パイロット講義: 計算科学・量子計算における情報圧縮

Data Compression in Computational Science and Quantum Computing

2022.01.25

#4 Quantum-Classical Hybrid Algorithms and Tensor Network

理学系研究科 量子ソフトウェア寄付講座

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Lecture materials: https://github.com/utokyo-qsw/data-compression

Outline

- Quantum Computer and Quantum Computation [review]
    - quantum circuits; quantum operations in quantum circuits; quantum measurement
- Quantum-classical Hybrid Algorithms
    - quantum computation on NIQS devices; variational quantum eigensolver; universal quantum gates; variational wave function
- Optimization of Quantum Circuit
    - gradient calculation; sequential optimization
- Machine Learning Based on Tensor Network
    - supervised learning with tensor network
- Qubit Efficient Implementation of Tensor-Network Machine Learning
    - converting MPS into quantum circuit; qubit-efficient implementation

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Quantum Computer and Quantum Computation

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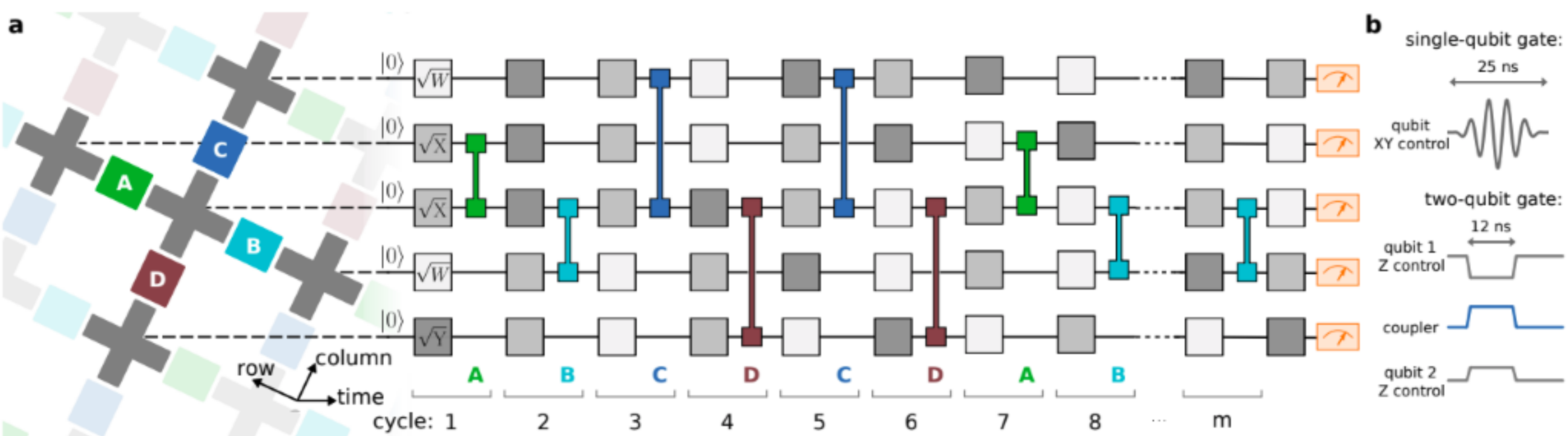
Quantum Circuits

- Prepare a set of quantum bits (qubits)
- A number of quantum gates (typically 1-qubit or 2-qubit gates) are applied to qubits in order
  - quantum gates are unitary operations
  - combination of quantum gates are also unitary operation
- Finally, perform measurements to extract information



Arute, F., Arya, K., Babbush, R. et al. Quantum supremacy using a programmable superconducting processor. Nature 574, 505–510 (2019). https://doi.org/10.1038/s41586-019-1666-5

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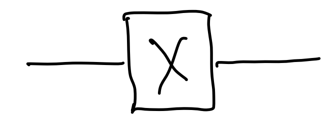
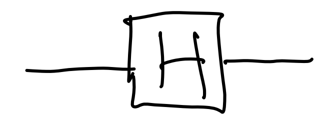
Typical Quantum Gates

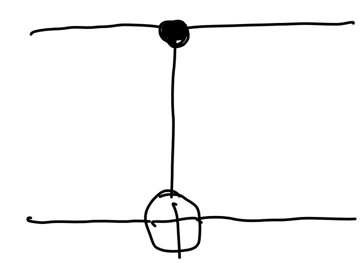
- One-qubit gates (2x2 matrix)
  - X gate (NOT) $$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$



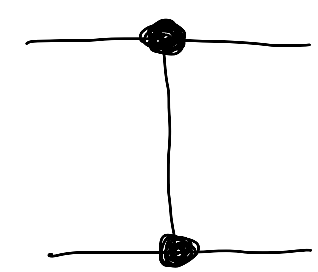
  - H gate (Hadamard) $$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$



- Two-qubit gates (4x4 matrix)
  - CX gate (controlled-NOT) $$CX = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$



  - CZ gate (controlled-Z) $$CZ = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$



Parameterized Quantum Gates

- One-qubit rotation gates (2x2 matrix)
  - RX gate (rotation around X axis)

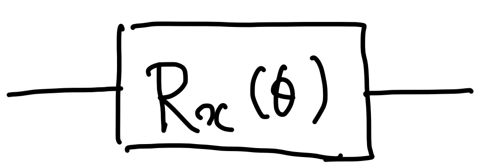
$$R_x(\theta) = e^{-i\theta\sigma_x/2} = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

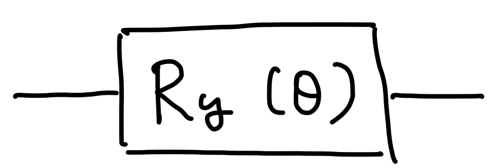
  - RY gate (rotation around Y axis)

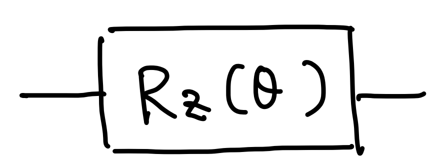
$$R_y(\theta) = e^{-i\theta\sigma_y/2} = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

