Introduction to
Machine Learning Methods in Condensed Matter Physics

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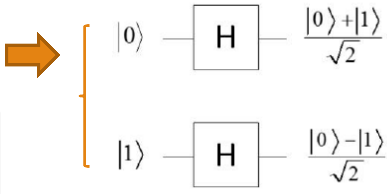
Quantum circuit and quantum computation

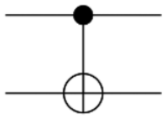
- Quantum circuit is a sequence of state initialization, quantum gates, and measurements.

Hadamard (H)

$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$$



CNOT

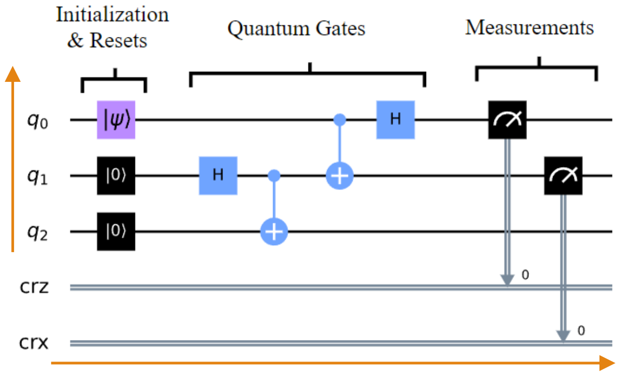


$$\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{bmatrix}$$

and more …

Qubits

(no projection operators, to be realized via interference)



Time (operation sequence)

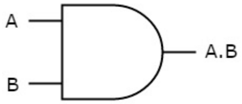
- All gates are unitary, as well as the entire quantum circuits.

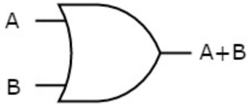
Feynman, Richard, "Quantum mechanical computers" (1986).

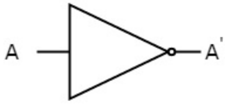
- Potential realizations:

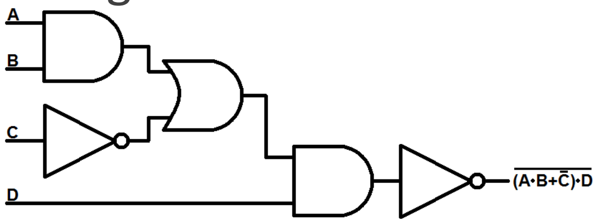
  Superconductors (Josephson junctions), trapped ions (optical lattices), quantum dots (NV centers), NMR, laser optics, etc.

- For comparison, our classical computers run on classical Boolean digital circuits:

AND gate: 

OR gate: 

NOT gate: 

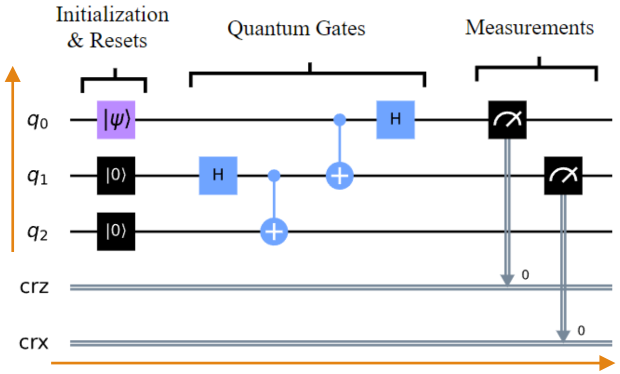


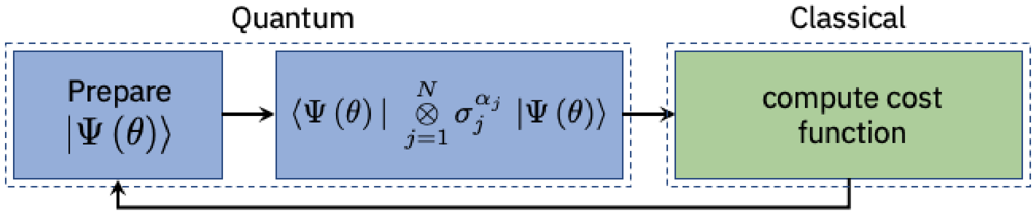
Note: ANN may also be regarded as a classical digital circuits.

