3rd Week of Quantum Information and String Theory 2019

Quantum-Classical Hybrid Algorithm: its advantage and methods for variational optimization

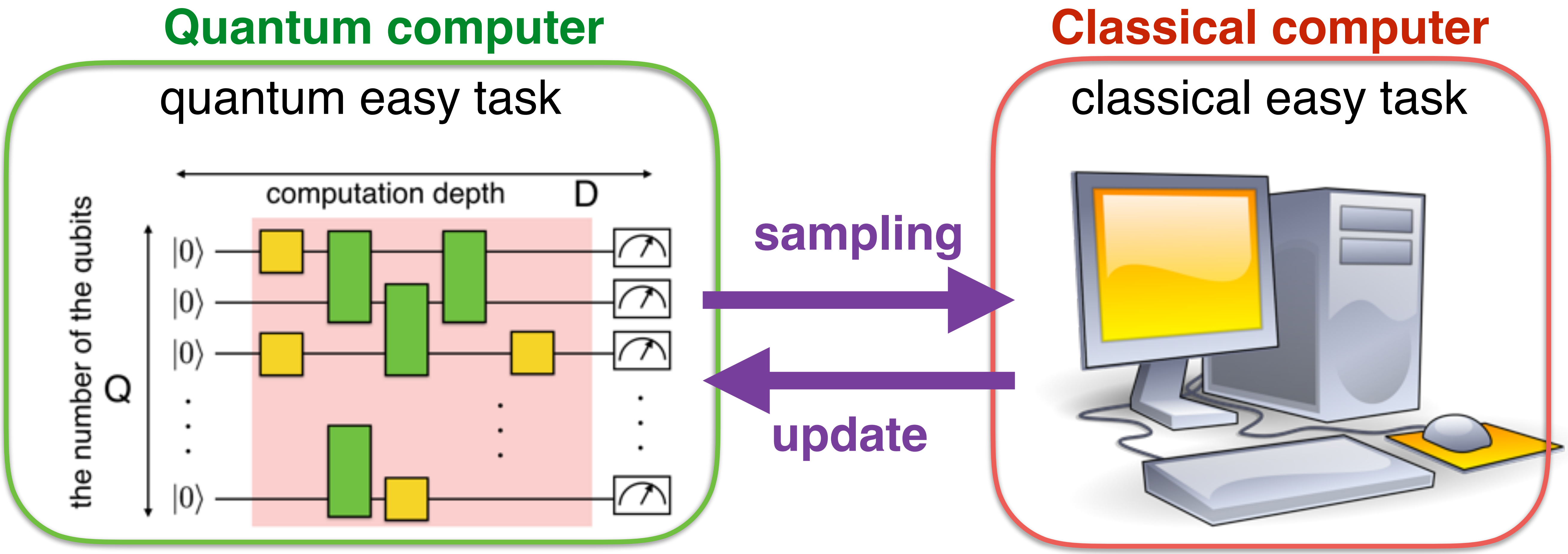
KF, arXiv:1803.09954
Mitarai-Negoro-Kitagawa-KF, Phys. Rev. A **98**, 032309 (2019)
Nakanishi-KF-Todo, arXiv:1903.12166

Keisuke Fujii
Graduate School of Science and Engineering,
Osaka University
JST PRESTO

大阪大学
OSAKA UNIVERSITY

さきがけ
PRESTO

Overview



Quantum computer

quantum easy task

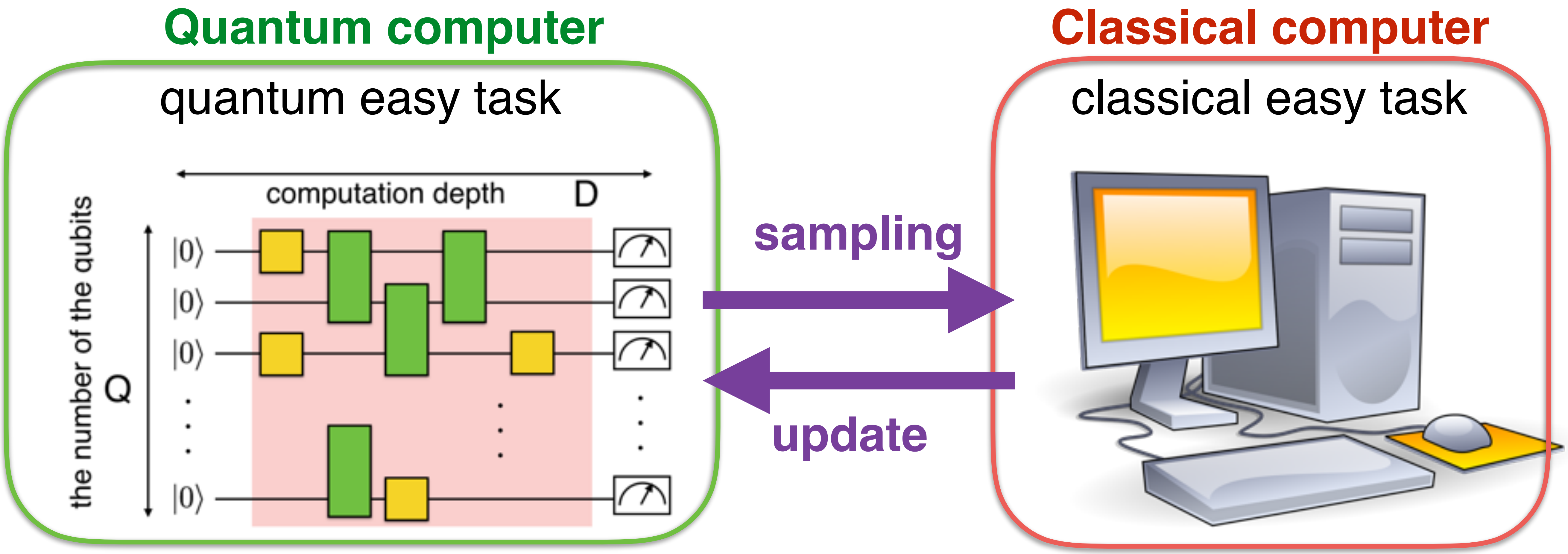
sampling

update

Classical computer

classical easy task

Overview



Quantum computer

quantum easy task

sampling

update

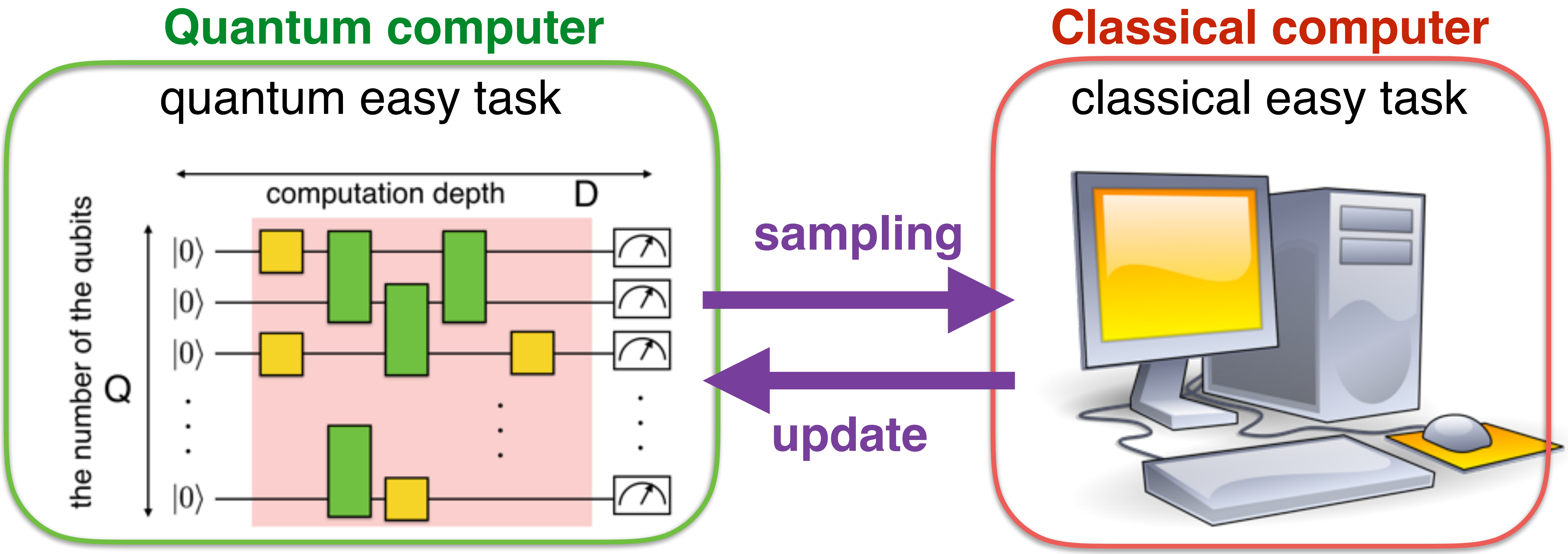
Classical computer

classical easy task

・Is there any situation where a quantum-classical hybrid approach provides a complexity theoretic advantage?

→*adiabatic quantum computation with stoquastic Hamiltonian*

Overview



Quantum computer

quantum easy task

sampling

update

Classical computer

classical easy task

・Is there any situation where a quantum-classical hybrid approach provides a complexity theoretic advantage?

→*adiabatic quantum computation with stoquastic Hamiltonian*

・How should we tune the parameters of (NISQ) quantum computers for quantum-classical variational algorithms.

→*gradient-based and -free optimizations*

Outline

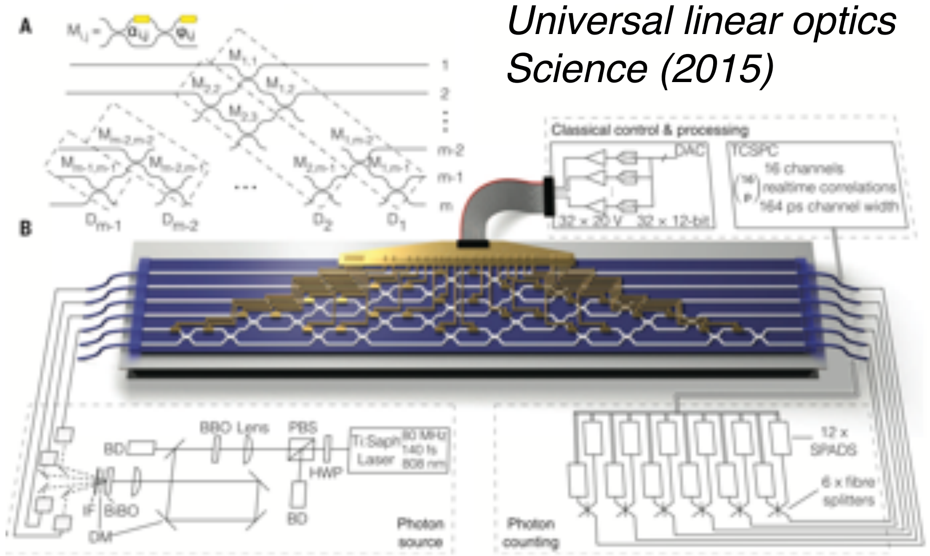
- **Advantage of quantum-classical hybrid algorithm**
  - Adiabatic quantum computation and quantum circuit model
  - Characterization of stoquastic adiabatic quantum computation
  - Quantum speedup in stoqAQC (sampling-based factoring & phase estimation)
- **Parameter tuning for quantum-classical variational algorithm**
  - Gradient-based optimization
  - Gradient-free optimization
  - Numerical comparisons of gradient-based and -free optimizations.

Quantum computational supremacy

non-universals model of quantum computation

Boson Sampling

Aaronson-Arkhipov ‘13



Universal linear optics
Science (2015)

Linear optical quantum computation

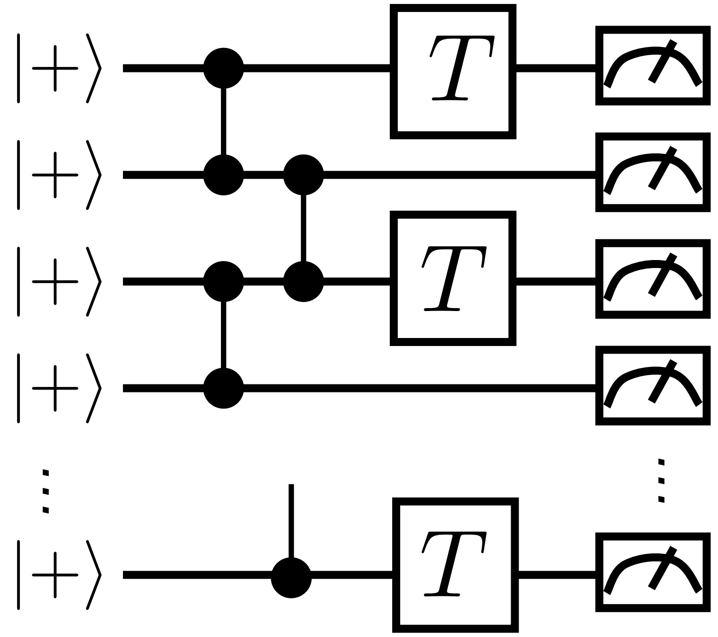
Experimental demonstrations

J. B. Spring *et al*. Science **339**, 798 (2013)
M. A. Broome, Science **339**, 794 (2013)
M. Tillmann *et al*., Nature Photo. **7**, 540 (2013)
A. Crespi *et al*., Nature Photo. **7**, 545 (2013)
N. Spagnolo *et al*., Nature Photo. **8**, 615 (2014)
J. Carolan *et al*., Science **349**, 711 (2015)

IQP

(commuting circuits)

Bremner-Jozsa-Shepherd ‘11



Ising type interaction

KF-Morimae ‘13

Bremner-Montanaro-Shepherd ‘15

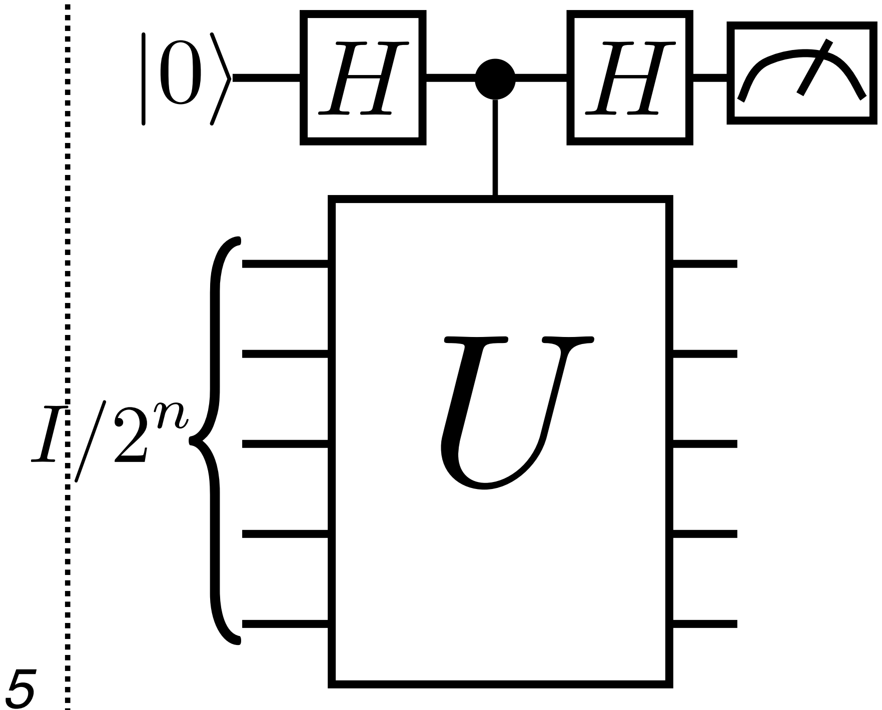
Gao-Wang-Duan ‘15

Farhi-Harrow ‘16

DQC1

(one-clean qubit model)

Knill-Laflamme ‘98
Morimae-KF-Fitzsimons ’14
KF et al, ‘18



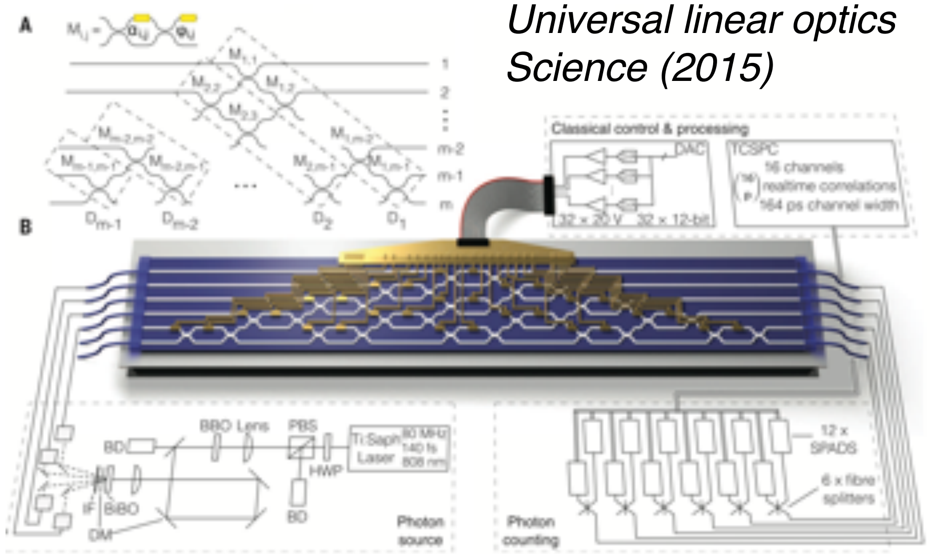
NMR spin ensemble

Quantum computational supremacy

non-universals model of quantum computation

Boson Sampling

Aaronson-Arkhipov '13



Universal linear optics
Science (2015)

Linear optical quantum computation

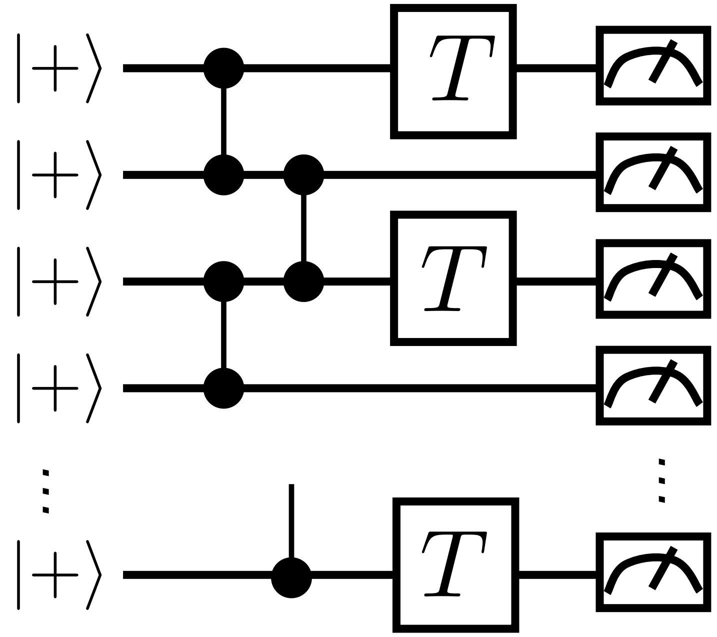
Experimental demonstrations

J. B. Spring *et al*. Science **339**, 798 (2013)
M. A. Broome, Science **339**, 794 (2013)
M. Tillmann *et al*., Nature Photo. **7**, 540 (2013)
A. Crespi *et al*., Nature Photo. **7**, 545 (2013)
N. Spagnolo *et al*., Nature Photo. **8**, 615 (2014)
J. Carolan *et al*., Science **349**, 711 (2015)

IQP

(commuting circuits)

Bremner-Jozsa-Shepherd '11



Ising type interaction

KF-Morimae '13

Bremner-Montanaro-Shepherd '15

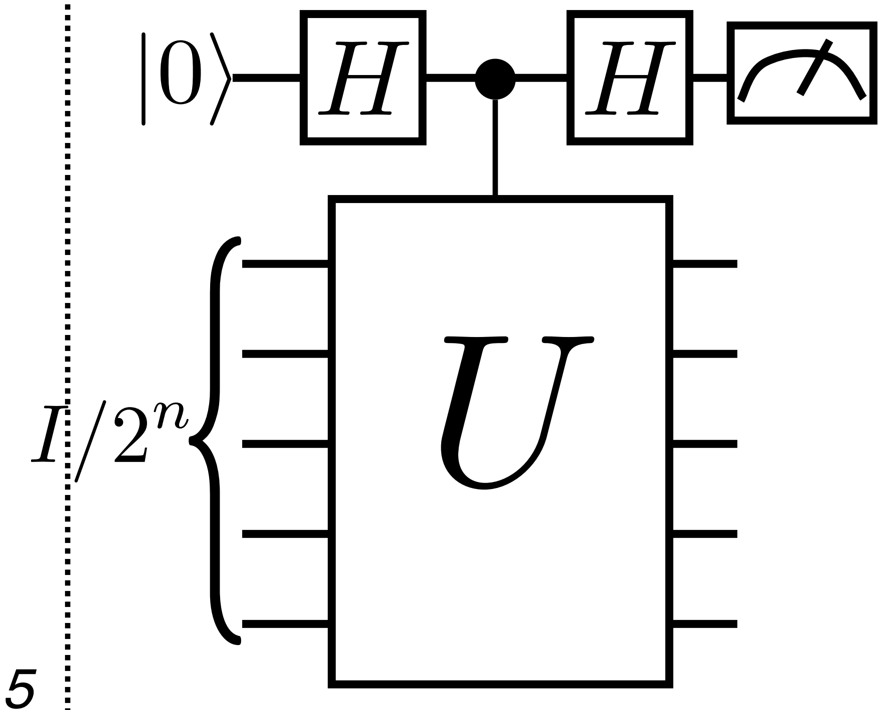
Gao-Wang-Duan '15

Farhi-Harrow '16

DQC1

(one-clean qubit model)

Knill-Laflamme '98
Morimae-KF-Fitzsimons '14
KF et al, '18



NMR spin ensemble

→ adiabatic quantum computation with **stoquastic** Hamiltonian

What is stoquastic Hamiltonian?