  - RZ gate (rotation around Z axis)

$$R_z(\theta) = e^{-i\theta\sigma_z/2} = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}$$







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Quantum Operations in Quantum Circuits

- Parallelism
    - inputting a state of superposition produces a superposition of the corresponding outputs.
- Bifurcation
    - states bifurcate (in terms of computational basis) when H-gates, etc. are applied
- Interference
    - superposition coefficients of the states are complex, and they may cancel each other out and vanish
- Collapse
    - collapse to one of the states in the basis used for the measurement

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Quantum Measurement

- Pure state
  - in a pure state, entropy is zero
    - density matrix: $\rho = |\Psi\rangle\langle\Psi|$ is rank-1
    - the largest eigenvalue is unity, all other eigenvalues are zero
    - Von Neumann entropy: $S(\rho) = -\operatorname{tr}(\rho \log \rho) = 0$
- Manipulation of states by quantum circuits
  - entropy does not change since operation are unitary transformations
    - if the initial state is a pure state, the entropy stays zero
    - $S(U\rho U^\dagger) = -\operatorname{tr}(U\rho U^\dagger \log U\rho U^\dagger) = -\operatorname{tr}(\rho \log \rho) = S(\rho) = 0$

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Quantum Measurement

- Non-selective projective measurement (= measure and don't see the result)
  - entropy always increases
    - projection operators $\{P_i\}$ $(\sum P_i = 1,\ (P_i)^2 = P_i)$
    - by projective measurement: $\rho \to \rho' = \sum P_i \rho P_i$
    - $S(\rho') \geq S(\rho)$ (Klein's theorem)
  - a pure state is converted into a mixed state
    - off-diagonal elements vanishes
- Selective projective measurement (measure and see the result)
  - a pure state is sampled according to the measurement probability
  - selection causes the state collapse and the entropy to be zero again

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Essence of Quantum Algorithm

- Prepare a superposition of many states, using Hadamard gates, etc.
  - if non-selective projective measurements is performed at this stage, the entropy is extensive (proportional to the number of qubits)
- Manipulate and interfere the states so that desired answer has large amplitude
  - entropy of the quantum state remains zero
    - interference reduces the entropy after non-selective projective measurement
    - a kind of data compression?
- Selective projective measurement (measure and see the result) to get the correct answer with high probability
  - sampling from the state with entropy as small as possible
    - a kind of information extraction?

Quantum-classical Hybrid Algorithms

Quantum Computation on NISQ Devices

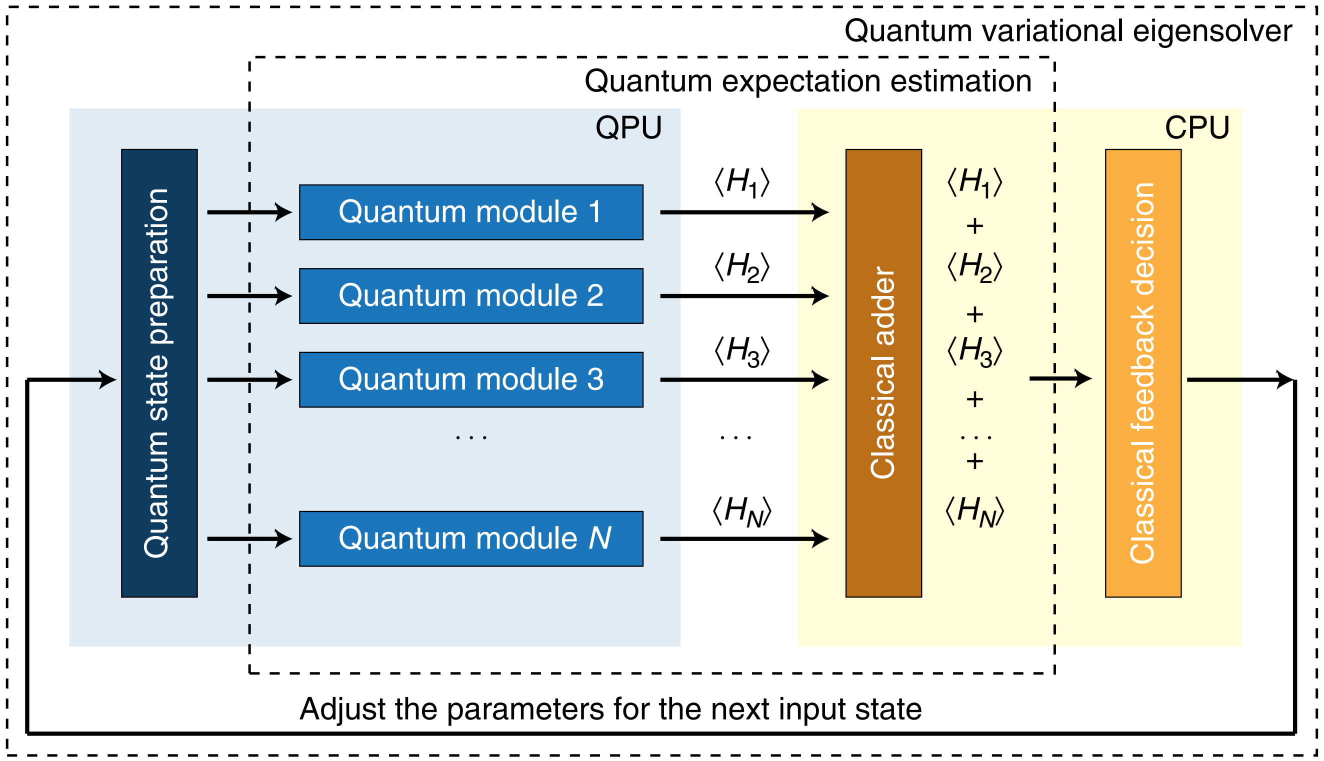
- Fault-tolerant quantum computing with quantum error correction
  - quantum phase estimation
    - prime factorization, eigenvalue problems, simultaneous linear equations (HHL)
    - Exponential speed improvement over classical computers
  - many *physical* qbits (100-1000) are needed for one *logical* qubits
- Today's NISQ (noisy intermediate-scale quantum) devices
  - only 50-100 qubits (not enough to implement quantum error correction)
  - at most 1000 quantum operations (due to large noise)

