Introduction to Quantum Computing

Lecture 3

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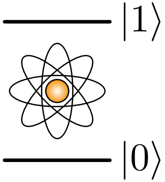
HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

Recap of the previous lecture

Qubits

- Quantum mechanical two-level systems $\mathcal{H} = \{|0\rangle, |1\rangle\}$
- Can be in superposition
- Mulitple qubits can be entangled



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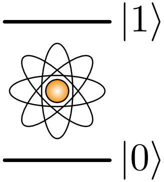
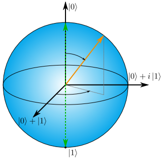


Quantum gates

- Quantum gates: unitary operations on a single/few qubits
- Combining quantum gates we can express any unitary operation



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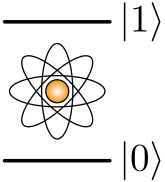

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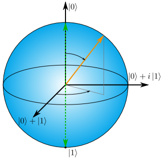
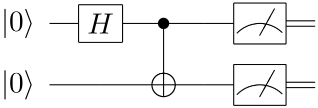


Quantum circuits

- Combining quantum gates we can express any unitary operation
- Measurement reveals information about the system



Outline

The Deutsch-Josza algorithm

Grover’s algorithm

Complexity theory

Hybrid quantum-classical algorithms

Challenges for hybrid quantum-classical algorithms

1.

The Deutsch-Josza algorithm

Grover's algorithm

Complexity theory

Hybrid quantum-classical algorithms

Challenges for hybrid quantum-classical algorithms

The Deutsch-Josza algorithm

Setting

- Given: a function $f : \mathbb{Z}_2^n \rightarrow \mathbb{Z}_2$ that is promised to be constant or balanced
- Task: find out if f is constant or balanced

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  - Classical computer: try more than half of the possible inputs
    $\Rightarrow \frac{1}{2} \times 2^n + 1 = 2^{n-1} + 1$ function calls

x_0	x_1	$f(x_0, x_1)$
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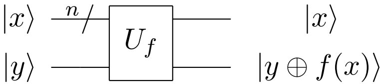
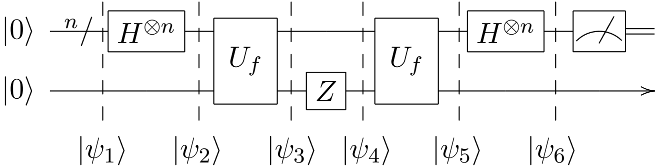
  - Classical computer: try more than half of the possible inputs
    $\Rightarrow \frac{1}{2} \times 2^n + 1 = 2^{n-1} + 1$ function calls
  - Let us assume we have a unitary $U_f \left|x\right\rangle \left|y\right\rangle = \left|x\right\rangle \left|y \oplus f(x)\right\rangle$



  - U_f is called an **oracle**

The Deutsch-Josza algorithm

Deutsch-Josza algorithm



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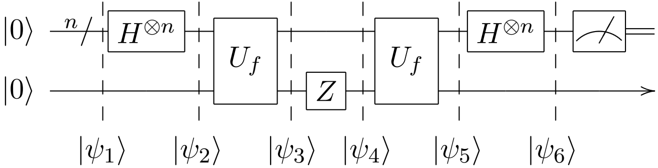
The Deutsch-Josza algorithm

Deutsch-Josza algorithm



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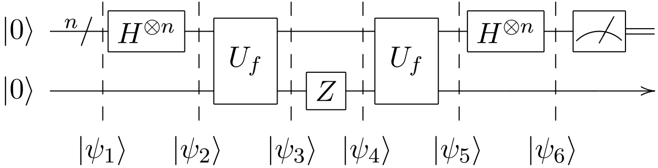

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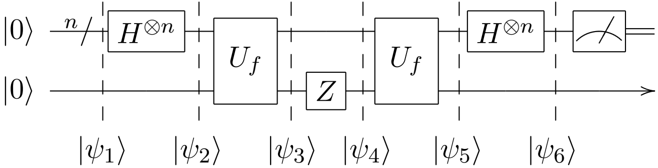

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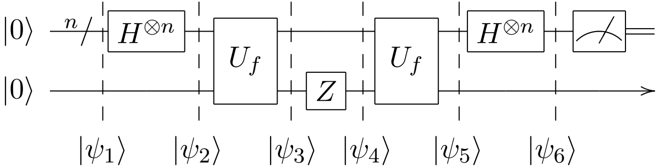

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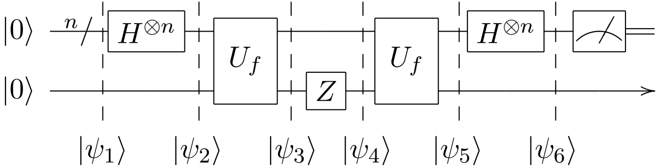

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$f(x)$ balanced

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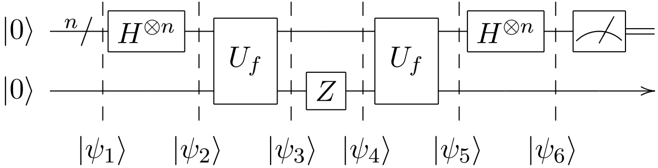

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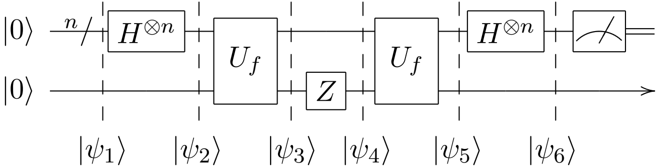

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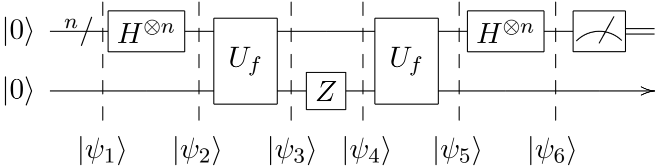

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7 $0 = \langle\phi|\psi_5\rangle = \langle\phi|H^{\otimes n}H^{\otimes n}|\psi_5\rangle = (\langle 0\ldots0|\langle 0|)|\psi_6\rangle$

The Deutsch-Josza algorithm

Deutsch-Josza algorithm

- Quantum algorithm allows for deciding whether f is balanced or not with **two calls to the oracle** (independent of n)
- Query the oracle in **superposition**
- Constructive **interference** (destructive interference) yields an unity (zero) amplitude in the constant (balanced) case

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The Deutsch-Josza algorithm needs exponentially fewer calls to the oracle than the classical algorithm.

The Deutsch-Josza algorithm

Deutsch-Josza algorithm on quantum hardware

- Example for $n = 2$ input bits and the following Boolean function

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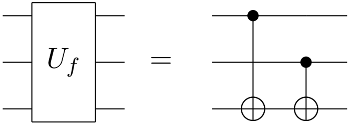

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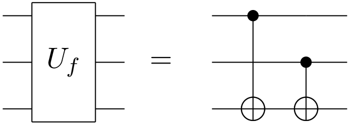
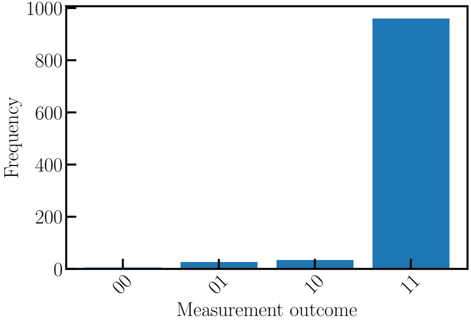


- Results on actual quantum hardware (`ibmq_lagos`)



2.

