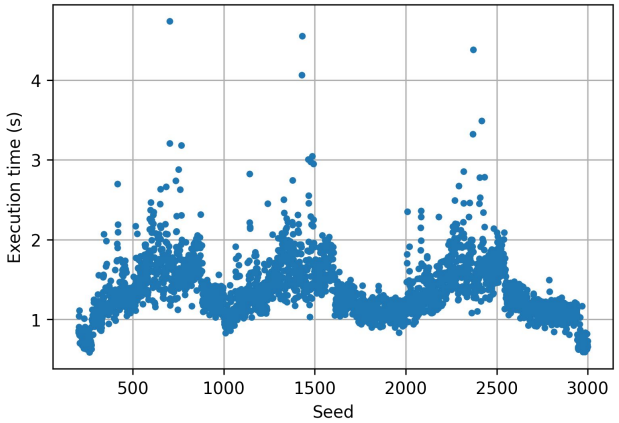
- COBYLA(maxiter = 400)
- All converged
- Apple M1



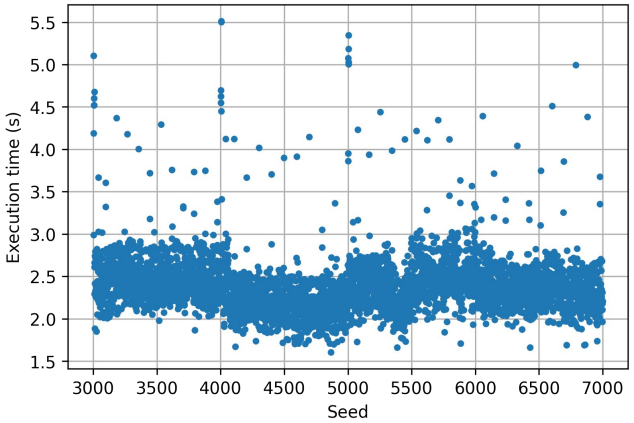




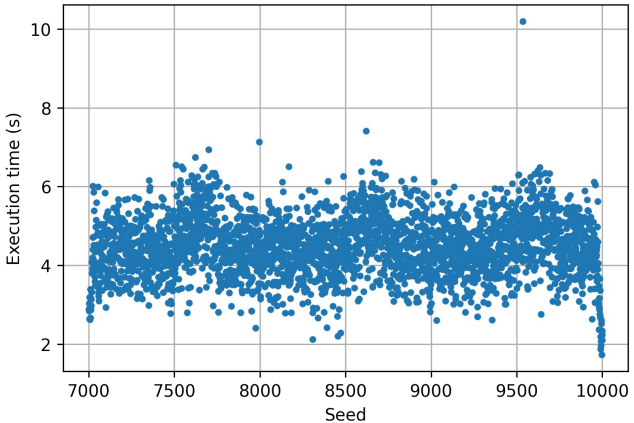
Benchmarking: 3x3
COBYLA(maxiter = 400)
Execution Time