Quantum-classical Hybrid Algorithms

- Combination of quantum and classical computation
    - evaluate "loss" by using quantum computer
    - optimize parameters of quantum circuit by using classical computer
- Examples of quantum-classical hybrid algorithms
    - variational quantum eigensolver (VQE)
    - quantum approximate optimization algorithm (QAOA)
    - variational quantum simulator (VQS)
    - variational quantum linear solver (VQLS)
    - quantum circuit learning (QCL)
    - etc

Variational Quantum Eigensolver

- Calculate ground state of quantum many-body system
  - represent variational wave function by parameterized quantum circuit
  - evaluate expectation value of Hamiltonian by using quantum computer
  - optimize parameters by using computer computer



- Peruzzo, A., et al (2014). A variational eigenvalue solver on a photonic quantum processor. *Nature Comm.* 5, 4213. https://doi.org/10.1038/ncomms5213 (arXiv:1304.3061)

An Example - Spin Dimer

- Interacting two spins
  - Hamiltonian: $H = JS_1 \cdot S_2 = \dfrac{J}{4}(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y + \sigma_1^z \sigma_2^z) \quad (J > 0)$
  - ground state: $|\Psi\rangle = \dfrac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$
- Variational wave function: $|\phi(\{\theta_i\})\rangle = U(\{\theta_i\})|00\rangle$
- Expectation value of Hamiltonian (energy):

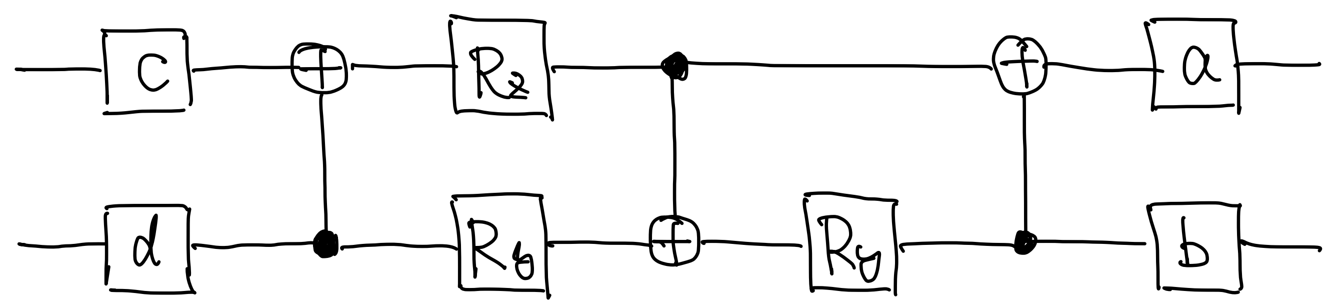
$$
\begin{aligned}
\langle\phi(\{\theta_i\})|H|\phi(\{\theta_i\})\rangle = \frac{J}{4}(&\langle\phi(\{\theta_i\})|\sigma_1^x\sigma_2^x|\phi(\{\theta_i\})\rangle + \langle\phi(\{\theta_i\})|\sigma_1^y\sigma_2^y|\phi(\{\theta_i\})\rangle \\
&+\langle\phi(\{\theta_i\})|\sigma_1^z\sigma_2^z|\phi(\{\theta_i\})\rangle
\end{aligned}
$$

Universal Quantum Gates

- *Universal* one-qubit unitary operation

$$U = \mathrm{R}_x(\theta_1)\mathrm{R}_y(\theta_2)\mathrm{R}_x(\theta_3)$$

- *Universal* two-qubit unitary operation

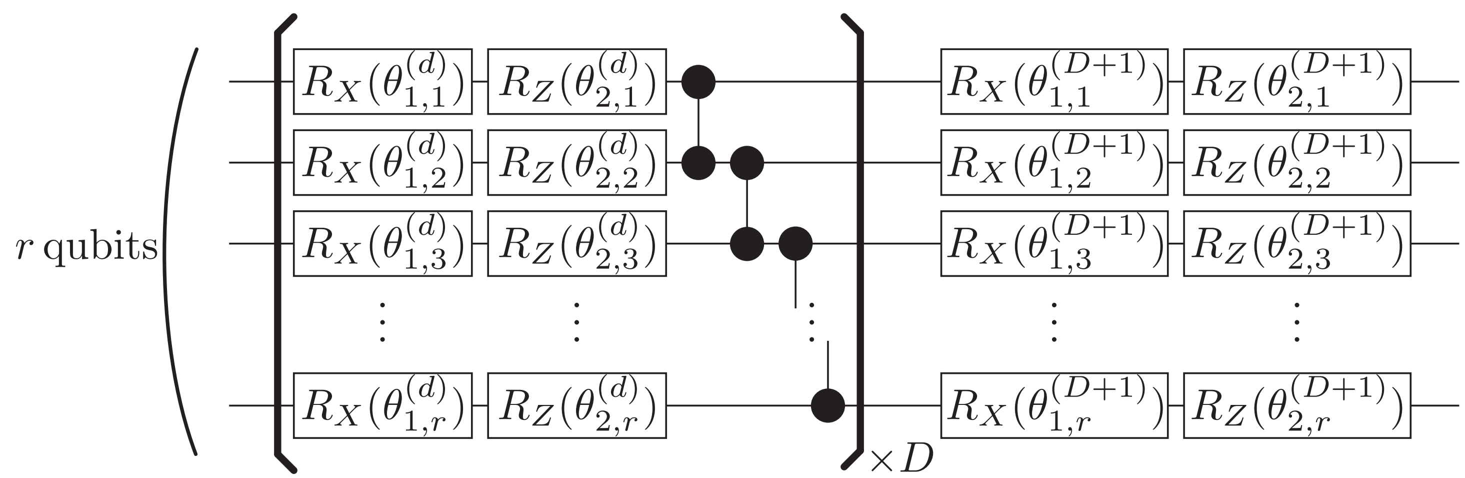


  - [a]-[d]: universal one-qubit unitary operations
  - 15 one-qubit rotations + 3 CNOTs