The Deutsch-Josza algorithm

Grover’s algorithm

Complexity theory

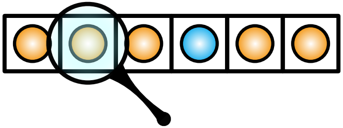
Hybrid quantum-classical algorithms

Challenges for hybrid quantum-classical algorithms

Setting

Description of the problem

> Goal: **find an element** in an **unstructured database**



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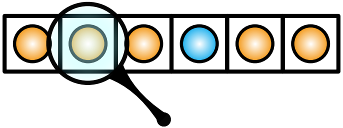

- Given:
  - A set of N elements $\{x_0, x_1, \ldots, x_{N-1}\}$
  - A function $f : \{x_0, x_1, \ldots, x_{N-1}\} \to \mathbb{Z}_2$
  - An element x_k is called iff **marked** $f(x_k) = 1$
- Task:
  - Find the marked element(s) in the data base

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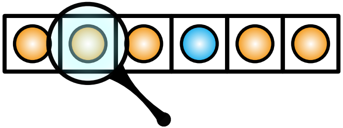

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- Task:
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- Best classical solution: go through the elements one by one or try elements randomly
  $\Rightarrow$ Access the database $\mathcal{O}(N)$ times

Setting

Comments

- If the database is sorted, the element can be found in $\mathcal{O}(\log N)$ time, however sorting the database takes $\mathcal{O}(N \log N)$
  $\Rightarrow$ Depending on the problem sorting might not pay off
- The problem essentially corresponds to function inversion: find the element that produces a certain output of the function
  $\Rightarrow$ Brute-force attack in symmetric cryptography
- Many problems can be cast into such a form, e.g. satisfiablity of a Boolean clause

Grover's search algorithm

Basic overview

- Quantum algorithm that allows for solving the problem described before with $\mathcal{O}(\sqrt{N})$ to an oracle implementing f
  $\Rightarrow$ **Polynomial speedup**

L.K. Grover, Proceedings of the twenty-eighth annual ACM symposium on Theory of Computing 212 – 219 (1996)

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- The different elements of the database are encoded in the different basis states

$$x_0 \equiv |x_0\rangle = |000\rangle \quad x_2 \equiv |x_2\rangle = |010\rangle \quad x_4 \equiv |x_4\rangle = |100\rangle \quad x_6 \equiv |x_6\rangle = |110\rangle$$
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- Starting from an equal-weight superposition of all basis states, one uses **amplitude amplification** to single out the marked element
  - Oracle
  - Diffusion operator

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- Starting from an equal-weight superposition of all basis states, one uses **amplitude amplification** to single out the marked element
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  - Diffusion operator
- Measure the final state to obtain a candidate for the marked element $|m\rangle$

L.K. Grover, Proceedings of the twenty-eighth annual ACM symposium on Theory of Computing 212 – 219 (1996)

Grover's search algorithm

The oracle

- We need to implement the function f on a quantum computer
- This is done in form of an **oracle**

$$U_f \left|x_i\right\rangle = (-1)^{f(x_i)} \left|x_i\right\rangle , \qquad U_f = \mathbb{1} - 2\left|m\right\rangle\left\langle m\right|$$

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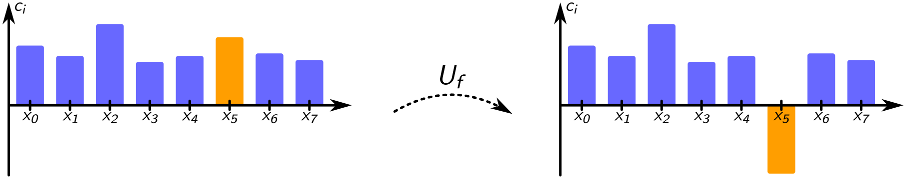
- Effect of the oracle on a wave function $|\psi\rangle = \sum_i c_i\,|x_i\rangle$



- While U_f has an effect on $|\psi\rangle$ this effect cannot be measured, as a measurement only reveals information about $|c_i|^2$

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Grover's search algorithm

The oracle

- To understand the effect of U_f further it is advantageous to separate the wave function $|\psi\rangle$ in a component parallel to $|m\rangle$ and one orthogonal to it

$$|\psi\rangle = c_i |m\rangle + \underbrace{\sum_{i \neq m} c_i |x_i\rangle}_{|t\rangle}$$

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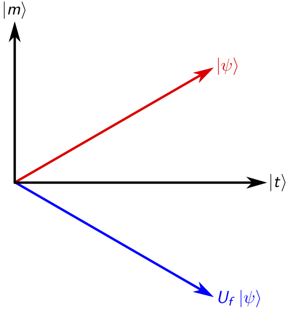

- U_f reflects $|\psi\rangle$ around $|t\rangle$

L. K. Grover, Proceedings of the twenty-eighth annual ACM symposium on Theory of Computing 212 – 219 (1996)

Grover's search algorithm

The diffusion operator

- Let $|u\rangle = H^{\otimes N} |0\dots0\rangle$
  $\Rightarrow$ Uniform superposition of all 2^N basis states
- Let R_0 be the reflection around $|0\dots0\rangle$

$$R_0 |y\rangle = \begin{cases} +|y\rangle & \text{iff } |y\rangle = |0...0\rangle \\ -|y\rangle, & \text{otherwise.} \end{cases}$$

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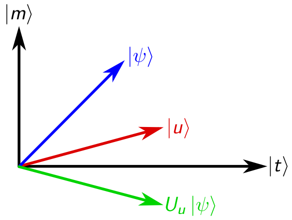

- Then $U_u = H^{\otimes N} R_0 H^{\otimes N}$ is a reflection around $|u\rangle$
- U_u is called **Grover's diffusion operator**
- It corresponds to a reflection of the amplitudes around the mean value $\mu = \frac{1}{N} \sum_i c_i$

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Grover's search algorithm

The Grover iteration

- Start from the equal-weight superposition state $|\psi\rangle = |u\rangle = H^{\otimes N} |0 \dots 0\rangle$
- Repeatedly apply the oracle and the diffusion operator $U_u U_f$ to the wave function

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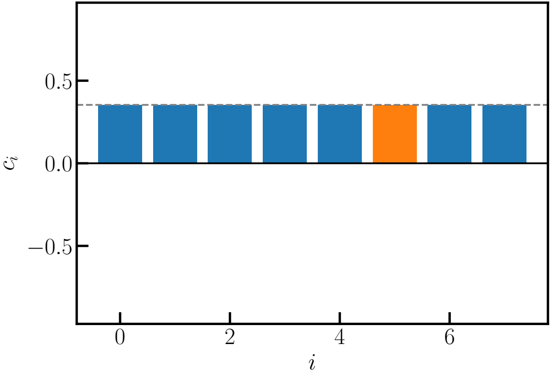

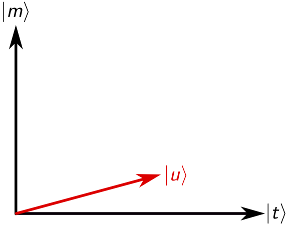

L.K. Grover, Proceedings of the twenty-eighth annual ACM symposium on Theory of Computing 212 – 219 (1996)

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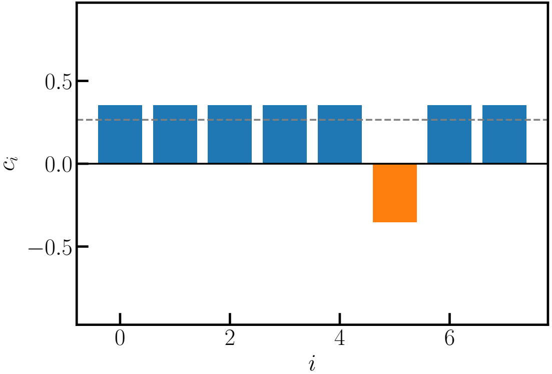

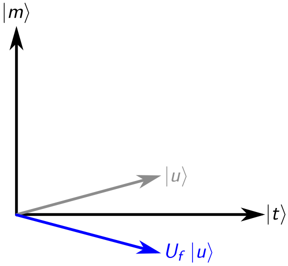

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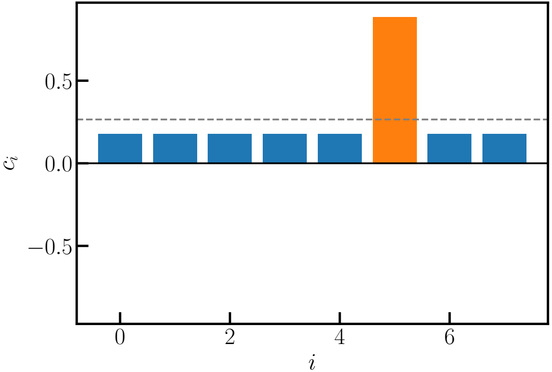

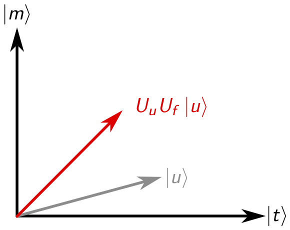

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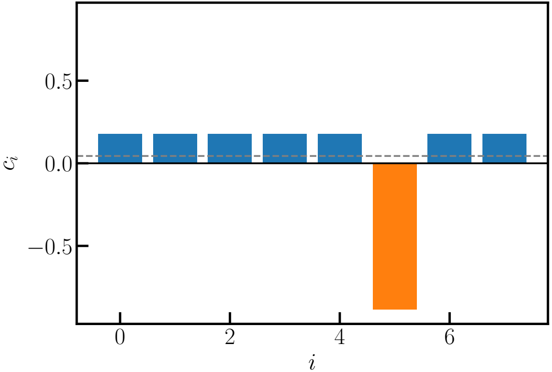