Apple M1



Google Colab



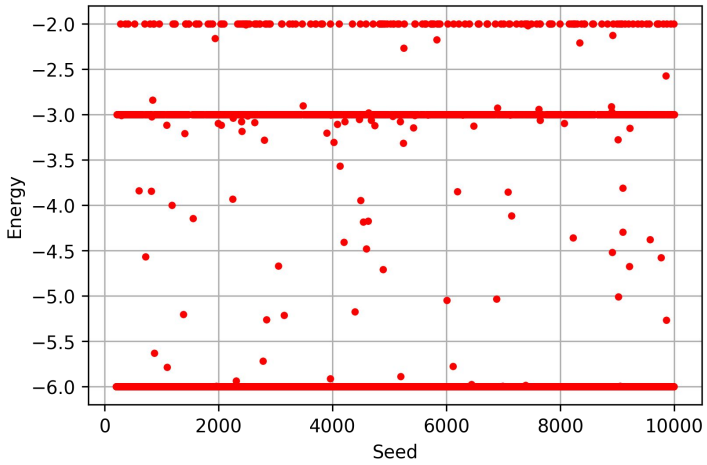
IBM Quantum Lab

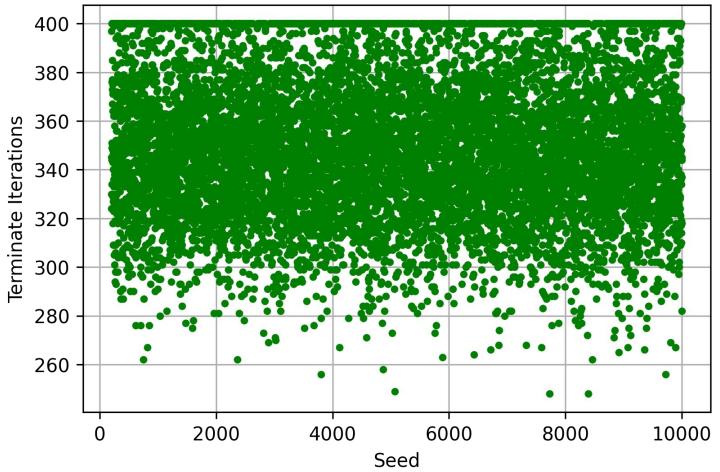
Periodic phenomenon: could the reason be the way of running the tests?

The tests are performed on 10 copies of the same code, each given 1000 seeds to test.

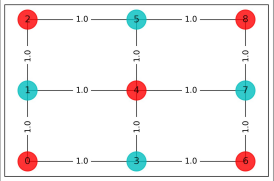
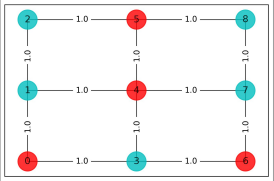
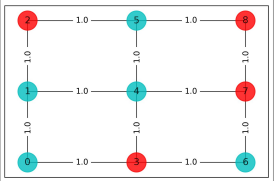
Compiler version? Interpreter version?

Benchmarking: 3x3
COBYLA(maxiter = 400)