  - Shende, V. V., Markov, I. L., & Bullock, S. S. (2004). *Minimal universal two-qubit controlled-NOT-based circuits*. Phys, Rev. A, 69, 1. https://doi.org/10.1103/PhysRevA.69.062321 (arXiv:quant-ph/0308033)

Variational Wave Function

- Universal multi-qubit unitary operation
  - number of elemental (one- and two-qubit) operations increases rapidly → the number of parameters that must be optimized also increases
- In practical VQE algorithms
  - use some heuristic parameterized quantum circuits, ex)



- For quantum chemical calculations
  - various high-precision variational wave functions have been proposed
  - ref) 杉崎「量子コンピュータによる量子化学計算入門」(講談社, 2020)

Optimization of Quantum Circuit

Optimization of Quantum Circuit

- Optimization is performed on classical computer
- Standard optimization algorithms can be used
  - Gradient-free algorithms
    - Nelder-Mead, Powell method
  - Optimization using gradient
    - Gradient descent, Adam, etc
- Gradient-based algorithms generally show better performance than gradient-free methods
  - How to calculate gradient of cost function using quantum computer?

Gradient Calculation

- Finite difference method
  - sensitive to noise
- Using special property of loss function
  - fix $(\theta_1, \theta_2, \cdots, \theta_{k-1}, \theta_{k+1}, \cdots, \theta_n)$
  - unitary transformation for generating variational wave function can be written as

$$U(\theta_k) = VU_k(\theta_k)W \qquad U_k(\theta_k) = e^{-i\sigma_k\theta_k/2}$$

  - expectation value of operator $\mathcal{O}$

$$\begin{aligned}\langle \mathcal{O}(\theta_k) \rangle &= \langle 0 | U^\dagger(\theta_k) \mathcal{O} U(\theta_k) | 0 \rangle \\ &= \langle 0 | W^\dagger U_k^\dagger(\theta_k) V^\dagger \mathcal{O} V U_k(\theta_k) W | 0 \rangle \\ &= \langle \Psi | U_k^\dagger(\theta_k) Q U_k(\theta_k) | \Psi \rangle \quad | \Psi \rangle = W | 0 \rangle,\ Q = V^\dagger \mathcal{O} V\end{aligned}$$

Derivative of Cost Function

- Using $U_k(\theta_k) = e^{-i\sigma_k\theta_k/2}$

$$\frac{\partial}{\partial\theta_k}\langle\mathcal{O}(\theta_k)\rangle = \frac{i}{2}\langle\Psi|\sigma_k U_k^\dagger(\theta_k) Q U_k(\theta_k)|\Psi\rangle - \frac{i}{2}\langle\Psi|U_k^\dagger(\theta_k) Q U_k(\theta_k)\sigma_k|\Psi\rangle$$

- On the other hand, since $(\sigma_k)^2 = I$

$$e^{i\sigma_k\theta/2} = I\cos\frac{\theta}{2} + i\sigma_k\sin\frac{\theta}{2} \quad \Rightarrow \quad e^{\pm i\sigma_k\pi/4} = \frac{\sqrt{2}}{2}(I \pm i\sigma_k)$$

- Stable derivative estimation

$$\frac{\partial}{\partial\theta_k}\langle\mathcal{O}(\theta_k)\rangle = \frac{1}{2}\left(\langle\mathcal{O}(\theta_k + \frac{\pi}{2})\rangle - \langle\mathcal{O}(\theta_k - \frac{\pi}{2})\rangle\right)$$

- Mitarai, K., Negoro, M., Kitagawa, M., & Fujii, K. (2018). *Quantum circuit learning*. Physical Review A, 98, 1. https://doi.org/10.1103/PhysRevA.98.032309 (arXiv:1803.00745)

Sequential Optimization

- Using $e^{i\sigma_k\theta/2} = I\cos\frac{\theta}{2} + i\sigma_k \sin\frac{\theta}{2}$

$$\langle \mathcal{O}(\theta'_k) \rangle = \langle \Psi \,|\, (I\cos\frac{\theta'_k}{2} + i\sigma_k \sin\frac{\theta'_k}{2}) Q (I\cos\frac{\theta'_k}{2} + i\sigma_k \sin\frac{\theta'_k}{2}) \,|\, \Psi \rangle$$
$$= a_1 \cos(\theta'_k - a2) + a_3$$