Variational quantum eigensolver

- VQE is a quantum/classical hybrid algorithm to solve ground state / minimum of cost function.

  1. Prepare a quantum state $|\Psi(\theta)\rangle$.
  2. Measure the expectation value and gradients of $\langle\Psi(\theta)|\hat{H}|\Psi(\theta)\rangle$.
  3. Minimize the expectation value by varying the parameters θ.
  4. Iterate until convergence (state and expectation value stabilize).

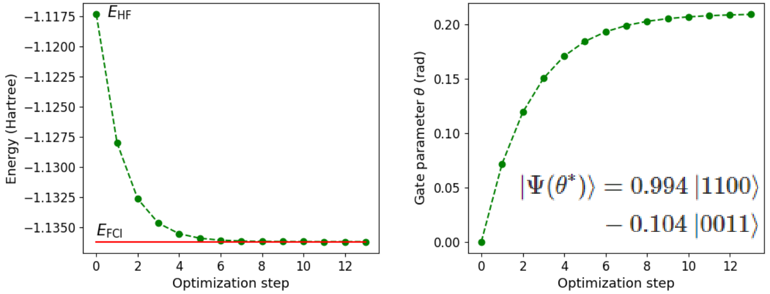




Reduce computation into smaller ones;
Reduce circuit depth and decoherence.

- VQE (also QAOA) is fundamentally a variational ansatz.
- Toy example: ground state of hydrogen molecule

$$|\Psi(\theta)\rangle = \cos(\theta/2)\,|1100\rangle - \sin(\theta/2)\,|0011\rangle$$



- Obstacle: costly optimization (lack of backpropagation and parallelization, barren plateaus).

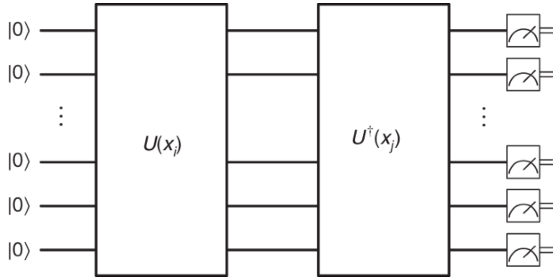
Quantum speed up and advantage?

- Quantum circuit has an advantage on expressivity over its classical counterpart.
- Example: Support vector machine (SVM) with quantum kernel versus classical kernel

Maps a classical data point $x \in \mathbb{R}^d$ to a quantum state $|\phi(x)\rangle = U(x)|0^n\rangle$

The Kernel: $K(x_i, x_j) = \left|\langle 0^n| U^\dagger(x_j) U(x_i) |0^n\rangle\right|^2$ is obtainable via:

1. Start with a state $|0\rangle^n$;
2. Run the circuit $U^{-1}(x_j)U(x_i)$;
3. Evaluate the probability of $|0\rangle^n$ in output.



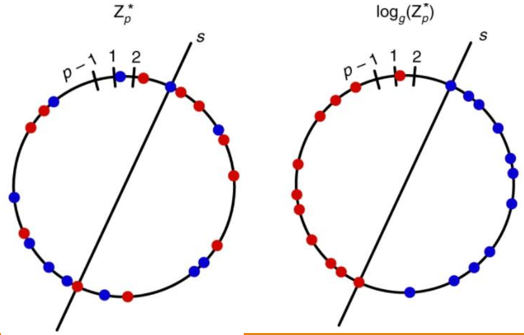
$$k(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i) \cdot \varphi(\mathbf{x}_j)$$

$$K(\boldsymbol{x}, \boldsymbol{x}') = \exp(-\gamma||\boldsymbol{x} - \boldsymbol{x}'||^2)$$

$$K(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x} \cdot \boldsymbol{x}')^d$$