- **Off-diagonal terms are non positive** in a standard basis.
- The ground state has positive coefficients in the standard basis.
- **No negative sign problem** → Quantum Monte-Carlo method.

What is stoquastic Hamiltonian?

- **Off-diagonal terms are non positive** in a standard basis.
- The ground state has positive coefficients in the standard basis.
- **No negative sign problem** → Quantum Monte-Carlo method.
    - **Transverse Ising model:**

$$H = \sum_{ij} J_{ij} Z_i Z_J - h \sum_i X_i$$

What is stoquastic Hamiltonian?

- **Off-diagonal terms are non positive** in a standard basis.
- The ground state has positive coefficients in the standard basis.
- **No negative sign problem** → Quantum Monte-Carlo method.
  - **Transverse Ising model:**

$$H = \sum_{ij} J_{ij} Z_i Z_J - h \sum_i X_i$$

  - **Bose-Hubbard model with negative hopping:**

$$H = -\omega \sum_{ij} (a_i^\dagger a_j + a_j^\dagger a_i) - \mu \sum_i n_i + U \sum_i n_i (n_i - 1)$$

What is stoquastic Hamiltonian?

- **Off-diagonal terms are non positive** in a standard basis.
- The ground state has positive coefficients in the standard basis.
- **No negative sign problem** → Quantum Monte-Carlo method.
  - **Transverse Ising model:**

$$H = \sum_{ij} J_{ij} Z_i Z_J - h \sum_i X_i$$

  - **Bose-Hubbard model with negative hopping:**

$$H = -\omega \sum_{ij} (a_i^\dagger a_j + a_j^\dagger a_i) - \mu \sum_i n_i + U \sum_i n_i(n_i - 1)$$

  - **Heisernberg anti-ferro magnetic on a bipartite graph:**

$$H = J \sum_{ij} (X_i X_j + Y_i Y_j + Z_i Z_j) \, .$$

What is stoquastic Hamiltonian?

- **Off-diagonal terms are non positive** in a standard basis.
- The ground state has positive coefficients in the standard basis.
- **No negative sign problem** → Quantum Monte-Carlo method.
  - **Transverse Ising model:**

$$H = \sum_{ij} J_{ij} Z_i Z_J - h \sum_i X_i$$

  - **Bose-Hubbard model with negative hopping:**

$$H = -\omega \sum_{ij} (a_i^\dagger a_j + a_j^\dagger a_i) - \mu \sum_i n_i + U \sum_i n_i (n_i - 1)$$

  - **Heisernberg anti-ferro magnetic on a bipartite graph:**

$$H = J \sum_{ij} (X_i X_j + Y_i Y_j + Z_i Z_j) \ .$$

How powerful is adiabatic quantum computation with these restricted types of Hamiltonians?

Take home messages

- ***Non standard basis measurements change the situation drastically***, *while they would be relatively easy on an actual quantum machine if it has true quantum coherence.*

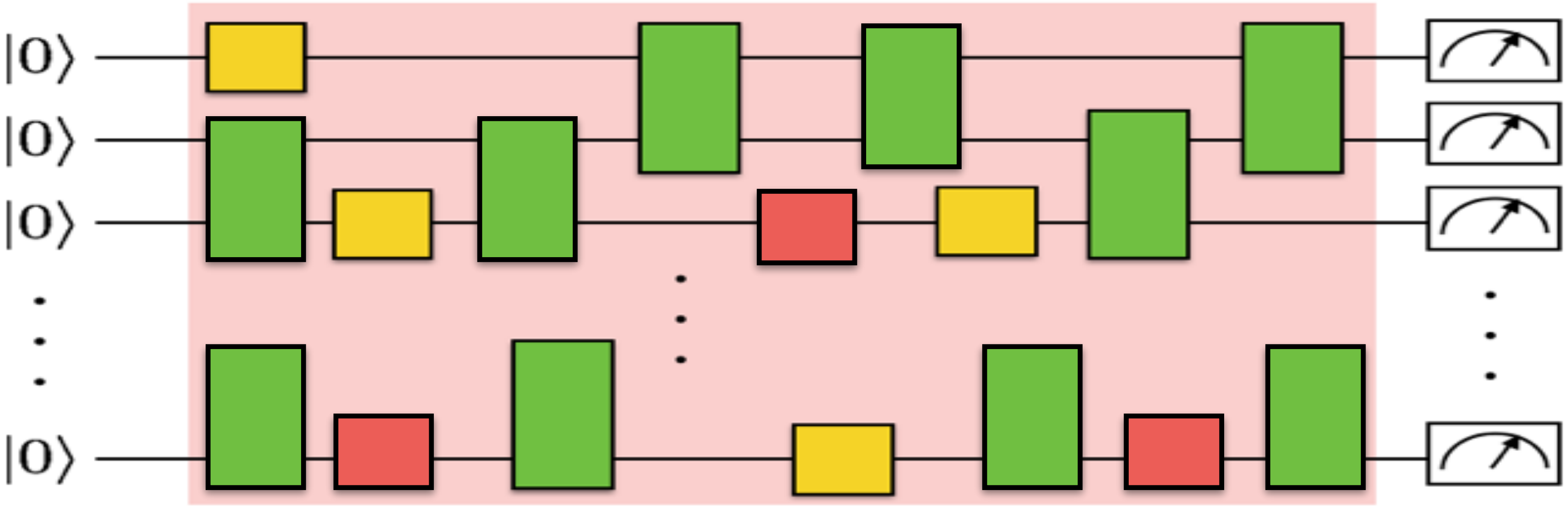
Take home messages

- ***Non standard basis measurements change the situation drastically****, while they would be relatively easy on an actual quantum machine if it has true quantum coherence.*

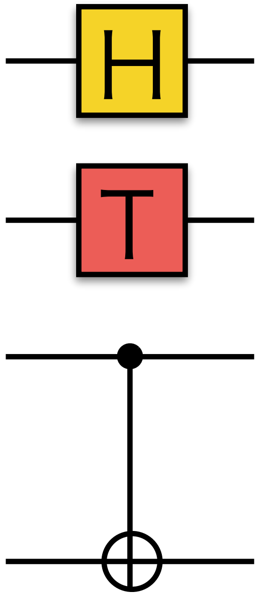
- ***StoqAQC with simultaneous measurements can solve meaningful and important problems like factoring with a quantum-classical hybrid algorithm.***

Circuit model and adiabatic model

Circuit model:

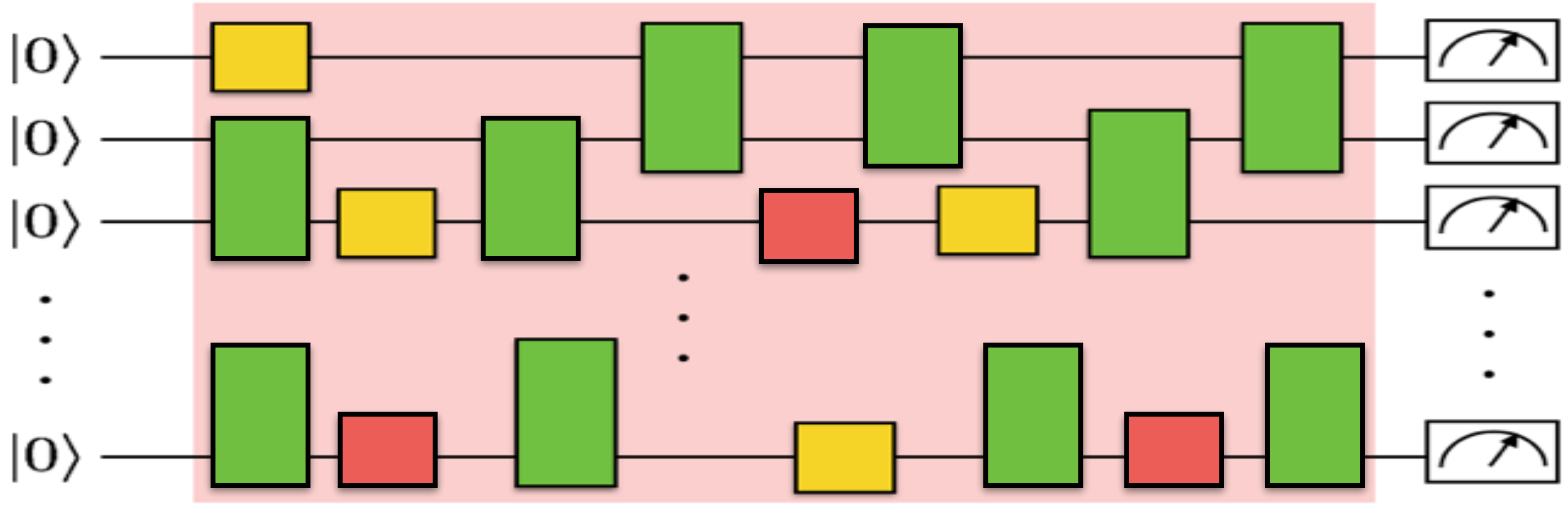


universal set of gate

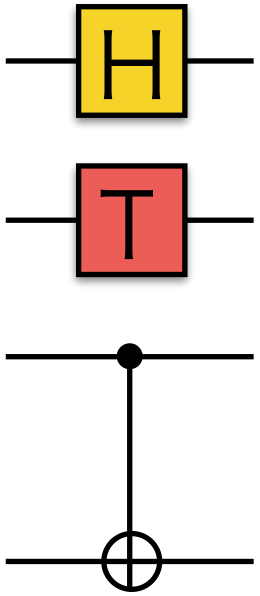


Circuit model and adiabatic model

Circuit model:



universal set of gate



Adiabatic quantum computation:

$$H(t) = a(t)H_{\text{initial}} + b(t)H_{\text{final}}$$

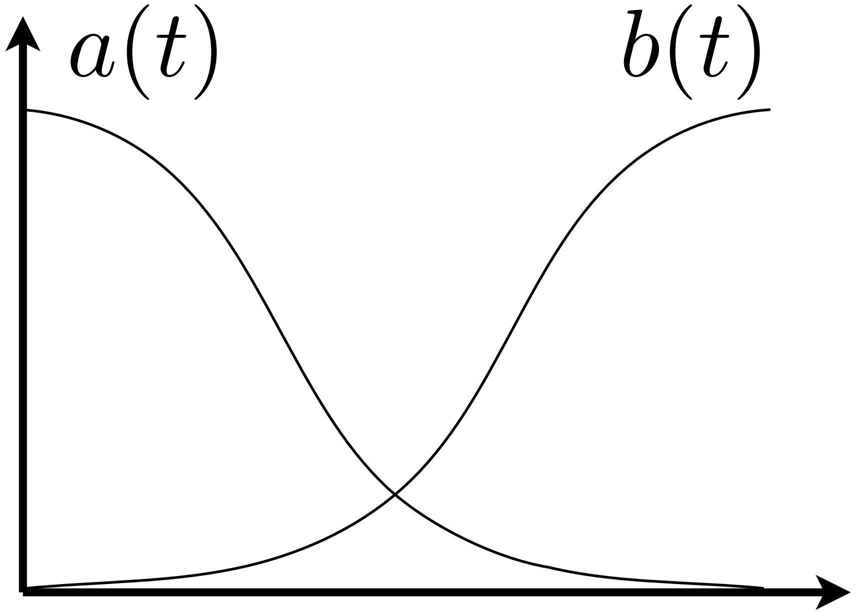
trivial state

solution

→→→→→

↑↓↓↑↓↑

adiabatic theorem



Feynman’s seminal idea ‘84

Mapping each step of quantum computation to each site!

$$\mathcal{H}_{\rm work} \otimes \mathcal{H}_{\rm clock}$$

working system for quantum computation

clock to track the step

Feynman's seminal idea '84

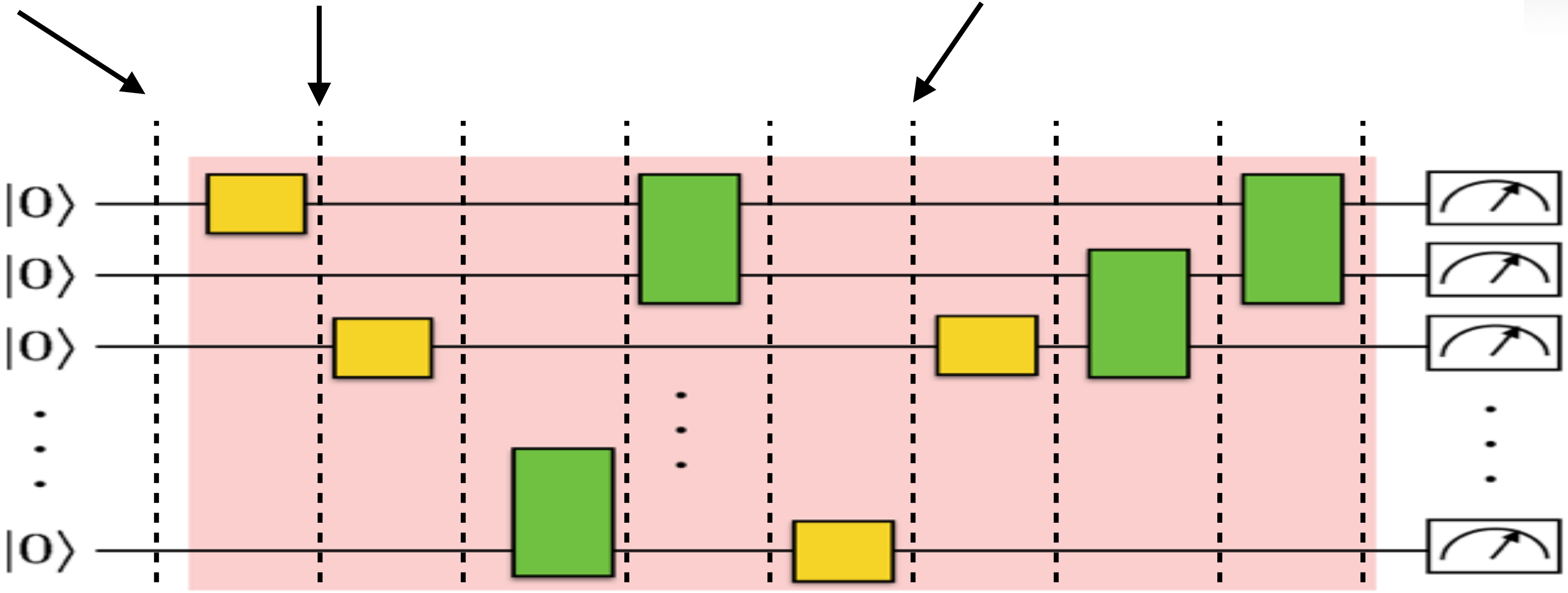
Mapping each step of quantum computation to each site!

$$\mathcal{H}_{\text{work}} \otimes \mathcal{H}_{\text{clock}}$$

working system for quantum computation

clock to track the step

$|0\rangle^{\otimes n}|0\rangle_{\text{c}}$ $\quad U_1|0\rangle^{\otimes n}|1\rangle_{\text{c}}$ $\quad \ldots \quad$ $U_t \cdots U_1|0\rangle^{\otimes n}|t\rangle_{\text{c}}$



Clock makes all theses intermediate states orthogonal!