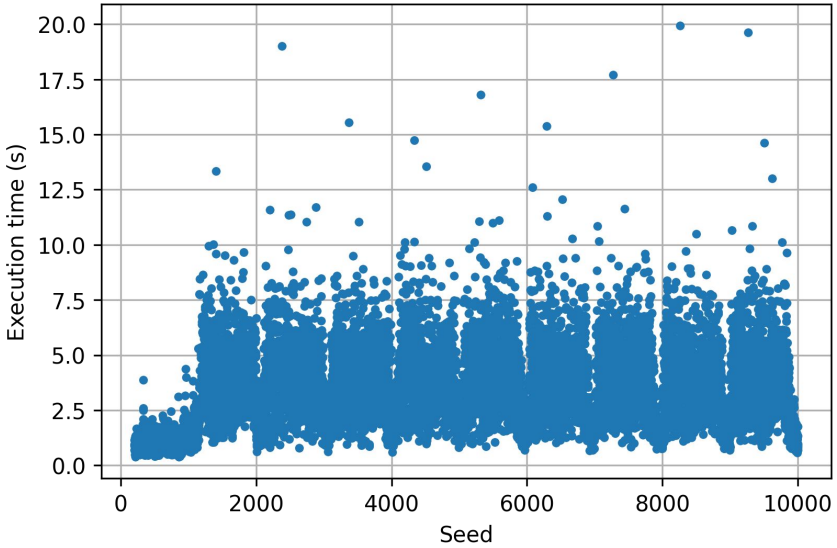


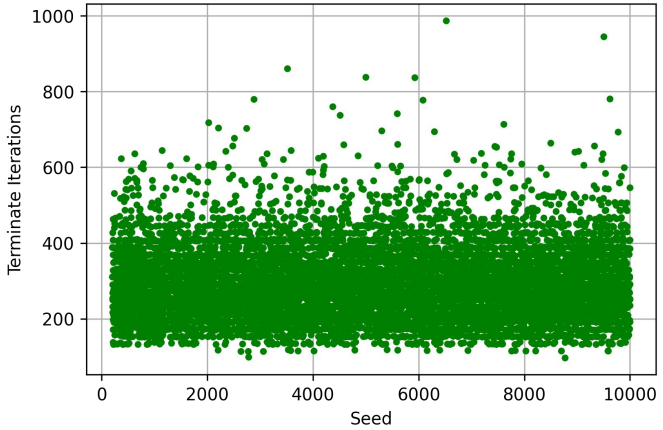


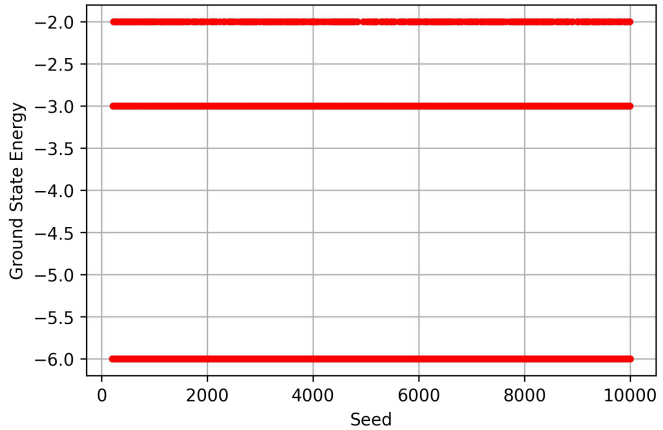
Typical Configs converged to

Seed	Optimizer	Terminate Iterations	Converged Energy	Time (s)	Solution	Visualization
201	COBYLA (maxiter = 2000)	324	-5.99999999512253	3.63391900062561	[0. 1. 0. 1. 0. 1. 0. 1. 0.]	
210	COBYLA (maxiter = 2000)	349	-2.99999999618755	3.40160894393921	[0. 1. 1. 1. 0. 0. 0. 1. 1.]	
277	COBYLA (maxiter = 2000)	418	-1.999999998	4.553569078	[1. 1. 0. 0. 1. 1. 1. 0. 0.]	

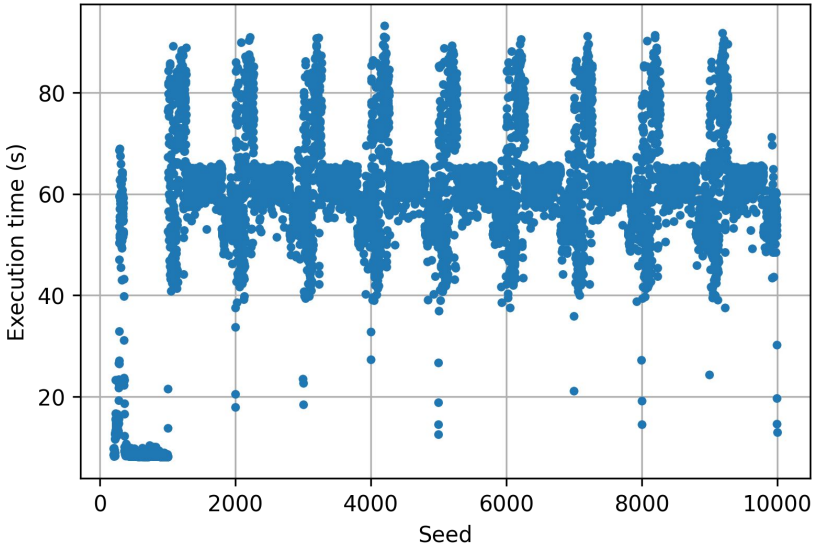
Benchmarking: 3x3 SLSQP(maxiter = 2000)