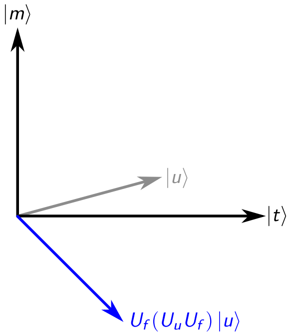

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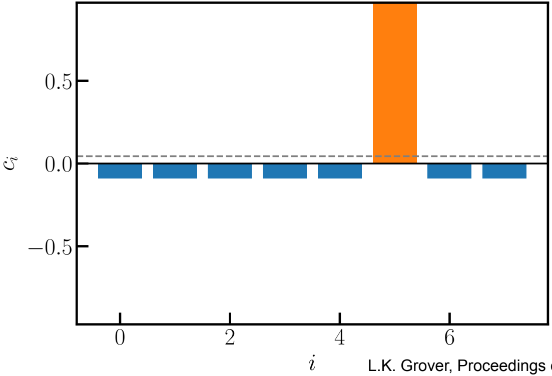
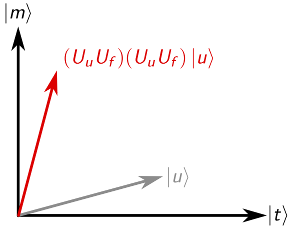




L.K. Grover, Proceedings of the twenty-eighth annual ACM symposium on Theory of Computing 212 – 219 (1996)

Grover's search algorithm

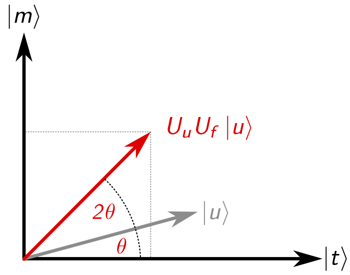
The Grover iteration

- After k iterations the wave function is of the form

$$
\begin{aligned}
|\psi_k\rangle &= (U_u U_f)^k |\psi\rangle = (U_u U_f)^k |u\rangle \\
&= \sin\big((2k+1)\theta\big)\,|m\rangle + \cos\big((2k+1)\theta\big)|t\rangle
\end{aligned}
$$

- If $\cos\big((2k+1)\theta\big)$ vanishes we are left with $|m\rangle$

$$
(2k+1)\theta = \frac{\pi}{2} \quad \Leftrightarrow \quad \theta = \frac{\pi}{2(2k+1)} \approx \frac{\pi}{4k}
$$



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Grover's search algorithm

Complexity of the algorithm

- How does the optimal k depend on N?

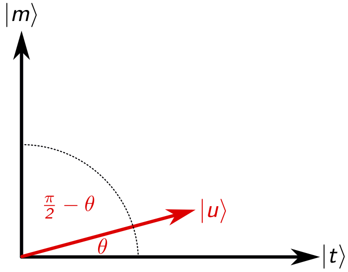
L.K. Grover, Proceedings of the twenty-eighth annual ACM symposium on Theory of Computing 212 – 219 (1996)

Grover's search algorithm

Complexity of the algorithm

- How does the optimal k depend on N?
- This can be determined with a simple geometrical picture

$$\sin(\theta) = \cos\left(\frac{\pi}{2} - \theta\right)$$
$$= \langle m|u\rangle = \langle m\middle|H^{\otimes n}\middle|00\ldots 0\rangle = \frac{1}{\sqrt{N}}$$



- For large values of N we can approximate

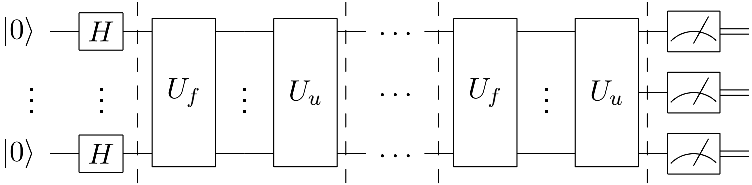
$$\theta \approx 1/\sqrt{N} \approx \pi/4k$$

- Overall complexity $\mathcal{O}(\sqrt{N})$

L.K. Grover, Proceedings of the twenty-eighth annual ACM symposium on Theory of Computing 212 – 219 (1996)

Grover's search algorithm

Quantum circuit for Grover's algorithm



$|u\rangle$ Grover iteration

- Initial layer of Hadamard gates prepares the equal-weight superposition $|u\rangle$
- Subsequent layers correspond do Grover iterations consisting of the oracle U_f and the diffusion operator U_u amplifying the amplitude of the marked element
- Final measurement reveals the probability distribution of basis states

Grover's search algorithm

Comments

> It is important to choose the right number of iterations, coefficient of $|m\rangle$ is given by

$$\sin\big((2k+1)\theta\big)$$

$\Rightarrow$ It oscillates periodically in k assuming a small value of θ

Grover's search algorithm

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- $|\psi\rangle$ will have a dominant component $|m\rangle$ at the end, but there might be small other components
- A single measurement at the end might not reveal the element, but a few repetitions should be sufficient
- We assume that we have f in form of the oracle U_f
  $\Rightarrow$ If we have to go through all the elements to construct U_f this is not helpful!
- If one has additional knowledge on how to implement f one can often do better using a classical algorithm

E. M. Stoudenmire, X. Waintal, Phys. Rev. X **14**, 041029 (2024)

3.

The Deutsch-Josza algorithm

Grover’s algorithm

Complexity theory

Hybrid quantum-classical algorithms

Challenges for hybrid quantum-classical algorithms

Complexity theory

Solving problems on a quantum computer

- Many more known quantum algorithms that (might) perform better than the best known classical algorithms
  - Shor's factoring algorithm
  - Grover's search algorithm
  - HHL algorithm for linear equations
  - Quantum Simulation
  - Bernstein–Vazirani algorithm
  - ...
- Exploiting quantum features such as superposition and entanglement these algorithms can outperform the best known classical algorithms

Catalog of quantum algorithms: `https://quantumalgorithmzoo.org/`

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Which problems can be solved efficiently on quantum computers?

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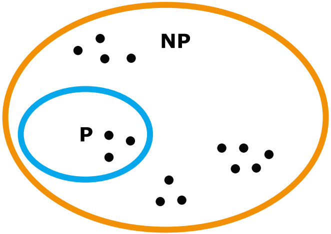
Complexity theory



- P: decision problems solvable by a deterministic Turing machine in **polynomial time**
- NP: decision problems solvable by a non-deterministic Turing machine in polynomial time
  - **Solution can be checked** on a deterministic Turing machine in **polynomial time**

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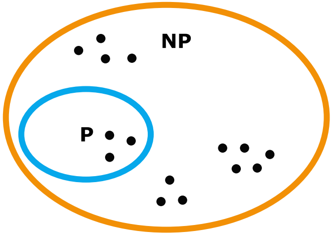

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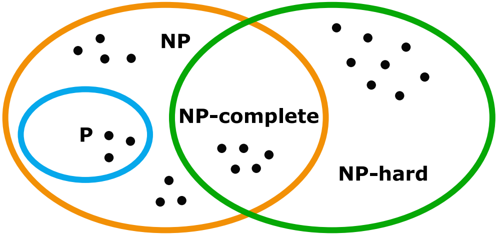

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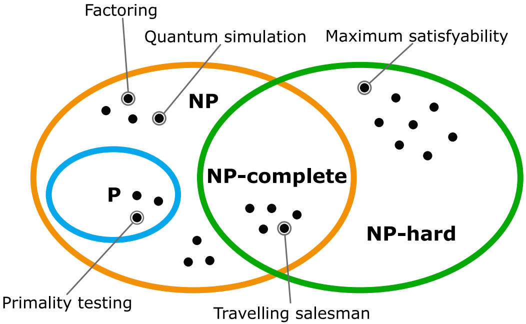

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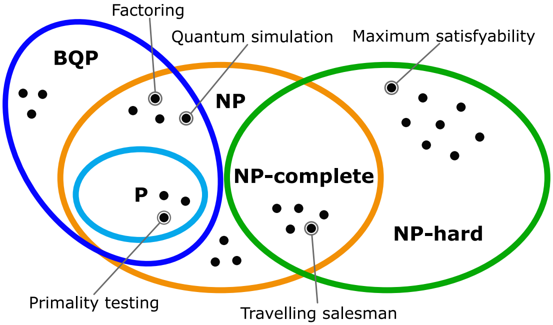
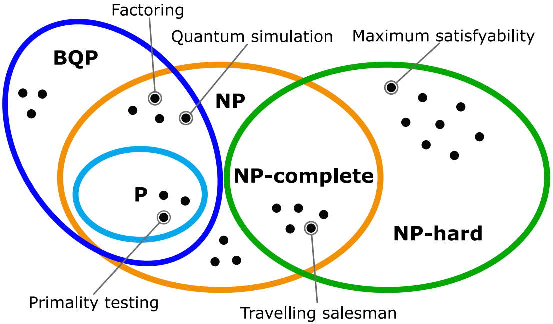


