Introduction to Machine Learning Methods in Condensed Matter Physics

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What is quantum machine learning?

- Why? Both quantum computation and machine learning are cutting-edge topics with a lot of interests and focuses (fundings, grants, jobs, etc.)

Method \ Data	Classical	Quantum
Classical	Classical ML	(1)
Quantum	(2)	(3)

Quantum-classical hybrid algorithm for noisy intermediate-scale quantum (NISQ) computer and devices

- (1) Application of classical Machine learning to meaningful quantum problems
  - ↘ A distinct perspective and a useful tool

  Examples: quantum phase identification, quantum compiling and control optimization, QMC speed up, renormalization group, quantum-state representation, quantum state tomography, etc.
- (2) Application of quantum methods to difficult classical problems
  - ↘ Practical utility, but true quantum advantage is difficult to establish

  Examples: Shor's factorization algorithm, quantum annealing, quantum generative adversarial network (QGAN), quantum approximate optimization algorithm (QAOA), variational quantum eigensolver (VQE), etc.
- (3) Quantum machine learning for quantum many-body problems ⇨ good utility yet to be established

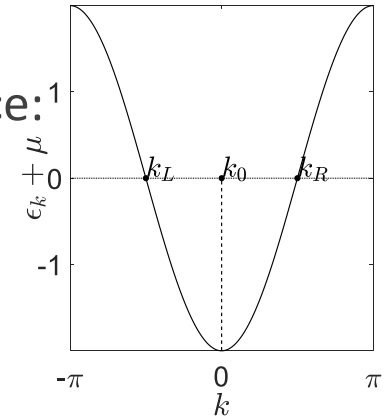
Quantum simulation?

A new perspective for quantum many-body problem

- Solve the ground-state properties of a tight-binding Hamiltonian (Solid state physics 101):

$$\hat{H} = \sum_x -t\left(c_{x+1}^\dagger c_x + \text{h. c.}\right) + \mu c_x^\dagger c_x$$

- Conventional strategy: (1) diagonalize the Hamiltonian in the momentum space:



and (2) fill the Fermi sea for the lowest-energy ground state:

$$|GS\rangle = \prod_{\epsilon_k+\mu<0} c_k^\dagger |vac\rangle$$

then (3) calculate the ground-state properties as expectation values:

$$\langle GS|c_x^\dagger c_x|GS\rangle, \langle GS|c_{x+1}^\dagger c_x|GS\rangle, \textit{etc.}$$

- Alternative strategy: given a quantum state with translation symmetry and a single Fermi sea:

$$\begin{cases} |\Phi\rangle = \prod_{k_L<k<k_R} c_k^\dagger |vac\rangle \\ k_{R(L)} = k_0 \pm k_F \end{cases} \Rightarrow \begin{cases} C_1 = \langle c_{x+1}^\dagger c_x\rangle = \langle c_x^\dagger c_{x-1}\rangle = \cdots = k_F/\pi \\ C_0 = \langle c_x^\dagger c_x\rangle = \langle c_{x-1}^\dagger c_{x-1}\rangle = \cdots = \sin(k_F)\, e^{ik_0}/\pi \end{cases} \Rightarrow \pm\pi|C_1| = \sin(\pi C_0)$$

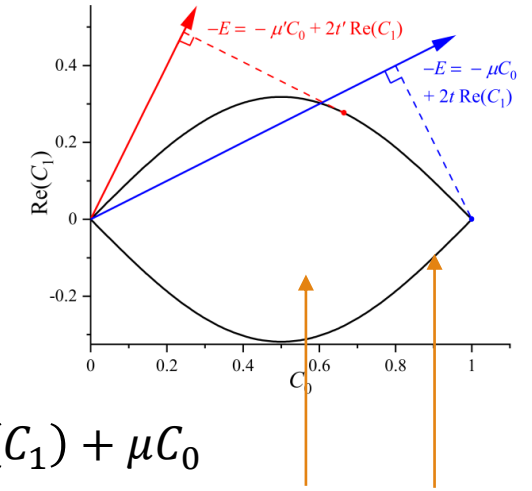
A new perspective for quantum many-body problem