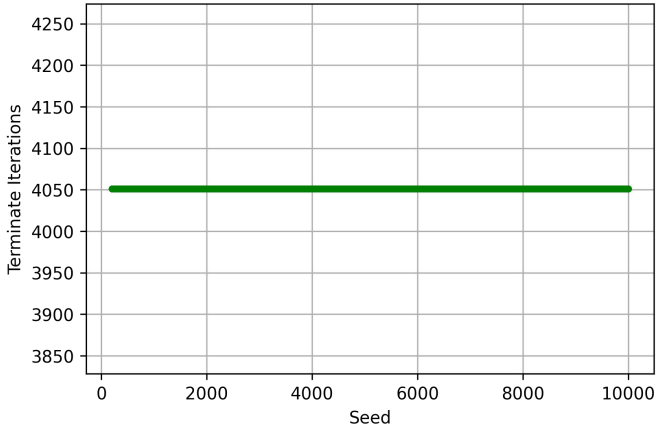


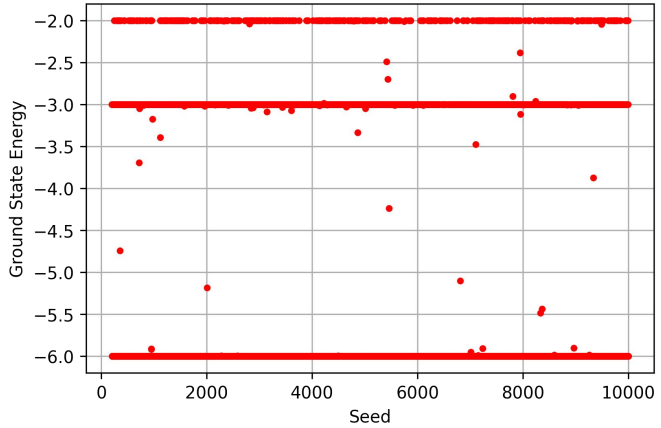




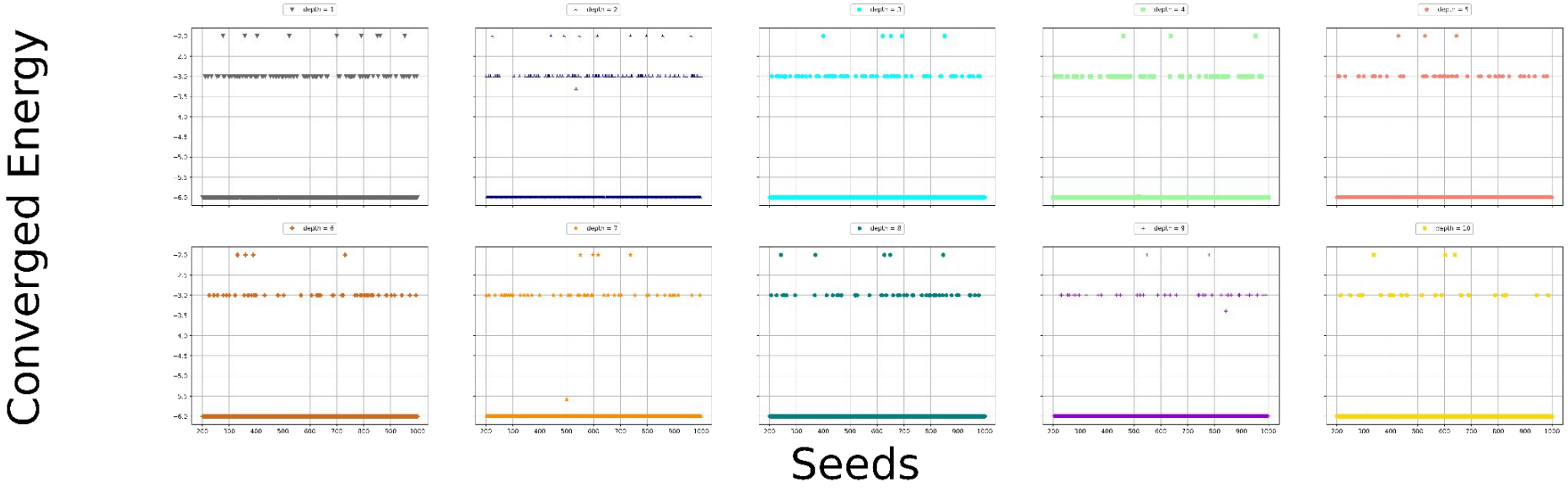
Benchmarking: 3x3 SPSA(maxiter = 2000)