BQP (bounded-error quantum polynomial time):

- Decision problems solvable by a quantum computer in **polynomial time** with error probability less than $1/3$
- Quantum equivalent to P, “easy problems”

Complexity theory



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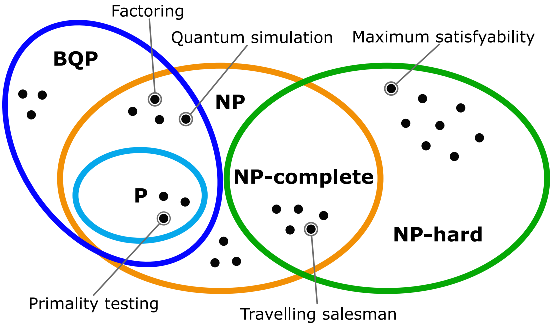
Take home message

- **Exponential speedup** on a quantum computer only for **very specific problems**
- **No exponential speedup** for **NP-complete problems**!

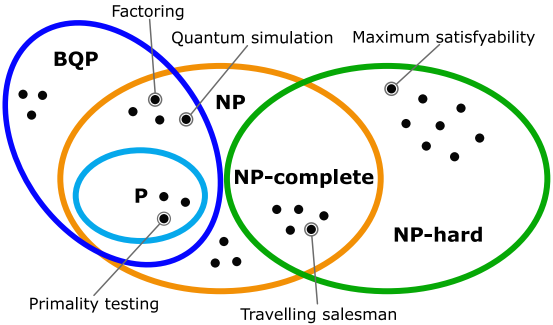
Complexity theory



> Not strictly proven, proving P $\neq$ NP is one of the millennium problems

https://www.claymath.org/millennium-problems/

Complexity theory



- Not strictly proven, proving P $\neq$ NP is one of the millennium problems
- If P $=$ NP then quantum computers would not allow for an exponential speedup
- Empirically, nobody has found a polynomial time algorithm for (all instances of) a problem in NP

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4.

The Deutsch-Josza algorithm

Grover's algorithm

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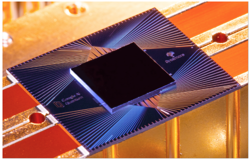
Challenges for hybrid quantum-classical algorithms

Variational hybrid quantum-classical algorithms

On the verge of the NISQ era

- Noisy intermediate-scale quantum computers with $\mathcal{O}(100)$ qubits are already available
- Noise significantly limits the circuit depths that can be executed reliably, no quantum error correction possible



J. Preskill, Quantum 2, 79 (2018)

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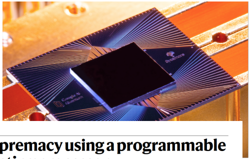

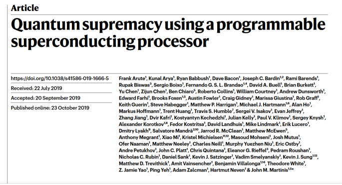

Article

Quantum supremacy using a programmable superconducting processor

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Frank Arute[1], Kunal Arya[1], Ryan Babbush[1], Dave Bacon[1], Joseph C. Bardin[1,2], Rami Barends[1], Rupak Biswas[3], Sergio Boixo[1], Fernando G. S. L. Brandao[1,4], David A. Buell[1], Brian Burkett[1], Yu Chen[1], Zijun Chen[1], Ben Chiaro[5], Roberto Collins[1], William Courtney[1], Andrew Dunsworth[1], Edward Farhi[1], Brooks Foxen[1,5], Austin Fowler[1], Craig Gidney[1], Marissa Giustina[1], Rob Graff[1], Keith Guerin[1], Steve Habegger[1], Matthew P. Harrigan[1], Michael J. Hartmann[1,6], Alan Ho[1], Markus Hoffmann[1], Trent Huang[1], Travis S. Humble[7], Sergei V. Isakov[1], Evan Jeffrey[1], Zhang Jiang[1], Dvir Kafri[1], Kostyantyn Kechedzhi[1], Julian Kelly[1], Paul V. Klimov[1], Sergey Knysh[1], Alexander Korotkov[1,8], Fedor Kostritsa[1], David Landhuis[1], Mike Lindmark[1], Erik Lucero[1], Dmitry Lyakh[9], Salvatore Mandrà[3,10], Jarrod R. McClean[1], Matthew McEwen[5], Anthony Megrant[1], Xiao Mi[1], Kristel Michielsen[11,12], Masoud Mohseni[1], Josh Mutus[1], Ofer Naaman[1], Matthew Neeley[1], Charles Neill[1], Murphy Yuezhen Niu[1], Eric Ostby[1], Andre Petukhov[1], John C. Platt[1], Chris Quintana[1], Eleanor G. Rieffel[3], Pedram Roushan[1], Nicholas C. Rubin[1], Daniel Sank[1], Kevin J. Satzinger[1], Vadim Smelyanskiy[1], Kevin J. Sung[1,13], Matthew D. Trevithick[1], Amit Vainsencher[1], Benjamin Villalonga[1,14], Theodore White[1], Z. Jamie Yao[1], Ping Yeh[1], Adam Zalcman[1], Hartmut Neven[1] & John M. Martinis[1,5*]

J. Preskill, Quantum 2, 79 (2018)
F. Arute et al., Nature 574, 5050 (2019)

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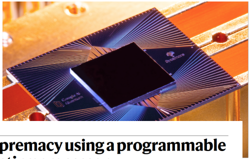

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RESEARCH

QUANTUM COMPUTING

Quantum computational advantage using photons

Han-Sen Zhong[1,2]*, Hui Wang[1,2]*, Yu-Hao Deng[1,2]*, Ming-Cheng Chen[1,2]*, Li-Chao Peng[1,2], Yi-Han Luo[1,2], Jian Qin[1,2], Dian Wu[1,2], Xing Ding[1,2], Yi Hu[1,2], Peng Hu[3], Xiao-Yan Yang[3], Wei-Jun Zhang[3], Hao Li[3], Yuxuan Li[4], Xiao Jiang[1,2], Lin Gan[4], Guangwen Yang[4], Lixing You[3], Zhen Wang[3], Li Li[1,2], Nai-Le Liu[1,2], Chao-Yang Lu[1,2]†, Jian-Wei Pan[1,2]†

Quantum computers promise to perform certain tasks that are believed to be intractable to classical computers. Boson sampling is such a task and is considered a strong candidate to demonstrate the quantum computational advantage. We performed Gaussian boson sampling by sending 50 indistinguishable single-mode squeezed states into a 100-mode ultralow-loss interferometer with full connectivity and random matrix—the whole optical setup is phase-locked—and sampling the output using 100 high-efficiency single-photon detectors. The obtained samples were validated against plausible hypotheses exploiting thermal states, distinguishable photons, and uniform distribution. The photonic quantum computer, *Jiuzhang*, generates up to 76 output photon clicks, which yields an output state-space dimension of 10^{30} and a sampling rate that is faster than using the state-of-the-art simulation strategy and supercomputers by a factor of ~10^{14}.

F. Arute et al., Nature 574, 5050 (2019)
H.-S. Zhong et al., Science 370, 1460 (2020)

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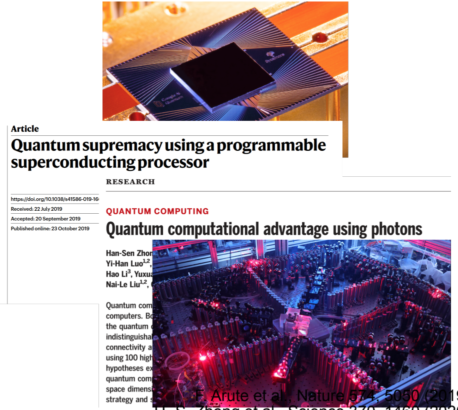

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Article

Evidence for the utility of quantum computing before fault tolerance

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Check for updates

Youngseok Kim[1,6✉], Andrew Eddins[2,6✉], Sajant Anand[3], Ken Xuan Wei[1], Ewout van den Berg[1], Sami Rosenblatt[1], Hasan Nayfeh[1], Yantao Wu[3,4], Michael Zaletel[3,5], Kristan Temme[1] & Abhinav Kandala[1✉]

Quantum computing promises to offer substantial speed-ups over its classical counterpart for certain problems. However, the greatest impediment to realizing its full potential is noise that is inherent to these systems. The widely accepted solution to this challenge is the implementation of fault-tolerant quantum circuits, which is out of reach for current processors. Here we report experiments on a noisy 127-qubit processor and demonstrate the measurement of accurate expectation values for circuit volumes at a scale beyond brute-force classical computation. We argue that this represents evidence for the utility of quantum computing in a pre-fault-tolerant era. These experimental results are enabled by advances in the coherence and calibration of a superconducting processor at this scale and the ability to characterize[1] and controllably manipulate noise across such a large device. We establish the accuracy of the measured expectation values by comparing them with the output of exactly verifiable circuits. In the regime of strong entanglement, the quantum computer provides correct results for which leading classical approximations such as pure-state-based 1D (matrix product states, MPS) and 2D (isometric tensor network states, isoTNS) tensor network methods[2,3] break down. These experiments demonstrate a foundational tool for the realization of near-term quantum applications[4,5].