Feynman’s seminal idea ‘84

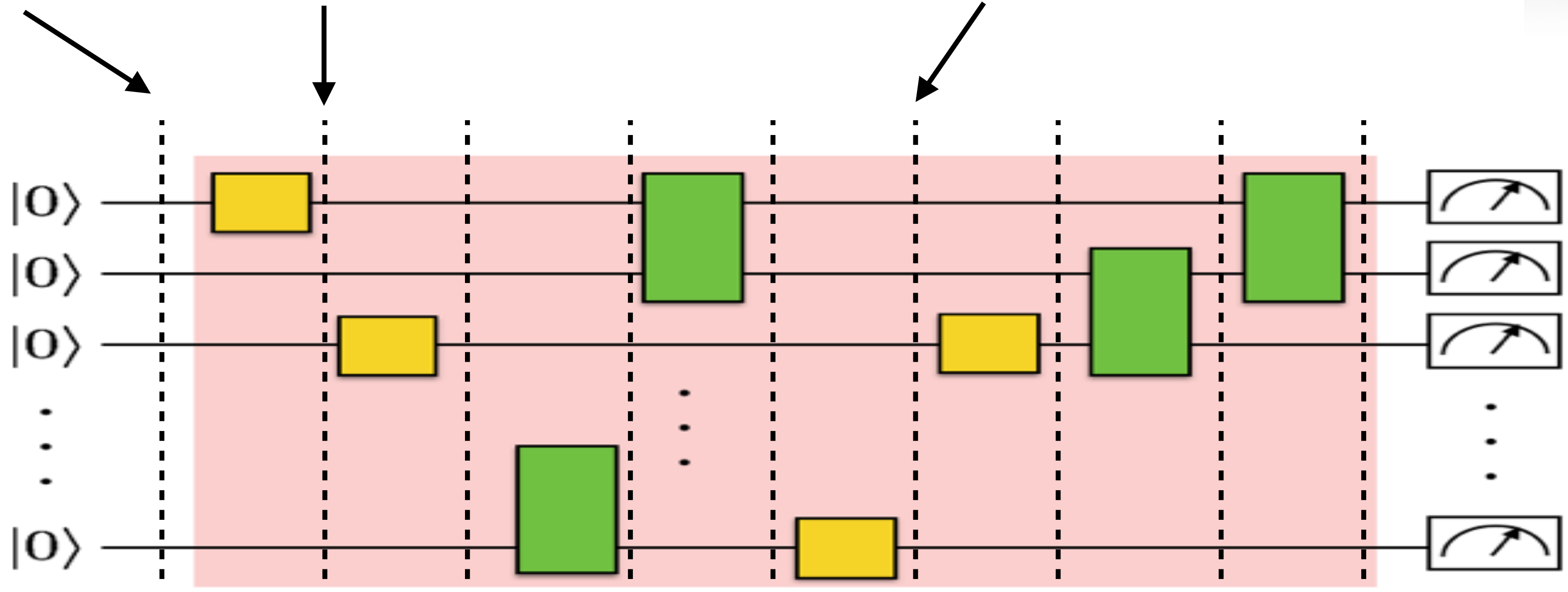
Mapping each step of quantum computation to each site!

$$\mathcal{H}_{\text{work}} \otimes \mathcal{H}_{\text{clock}}$$

working system for quantum computation

clock to track the step

$$|0\rangle^{\otimes n}|0\rangle_{\text{c}} \quad U_1|0\rangle^{\otimes n}|1\rangle_{\text{c}} \quad \ldots \quad U_t\cdots U_1|0\rangle^{\otimes n}|t\rangle_{\text{c}}$$



Clock makes all theses intermediate states orthogonal!

tight-binding Hamiltonian: $H = \frac{1}{2}\sum_i [(|i\rangle\langle i| + |i-1\rangle\langle i-1|) - (|i\rangle\langle i-1| + \text{h.c})]$

→ground state: $|\Psi\rangle = \frac{1}{\sqrt{N}}\sum_i |i\rangle$

Universality of non-stoqAQC

Aharonov et al ‘04

- energy penalty for the initial clock state:

$$H_{\text{initial}} = H_{\text{in}} + (I_c - |0\rangle\langle 0|_c),$$

- energy penalty for the initial state of the working system:

$$H_{\text{in}} = \sum_{i=1}^{n} |1\rangle\langle 1|_i \otimes |0\rangle\langle 0|_c$$

imposing initial state should be all 0s

Universality of non-stoqAQC

Aharonov et al ‘04

- energy penalty for the initial clock state:

$$H_{\text{initial}} = H_{\text{in}} + (I_c - |0\rangle\langle 0|_c),$$

- energy penalty for the initial state of the working system:

$$H_{\text{in}} = \sum_{i=1}^{n} |1\rangle\langle 1|_i \otimes |0\rangle\langle 0|_c$$

imposing initial state should be all 0s

- tight-binding Hamiltonian (Kitaev-Shen-Vyalyi ’02) :

site energy

hopping term

$$H_{\text{final}} = H_{\text{in}} + \sum_{t=1}^{T} \frac{1}{2}\left[|t\rangle\langle t|_c + |t-1\rangle\langle t-1|_c - \boxed{(U_t|t\rangle\langle t-1|_c + U_t^{\dagger}|t-1\rangle\langle t|_c)]}\right.$$

Feynman’s Hamiltonian

Universality of non-stoqAQC

Aharonov et al ‘04

- energy penalty for the initial clock state:

$$H_{\text{initial}} = H_{\text{in}} + (I_c - |0\rangle\langle 0|_c),$$

- energy penalty for the initial state of the working system:

$$H_{\text{in}} = \sum_{i=1}^{n} |1\rangle\langle 1|_i \otimes |0\rangle\langle 0|_c$$

imposing initial state should be all 0s

- tight-binding Hamiltonian (Kitaev-Shen-Vyalyi ’02) :

site energy

hopping term

$$H_{\text{final}} = H_{\text{in}} + \sum_{t=1}^{T} \frac{1}{2}[|t\rangle\langle t|_c + |t-1\rangle\langle t-1|_c - \boxed{(U_t|t\rangle\langle t-1|_c + U_t^{\dagger}|t-1\rangle\langle t|_c)]},$$

Feynman’s Hamiltonian

- adiabatic quantum computation:

$$H(s) = (1-s)H_{\text{initial}} + sH_{\text{final}},$$

The lowest energy gap is always lower bounded by an inverse of polynomial.

Universality of non-stoqAQC

Aharonov et al ‘04

- tight-binding Hamiltonian (Kitaev-Shen-Vyalyi ’02) :

$$H_{\text{final}} = H_{\text{in}} + \sum_{t=1}^{T} \frac{1}{2}\left[|t\rangle\langle t|_c + |t-1\rangle\langle t-1|_c - \boxed{(U_t|t\rangle\langle t-1|_c + U_t^{\dagger}|t-1\rangle\langle t|_c)]}\right.,$$

Feynman’s Hamiltonian

The ground state of the final Hamiltonian (history state):

$$|\Psi\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^{T} U_t \cdots U_1 |0\rangle^{\otimes n} |\, t \,\rangle_{\mathrm{c}}$$

Universality of non-stoqAQC

Aharonov et al ‘04

- tight-binding Hamiltonian (Kitaev-Shen-Vyalyi ’02) :

$$H_{\text{final}} = H_{\text{in}} + \sum_{t=1}^{T} \frac{1}{2}[|t\rangle\langle t|_c + |t-1\rangle\langle t-1|_c - \boxed{(U_t|t\rangle\langle t-1|_c + U_t^{\dagger}|t-1\rangle\langle t|_c)],}$$

Feynman’s Hamiltonian

The ground state of the final Hamiltonian (history state):

$$|\Psi\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^{T} U_t \cdots U_1 |0\rangle^{\otimes n} |\, t \,\rangle_{\mathrm{c}}$$

If the propagator Hamiltonian is restricted into stoquastic terms, how quantum computation would be changed?

Restriction to stoquastic Hamiltonians

off-diagonal terms:

$$-\left(U_t|t\rangle\langle t-1|_c + U_t^\dagger|t-1\rangle\langle t|_c\right)$$

Each element of U should be non negative!

Restriction to stoquastic Hamiltonians

off-diagonal terms:

$$-\left(U_t|t\rangle\langle t-1|_c + U_t^\dagger|t-1\rangle\langle t|_c\right)$$

Each element of U should be non negative!

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \mathrm{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

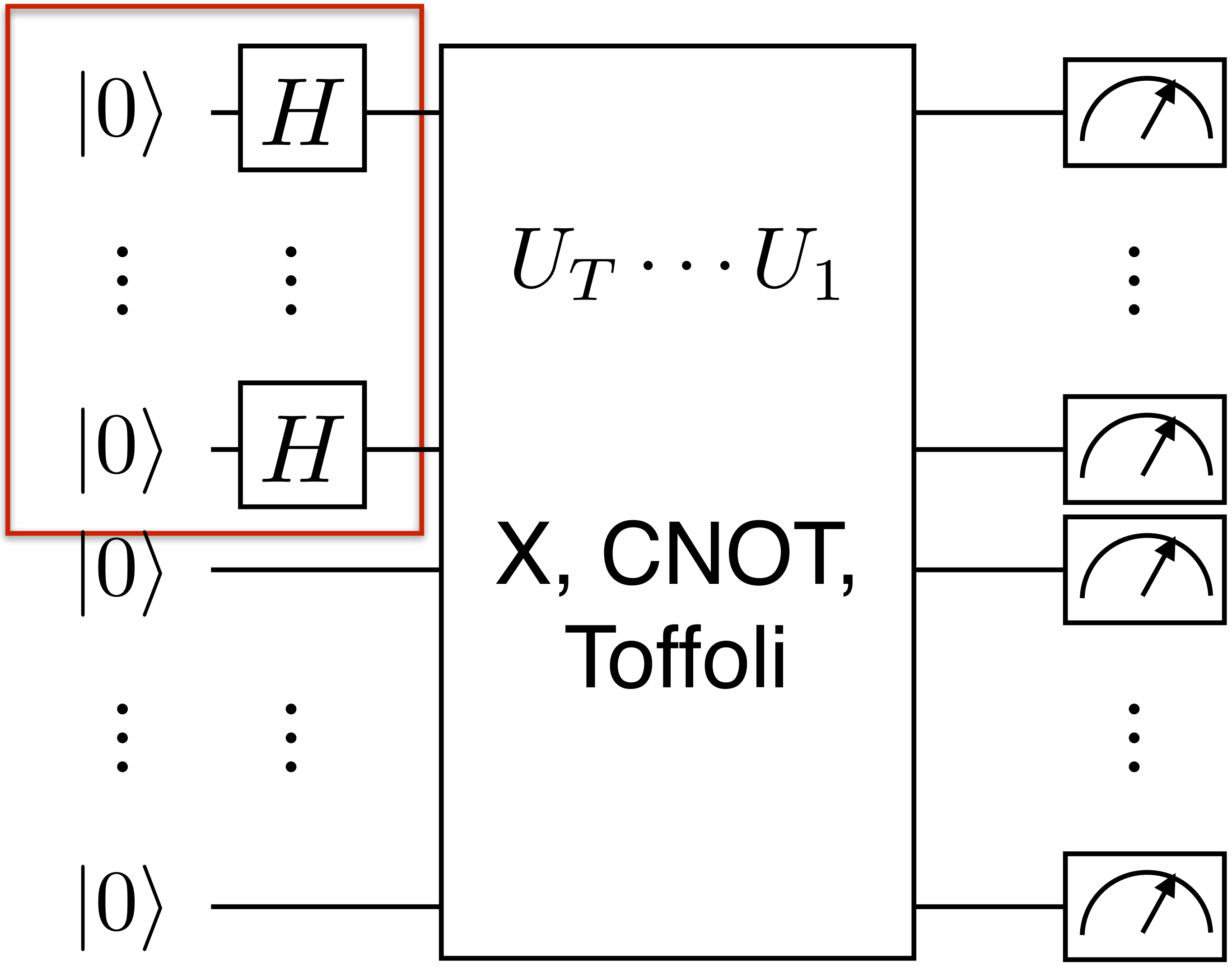
$$\text{Toffoli} \quad (I^{\otimes 2} - |11\rangle\langle 11|) \otimes I + |11\rangle\langle 11| \otimes X$$

Elements of *U* are non negative, iff *U* is a unitary version of reversible classical computation.

Hamiltonian complexity of stoquastic Hamiltonian [Bravyi, DiVencenzo, Oliveira, and Terhal (2008)]

Stoquastic AQC as a sampling problem

Quantum circuit that can be simulated by stoqAQC.

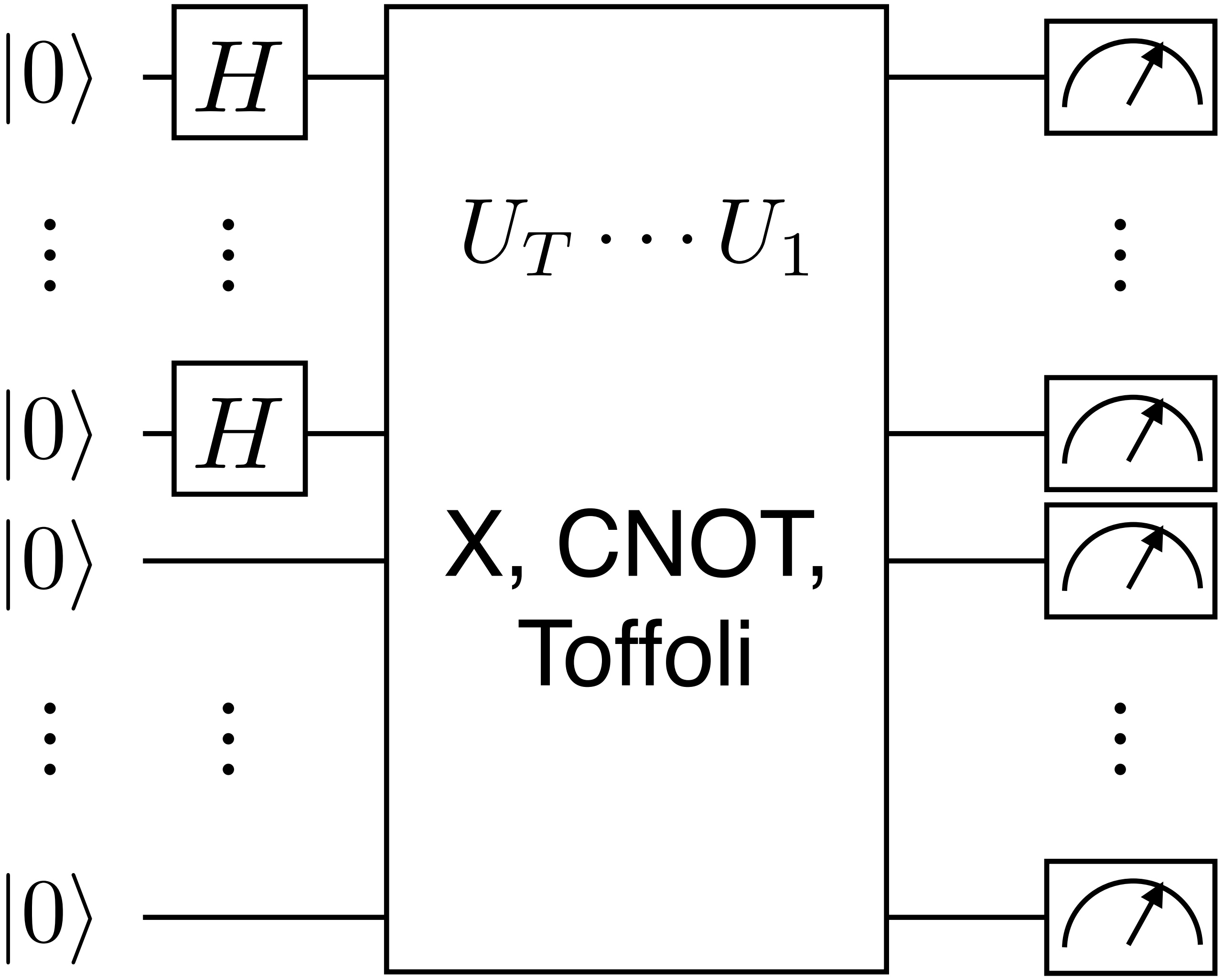


Initial Hadamard transformations are allowed.

Arbitrary single-qubit measurements!

Unitary gates for reversible classical computation.