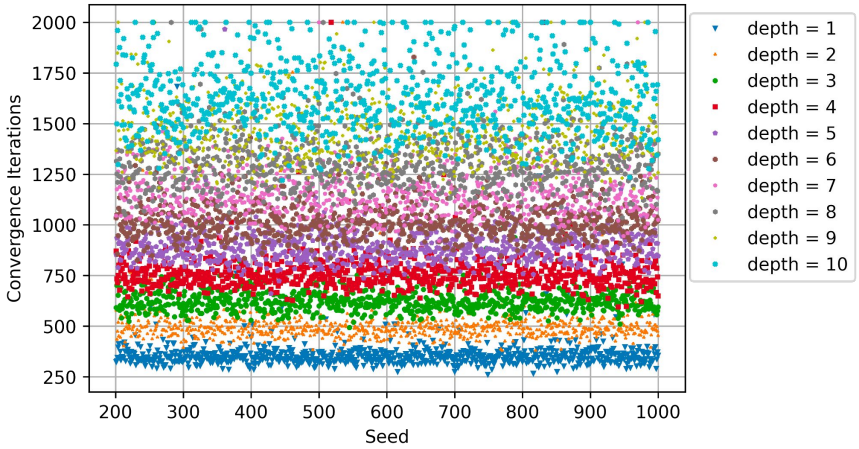


3x3 different ansatz depth

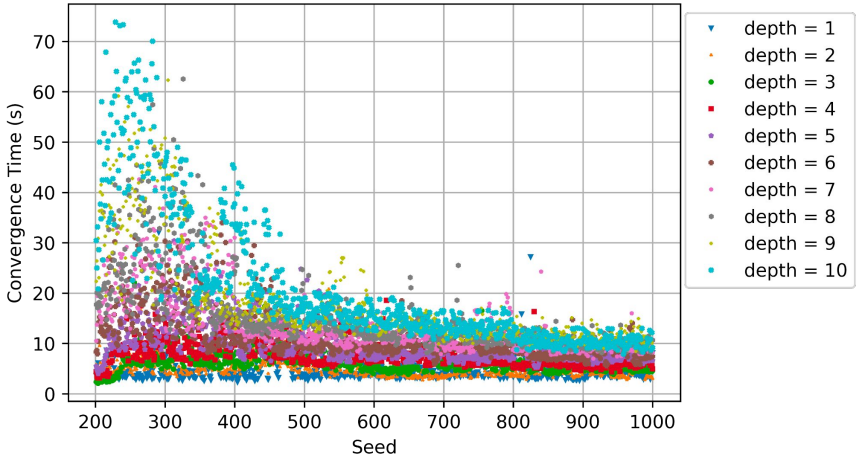


Greater circuit depths does not improve convergence

3x3 different ansatz depth
COBYLA(maxiter = 2000)



- Depth↑, iterations↑
- Depth↑, noise↑



- Depth↑, convergence time↓
  - Seeds 201 - 1000

VQE convergence

global minimum. The situation in practice may be even worse: practical VQEs are optimized using gradient-based algorithms, and in general there is no guarantee that such algorithms converge to a global minimum *at all*, the algorithm may get trapped in suboptimal local minima or saddle points.

[1]

First, the optimization could get stuck in a local minimum that would correspond to an excited state of the system. Using a suitable optimization routine can prevent finding such false minima. Gradient-descent methods may be combined with simulated annealing steps or strategies that involve starting from multiple initial points. In this context, in [38] a greedy search with multiple starting points is alternated with a Powell search, showing good performances on Hubbard lattices of up to twelve sites.

[2]

Results may also depend on the specific steps taken by VQE

Seed	Optimizer	state after 1st iteration	probability for the 1st state	terminate iterations	energy	circuit depth
201	COBYLA (maxiter = 2000)	011111101	0.421	577	-2.9999999834840 2	2
375	COBYLA (maxiter = 2000)	011111101	0.256	494	-5.999999994	2

Prob of Convergence (Seeds 201-10000)

	Energy		
Simulator	-6	-3	-2
COBYLA(maxiter = 400)	85.06%	13.39%	1.55%
SLSQP(maxiter = 2000)	74.77%	20.17%	5.06%
SPSA(maxiter = 2000)	80.08%	16.39%	3.53%

Conclusion

- 2x2 converges perfectly
- 3x3 typically converges to energies of -2 and -3 if not ground
- Results depends on seed, optimizer, and specific steps taken by the VQE
- Possible solution: use a random number generator (such as time of the day) to randomly select several different seeds and choose the lowest energy produced. COBYLA would be best suited for this.
- Report

References

1. X. You, S. Chakrabarti **and** X.Wu, *A convergence theory for over-parameterized variational quantum eigensolvers*. DOI:10 48550 /ARXIV.2205 12481. [Online]. Available:https //arxiv.org/a6s2205.12481.

2. N.Moll,P.Barkoutsos,L.S.Bishop et al., "Quantum optimization using variational algorithms on near-term quantum devices, "Quantum Science and Technology, **jourvol** 3, **number** 3, **page** 030 503,Jun.2018.DOI:10.1088 /2058-9565 /aab822.[Online].Available:https /doi.org/10.1088%2F2058-9565÷2Faa6822