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Y. Kim et al., Nature 618, 500 (2023)

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- Larger quantum devices in the near future with error correction are announced future

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`https://www.ibm.com/quantum/technology#scaling-quantum-computing`, `https://blog.google/technology/ai/unveiling-our-new-quantum-ai-campus/`

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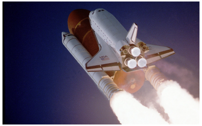
Solving “useful” problems

- Large number of qubits
- Deep circuits
- Quantum error correction necessary
- So far only proof of principle demonstrations

Variational hybrid quantum-classical algorithms



Current NISQ devices

- Small or intermediate scale
- Considerable amount of noise
- Only shallow circuits can be executed faithfully/no error correction
- Quantum advantage demonstrated

Solving “useful” problems

- Large number of qubits
- Deep circuits
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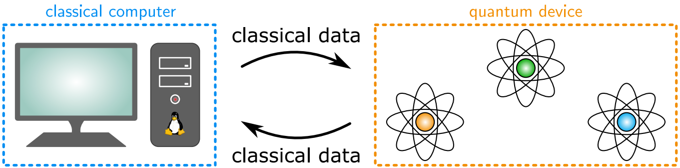
- So far only proof of principle demonstrations

How can we utilize existing quantum hardware in a beneficial way?

Variational hybrid quantum-classical algorithms

The basic idea of hybrid quantum-classical algorithms

- Combine classical and quantum devices
- Rely on classical computing where possible
- Use the quantum device as a coprocessor
  - Tackle the classically hard/intractable part of the problem
  - Feed the classical data obtained from a measurement back to the classical computer



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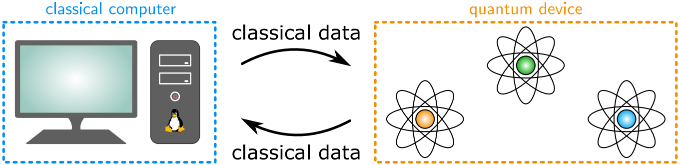


Even modest quantum hardware can yield advantages

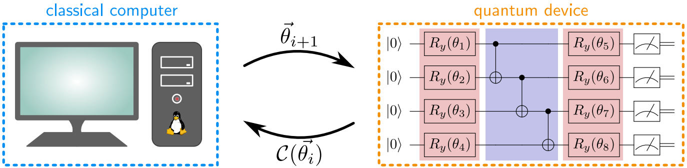
Variational hybrid quantum-classical algorithms

Variational quantum-classical algorithms

- Focus on optimization problems trying to minimize a cost function $\mathcal{C}(\vec{\theta})$

$$\min_{\vec{\theta}} \mathcal{C}(\vec{\theta}) = \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle, \qquad \vec{\theta} = \mathbb{R}^n$$

- Solve them iteratively using a parametric ansatz
  - Quantum coprocessor: prepare the **variational ansatz** $|\psi(\vec{\theta}_i)\rangle$ and evaluate $\mathcal{C}(\vec{\theta}_i)$
  - Classical computer: given $\mathcal{C}(\vec{\theta}_i)$, find optimized $\vec{\theta}_{i+1}$



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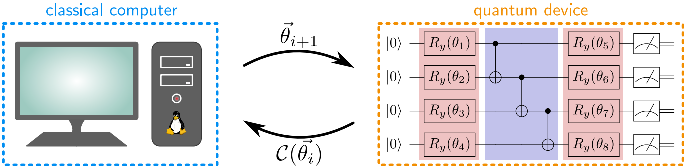
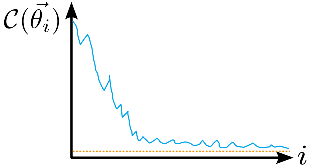




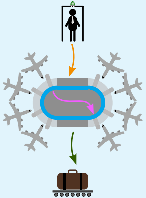
$\Rightarrow$ Run **feedback loop** between the classical computer and the quantum device until convergence

Variational hybrid quantum-classical algorithms

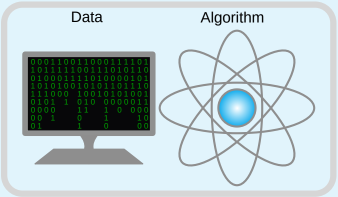
Why variational quantum algorithms?

> A large class of problems is naturally of that form or can be recast into such a form

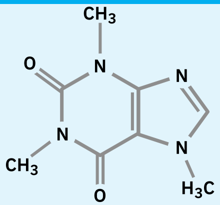
Optimization



Machine learning



Physics/Chemistry



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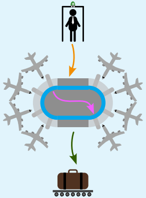

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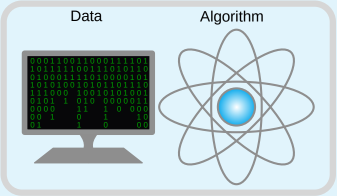

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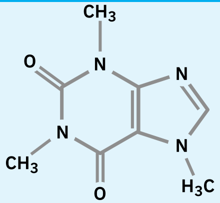


> Evaluating $\langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle$ is in general exponentially costly on classical computers

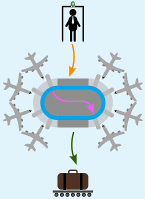
> Given that the ansatz $|\psi(\vec{\theta})\rangle$ is expressive enough at the end of the optimization

- $\mathcal{C}(\vec{\theta})$ corresponds to the smallest eigenvalue E_0 of H
- $|\psi(\vec{\theta})\rangle$ is the corresponding eigenstate, i.e. the ground state of H

Variational hybrid quantum-classical algorithms

How to implement variational quantum algorithms?

Optimization



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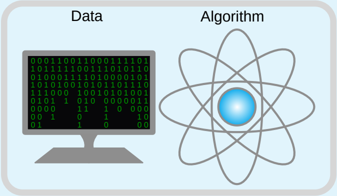

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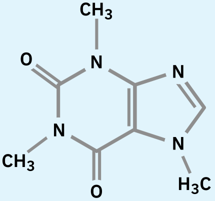

- How do we measure the cost function?
- How can we cast problems in such a form?
- How can we choose a suitable ansatz?

Measuring observables on a quantum device

Variational hybrid quantum-classical algorithms

Measuring observables

- Given an observable O we want to compute $\langle\psi| O |\psi\rangle$
- State can only be measured in the computational basis

$$\langle\psi| O |\psi\rangle = \langle\psi| U^\dagger U O U^\dagger U |\psi\rangle = \left\langle\psi'\right| U O U^\dagger \left|\psi'\right\rangle = \left\langle\psi'\right| D \left|\psi'\right\rangle$$

Variational hybrid quantum-classical algorithms

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- Choose U such that $D = UOU^\dagger = \text{diag}(\lambda_0, \dots, \lambda_{2^N-1}) = \sum_x \lambda_x |x\rangle\langle x|$ in the computational basis
- Expand $|\psi'\rangle$ in the computational basis: $|\psi'\rangle = \sum_x c'_x |x\rangle$

$$\langle\psi| O |\psi\rangle = \langle\psi'| D |\psi'\rangle = \sum_{x=0}^{2^N-1} \lambda_x \langle\psi' \underbrace{|x\rangle\langle x|}_{P_x} \psi'\rangle = \sum_{x=0}^{2^N-1} \lambda_x \langle\psi'|P_x|\psi'\rangle = \sum_{x=0}^{2^N-1} |c'_x|^2 \lambda_x$$