- Physical expectation values (classical number):

$$\pm\pi|C_1| = \sin(\pi C_0)$$

- For the ground state, minimize energy (Hamiltonian expectation value) with a classical constrained optimization:

$$\min \bar{E} \ \text{ s.t. } \pm\pi|C_1| = \sin(\pi C_0)$$



unphysical vs physical

- Example: $\hat{H} = \sum_x -t\left(c_{x+1}^\dagger c_x + \text{h. c.}\right) + \mu c_x^\dagger c_x$ ➡ $\bar{E} = E/N = -2t\mathrm{Re}(C_1) + \mu C_0$

t is Real ➡ $\mathrm{Im}(C_1) = 0$

- The quantum many-body system $\hat{H}$ ➡ The ground-state properties $\langle \hat{\boldsymbol{O}} \rangle_{GS}$

$$\hat{H} \not\rightarrow |\Phi\rangle_{GS} \Rightarrow \langle \hat{\boldsymbol{O}} \rangle_{GS}$$

- The Hamiltonian is also but an operator (linear combination of operators):

$$\hat{H} = \sum_i c_i \hat{O}_i \quad \Rightarrow \quad E = \sum_i c_i \langle \hat{O}_i \rangle$$

Its role?

Minimum energy criteria.

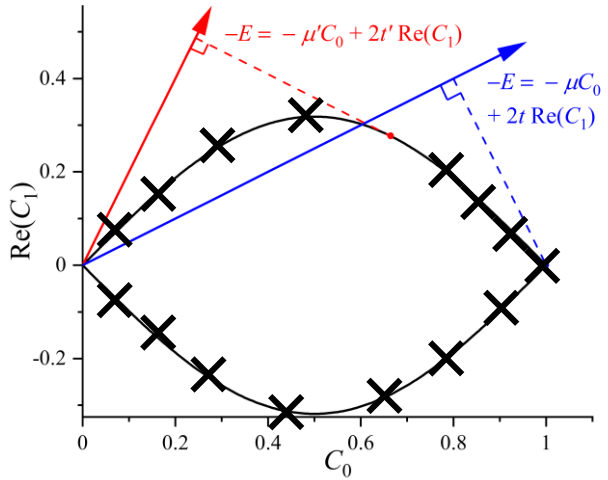
Pei-lin Zheng, Si-Jing Du, YZ, arXiv: 2105.09947

Classical-machine-learning-invigorated quantum strategy

- How do we get such function $f(\langle\hat{\boldsymbol{O}}\rangle)$ that can distinguish physical and unphysical expectation values?
  - Sample $|\Phi\rangle$ consistent with the *presumptions* of the ground states.
  - Evaluate $\langle\hat{\boldsymbol{O}}\rangle$ as one sample, so on so forth.
  - Apply supervised machine learning for an approximate $f(\langle\hat{\boldsymbol{O}}\rangle)$.

Expectation values → Machine learning → $\mathbf{H} = a_j\hat{O}_j$

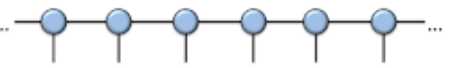
$$\{|\boldsymbol{\Phi}\rangle\} \rightarrow \{\langle\hat{\boldsymbol{O}}_{\boldsymbol{j}}\rangle\} \rightarrow f_{\mathrm{ANN}}(\langle\hat{\boldsymbol{O}}_{\boldsymbol{j}}\rangle) \rightarrow \{\langle\hat{\boldsymbol{O}}\rangle\}_{\min(a_j\langle\hat{O}_j\rangle)\ in\ f}$$



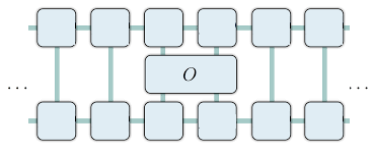
- Advantages: thermodynamic limit, strongly correlated systems, etc.