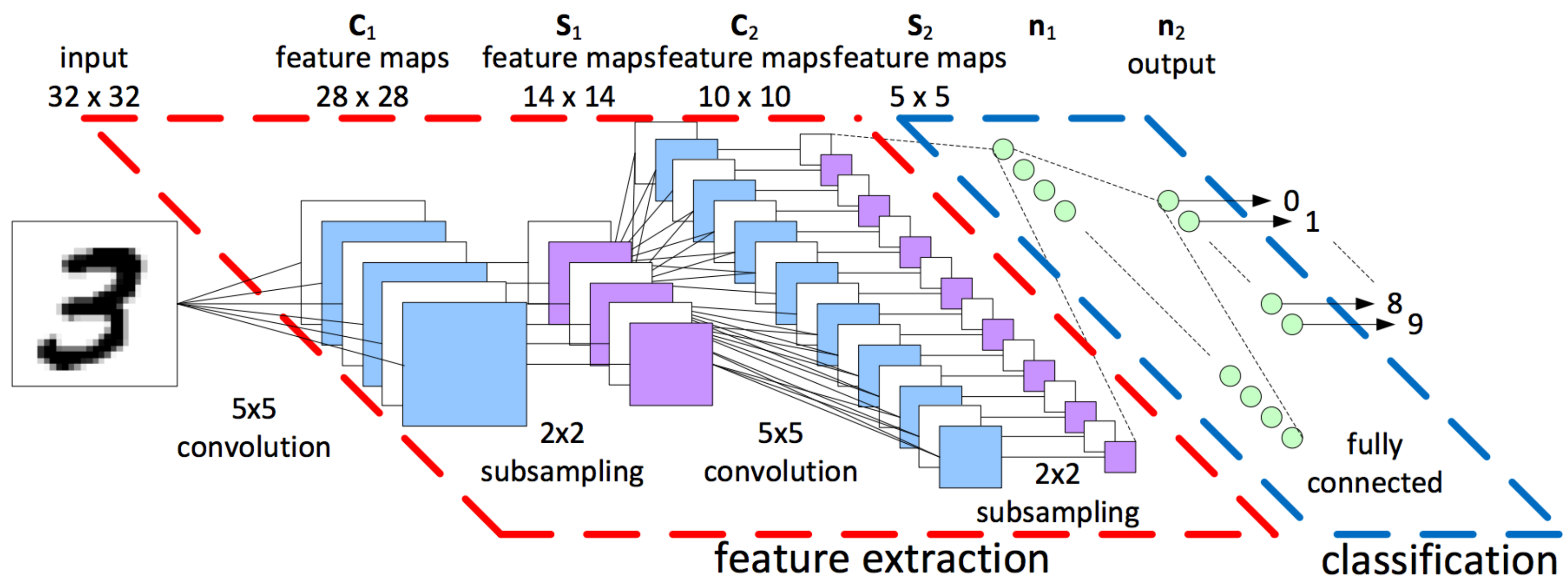
- Coefficients a_1, a_2, a_3 can be determined from $\langle \mathcal{O}(\theta_k) \rangle$, $\langle \mathcal{O}(\theta_k + \frac{\pi}{2}) \rangle$, $\langle \mathcal{O}(\theta_k - \frac{\pi}{2}) \rangle$
- $\langle \mathcal{O}(\theta'_k) \rangle$ can be minimized by choosing $\theta'_k = a_2$ or $\theta'_k = -a_2$ (depending on the sign of a_1)

- Nakanishi, K. M., Fujii, K., & Todo, S. (2020). *Sequential minimal optimization for quantum-classical hybrid algorithms*. Phys. Rev. Research, 2, 1. https://doi.org/10.1103/PhysRevResearch.2.043158 (arXiv:1903.12166)

Machine Learning Based on Tensor Network

Handwritten Character Recognition

- Machine learning based on convolutional neural network (CNN)



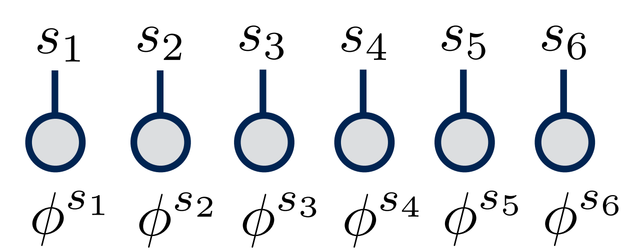
https://www.kaggle.com/cdeotte/how-to-choose-cnn-architecture-mnist

  - input: gray scale image
  - output: 10-dimensional vector
- Accuracy > 99.5% for MNIST
  - c.f. Gao, Z. F., Cheng, S., He, R. Q., Xie, Z. Y., Zhao, H. H., Lu, Z. Y., & Xiang, T. (2020). Compressing deep neural networks by matrix product operators. *Phys. Rev. Research*, *2*(2), 23300. https://doi.org/10.1103/PhysRevResearch.2.023300 (arXiv:1904.06194)

Supervised Leaning with Tensor Networks

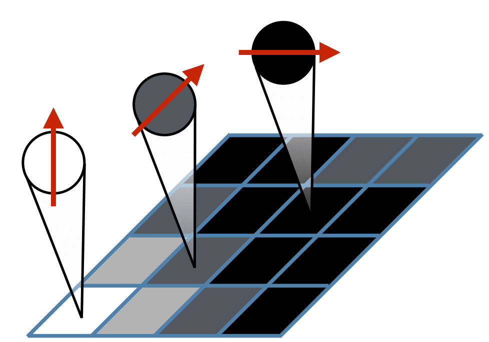
- Tensor network has multi-linear property
  - how to introduce non-linearity and increase expressive power?
- Encode of input data
  - convert N-dimensional vector (N-pixel image) into 2^N-dimensional feature map

$$\Phi^{s_1 s_2 \cdots s_N}(\mathbf{x}) = \phi^{s_1}(x_1) \otimes \phi^{s_2}(x_2) \otimes \cdots \phi^{s_N}(x_N) =$$



  - $\Phi(x)$ is a tensor product of (2-dimensional) local feature map

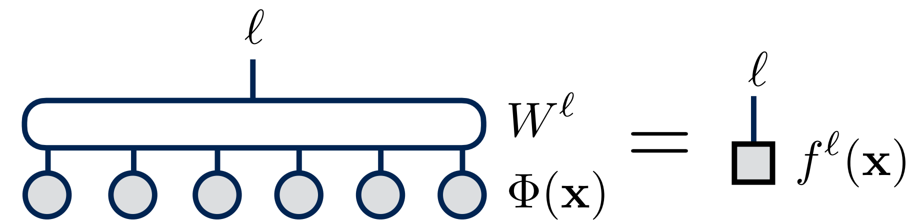
$$\phi^{s_j}(x_j) = \left[\cos\left(\frac{\pi}{2}x_j\right),\ \sin\left(\frac{\pi}{2}x_j\right)\right]$$



- Stoudenmire, E. M., & Schwab, D. J. (2016). Supervised Learning with Quantum-Inspired Tensor Networks. Advances in Neural Information Processing Systems, 29, 4799. (arXiv:1605.05775)