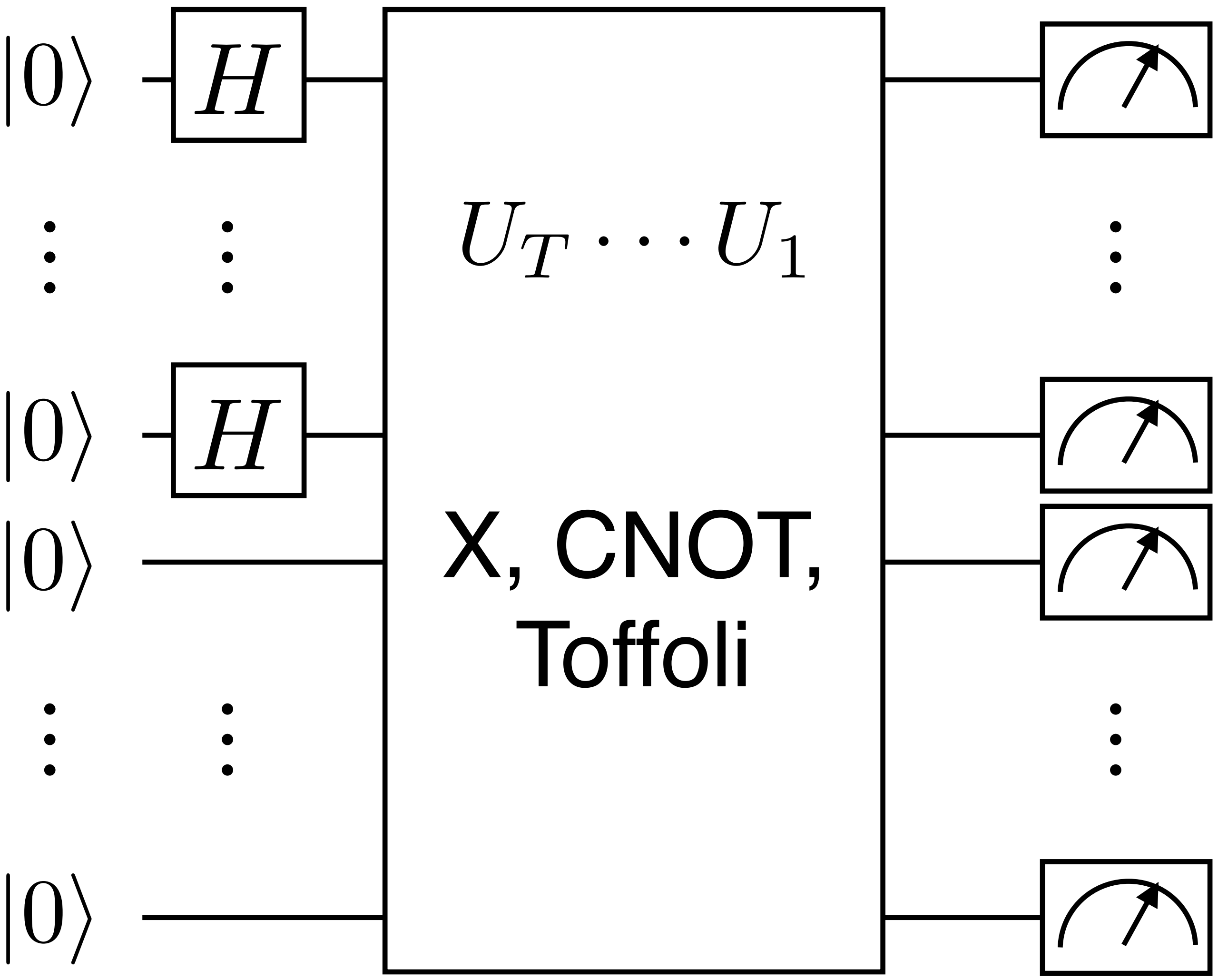
Universal QC with stoqAQC

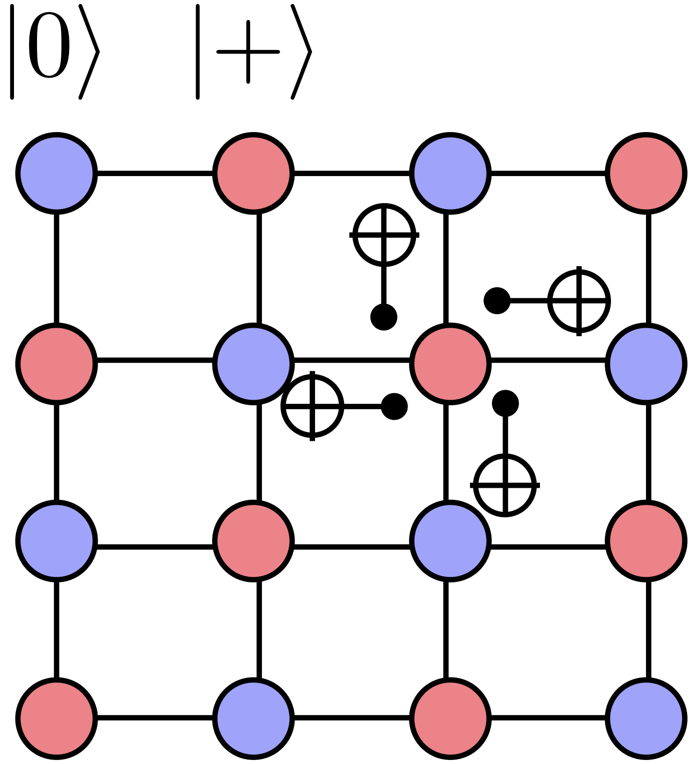


arbitrary single-qubit measurements

measurement-based quantum computation（Graph state, hyper graph state）

Universal QC with stoqAQC

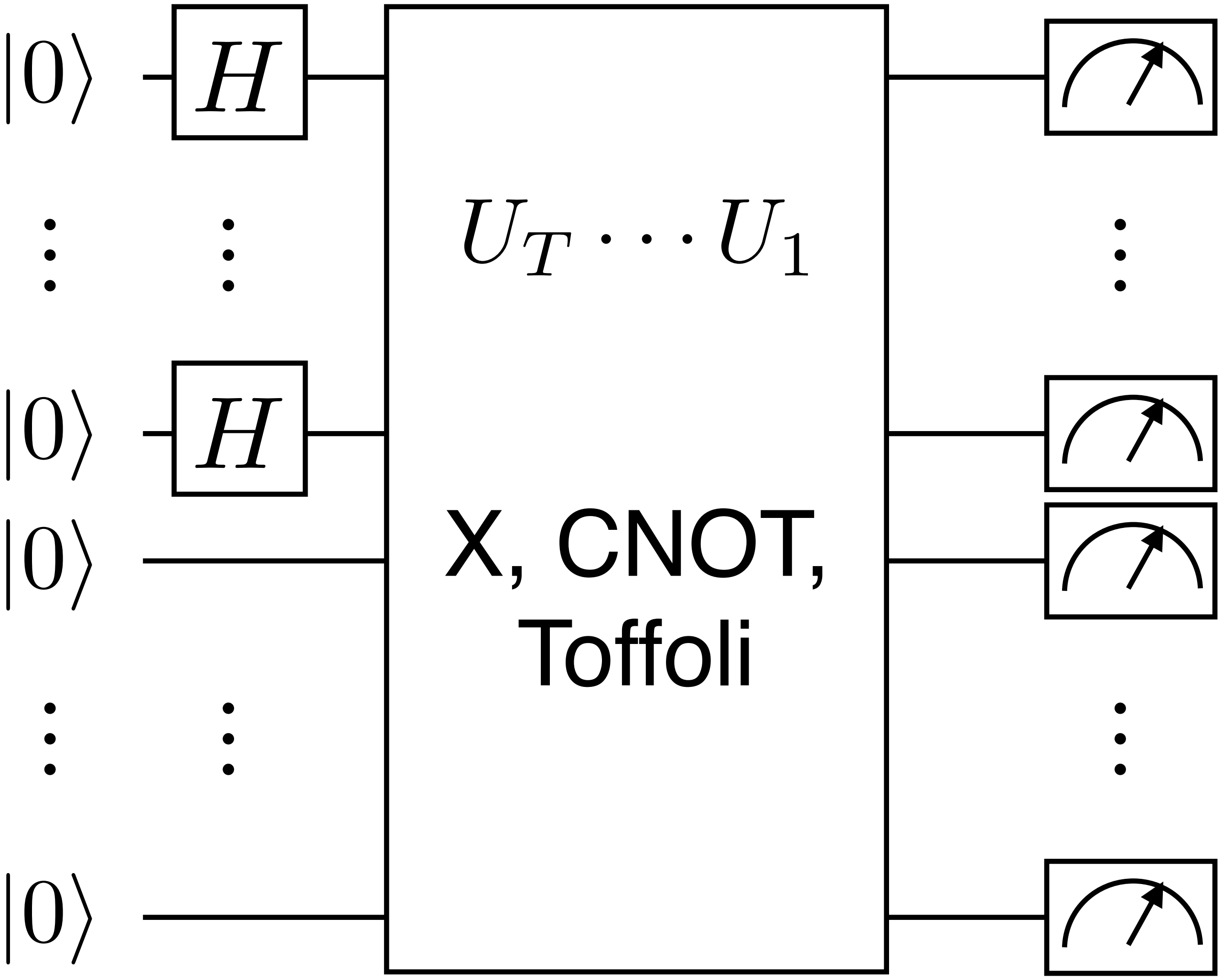




cluster state on a square lattice = universal resource for MBQC

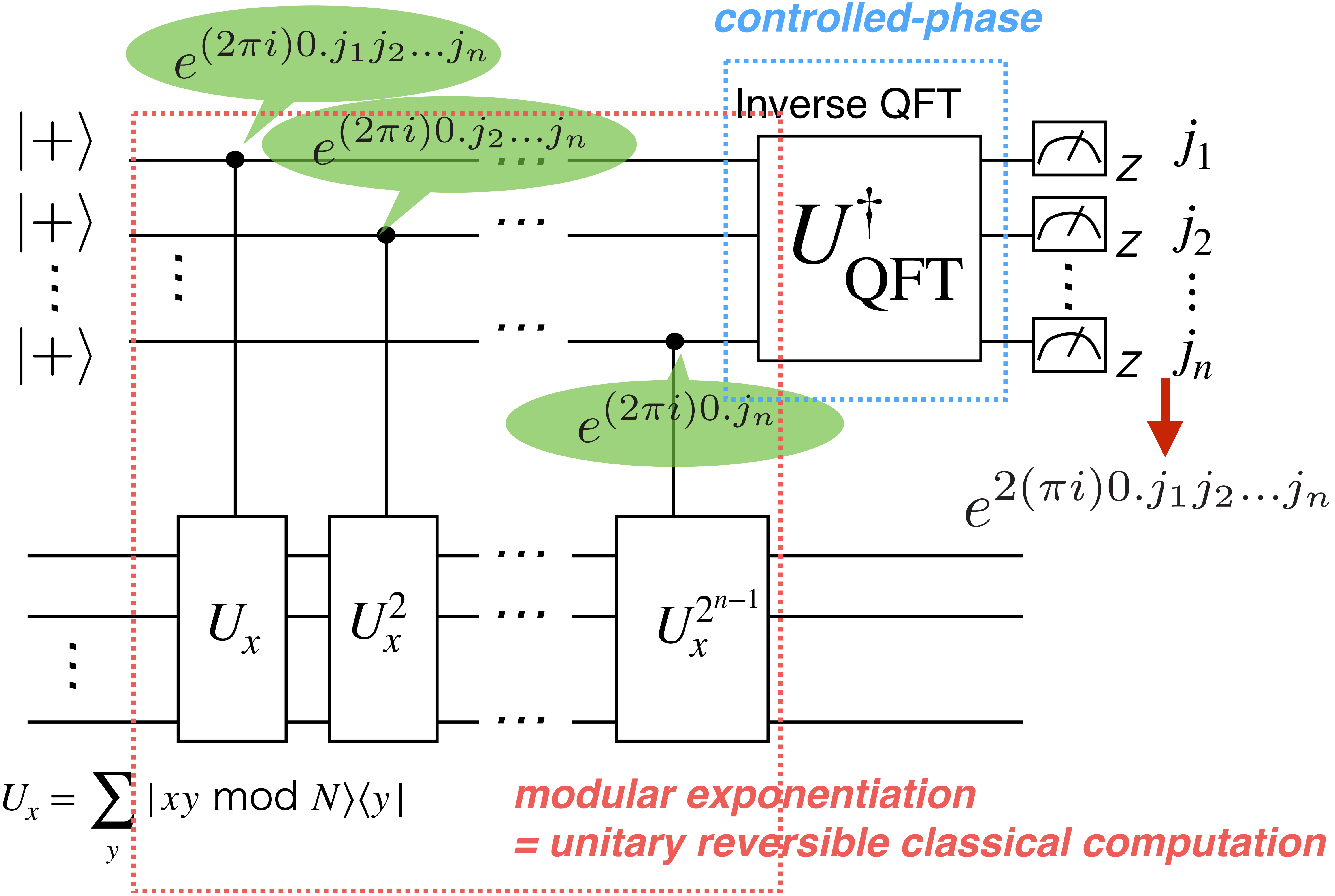
StoqAQC with adaptive measurements is can simulate universal QC.

Universal QC with stoqAQC



With **non-adaptive**
single-qubit measurements?

Kitaev's Phase estimation and Shor's algorithm



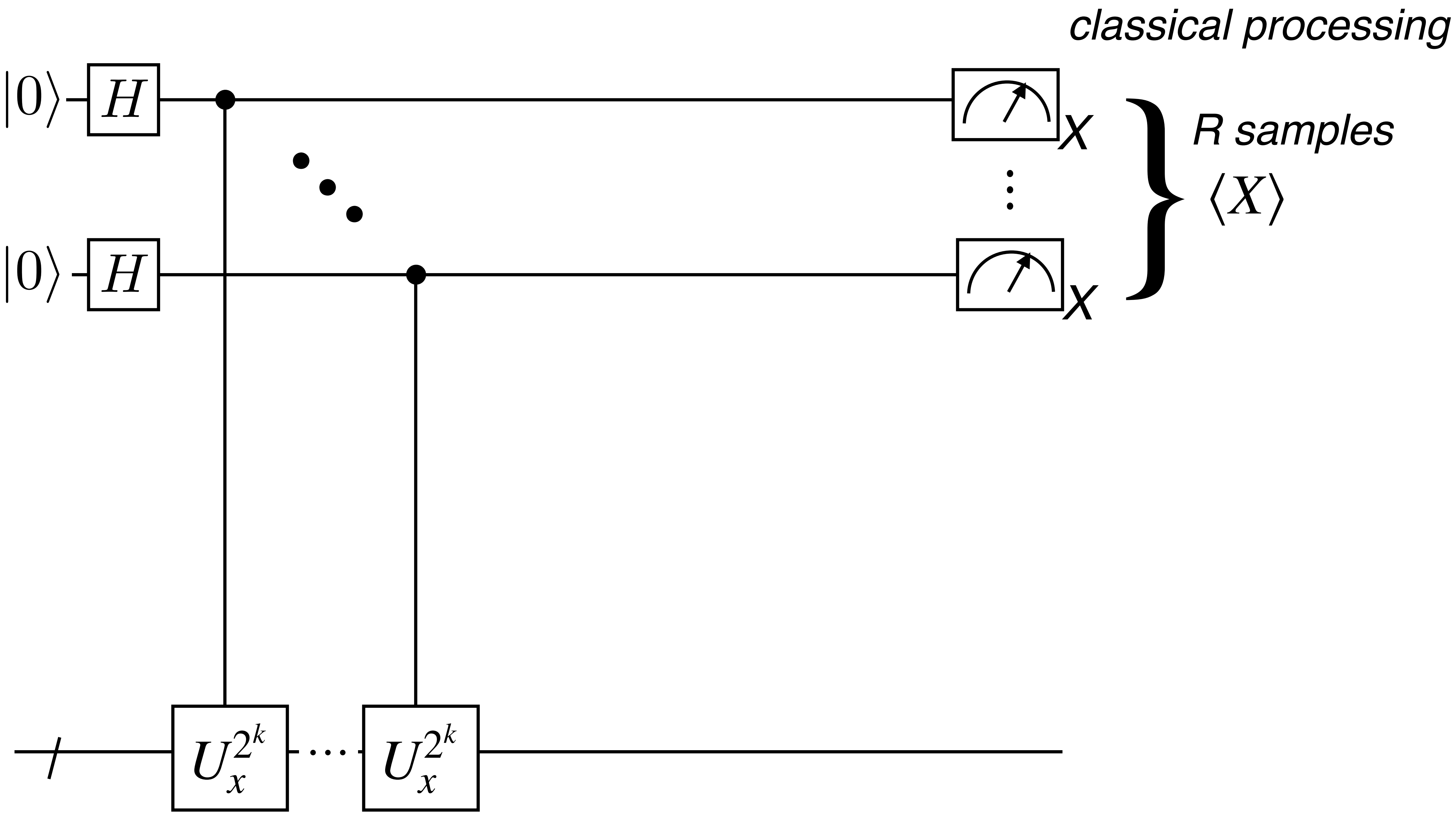
controlled-phase

Inverse QFT

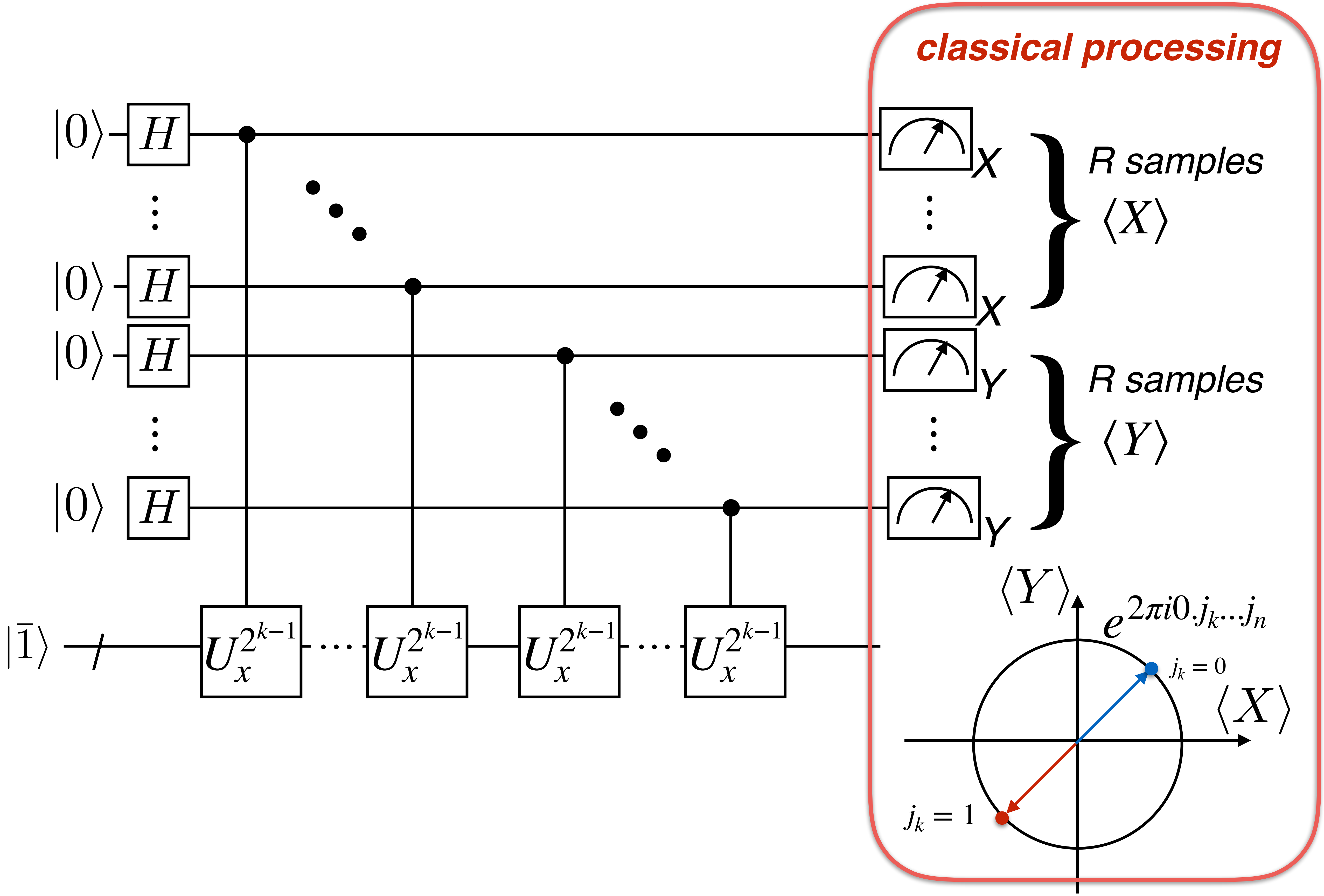
$U_x = \sum_y |xy \text{ mod } N\rangle\langle y|$

modular exponentiation
= unitary reversible classical computation

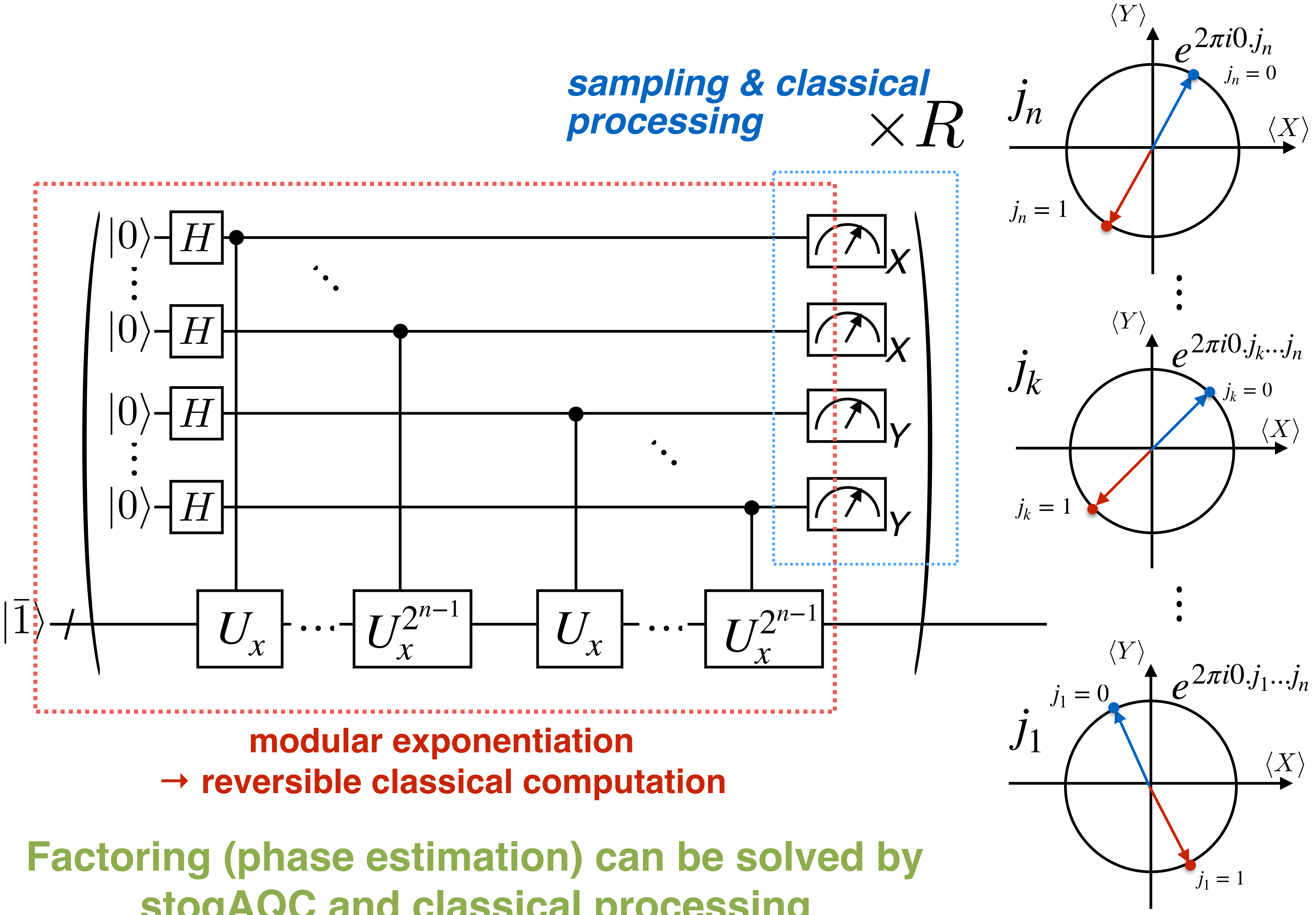
Quantum-classical hybrid phase estimation



Quantum-classical hybrid phase estimation



Quantum-classical hybrid phase estimation



sampling & classical processing

modular exponentiation
→ reversible classical computation

Factoring (phase estimation) can be solved by stoqAQC and classical processing

Quantum-classical hybrid phase estimation

StoqAQC with simultaneous single-qubit measurements
→ non-universal model quantum computation

Quantum-classical hybrid algorithm allows us to
solve nontrivial problems like factoring etc.
(Without classical processing, stoqAQC with
simultaneous non-standard basis measurements
could not decide the problem.)