fully translation-invariant *iMPS*

$$|\Psi\rangle = \sum_{\cdots,s_n,\cdots} \cdots M_{s_n} \cdots \times |\cdots, s_n, \cdots\rangle$$

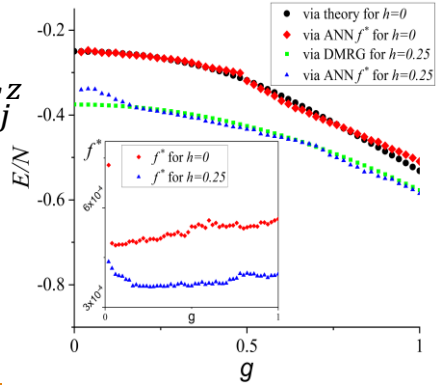


Evaluate expectation value of $S_r^{\lambda}, S_r^{\lambda}S_{r+l}^{\lambda'}\Big|_{l=1,\cdots,l_{max}}^{\lambda,\lambda'=x,y,z}$



$$H = \sum_j -JS_j^zS_{j+1}^z - gS_j^x - hS_j^z$$

$$\min_{\langle\hat{\boldsymbol{o}}\rangle} L = \bar{E} + \eta f^*$$



Pei-lin Zheng, Si-Jing Du, YZ, arXiv: 2105.09947

Classical-machine-learning-invigorated quantum strategy

- Another advantage: property design, for example, maximize $(C_1^{AA}-C_1^{BB})^{\epsilon}(C_{1/2}^{AB}+C_{-1/2}^{AB})$

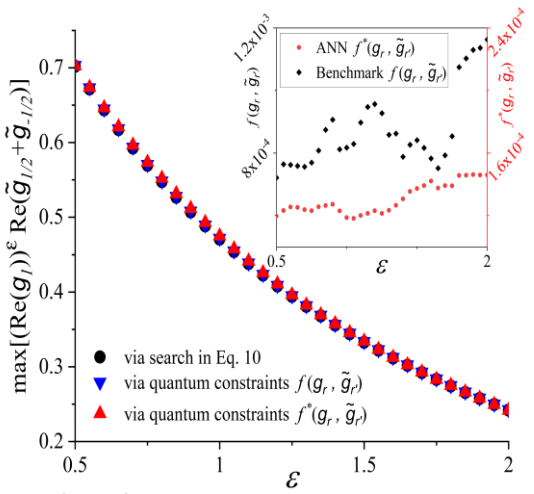
Conventionally, we can search within a variational model:

$$\widehat{H}_{var}=\sum_x -t\left(c_{x+1}^{\dagger}c_x+\text{h. c.}\right)+(-1)^x\Delta\left(c_{x+2}^{\dagger}c_x+\text{h. c.}\right)\ \boxed{?\ +\cdots}$$

Generally, we need a larger search space for better outcome, and solve the ground state for each attempted Hamiltonian.

- With the new perspective, we simply need to apply classical optimizations:

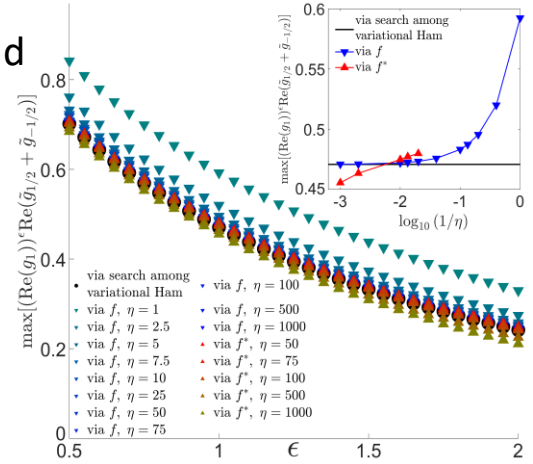
$$\min_{g_r,\tilde{g}_{r'}} \quad L=-(C_1^{AA}-C_1^{BB})^{\epsilon}(C_{1/2}^{AB}+C_{-1/2}^{AB})\ +\eta f$$