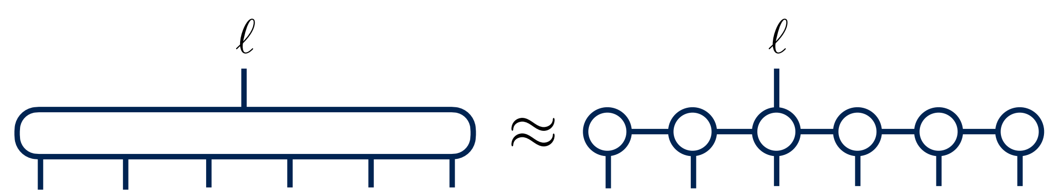
Classification Model

- $f^{\ell}(\mathbf{x}) = W^{\ell} \cdot \Phi(\mathbf{x})$
  - W is a 10×2^N matrix



- Decompose W into tensor network (matrix product) state

$$W^{\ell}_{s_1 s_2 \cdots s_N} = \sum_{\{\alpha\}} A^{\alpha_1}_{s_1} A^{\alpha_1 \alpha_2}_{s_2} \cdots A^{\ell;\alpha_j \alpha_{j+1}}_{s_j} \cdots A^{\alpha_{N-1}}_{s_N}$$



  - each tensor has $2m^2$ elements (m: bond dimension between tensors)

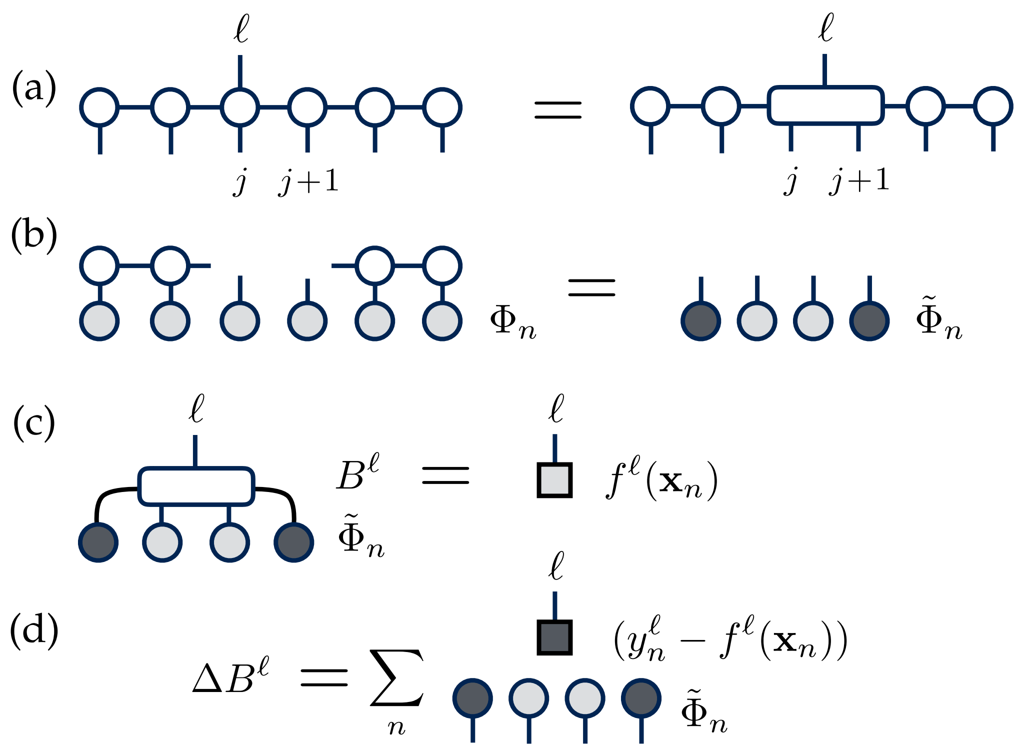
- Stoudenmire, E. M., & Schwab, D. J. (2016). Supervised Learning with Quantum-Inspired Tensor Networks. Advances in Neural Information Processing Systems, 29, 4799. (arXiv:1605.05775)

Cost Function and Gradient

- Cost: $C = \frac{1}{2} \sum_{n=1}^{N_T} \sum_{\ell} (f^{\ell}(\mathbf{x}_n) - y_n^{\ell})^2$
    - N_T : number of training data
    - $f^{\ell}(\mathbf{x_n})$: contraction result of tensor network (10-dimensional vector)
    - y_n^{ℓ} : correct label (one-hot representation)

- Gradient:

$$\Delta B^{\ell} = -\frac{\partial C}{\partial B^{\ell}} = \sum_{n=1}^{N_T} (y_n^{\ell} - f^{\ell}(\mathbf{x}_n)) \tilde{\Phi}_n$$



- Stoudenmire, E. M., & Schwab, D. J. (2016). Supervised Learning with Quantum-Inspired Tensor Networks. Advances in Neural Information Processing Systems, 29, 4799. (arXiv:1605.05775)

Qubit Efficient Implementation of Tensor-Network Machine Learning

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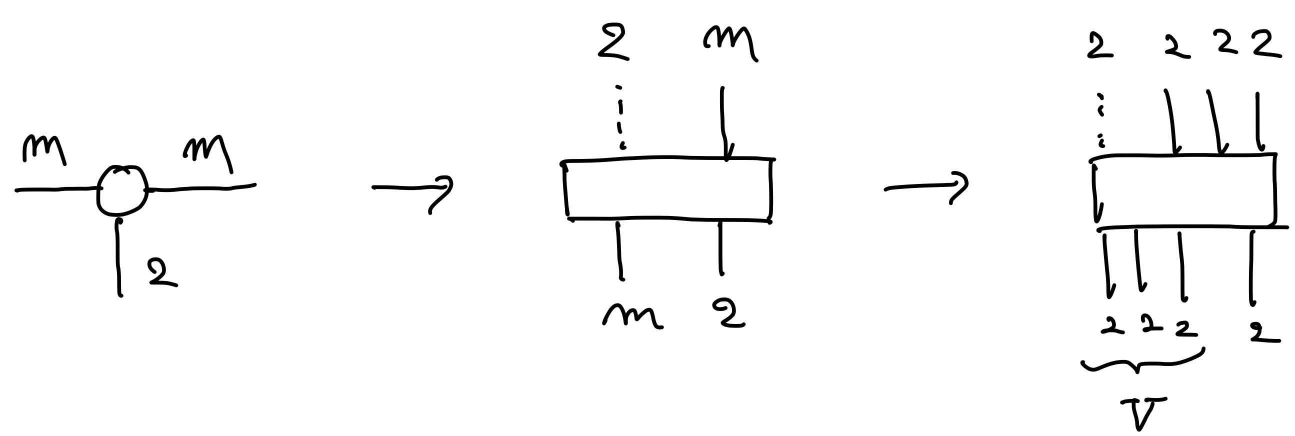
Tensor Network Representation of Quantum Circuits