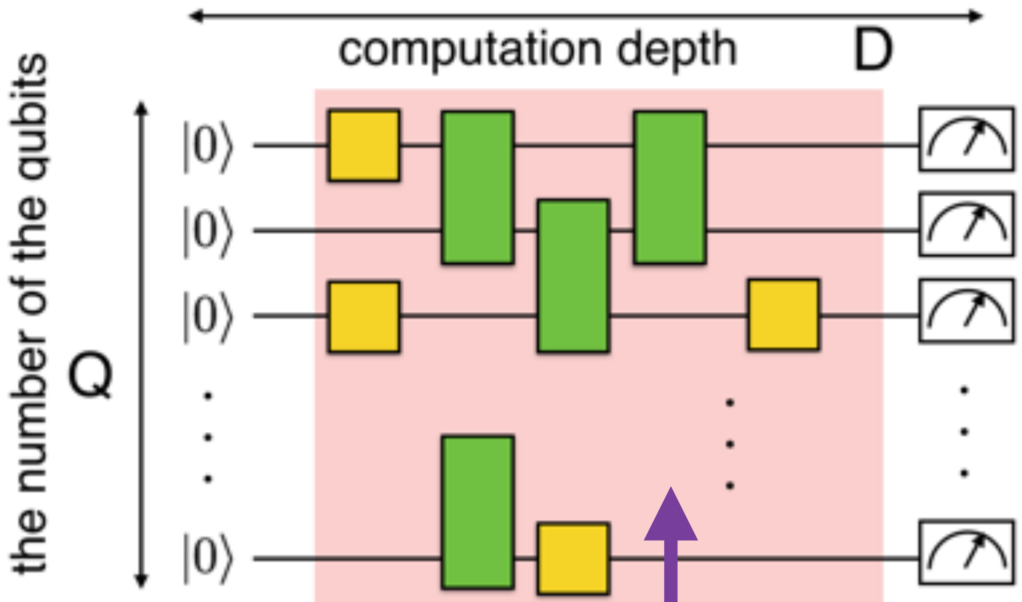
Outline

- **Advantage of quantum-classical hybrid algorithm**
  - Adiabatic quantum computation and quantum circuit model
  - Characterization of stoquastic adiabatic quantum computation
  - Quantum speedup in stoqAQC (sampling-based factoring & phase estimation)
- **Parameter tuning for quantum-classical variational algorithm**
  - gradient-based optimization
  - gradient-free optimization designed for hardware efficient ansatz
  - Numerical comparisons of gradient-based and -free optimizations.

Quantum-classical hybrid algorithm

Quantum computer

trial function of variational methods



sampling

classical computer

classical easy task

parameter update

Approximated optimization：QAOA (quantum approximate optimization algo

E. Farhi, J. Goldstone, and S. Gutmann, arXiv preprint arXiv:1411.4028 (2014).

Ground state：VQE (variational quantum eigensolver)

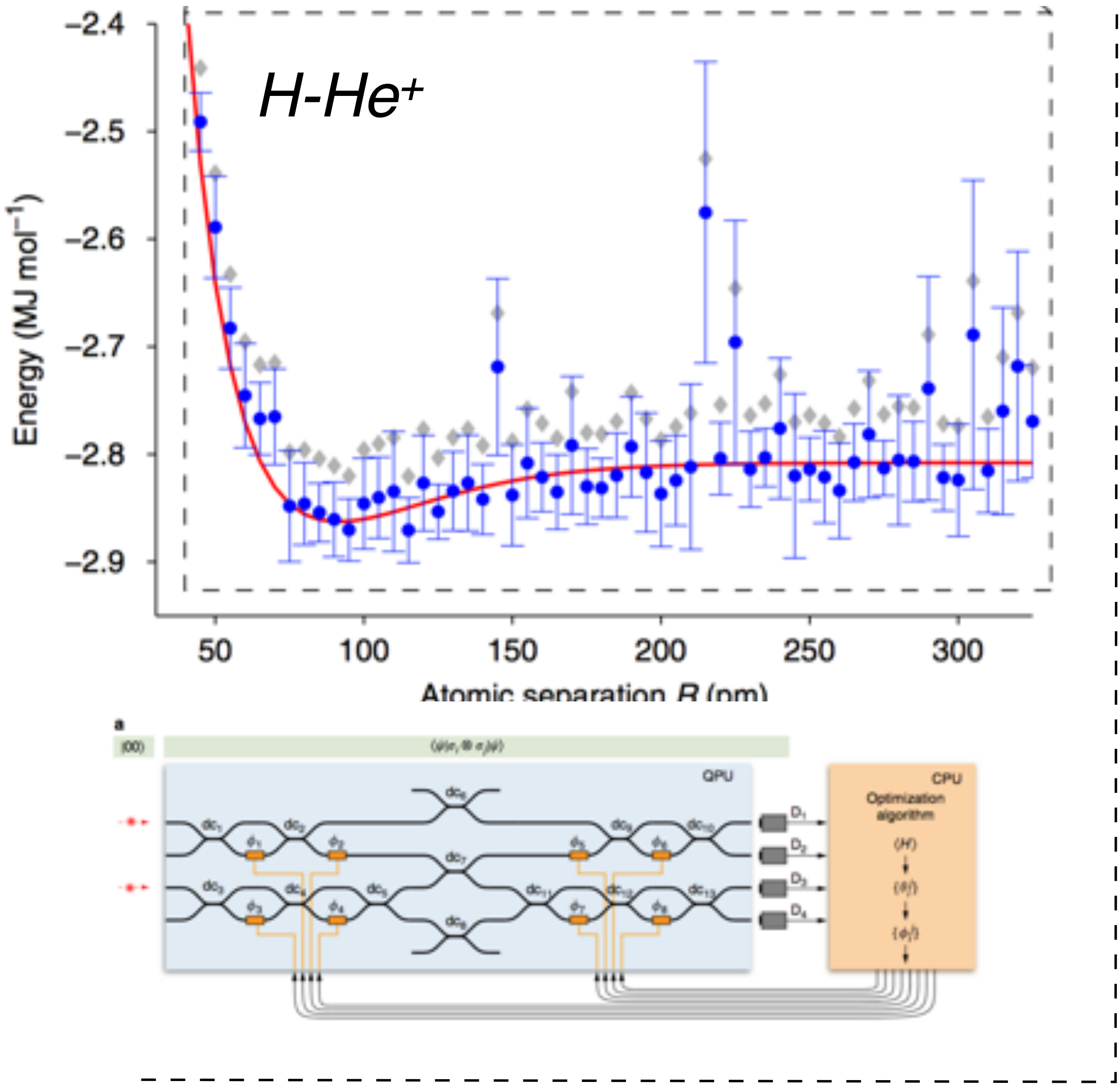
A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'brien, Nature Communications 5, 4213 (2014).

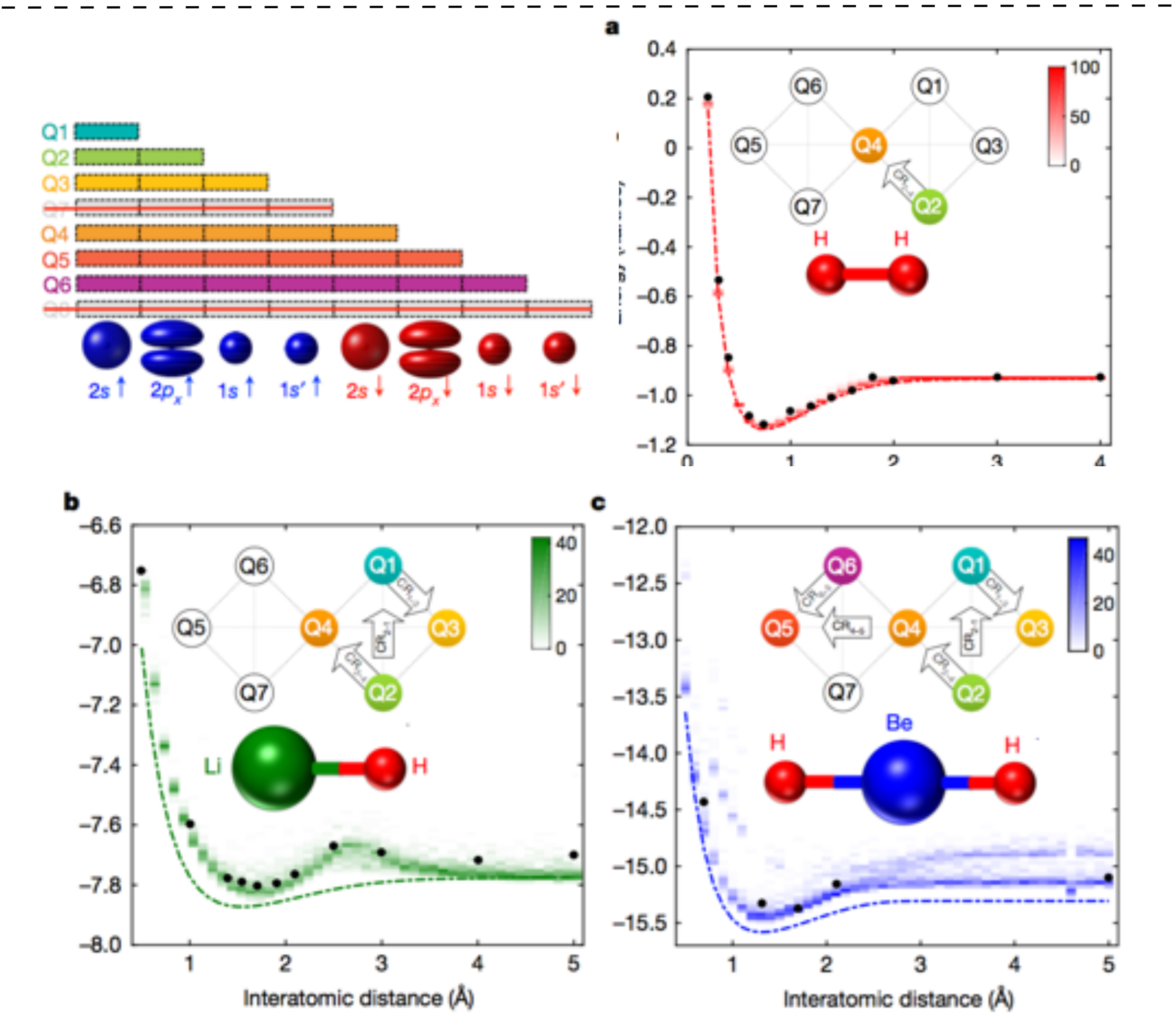
Supervised machine learning：QCL (quantum circuit learning)

K. Mitarai, M. Negoro, M. Kitagawa, and K. Fujii Phys. Rev. A **98**, 032309 (2018).

Quantum-classical hybrid algorithm: variational quantum eigensolver

“A variational eigenvalue solver on a photonic quantum processor”
Peruzzo, McClean *et al,* Nature Communication **5**:4213 (2014)





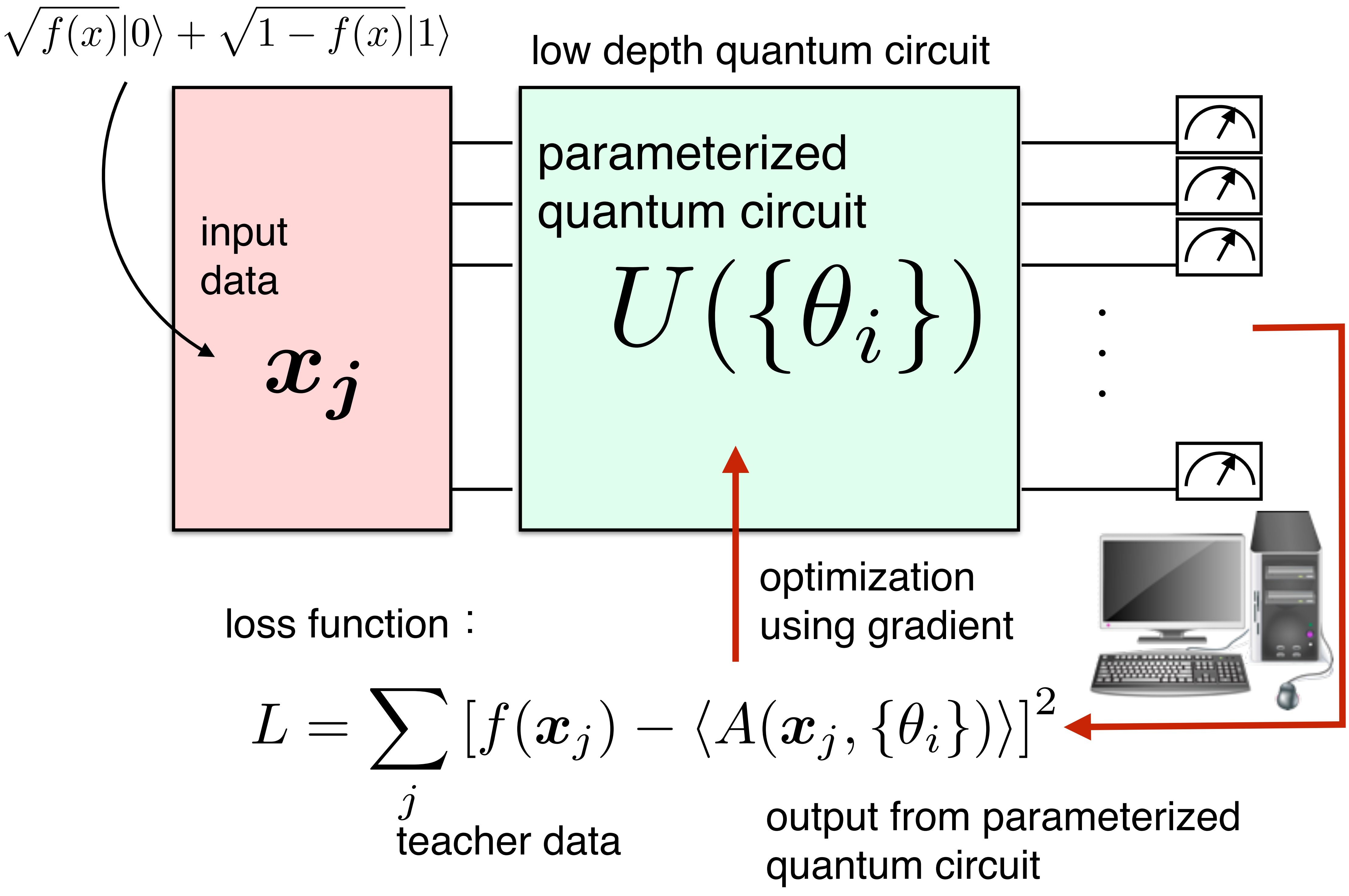
“Hardware-efficient Quantum Optimizer for Small Molecules and Quantum Magnets”
Kandala, Mezzacapo *et al,* Nature **549** 242 (2017)

Variational algorithms

	model・ trial function	**tuning・ optimization**	**task**
Neural netwrok	W, tanh()	backpropagation (gradient)	machine learning
Rayleigh-Ritz (Hartree-Fock)	orthogonal functions (Slater determinant)	diagonalization of Hermitian matrix (HF equation)	ground state
Tensor network (MPS, PEPS, MERA)	tensor network	singular value decomposition	ground state (dynamics)
Variational quantum algorithms	parameterized quantum circuit	**gradient?** [Mitarai-Negoro-Kitagawa-KF '18] **other?** [Nakanishi-KF-Todo '19]	machine learning ground state dynamics

Quantum circuit learning: supervised learning on near-term quantum devices

K. Mitarai, M. Negoro, M. Kitagawa, and **KF** Phys. Rev. A **98**, 032309 (2018).
and many others



$\sqrt{f(x)}|0\rangle + \sqrt{1-f(x)}|1\rangle$

low depth quantum circuit

input data

$\boldsymbol{x}_{\boldsymbol{j}}$

parameterized quantum circuit

$U(\{\theta_i\})$

optimization using gradient

loss function :