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- U is often called **post rotation**
- Instead of $|\psi\rangle$ we prepare $|\psi'\rangle$ and measure the probability distribution $|c'_x|^2$

Variational hybrid quantum-classical algorithms

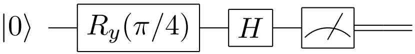
Example

- State $|\psi\rangle = R_y(\pi/4)\,|0\rangle$
- Observable we want to measure $O = X$

$$D = UOU^\dagger = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\; X\; \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$
$$= HXH = Z$$

- Circuit to prepare and measure

$$|\psi'\rangle = U\,|\psi\rangle = HR_y(\pi/4)\,|0\rangle$$



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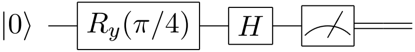

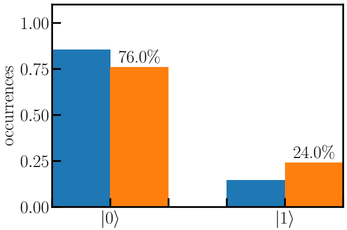

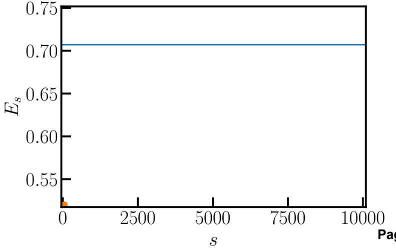

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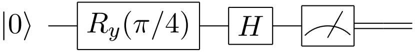

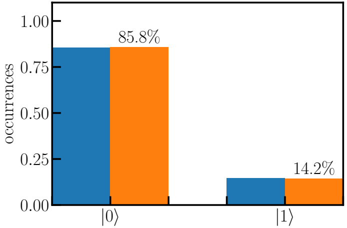

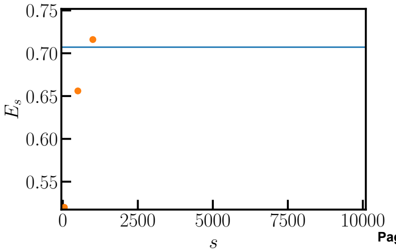

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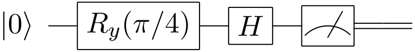

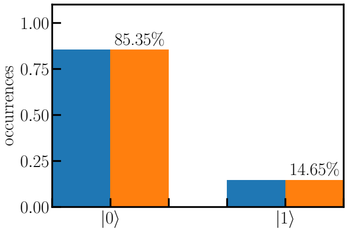

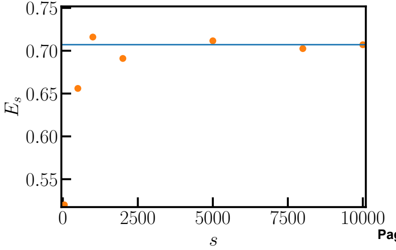

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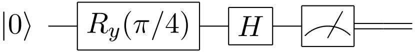

$\Rightarrow$ Error is $\propto 1/\sqrt{s} \to 0$ for $s \to \infty$

Quantum Approximate Optimization Algorithm (QAOA)

Variational hybrid quantum-classical algorithms

Combinatorial optimization problems

- Algorithm for approximating (binary) combinatorial optimization problems

$$\min_{x \in V} C(x)$$
$$\text{subject to } x \in S$$

- x: binary string in $V = \{0,1\}^n$ encoding a solution
- $S \subseteq V$: feasible solutions
- $C : V \to \mathbb{R}$ cost function
- Objective is to find the optimal solution

Variational hybrid quantum-classical algorithms

The Max-Cut problem

Max-Cut

- **Input:** undirected graph $G = (V, E)$
- **Task:** find a bipartition of $V = A \cup B$ such that the number of edges between A and B is maximal

Variational hybrid quantum-classical algorithms

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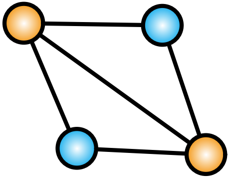


- Max-Cut is NP-complete

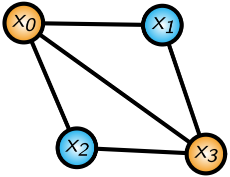
$\Rightarrow$ We cannot find a (quantum) algorithm which solves it polynomial time

- We can however try to find a good approximation to the exact solution in polynomial time

Variational hybrid quantum-classical algorithms

Max-Cut as combinatorial optimization problem

- Max-Cut on a Graph $G = (V, E)$ can be expressed as combinatorial optimization problem
- Label the vertices as x_i define a function w_{ij}



$$x_i = \begin{cases} 0 & \text{if } i \in A \\ 1 & \text{if } i \in B \end{cases} \qquad w_{ij} = \begin{cases} 1 & \text{iff } (i,j) \in E \\ 0 & \text{otherwise} \end{cases}$$

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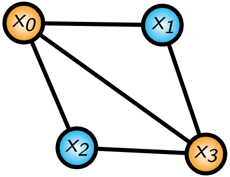

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- Cost function

$$C(x) = \sum_{i,j=0}^{n-1} w_{ij} x_i (x_j - 1) = \sum_{(i,j)\in E} (x_i(x_j - 1) + x_j(x_i - 1))$$

$\Rightarrow$ Contribution of -1 iff endpoints of edge (i, j) belong to different subsets

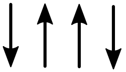
- Finding the Max-Cut for G is equivalent to minimizing $C(x)$

Variational hybrid quantum-classical algorithms

Max-Cut as Hamiltonian problem

- Cost function can be turned into a Hamiltonian using the mapping $x_i \rightarrow \frac{1}{2}(1 - Z_i)$

$$H_c = \frac{1}{2} \sum_{(i,j) \in E} (Z_i Z_j - 1)$$



- Diagonal Hamiltonian of Ising type, summands commute

Variational hybrid quantum-classical algorithms

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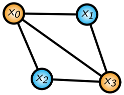

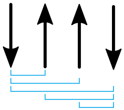

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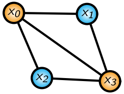

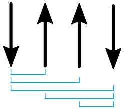

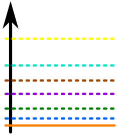

- Diagonal Hamiltonian of Ising type, summands commute
- The eigenstates of H are **computational basis states which encode graph cuts**
- The lower the energy, the larger the number of edges between the subsets
- The **ground state** $|x^*\rangle$ encodes the bit string of the **optimal solution** x^*

Variational hybrid quantum-classical algorithms

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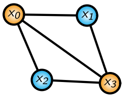

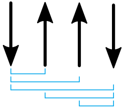

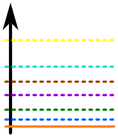

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How to choose a suitable ansatz to find a low energy state of H?

Variational hybrid quantum-classical algorithms

The Quantum Approximate Optimization Algorithm (QAOA)

- We want to find a parametric quantum state $|\psi_p(\vec{\gamma},\vec{\beta})\rangle$, $\vec{\gamma}$, $\vec{\beta} \in \mathbb{R}^p$ which minimizes

$$\mathcal{C}(\vec{\gamma},\vec{\beta}) = \langle\psi_p(\vec{\gamma},\vec{\beta})|H_c|\psi_p(\vec{\gamma},\vec{\beta})\rangle$$

E. Farhi, J. Goldstone, S. Gutmann, arXiv:1411.4028

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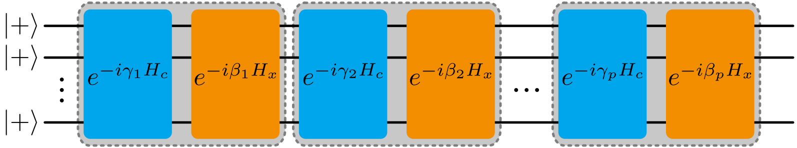
- Mixing Hamiltonian $H_x = \sum_i X_i$
- Ansatz structure

$|\psi_p(\vec{\gamma},\vec{\beta})\rangle =$



- $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ is an eigenstate of X, $X|+\rangle = +1|+\rangle$

E. Farhi, J. Goldstone, S. Gutmann, arXiv:1411.4028

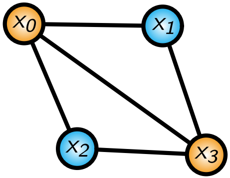
Variational hybrid quantum-classical algorithms

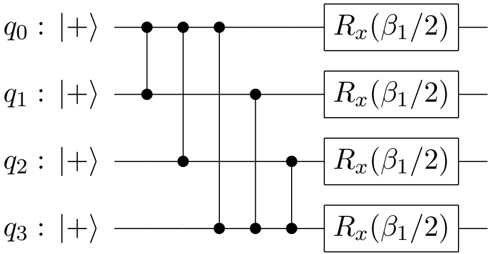
The Quantum Approximate Optimization Algorithm (QAOA)