Variational strategy:
incomplete search space
→ underestimate

Quantum constraints strategy:
exaggerated search space
→ overestimate

Extrapolation and impact of η:



Pei-lin Zheng, Si-Jing Du, YZ, arXiv: 2105.09947

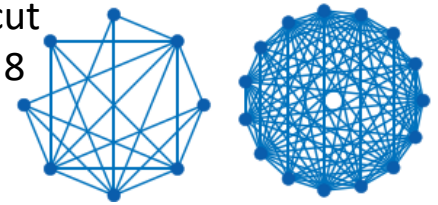
‘Simple’ yet difficult classical optimization problems

- Globally optimal solutions of classical spin glass problems are difficult (NP-hard):

$$\hat{H}_C = \sum_{i<j} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z + \sum_{i=1}^{n} h_i\hat{\sigma}_i^z$$

Examples: number partition, max cut, 3-SAT, exact cover, etc.

Example max-cut problems with 8 and 15 nodes:



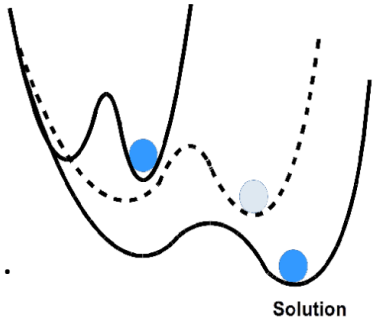
- Conventional methods: simulated annealing (Classical Monte Carlo), quantum annealing

$$H = \lambda H_C + (1-\lambda)\, H_M, \lambda = 0 \to 1$$

from a trivial initial H_M with a simple ground state.

Example: $\hat{H}_M \equiv \sum_{i=1}^{n} \hat{\sigma}_i^x$ and $|+\rangle^{\otimes n}$

Need quantum experiment, since the real-time evolution is very expensive to calculate.

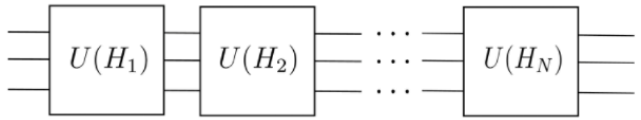


Quantum annealing needs to be sufficiently slow to keep the system at ground state.

- Time evolution operator: time-independent $U(H,\, t) = e^{-iHt/\hbar}$

time-dependent: Trotter-Suzuki decomposition when $n \gg 1$

$$U(H,t) = \prod_{k=1}^{n} e^{-iH_k t/n}$$



Quantum approximate optimization algorithm

- Instead of an infinite number of (time) steps, we approximate the process with p discrete steps:

$$|\psi_p(\vec{\gamma},\vec{\beta})\rangle \equiv \hat{V}(\beta_p)\hat{U}(\gamma_p)\ldots\hat{V}(\beta_1)\hat{U}(\gamma_1)|+\rangle^{\otimes n} \qquad \hat{V}(\beta) \equiv e^{-i\beta\hat{H}_M} \qquad \hat{U}(\gamma) \equiv e^{-i\gamma\hat{H}_C}$$

and treat it as a variational state and optimize the energy with respect to its parameters:

$$E_p(\vec{\gamma},\vec{\beta}) \equiv \langle\psi_p(\vec{\gamma},\vec{\beta})|\hat{H}_C|\psi_p(\vec{\gamma},\vec{\beta})\rangle$$

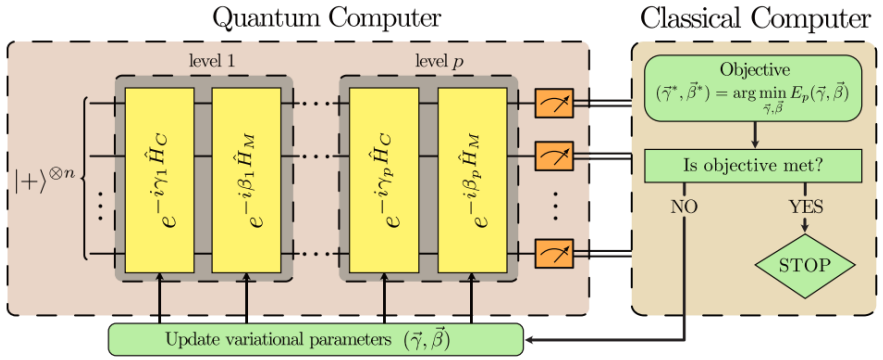
$$(\vec{\gamma}^*,\vec{\beta}^*) = \arg\min_{\vec{\gamma},\vec{\beta}} E_p(\vec{\gamma},\vec{\beta})$$