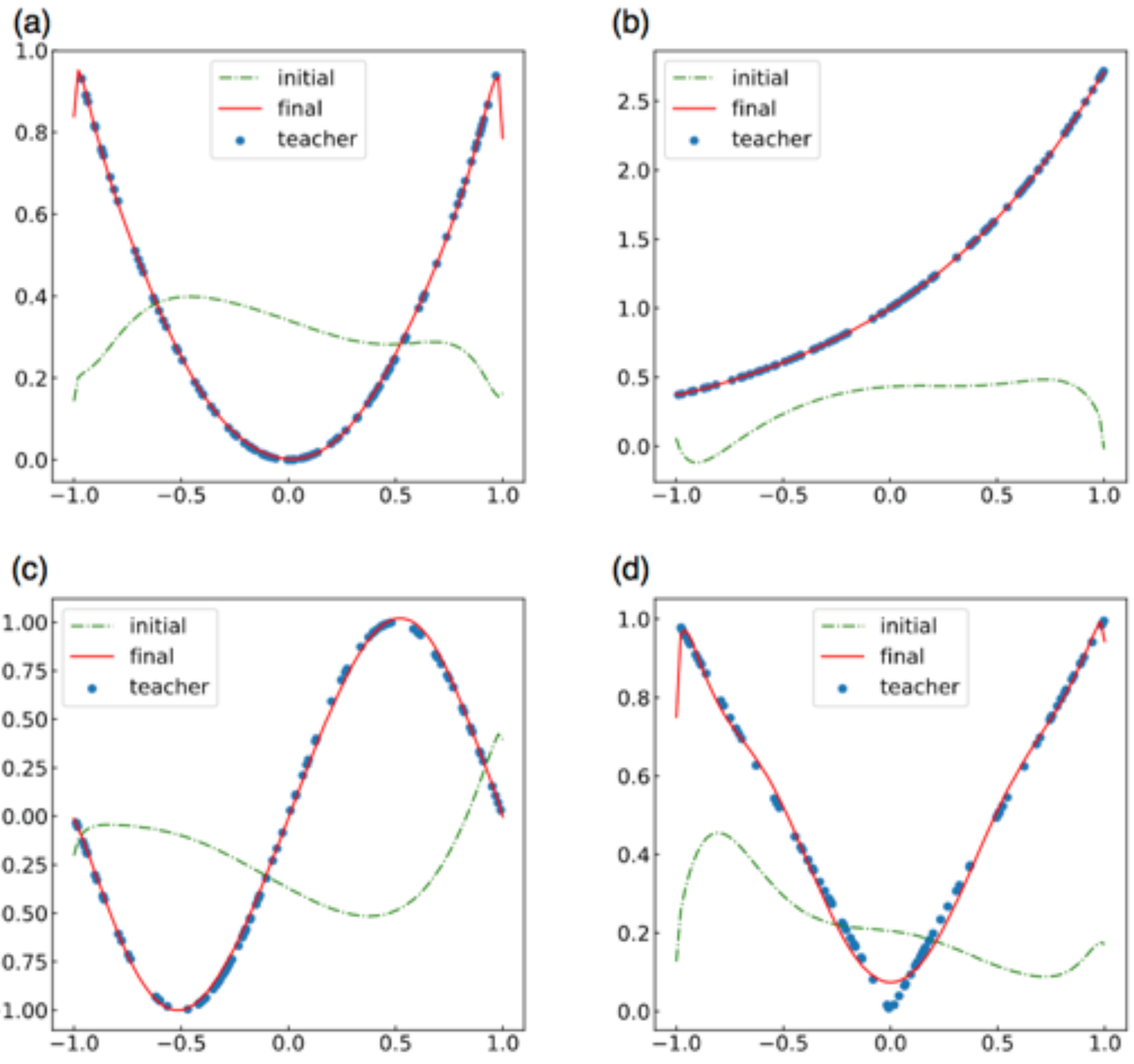
$$L = \sum_j [f(\boldsymbol{x}_j) - \langle A(\boldsymbol{x}_j, \{\theta_i\})\rangle]^2$$

teacher data

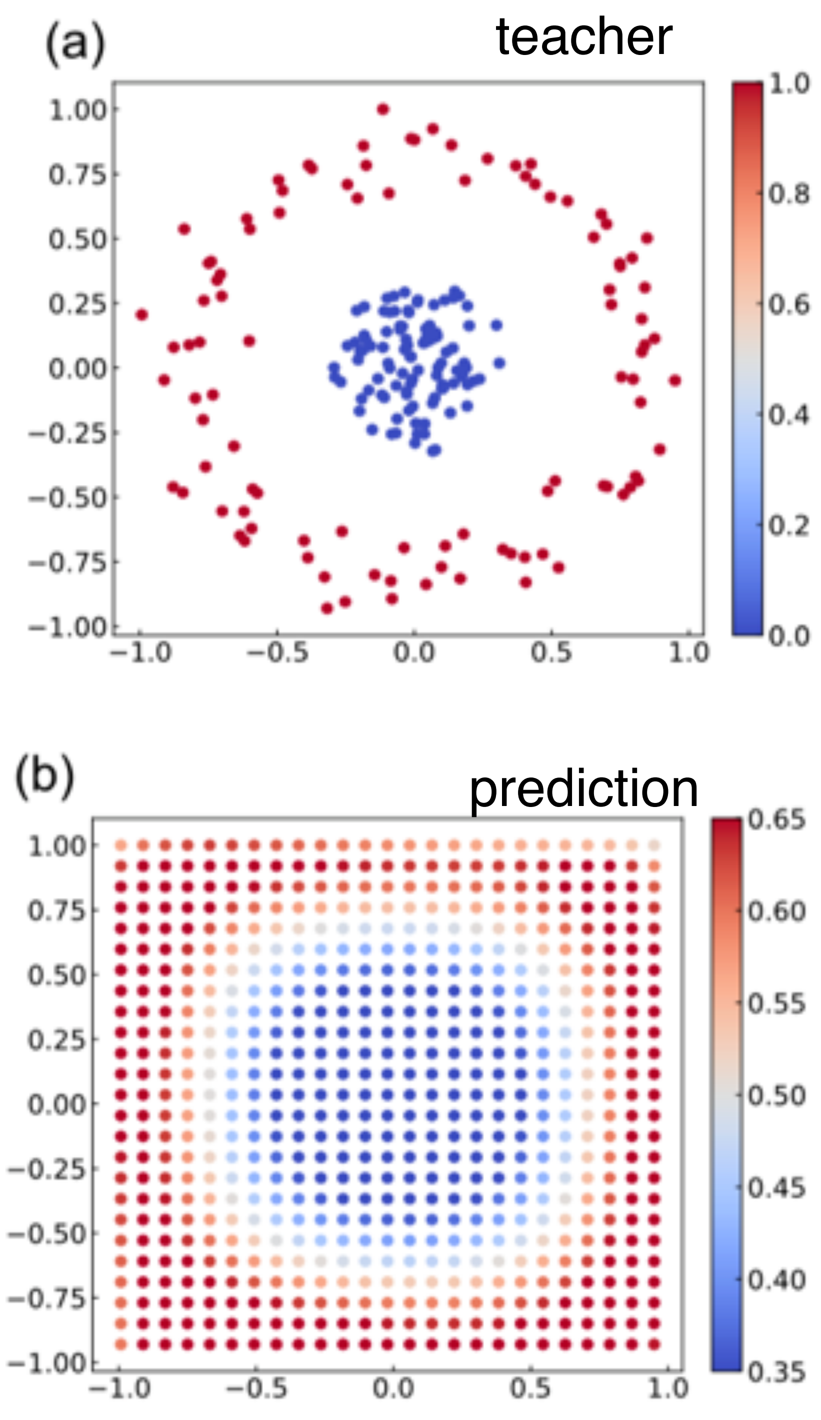
output from parameterized quantum circuit

Quantum circuit learning: supervised learning on near-term quantum devices

K. Mitarai, M. Negoro, M. Kitagawa, and **KF** Phys. Rev. A **98**, 032309 (2018).
and many others



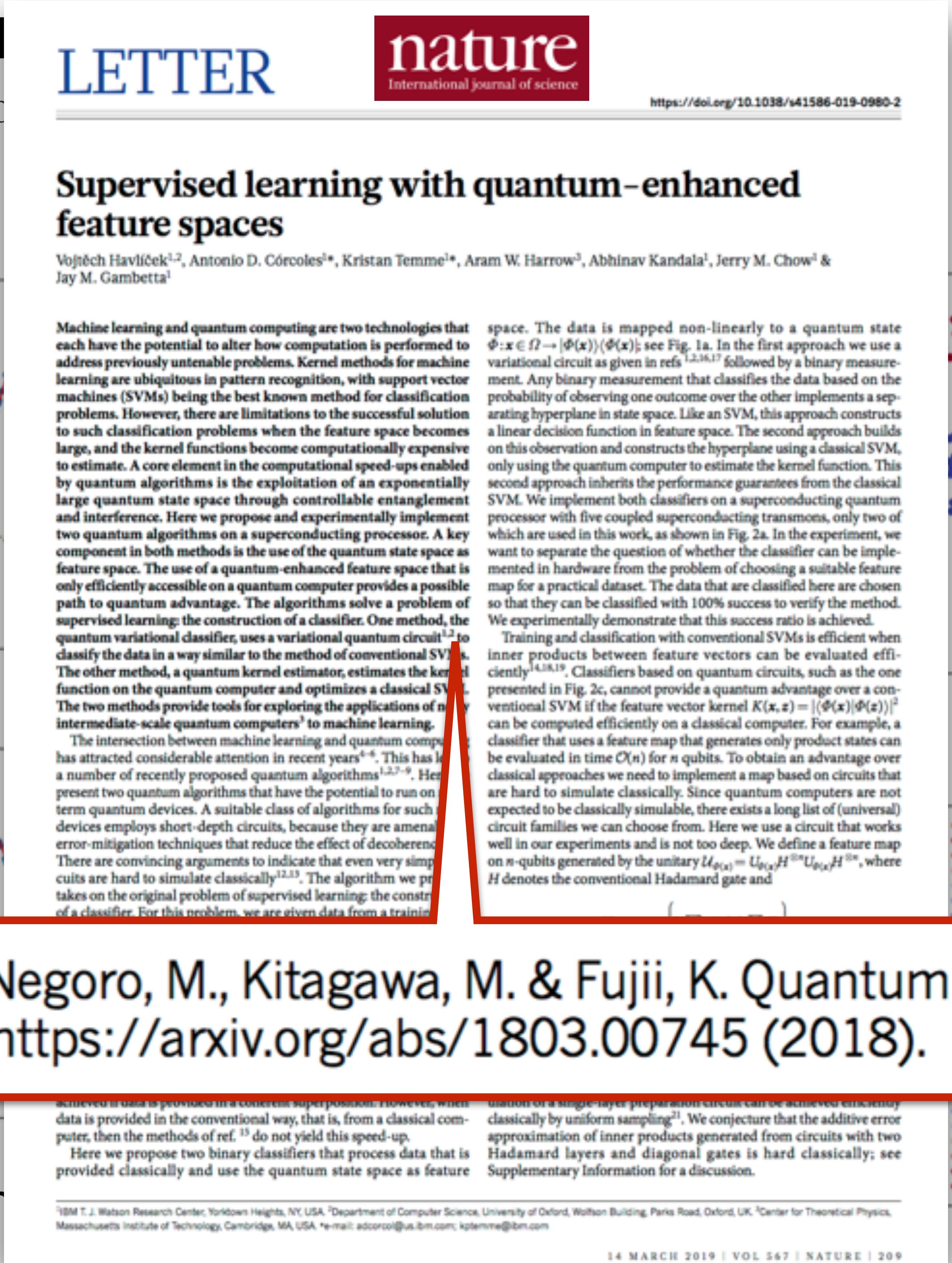
Generalization of nonlinear functions



nonlinear classification

Quantum circuit learning: supervised learning on near-te

K. Mitarai, M. Nego (2018).
and many others



LETTER

nature
International journal of science

https://doi.org/10.1038/s41586-019-0980-2

Supervised learning with quantum-enhanced feature spaces

Vojtěch Havlíček[1,2], Antonio D. Córcoles[1]*, Kristan Temme[1]*, Aram W. Harrow[3], Abhinav Kandala[1], Jerry M. Chow[1] &
Jay M. Gambetta[1]

Machine learning and quantum computing are two technologies that each have the potential to alter how computation is performed to address previously untenable problems. Kernel methods for machine learning are ubiquitous in pattern recognition, with support vector machines (SVMs) being the best known method for classification problems. However, there are limitations to the successful solution to such classification problems when the feature space becomes large, and the kernel functions become computationally expensive to estimate. A core element in the computational speed-ups enabled by quantum algorithms is the exploitation of an exponentially large quantum state space through controllable entanglement and interference. Here we propose and experimentally implement two quantum algorithms on a superconducting processor. A key component in both methods is the use of the quantum state space as feature space. The use of a quantum-enhanced feature space that is only efficiently accessible on a quantum computer provides a possible path to quantum advantage. The algorithms solve a problem of supervised learning: the construction of a classifier. One method, the quantum variational classifier, uses a variational quantum circuit[1,2] to classify the data in a way similar to the method of conventional SV s. The other method, a quantum kernel estimator, estimates the ker el function on the quantum computer and optimizes a classical SV . The two methods provide tools for exploring the applications of n y intermediate-scale quantum computers[3] to machine learning.

The intersection between machine learning and quantum compu has attracted considerable attention in recent years[4–6]. This has l a number of recently proposed quantum algorithms[1,2,7–9]. He present two quantum algorithms that have the potential to run on term quantum devices. A suitable class of algorithms for such devices employs short-depth circuits, because they are amena error-mitigation techniques that reduce the effect of decoherenc There are convincing arguments to indicate that even very simp cuits are hard to simulate classically[12,13]. The algorithm we pr takes on the original problem of supervised learning: the constr of a classifier. For this problem, we are given data from a trainin

data is provided in the conventional way, that is, from a classical computer, then the methods of ref. [15] do not yield this speed-up.

Here we propose two binary classifiers that process data that is provided classically and use the quantum state space as feature space. The data is mapped non-linearly to a quantum state $\Phi: x \in \Omega \rightarrow |\Phi(x)\rangle\langle\Phi(x)|$; see Fig. 1a. In the first approach we use a variational circuit as given in refs [1,2,16,17] followed by a binary measurement. Any binary measurement that classifies the data based on the probability of observing one outcome over the other implements a separating hyperplane in state space. Like an SVM, this approach constructs a linear decision function in feature space. The second approach builds on this observation and constructs the hyperplane using a classical SVM, only using the quantum computer to estimate the kernel function. This second approach inherits the performance guarantees from the classical SVM. We implement both classifiers on a superconducting quantum processor with five coupled superconducting transmons, only two of which are used in this work, as shown in Fig. 2a. In the experiment, we want to separate the question of whether the classifier can be implemented in hardware from the problem of choosing a suitable feature map for a practical dataset. The data that are classified here are chosen so that they can be classified with 100% success to verify the method. We experimentally demonstrate that this success ratio is achieved.

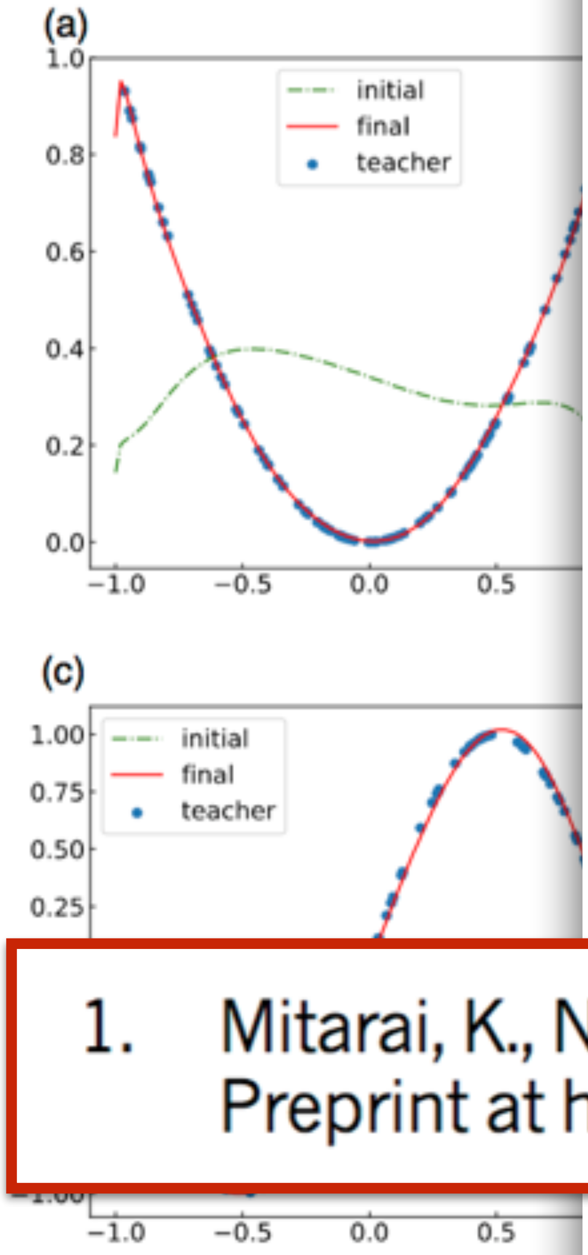
Training and classification with conventional SVMs is efficient when inner products between feature vectors can be evaluated efficiently[14,18,19]. Classifiers based on quantum circuits, such as the one presented in Fig. 2c, cannot provide a quantum advantage over a conventional SVM if the feature vector kernel $K(x,z) = |\langle\Phi(x)|\Phi(z)\rangle|^2$ can be computed efficiently on a classical computer. For example, a classifier that uses a feature map that generates only product states can be evaluated in time $\mathcal{O}(n)$ for n qubits. To obtain an advantage over classical approaches we need to implement a map based on circuits that are hard to simulate classically. Since quantum computers are not expected to be classically simulable, there exists a long list of (universal) circuit families we can choose from. Here we use a circuit that works well in our experiments and is not too deep. We define a feature map on n-qubits generated by the unitary $\mathcal{U}_{\Phi(x)} = U_{\Phi(x)}H^{\otimes n}U_{\Phi(x)}H^{\otimes n}$, where H denotes the conventional Hadamard gate and

classically by uniform sampling[21]. We conjecture that the additive error approximation of inner products generated from circuits with two Hadamard layers and diagonal gates is hard classically; see Supplementary Information for a discussion.

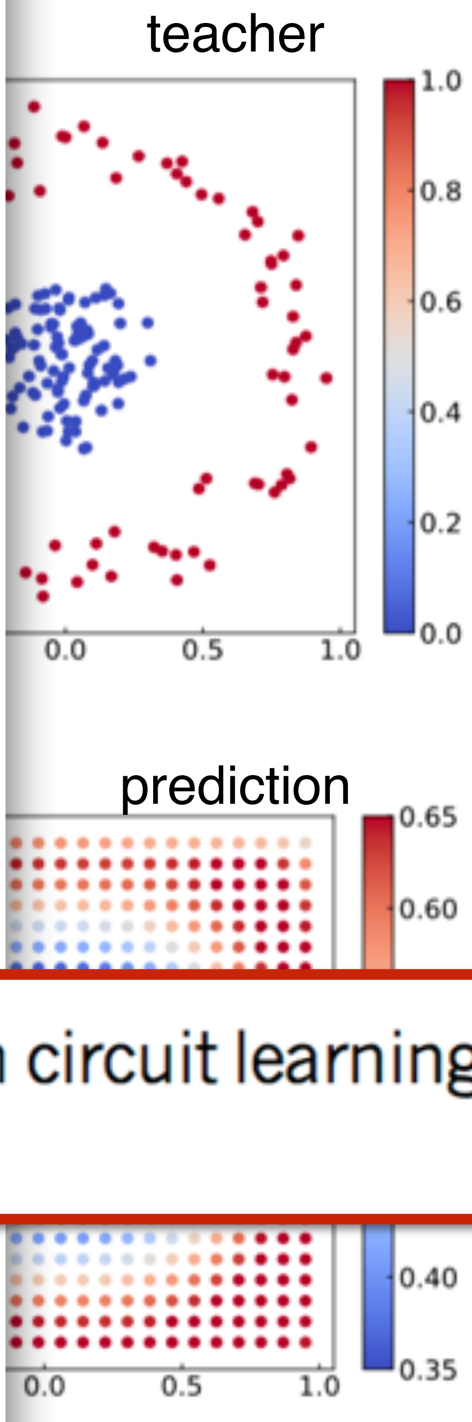
---

[1]IBM T. J. Watson Research Center, Yorktown Heights, NY, USA. [2]Department of Computer Science, University of Oxford, Wolfson Building, Parks Road, Oxford, UK. [3]Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA, USA. *e-mail: adcorcol@us.ibm.com; kptemme@ibm.com

1. Mitarai, K., Negoro, M., Kitagawa, M. & Fujii, K. Quantum circuit learning. Preprint at https://arxiv.org/abs/1803.00745 (2018).