The discrete logarithm problem

$$f_s(x) = \begin{cases} +1, & \text{if } \log_g x \in [s, s + \frac{p-3}{2}], \\ -1, & \text{else.} \end{cases}$$



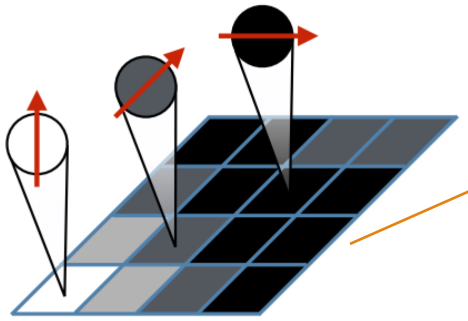
- Quantum feature maps are more expressive than classical counterparts:

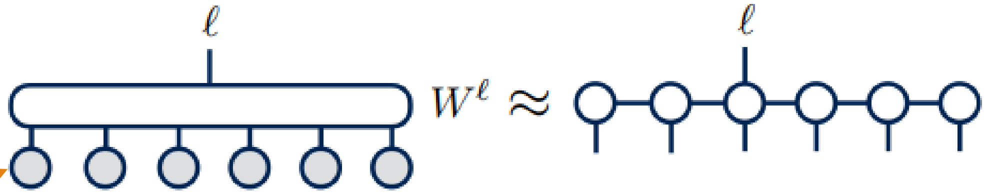
Examples: indistinguishable and not separable by classical kernel, yet linearly and straightforwardly separable in high-dimensional Hilbert space:

Yunchao Liu, Srinivasan Arunachalam, Kristan Temme, Nature Physics ***17****, 1013–1017 (2021).*

Quantum many-body methods for classical machine learning

- Map the classification problem to a quantum many-body state under MPS representation:





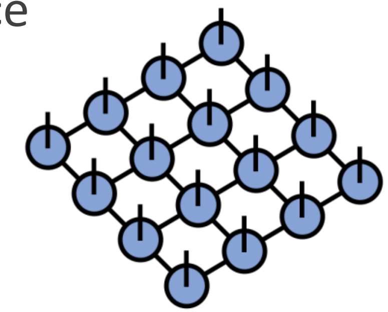
$$W^\ell_{s_1 s_2 \cdots s_N} = \sum_{\{\alpha\}} A^{\alpha_1}_{s_1} A^{\alpha_1 \alpha_2}_{s_2} \cdots A^{\ell;\alpha_j \alpha_{j+1}}_{s_j} \cdots A^{\alpha_{N-1}}_{s_N}$$

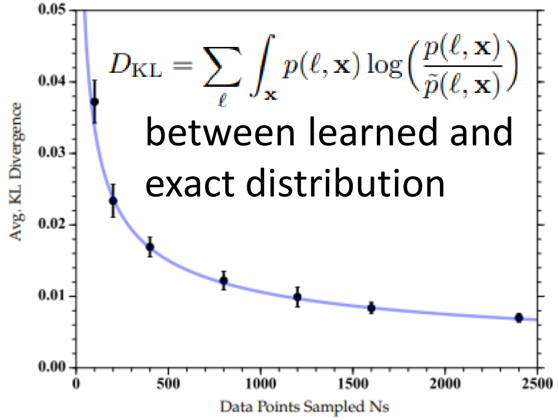
The ordering matters: keep as much locality when reducing from 2D to 1D, especially in regions of meaningful data

Then, optimize the cost function with DMRG: $C = \frac{1}{2} \sum_{n=1}^{N_T} \sum_{\ell} (f^\ell(\mathbf{x}_n) - \delta^\ell_{L_n})^2$