$$\hat{H}_C = \sum_{i<j} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z + \sum_{i=1}^{n} h_i\hat{\sigma}_i^z$$

$$\hat{H}_M \equiv \sum_{i=1}^{n}\hat{\sigma}_i^x$$

$|\psi_p\rangle$ is a linear superposition of classical configurations, which can be measured for the optimal solution as long as it has a notable weight.

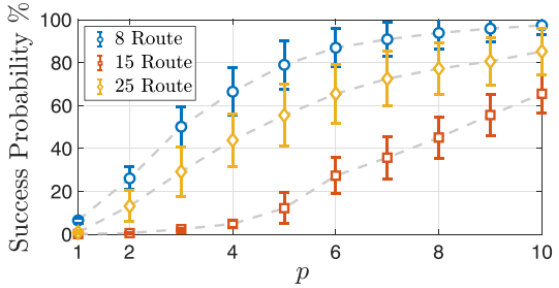
- QAOA as a hybrid algorithm:
  - Quantum computer/circuit: evaluate E_p
  - Classical computer: classical optimization problem

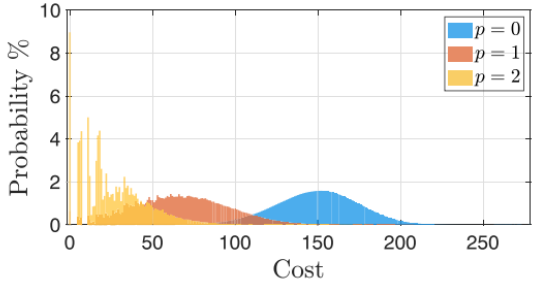


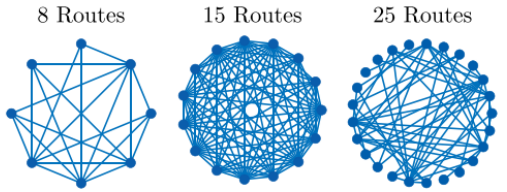
Edward Farhi and Jeffrey Goldstone, arXiv: 1411.4028; Pontus Vikstal, et al., Phys. Rev. Applied 14, 034009 (2020).

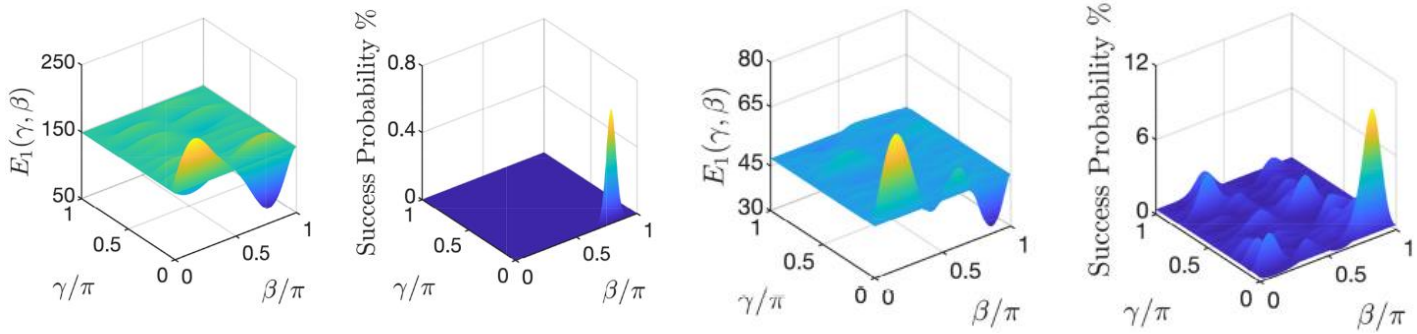
Quantum approximate optimization algorithm