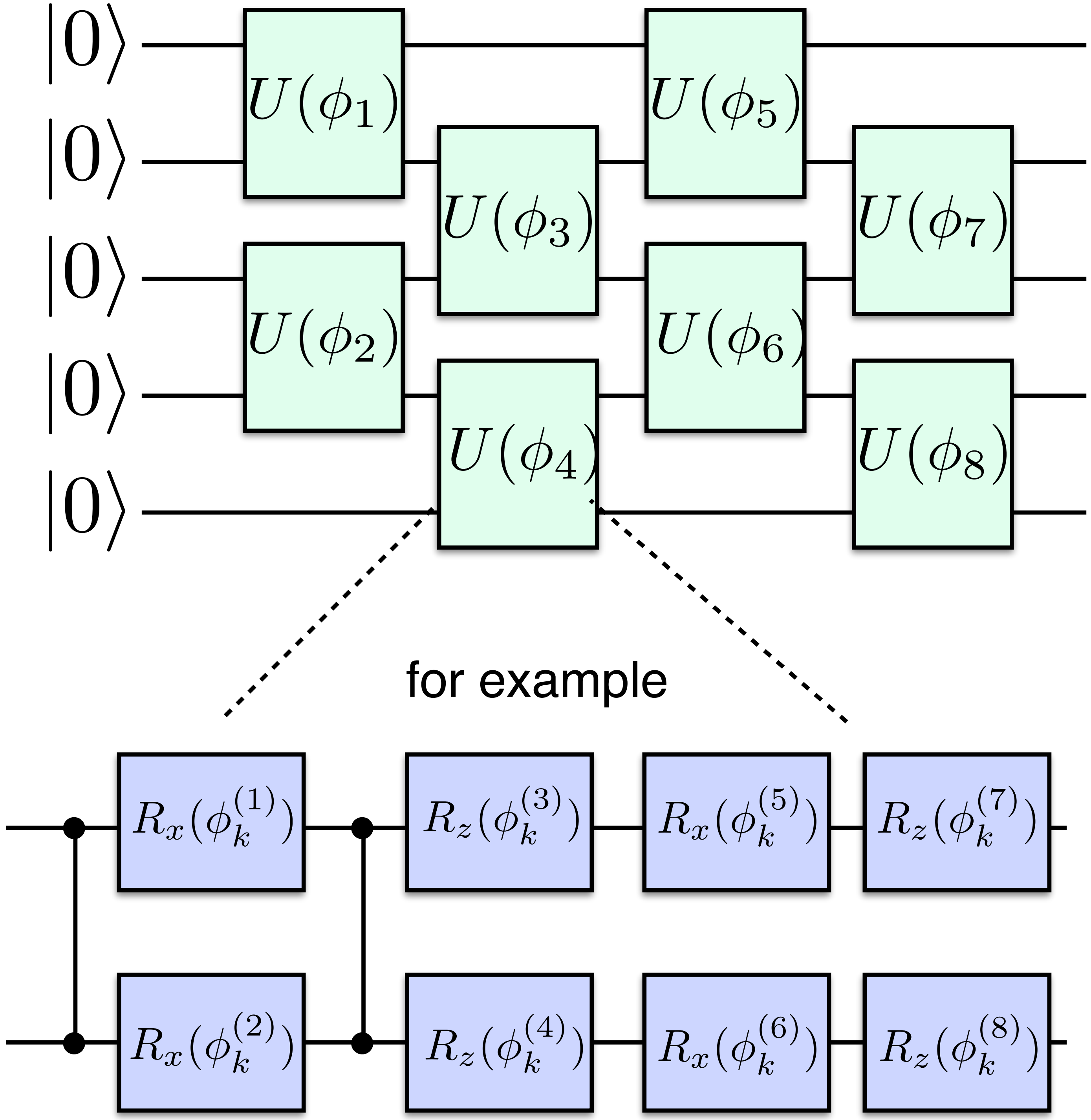


Generalization



nonlinear classification

Variational quantum algorithms and parameterized quantum circuit



for example

trial function
or
ansatz

$$|\psi(\{\phi_k\})\rangle$$

variational optimization:

$$\min_{\{\phi_k\}}\langle\psi(\{\phi_k\})|H|\psi(\{\phi_k\})\rangle$$

$$R_z(\phi) = e^{-i(\phi/2)Z}$$
$$R_x(\phi) = e^{-i(\phi/2)X}$$

How can we obtain the gradient $\frac{\partial}{\partial\phi_k}\langle\psi(\{\phi_k\})|H|\psi(\{\phi_k\})\rangle$?

Analytical differentiation of quantum circuits

Parameterized quantum circuit: $U(\{\phi_k\}) = \prod_k W_k e^{-i(\phi_k/2)P_k}$

hermitian & unitary
such as Pauli operators

fixed unitary

Analytical differentiation of quantum circuits

Parameterized quantum circuit: $U(\{\phi_k\}) = \prod_k W_k e^{-i(\phi_k/2)P_k}$

fixed unitary

hermitian & unitary
such as Pauli operators

Expectation value: $\langle A(\{\phi_k\})\rangle = \langle \psi(\{\phi_k\})|A|\psi(\{\phi_k\})\rangle$

where $|\psi(\{\phi_k\})\rangle = U(\{\phi_k\})|0\rangle^{\otimes n}$

Analytical differentiation of quantum circuits

Parameterized quantum circuit: $U(\{\phi_k\}) = \prod_k W_k e^{-i(\phi_k/2)P_k}$

fixed unitary

hermitian & unitary
such as Pauli operators

Expectation value: $\langle A(\{\phi_k\})\rangle = \langle\psi(\{\phi_k\})|A|\psi(\{\phi_k\})\rangle$

where $|\psi(\{\phi_k\})\rangle = U(\{\phi_k\})|0\rangle^{\otimes n}$

Analytical differentiation:

$$\frac{\partial}{\partial\phi_l}\langle A(\{\phi_k\})\rangle = \frac{\langle A(\{\phi_1, ..., \phi_l + \epsilon, \phi_{l+1}, ...\}\rangle - \langle A(\{\phi_1, ..., \phi_l - \epsilon, \phi_{l+1}, ...\}\rangle}{2\sin\epsilon}$$

$$\epsilon = \pi/2$$

Analytical differentiation of quantum circuits

Parameterized quantum circuit: $U(\{\phi_k\}) = \prod_k W_k e^{-i(\phi_k/2)P_k}$

fixed unitary

hermitian & unitary
such as Pauli operators

Expectation value: $\langle A(\{\phi_k\})\rangle = \langle\psi(\{\phi_k\})|A|\psi(\{\phi_k\})\rangle$

where $|\psi(\{\phi_k\})\rangle = U(\{\phi_k\})|0\rangle^{\otimes n}$

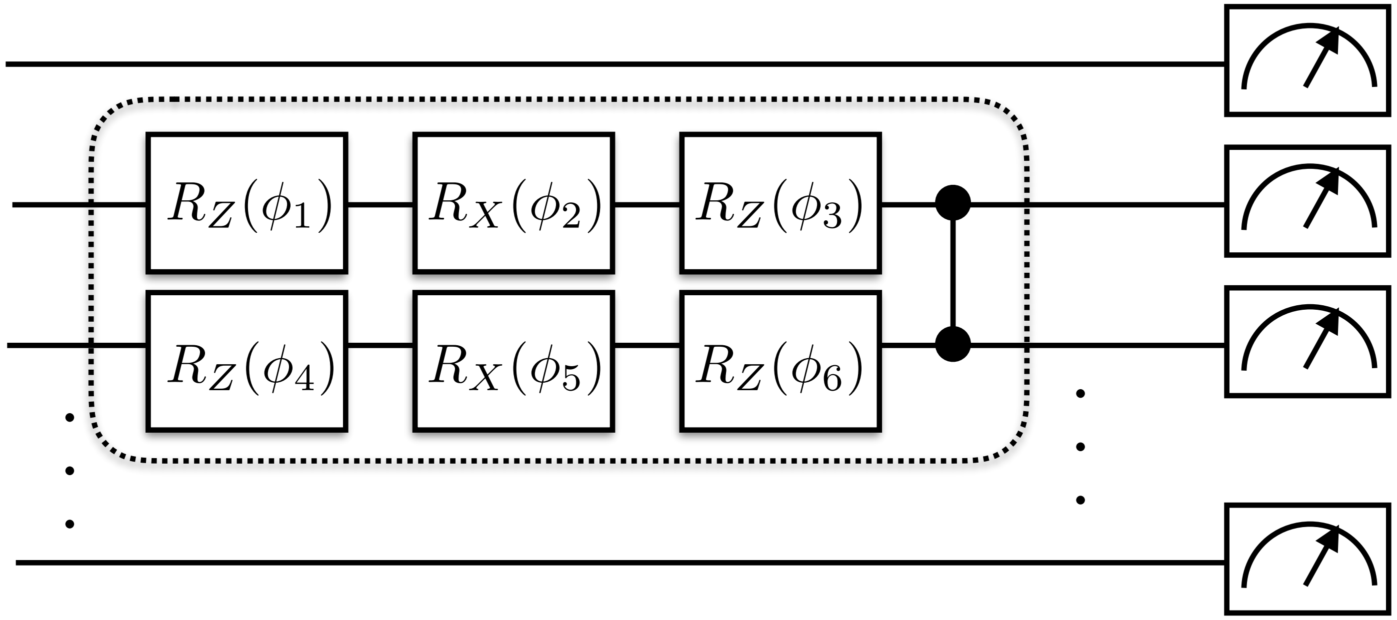
Analytical differentiation:

$$\frac{\partial}{\partial\phi_l}\langle A(\{\phi_k\})\rangle = \frac{\langle A(\{\phi_1, ..., \phi_l + \epsilon, \phi_{l+1}, ...\}\rangle - \langle A(\{\phi_1, ..., \phi_l - \epsilon, \phi_{l+1}, ...\}\rangle}{2\sin\epsilon}$$

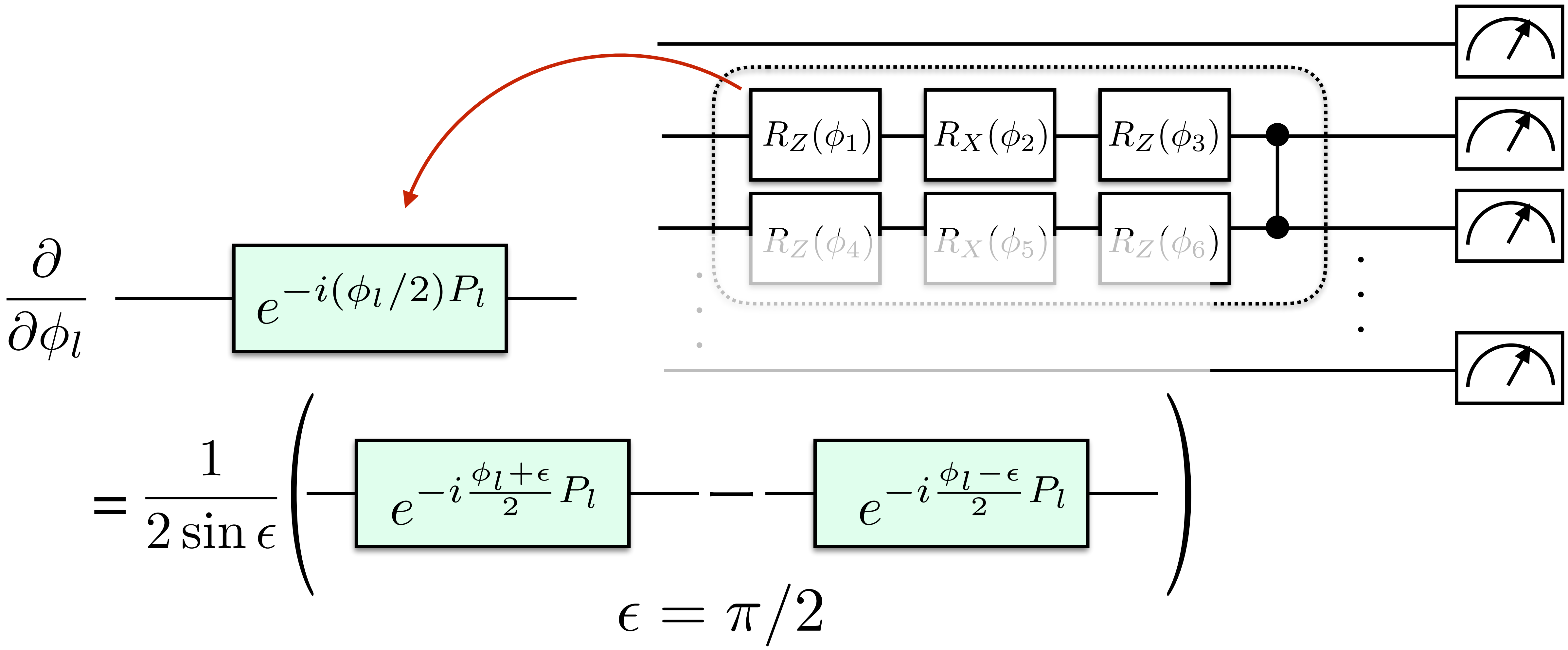
$$\epsilon = \pi/2$$

$$\left(\begin{aligned}
\langle A(\theta)\rangle &= \langle\psi|e^{-i(\theta/2)P} A e^{i(\theta/2)P}|\psi\rangle \\
\frac{\partial}{\partial\theta}\langle A(\theta)\rangle &= \langle\psi|(-iP/2)\tilde{A}|\psi\rangle + \langle\psi|\tilde{A}(iP/2)|\psi\rangle \qquad \tilde{A} = e^{-i(\theta/2)P} A e^{i(\theta/2)P} \\
&= -i(1/2)(\langle\psi|P\tilde{A}|\psi\rangle - \langle\psi|\tilde{A}P|\psi\rangle) \\
\langle A(\theta+\epsilon)\rangle &= \cos^2(\epsilon/2)\langle\tilde{A}\rangle + \sin^2(\epsilon/2)\langle P\tilde{A}P\rangle \\
&\quad - i\sin(\epsilon/2)\cos(\epsilon/2)\langle P\tilde{A}\rangle + i\cos(\epsilon/2)\sin(\epsilon/2)\langle\tilde{A}P\rangle
\end{aligned}\right)$$

Analytical differentiation of quantum circuits



Analytical differentiation of quantum circuits



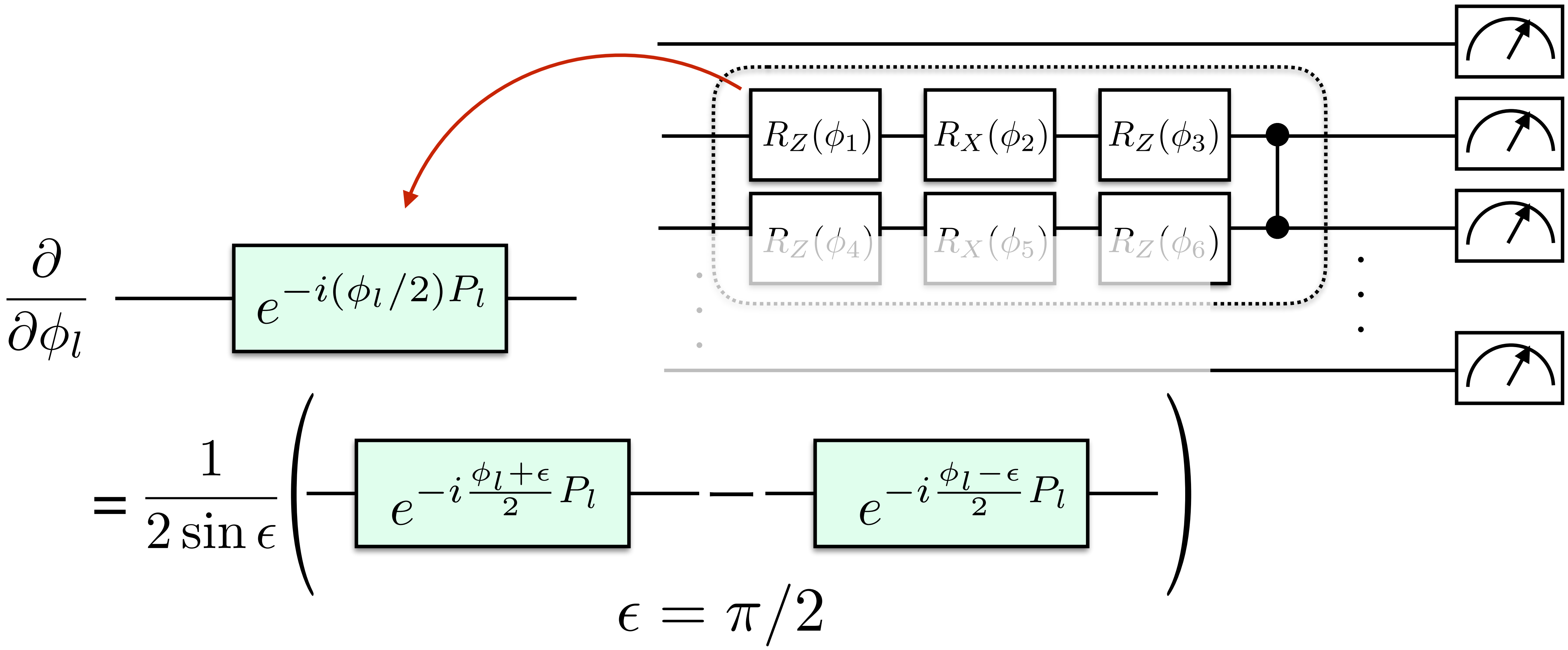
$$\frac{\partial}{\partial \phi_l} \boxed{e^{-i(\phi_l/2)P_l}}$$

$$= \frac{1}{2\sin\epsilon}\left(\boxed{e^{-i\frac{\phi_l+\epsilon}{2}P_l}} - \boxed{e^{-i\frac{\phi_l-\epsilon}{2}P_l}} \right)$$

$$\epsilon = \pi/2$$

→ The gradient can be obtain differently from measurements of two observables.

Analytical differentiation of quantum circuits



→ The gradient can be obtain differently from measurements of two observables.

See also

M. Schuld, *et al.* (Xanadu) "Evaluating analytic gradients on quantum hardware." *Physical Review A* 99, 032331 (2019) → PennyLane

Z. Y. Chen, et al. "VQNet: Library for a Quantum-Classical Hybrid Neural Network." *arXiv preprint arXiv:1901.09133* (2019). → 本源量子

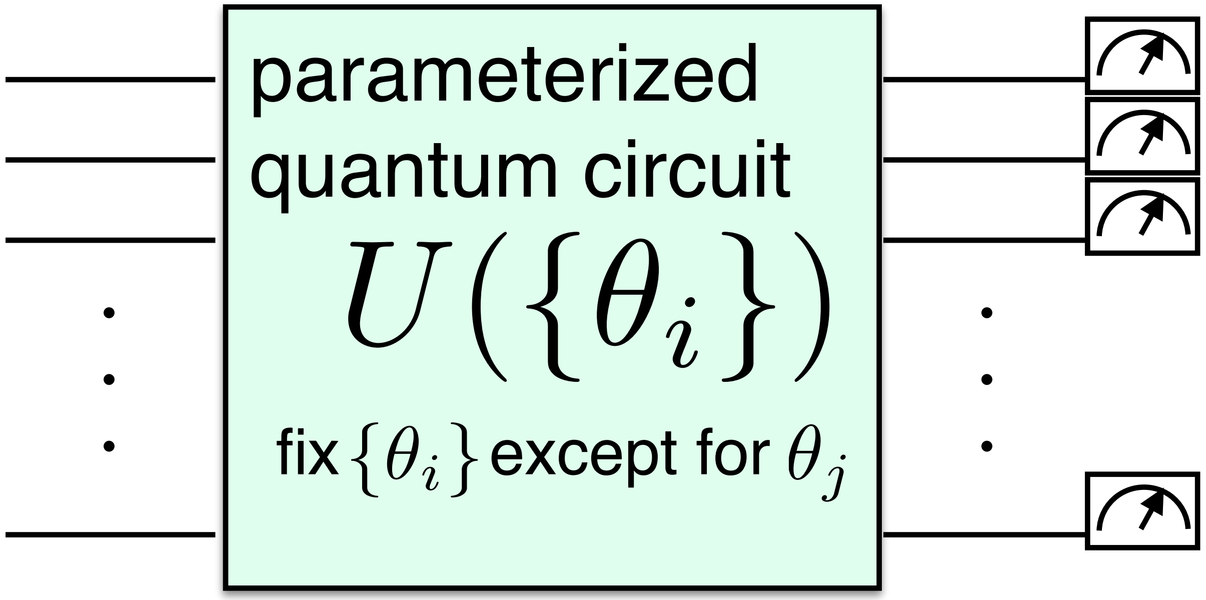
K. Mitarai, and K. Fujii. "Methodology for replacing indirect measurements with direct measurements." *arXiv preprint arXiv:1901.00015* (2018).