- Test on MNIST data: good and quick convergence

MPS bond dimension	10	20	120
Test error rate	~5%	~2%	0.97%



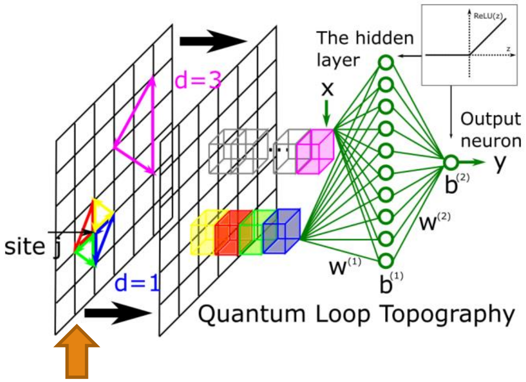


- Also available: PEPS (but harder to train)

*E. Miles Stoudenmire, David J. Schwab, Advances in Neural Information Processing Systems **29**, 4799 (2016).*

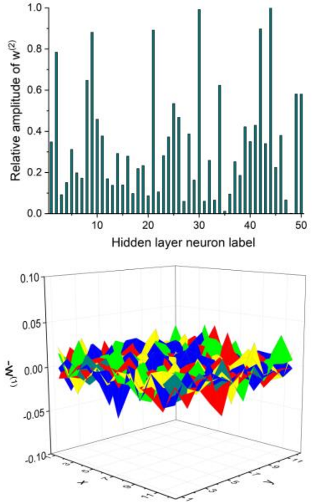
How “scientific” is machine learning?

- Physics is science, not engineering. “AlphaGo knows how, but not why.”
- Use simple ANN, RELU activation, and L1 regularization for interpretability:

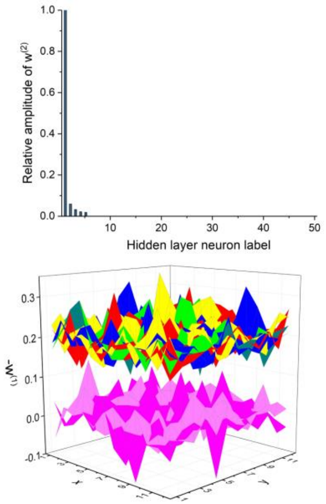


Monte Carlo sampled data with quantum fluctuations

Yi Zhang, Paul Ginsparg, and Eun-Ah Kim, Phys. Rev. Research 2, 023283 (2020).



before learning



after learning

$$-4.84\max\left[-0.208\sum_{d_{\triangle jkl}=1}\mathrm{Im}P_{jk}P_{kl}P_{l\,j}+3.73,\,0\right]+9.03>0$$

$$\Leftrightarrow\ \frac{4\pi}{N}\sum_{d_{\triangle jkl}=1}-\mathrm{Im}P_{jk}P_{kl}P_{l\,j}/2>0.4,$$

Kubo formula emerges from the ANN

$$\sigma_{xy}=\frac{e^2}{h}\frac{1}{N}\sum_{\triangle jkl}4\pi\, iP_{jk}P_{kl}P_{l\,j}S_{\triangle jkl}$$

Translation and rotation symmetries emerge from the ANN

- For machine learning, interpretability and expressivity seem to be confronting attributes.
- Keep it simple, use shallow ANN, SVM, etc. when adequate / conditions suffice.

When NOT to use machine learning

- Problems we have exact solutions or methods (other than benchmark purposes).
- Problems we require absolute precision and safety.
- Problems where bottleneck is the data samples themselves.
- Problems that are full details and lack universality.

- Machine learning is not guaranteed to converge: lack of information, noises, model architecture, hyperparameters, overly large data manifold, etc.

  - Luckily, it fails rather than lies most of the time, at least when voluntarily.

- Still, it offers powerful tools: nonlinearity and big data, both are common in condensed matter physics. Therefore, we can consider their potentials when:
  - Exact solutions are unavailable or expensive, and we can tolerate approximations, especially at first.
  - Optimal solutions known to exist, and we aim to improve the maybe existing but terrible solutions.
  - We have intuitions, which are too abstract, elusive, or complicated to summarize.
  - Change the perspective and attack the problem from a different angle.

Use the knowledge and intuition to improve the learning, every bit helps!