- When the depth/level $p \to \infty$, we should approach the expressibility of the true solution.
- Good-enough approximation to the true solution is good enough.
- All potential solutions are considered equally in the initial state.
- When the energy is low, the true solution's weight should be high.
- The optimization problem is with respect to the parameters $\vec{\lambda}$ and $\vec{\beta}$, and can be carried out using gradient descent, etc.









Single layer ($p = 1$) QAOA's energy landscape for $n = 25$ and $n = 8$ max-cut problems

Edward Farhi and Jeffrey Goldstone, arXiv: 1411.4028; Pontus Vikstal, et al., Phys. Rev. Applied 14, 034009 (2020).

QAOA for quantum states

- QAOA as an efficient way for state preparation:

$$|\psi(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle_p = e^{-i\beta_p H_1} e^{-i\gamma_p H_2} \cdots e^{-i\beta_1 H_1} e^{-i\gamma_1 H_2} |\psi_1\rangle$$

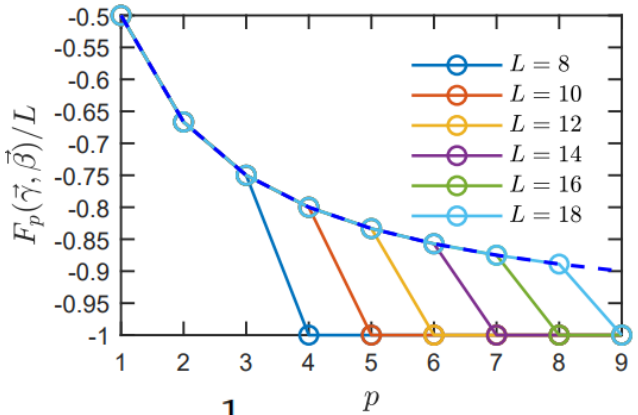
$$|\psi_1\rangle = \otimes |X=1\rangle$$

$$H_1 = -\sum_{i=1}^{L} X_i$$

$$H_2 = -\sum_{i=1}^{L} Z_i Z_{i+1}$$

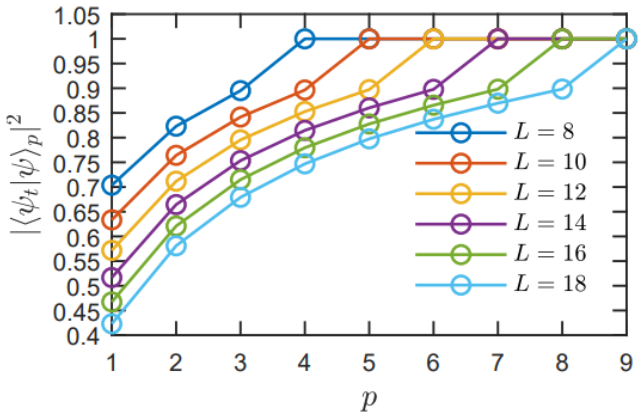
- Examples on the GHZ state and TFIM critical state:

$$H_T = -\sum_{i=1}^{L} Z_i Z_{i+1}$$



$$|\mathrm{GHZ}\rangle \equiv \frac{1}{\sqrt{2}}(\otimes|Z=1\rangle + \otimes|Z=-1\rangle)$$

$$H_T = -\sum_{i=1}^{L} Z_i Z_{i+1} - \sum_{i=1}^{L} X_i$$



Duality between the Ising model and Z_2 lattice gauge theory

Also for certain topological states

However, QAOA is still approximate in general, and can be most/more useful determine ground-state properties that are discrete, robust, e.g. topological invariants.

Wen Wei Ho, Timothy H. Hsieh, SciPost Phys. 6, 029 (2019).