- Tensor representation of quantum gates and states
  - 1-qubit gate:
    - 2×2 matrix → 2-leg tensor
  - 2-qubit gate:
    - 4×4 matrix → $2 \times 2 \times 2 \times 2$ tensor → 4-leg tensor
  - r-qubit gate:
    - $2^r \times 2^r$ matrix → $2 \times 2 \times \cdots \times 2$ tensor → $2r$-leg tensor
  - initial quantum states
    - product state, e.g., $|0\rangle \otimes |0\rangle \otimes \cdots \otimes |0\rangle$
      → a set of n 1-leg tensors (vectors)

Converting Tensor into Quantum Gate

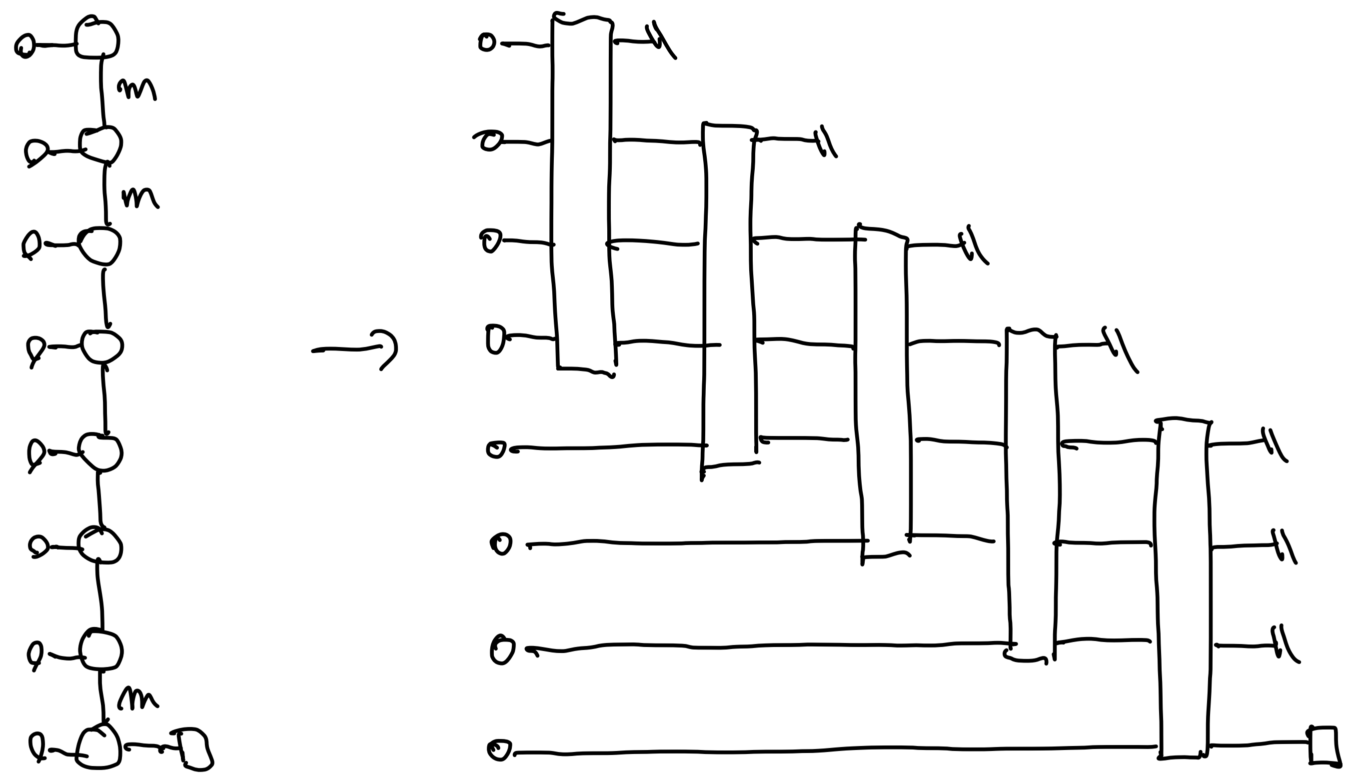
- Quantum gate is tensor
  - Tensor is quantum gate?
  - Yes, but quantum gate should be unitary operator
- $m = 2^V$ $(V = 3)$ case



- Huggins, W., Patil, P., Mitchell, B., Birgitta Whaley, K., & Miles Stoudenmire, E. (2019). Towards quantum machine learning with tensor networks. *Quantum Science and Technology*, *4*, 1. https://doi.org/10.1088/2058-9565/aaea94 (arXiv:1803.11537)