- Ansatz for $|\psi_p(\vec{\gamma}, \vec{\beta})\rangle$

$$|\psi_p(\vec{\gamma}, \vec{\beta})\rangle = e^{-i\beta_p H_x} e^{-i\gamma_p H_c} \dots e^{-i\beta_1 H_x} e^{-i\gamma_1 H_c} |+\rangle^{\otimes n}$$

- Circuit for $p = 1$



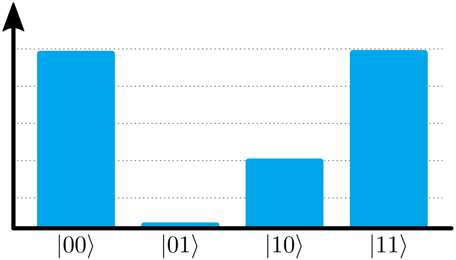


E. Farhi, J. Goldstone, S. Gutmann, arXiv:1411.4028

Variational hybrid quantum-classical algorithms

The Quantum Approximate Optimization Algorithm (QAOA)

- $|\psi_p(\vec{\gamma}, \vec{\beta})\rangle$ is in general an (entangled) superposition of basis states
- After minimizing $\mathcal{C}(\vec{\gamma}, \vec{\beta})$ the wave function $|\psi_p(\vec{\gamma}, \vec{\beta})\rangle$ has dominant component(s) of low energy states of H_c
- Measuring $|\psi_p(\vec{\gamma}, \vec{\beta})\rangle$ reveals the a bit string(s) x corresponding to low energy states



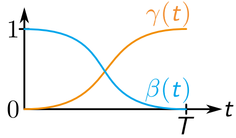
E. Farhi, J. Goldstone, S. Gutmann, arXiv:1411.4028

Variational hybrid quantum-classical algorithms

The Quantum Approximate Optimization Algorithm (QAOA)

- Ansatz is inspired by trotterized adiabatic time evolution
- Choose functions $\gamma(t)$, $\beta(t)$ such that

$$\gamma(t) \to \begin{cases} 0 & \text{for } t \to 0 \\ 1 & \text{for } t \to T \end{cases} \qquad \beta(t) \to \begin{cases} 1 & \text{for } t \to 0 \\ 0 & \text{for } t \to T \end{cases}$$



and set $\gamma_k = \gamma(k\Delta t)\Delta t$, $\beta_k = \beta(k\Delta t)\Delta t$

$\Rightarrow$ QAOA ansatz is a stroboscopic version of the adiabatic evolution

B. Barak et al., arXiv:2106.05900
E. Farhi, A. Harrow, arXiv:1602.07674
E. Farhi, J. Goldstone, S. Gutmann, arXiv:1411.4028
V. Akshay, H Philathong, M. E. S. Morales, J. D. Biamonte, Phys. Rev. Lett 124, 090504 (2020)

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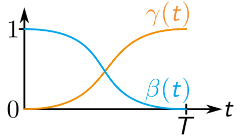

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$\Rightarrow$ QAOA ansatz is a stroboscopic version of the adiabatic evolution

- Even $p = 1$ can in general not be simulated on a classical computer efficiently
- For some problems classical algorithms got a better approximation ratios

$\Rightarrow$ Theoretically it is not entirely clear how QAOA performs

B. Barak et al., arXiv:2106.05900
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Variational Quantum Eigensolver (VQE)

Variational hybrid quantum-classical algorithms

Variational Quantum Algorithms

- Same principle can be used to find ground states of general quantum Hamiltonians
- Define a cost function

$$\mathcal{C}(\vec{\theta}) = \langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle$$

- $|\psi(\vec{\theta})\rangle$ ansatz realized by a parametric quantum circuit
- In practice ansätze are often built by repeating a layered structure

A. Peruzzo et al., Nat. Commun. 5, 1 (2014)
J. R. McClean et al., New J. Phys. 18, 023023 (2016)

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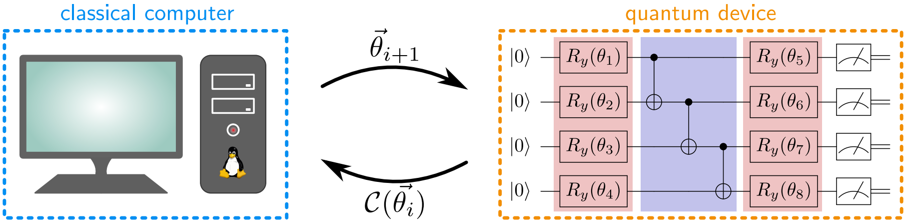

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Variational hybrid quantum-classical algorithms

Variational Quantum Eigensolver (VQE)

- To measure a general N-qubit Hamiltonian, we translate it into a sum of Pauli terms

$$H = \sum_i c_i P_i$$

  with $P_i \in \{\mathbb{1}, X, Y, Z\}^{\otimes N}$ a Pauli string and real coefficients c_i
- This can always be done, as the Pauli matrices form a basis for the real vector space of Hermitian matrices (see exercises)

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- The cost function is then given by

$$\mathcal{C}(\vec{\theta}) = \sum_i c_i \langle \psi(\vec{\theta}) | P_i | \psi(\vec{\theta}) \rangle$$

- The individual terms $\langle \psi(\vec{\theta}) | P_i | \psi(\vec{\theta}) \rangle$ can be measured as discussed before

$\Rightarrow$ This is efficient as long there is only on number of $\mathcal{O}(\text{poly}(N))$ terms with nonvanishing coefficients in H

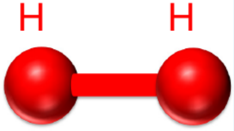
J. R. McClean et al., New J. Phys. 18, 023023 (2016)
A. Peruzzo et al., Nat. Commun. 5, 1 (2014)

Variational hybrid quantum-classical algorithms

Example: VQE for molecules

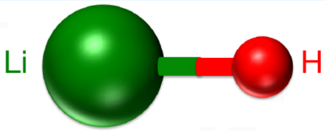
- Use the VQE for finding the potential energy surface of molecules

H_2



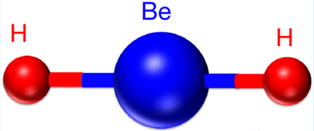
$$H = 0.011280ZZ + 0.397936ZI + 0.397936IZ + 0.180931XX$$

LiH



$$H = -0.096022ZIII - 0.206128ZZII + 0.364746IZII + \dots$$

BeH_2



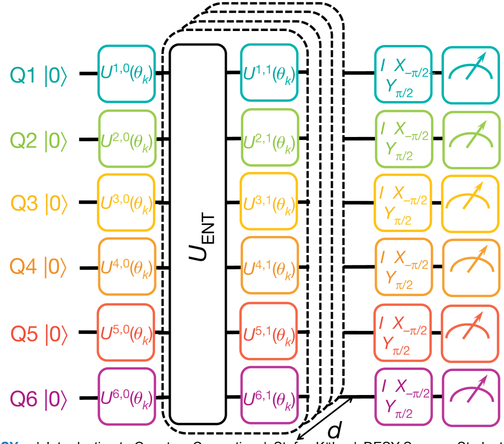
$$H = -0.143021ZIIIII + 0.104962ZZIIII + 0.038195IZZIII + \dots$$

A. Kandala et al., Nature 549, 242 (2017)

Variational hybrid quantum-classical algorithms

Example: VQE for molecules

> Ansatz circuit: layered structure of single-qubit gates and entangling layers



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Variational hybrid quantum-classical algorithms

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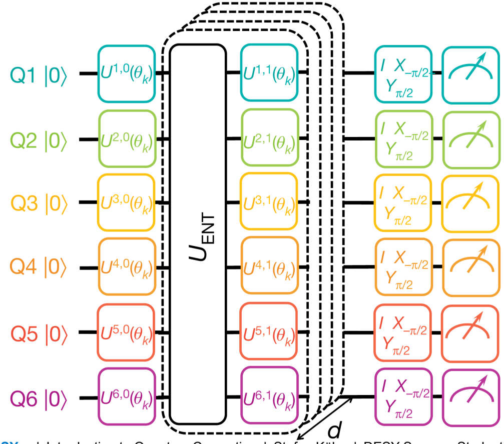
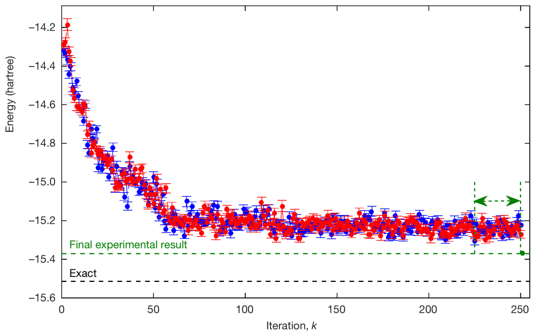