Outline

- Advantage of quantum-classical hybrid algorithm
  - Adiabatic quantum computation and quantum circuit model
  - Characterization of stoquastic adiabatic quantum computation
  - Quantum speedup in stoqAQC (sampling-based factoring & phase estimation)
- Parameter tuning for quantum-classical variational algorithm
  - gradient-based optimization
  - gradient-free optimization designed for hardware efficient ansatz
  - Numerical comparisons of gradient-based and -free optimizations.

Sequential minimal optimization for quantum-classical hybrid algorithms

Ken M. Nakanishi, Keisuke Fujii, Synge Todo, arXiv:1903.12166



parameterized quantum circuit

$U(\{\theta_i\})$

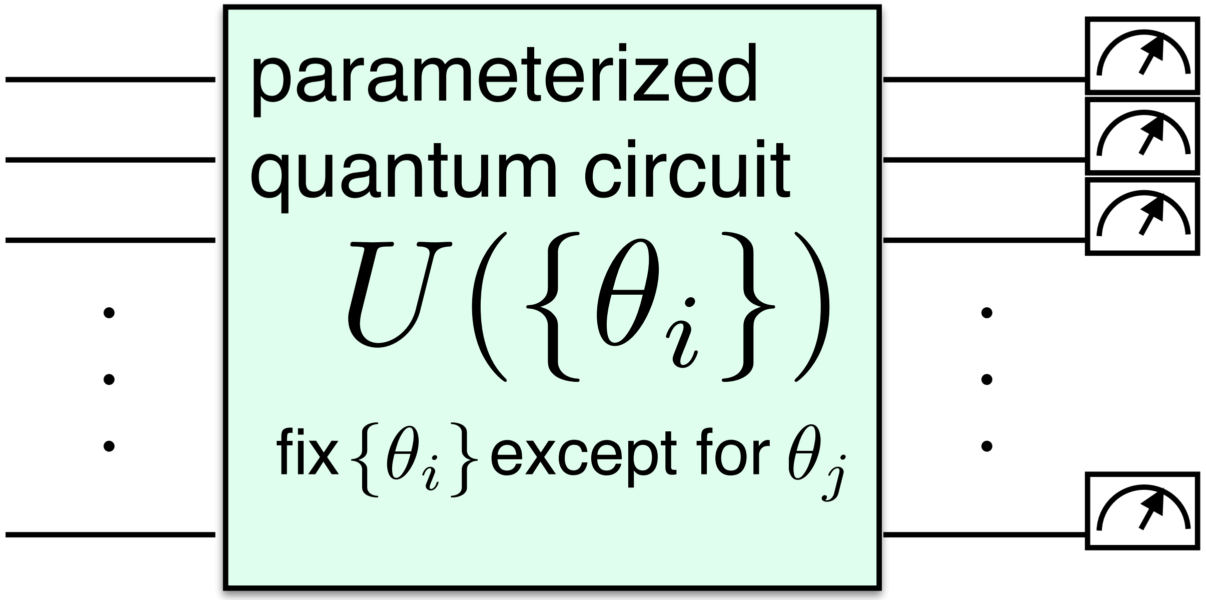
fix $\{\theta_i\}$ except for θ_j

$$\begin{aligned}\langle A(\theta)\rangle &= \langle\psi|e^{-i(\theta/2)P}Ae^{i(\theta/2)P}|\psi\rangle \\ &= \cos^2(\theta/2)\langle A\rangle + \sin^2(\theta/2)\langle PAP\rangle + \cos(\theta/2)\sin(\theta/2)i\langle[A,P]\rangle \\ &= \alpha\sin(\theta+\beta)+\gamma\end{aligned}$$

Unknown parameters are only three.

Sequential minimal optimization for quantum-classical hybrid algorithms

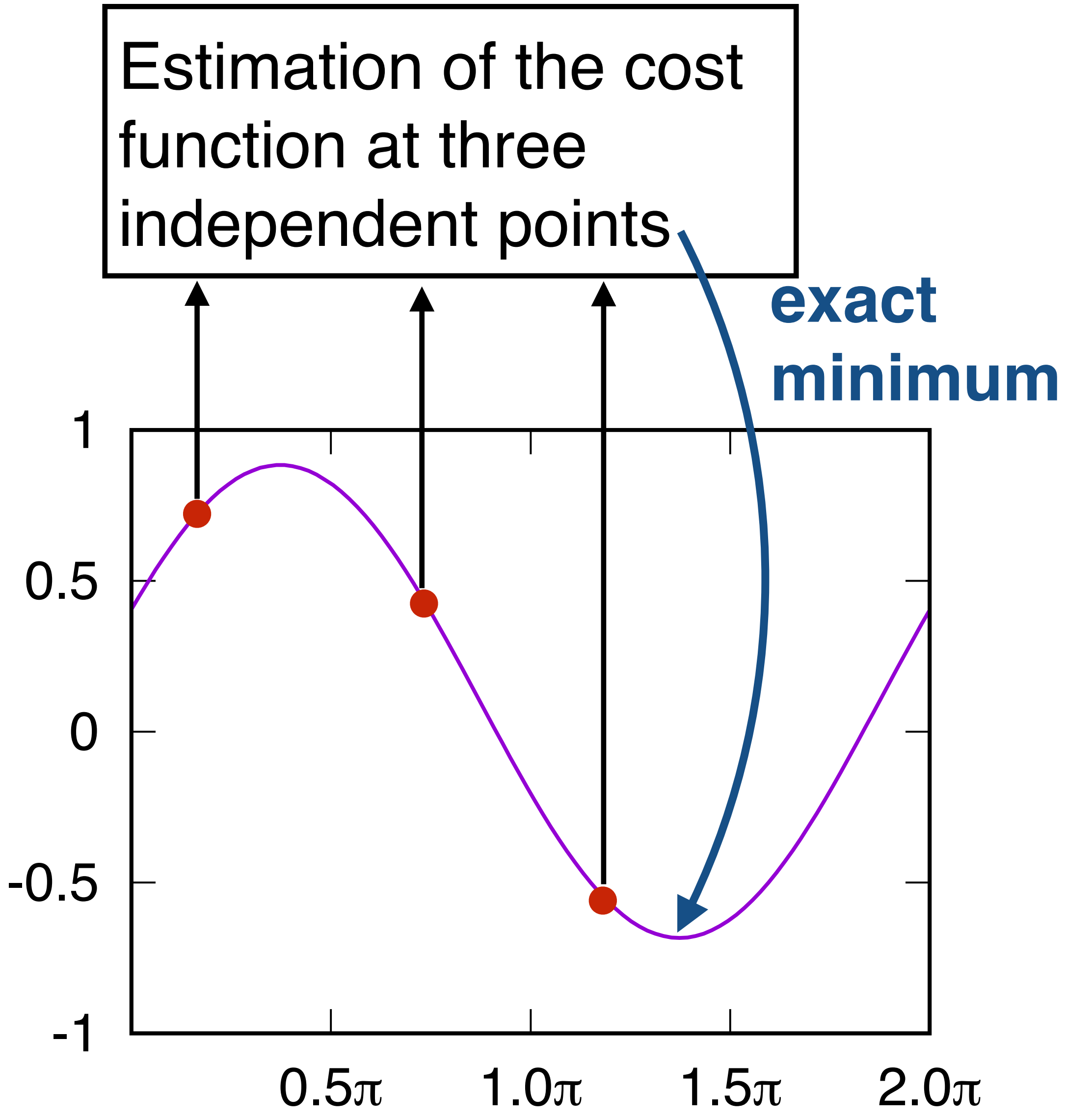
Ken M. Nakanishi, Keisuke Fujii, Synge Todo, arXiv:1903.12166



parameterized quantum circuit

$U(\{\theta_i\})$

fix $\{\theta_i\}$ except for θ_j



Estimation of the cost function at three independent points

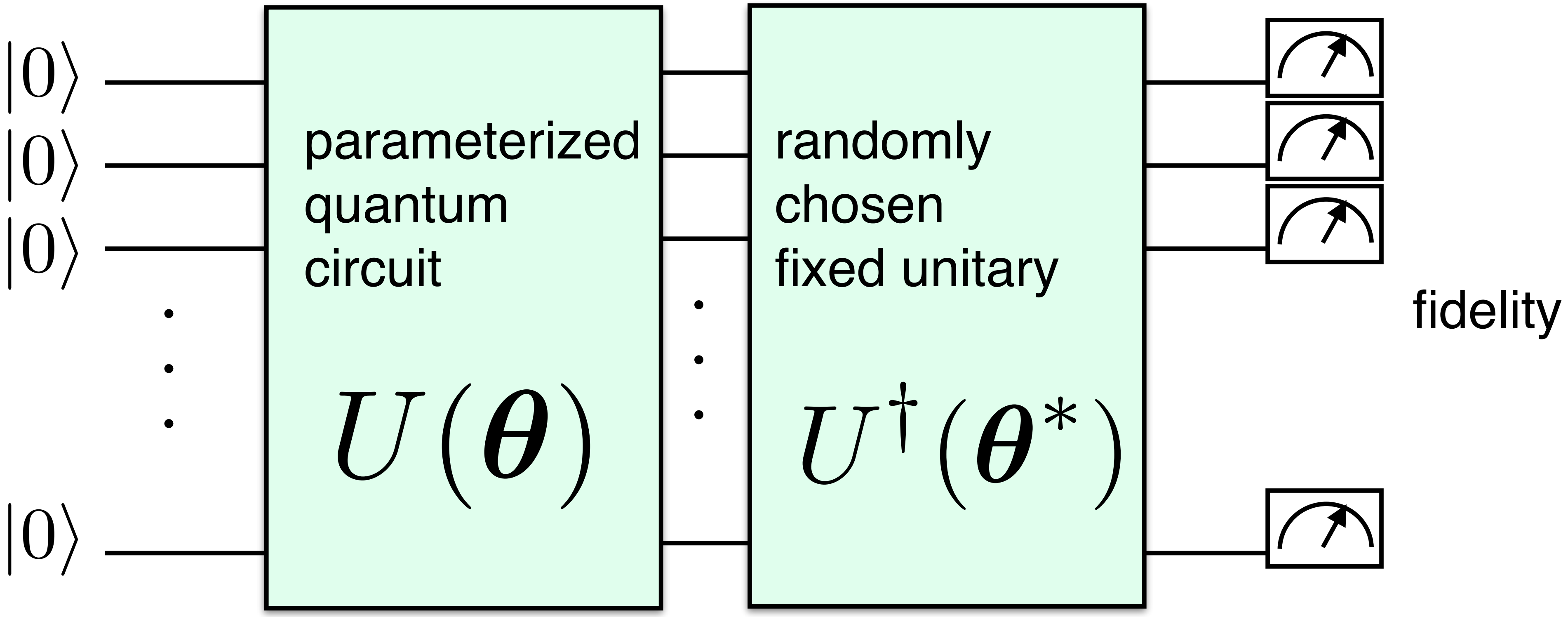
exact minimum

$$
\begin{aligned}
\langle A(\theta)\rangle &= \langle\psi|e^{-i(\theta/2)P}Ae^{i(\theta/2)P}|\psi\rangle \\
&= \cos^2(\theta/2)\langle A\rangle + \sin^2(\theta/2)\langle PAP\rangle + \cos(\theta/2)\sin(\theta/2)i\langle[A,P]\rangle \\
&= \alpha\sin(\theta+\beta)+\gamma
\end{aligned}
$$

Unknown parameters are only three.

Comparison between gradient-based and -free optimizations

Benchmark task：5qubit, 100 parameters $\mathcal{L}(\boldsymbol{\theta}) = -\left|\langle 0|^{\otimes r} U^\dagger(\boldsymbol{\theta}^*)U(\boldsymbol{\theta})\,|0\rangle^{\otimes r}\right|^2$



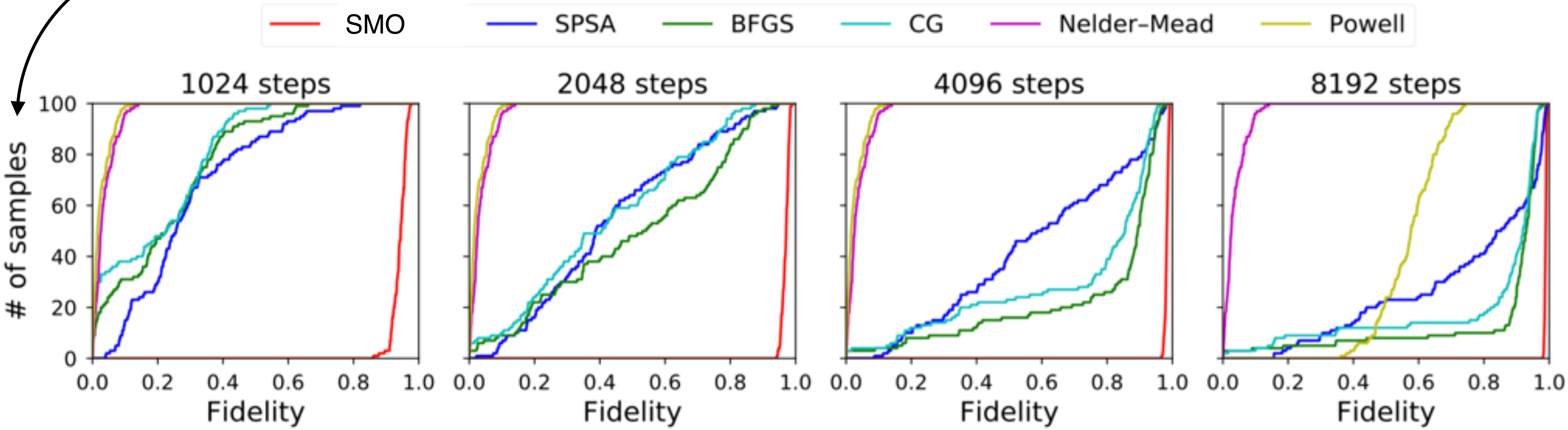
Optimization methods:

- Gradient based: BFGS, CG
- Gradient like: SPSA
- Gradient free: sequential minimum optimization(SMO) , Nelder-Mead, Powell

Comparison between gradient-based and -free optimizations

of steps (= # of observables estimated on QC) are changed.

initial random choice of the parameter

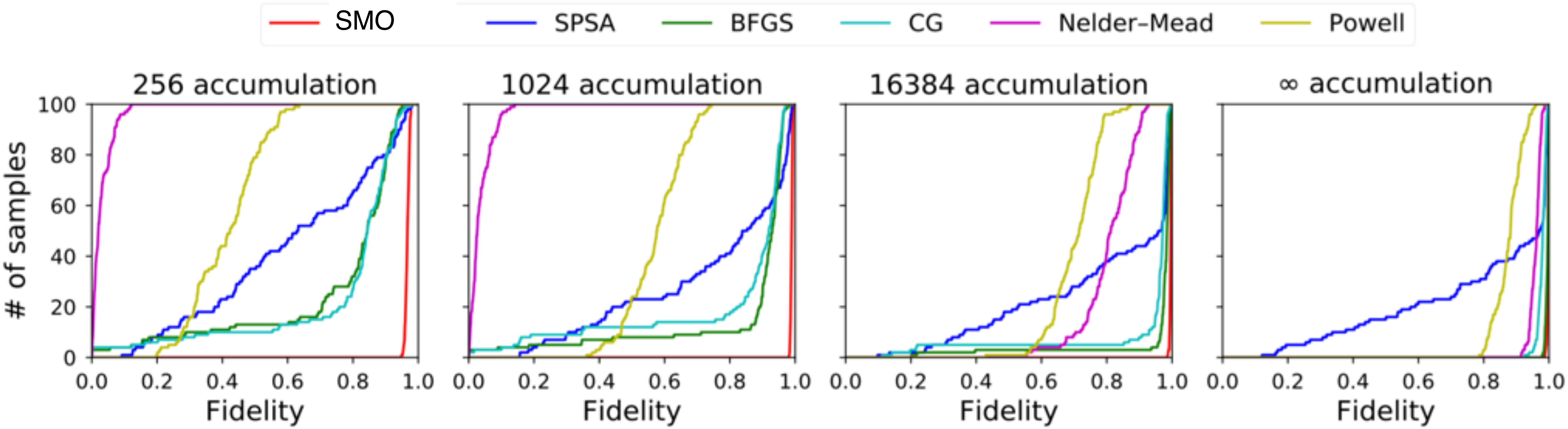


- (steps) counts the total number of call of a quantum computer.
- Gradient based methods outperforms NealderMead, Powell, and SPSA .
- Sequential minimal optimization substantially outperforms others especially in the presence of statistical error.

Ken M. Nakanishi, Keisuke Fujii, Synge Todo, arXiv:1903.12166

Comparison between gradient-based and -free optimizations

of samples to estimate an observable is changed.



- (steps) counts the total number of call of a quantum computer.
- Gradient based methods outperforms NealderMead, Powell, and SPSA .
- Sequential minimal optimization substantially outperforms others especially in the presence of statistical error.

Ken M. Nakanishi, Keisuke Fujii, Synge Todo, arXiv:1903.12166

Variations of variational approaches:

	model • **trial function**	**tuning •** **optimization**	**task**
Neural netwrok	W, tanh()	backpropagation (gradient)	machine learning
Rayleigh-Ritz (Hartree-Fock)	orthogonal functions (Slater determinant)	diagonalization of Hermitian matrix (HF equation)	ground state
Tensor network (MPS, PEPS, MERA)	tensor network	singular value decomposition	ground state (dynamics)
Variational quantum algorithms	parameterized quantum circuit **which kind?**	**gradient?** [Mitarai-Negoro-Kitagawa-KF '18] **other?** [Nakanishi-KF-Todo '19]	machine learning ground state dynamics **advantage?**

Summary

- We have seen an example where a non-universal model of quantum computation can solve non-trivial problem by a quantum-classical hybrid approach.

- Gradient can be directly obtained from analytical differentiation of parameterized quantum circuits.

- We can design a new optimization scheme, which is robust against the statistical error, based on the property of the parameterized quantum circuits.

Collaborators:

Todo, Nakanishi@UTokyo Mitarai, Negoro, Kitagawa @ Osaka U