Converting MPS into Quantum Circuit

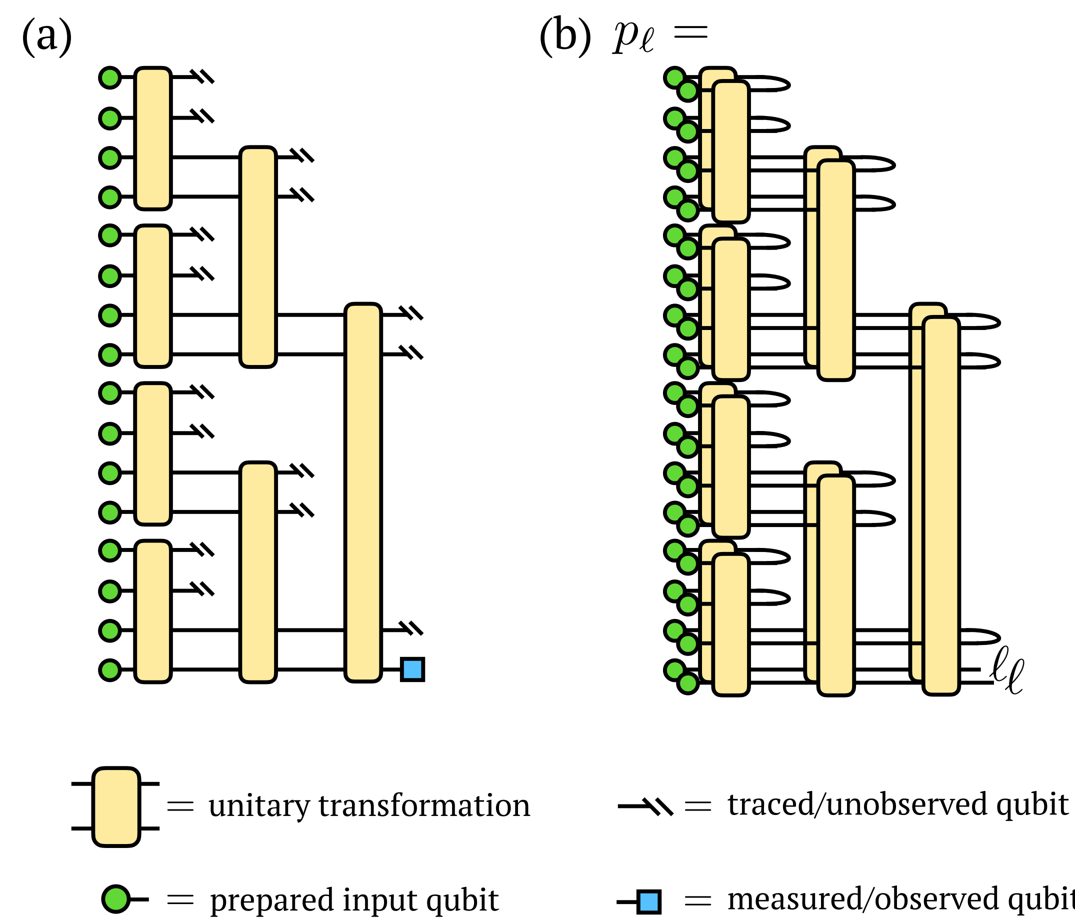
- $N = 8,\ m = 8$ case



- Optimization of tensors → optimization of parameters in parameterized quantum circuit → quantum-classical hybrid algorithm
    - Huggins, W., Patil, P., Mitchell, B., Birgitta Whaley, K., & Miles Stoudenmire, E. (2019). Towards quantum machine learning with tensor networks. *Quantum Science and Technology*, *4*, 1. https://doi.org/10.1088/2058-9565/aaea94 (arXiv:1803.11537)

Unobserved Qubits

- In classical simulation
  - take a partial trace on unobserved qubits
- On quantum computer
  - just ignore or reset qubits
  - → we can reuse discarded qubits!



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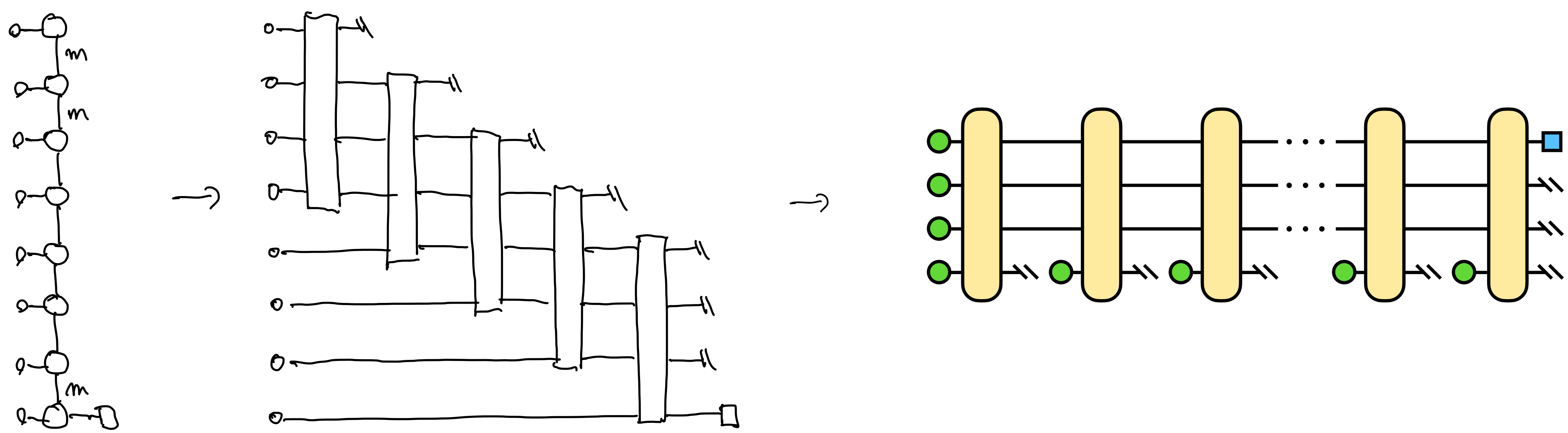
Qubit-efficient Implementation

- Reset and reuse discarded qubits



- Number of physical qubits required is independent of input size N

- Huggins, W., Patil, P., Mitchell, B., Birgitta Whaley, K., & Miles Stoudenmire, E. (2019). Towards quantum machine learning with tensor networks. *Quantum Science and Technology*, *4*, 1. https://doi.org/10.1088/2058-9565/aaea94 (arXiv:1803.11537)
- Liu, J.-G., Zhang, Y.-H., Wan, Y., & Wang, L. (2019). Variational quantum eigensolver with fewer qubits. *Phys. Rev. Research*, 1, 23025. https://doi.org/10.1103/physrevresearch.1.023025 (arXiv:1902.02663)