Results for BeH_2 at a given distance, 1000 measurements for each point

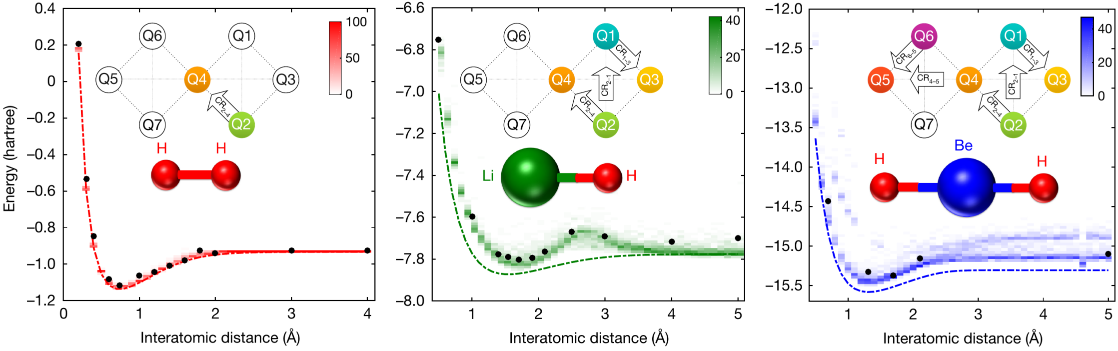


A. Kandala et al., Nature 549, 242 (2017)

Variational hybrid quantum-classical algorithms

Example: VQE for molecules

- Results from the VQE for $d = 1$ layer of the ansatz



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Variational hybrid quantum-classical algorithms

QAOA

- Combinatorial optimization problems
- Problem Hamiltonian is diagonal in the computational basis
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- Efficient as long as H has only a polynomial number of terms
- Hamiltonian exists only as a measurement
- Great freedom choosing the circuit
  - Problem requirements
  - Available hardware
  - Expressiveness

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  - Available hardware
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- Best answer for the given set of resources
- Largely resilient to systematic errors of the device

Variational hybrid quantum-classical algorithms

Remarks on VQE and QAOA

- QAOA can be seen as specific type of ansatz for the VQE
- Although QAOA was originally developed for combinatorial optimization problems it can be applied to arbitrary Hamiltonians

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J. R. McClean, S. Boixo, V. N. Smelyanskiy, R. Babbush, H. Neven, Nat. Commun. **9**, 4812 (2018)
A. Arrasmith, M. Cerezo, P. Czarnik, L. Cincio, P. J. Coles, Quantum **5**, 558 (2022)
A. Arrasmith, Z. Holmes, M. Cerezo, P. J. Coles, Quantum Science and Technology **7**, 045015 (2022)

5.

The Deutsch-Josza algorithm

Grover's algorithm

Complexity theory

Hybrid quantum-classical algorithms

Challenges for hybrid quantum-classical algorithms

Challenges for hybrid quantum-classical algorithms

Barren plateaus

> Optimizing the parameters using a classical algorithms turns out to be challenging

> For a wide class of parametrized circuits the **probability to have a non-vanishing gradient** along any direction **vanishes exponentially** with the number of qubits

$\Rightarrow$ **Barren plateaus**, gradient-based optimizers will fail

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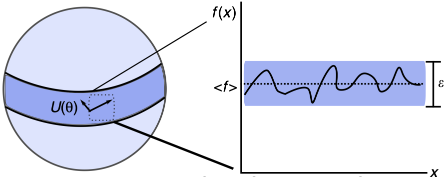
- Optimizing the parameters using a classical algorithms turns out to be challenging
- For a wide class of parametrized circuits the **probability to have a non-vanishing gradient** along any direction **vanishes exponentially** with the number of qubits

⇒ **Barren plateaus**, gradient-based optimizers will fail

- Mathematical reason: concentration of measure, sufficiently smooth function is concentrated in an exponentially small region around the mean



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Challenges for hybrid quantum-classical algorithms

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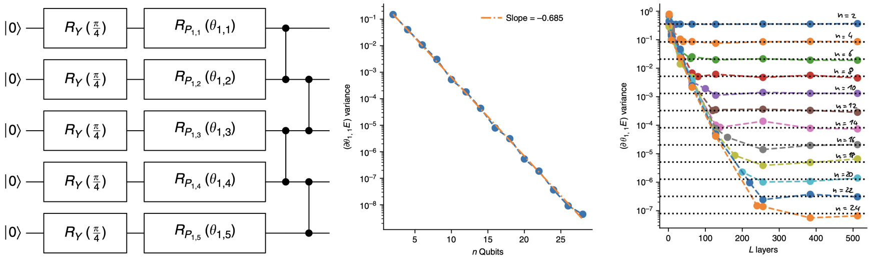
- This happens for sufficiently random circuits (match the Haar distribution up to the second moment)
- In practice this phenomena is already observed for relative simple ansatz circuits



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Challenges for hybrid quantum-classical algorithms

Barren plateaus

- It was shown that not only does the gradient vanish, but also the **cost function** has **exponentially narrow minima**
- Not only the gradients vanish exponentially, but also the variance of the cost function itself

⇒ Switching to a **gradient free optimization algorithm** does **not avoid the problem**

A. Arrasmith, M. Cerezo, P. Czarnik, L. Cincio, P. J. Coles, Quantum **5**, 558 (2022)
A. Arrasmith, Z. Holmes, M. Cerezo, P. J. Coles, Quantum Science and Technology **7**, 045015 (2022)
M. Larocca, S. Thanasilp, S. Wang, K. Sharma, J. Biamonte, P. J. Coles, L. Cincio, J. R. McClean, Z. Holmes, M. Cerezo, arXiv:2405.00781

Challenges for hybrid quantum-classical algorithms

Causes for barren plateaus

- Ansätze that are **too expressive** in a sense that they are able to relatively how uniformly it explores the unitary space exhibit barren plateaus

Z. Holmes et al., PRX Quantum **3**, 010313 (2022); J. Tangpanitanon et al., Phys. Rev. Research **2**, 043364 2020

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M. Cerezo et al., Nat. Commun. **12**, 1791, (2021)

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- Nature of the cost function, **global cost functions** are introducing barren plateaus, local cost functions only after a depth polynomial in the number of qubits
- **Noise** in the quantum device can wash out the features of the energy landscape leading to barren plateaus

Z. Holmes et al., PRX Quantum **3**, 010313 (2022); J. Tangpanitanon et al., Phys. Rev. Research **2**, 043364 2020
C. Ortiz Marrero et al., PRX Quantum **2**, 040316 (2021); T. L. Patti et al., Phys. Rev. Research **3**, 033090 (2021); K. Sharma et al., Phys. Rev. Lett. **128** 180505 (2022)
M. Cerezo et al., Nat. Commun. **12**, 1791, (2021)
S. Wang et al., Nat. Commun. 12, 6961 (2021); D. Stilck França, R. García-Patrón, Nat. Phys. **17**, 1221 (2021)

Challenges for hybrid quantum-classical algorithms

Avoiding/mitigating barren plateaus

- If possible, one can avoid the causes of barren plateaus, however this does not necessarily result in a trainable ansatz
- There is a plethora of proposals how to avoid/mitigate barren plateaus
  - Using modified cost functions

    A. Wu, G. Li, Y. Ding, Y. Xie, arXiv:211:13209
  - Special choices of the initial variational parameters

    Z. Holmes et al., PRX Quantum **3**, 010313 (2022)
    K. Zhang et al., arXiv2203:09376
  - Monitoring the entanglement during a gradient descent optimization in small subregions and adapting to learning rate to avoid uncontrolled entanglement growth

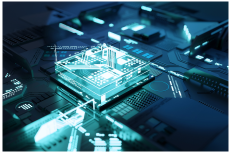
    S. H. Sack et al., PRX Quantum **3**, 020365 (2022)
  - ...

So far it seems that there is not simple way to avoid barren plateaus!

Thank you for your attention!

Further reading

- M. A. Nielsen and I. L. Chuang, Quantum computation and quantum information, Cambridge university press (2010)
- J. R. McClean, J. Romero, R. Babbush, A. A. Guzik, New J. Phys. **18**, 023023 (2016)
- J. Tilly et al., Physics Reports **986**, 1-128 (1011)
- `https://learning.quantum-computing.ibm.com/`



Contact

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