Introduction to Machine Learning Methods in Condensed Matter Physics

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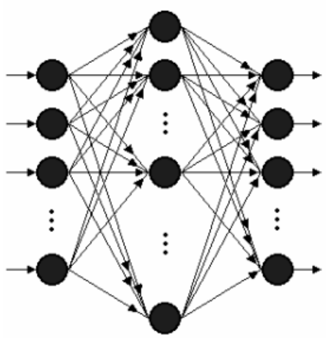
Yi Zhang (张亿)

International Center for Quantum Materials, School of Physics
Peking University, Beijing, 100871, China

Email: frankzhangyi@pku.edu.cn

What is and why reinforcement learning?

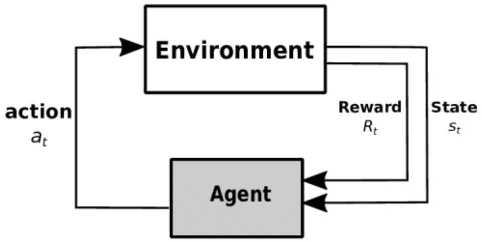
- An agent (strategy) that interacts with an environment and maximizes reward (minimize) penalty – value functions approximated by ANNs.
  - $V(S)$: the approximate most accumulated reward from state S. Then, given S, we can choose then optimal action $\mathrm{argmax}[V(S' = S(A)]$
  - $Q(S, A)$: the approximate most accumulated reward from state S after choosing action A. Then, given S, we can choose the optimal action $\mathrm{argmax}[Q(S, A)]$



- General setup: S: current state; A: action upon state; R: reward

$S \xrightarrow{A} S' \xrightarrow{A'} S'' \xrightarrow{A''} \cdots \rightarrow$ end, where the *accumulated reward* is determined

- Good for control problems where an optimal-strategy solution simply does not exist.
  - E.g. competing interests in experimental or numerical tunings

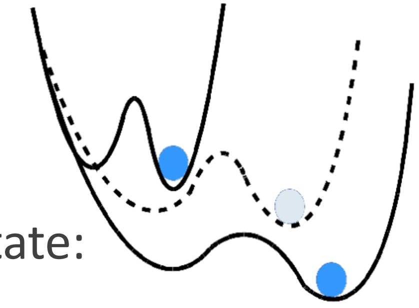


Reinforcement learning for Quantum Adiabatic Algorithm

- Calculating the ground state of a target Hamiltonian H_t via adiabatic evolution:

$$H = \lambda H_t + (1 - \lambda)\, H_0$$

from a trivial initial H_0 with a simple ground state, $\lambda = 0 \rightarrow 1$.



- The process needs to be sufficiently slow to keep the system at its ground state:
- More generally, we can have a path $H_{tar} \rightarrow H_1 \rightarrow H_2 \rightarrow \cdots \rightarrow H_0$:

S: current H_i;

A: ΔH_i, change $H_{i+1} = H_i + \Delta H_i$;

R: minimum gap or fidelity $\langle \Phi_i | \Phi_{i+1} \rangle$ along the path,

only available at the end of the path (arriving at H_0).

Compared with Goal:

Board configuration

Next move

Win rate / advantage

However, we have not achieved good convergence yet.

- Also, value function offers an estimate of the difficulty level of the target Hamiltonian.

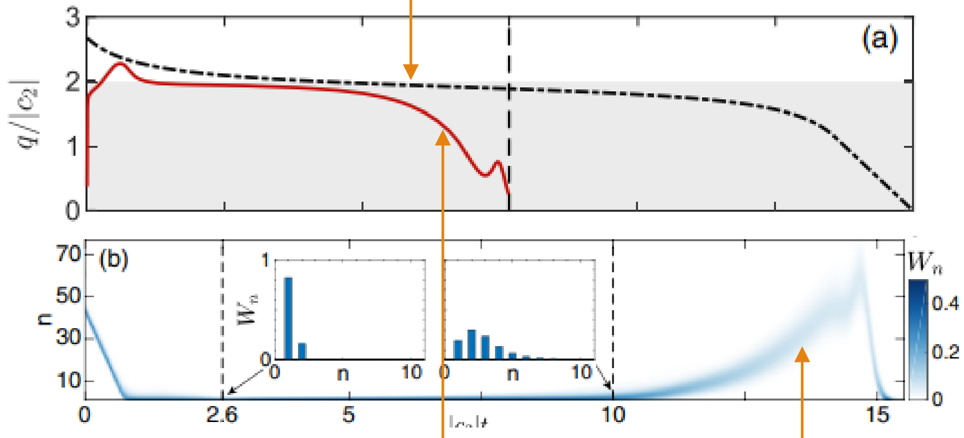
Reinforcement learning for fast state preparation

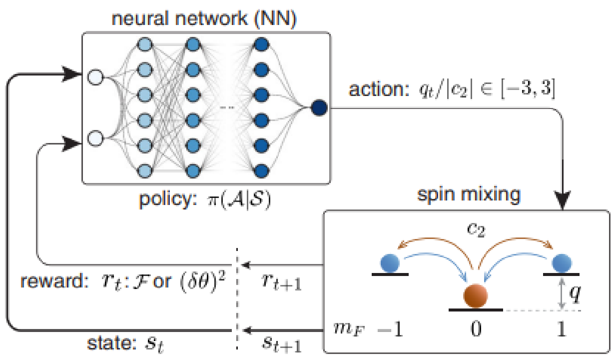
- Preparing the Dicke state through evolution ($q(t) \to 0$): (One target state only)

$$H = \frac{c_2}{2N}\mathbf{L}^2 - q(t)N_0$$

Conventional adiabatic evolution keeps the system at ground state.

takes longer, especially when system is gapless





$$\mathcal{F} = |\langle \psi(t) | \psi^{(0)}_{\text{Dicke}} \rangle|^2$$

An unconventional route by reinforcement learning forsakes the adiabaticity requirement.

Shuai-Feng Guo#, Feng Chen#, et al., Phys. Rev. Lett. ***126****, 060401 (2021).*

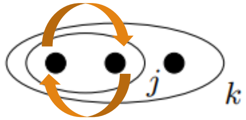
Universal quantum compiling

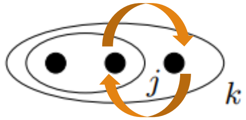
- Given a universal set of elementary gates, one can obtain any given unitary via a sequence:

For example, U_1 U_2

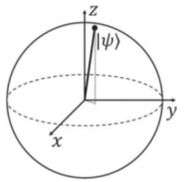
$\pi/8$ (T) $\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$ Hadamard (H) $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$

or by braiding topological quasiparticles:





$$\sigma_1 = \begin{pmatrix} \eta^{-4} & 0 \\ 0 & \eta^3 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} -\phi^{-1}\eta^{-1} & \phi^{-\frac{1}{2}}\eta^{-3} \\ \phi^{-\frac{1}{2}}\eta^{-3} & -\phi^{-1} \end{pmatrix}$$

System		
Initial state	The unitary to be approximated	The scrambled cube
Target state	The identity matrix	The solved cube
Basic move	A gate from the universal set	Rotation of one face

$$U \approx U_1^{n_1} U_2^{n_2} U_1^{n_3} U_2^{n_4} \cdots$$

Chetan Nayak, et al., Rev. Mod. Phys. ***80****, 1083 (2008).*

$\eta = e^{i\pi/5}$ $\quad \phi = (\sqrt{5}+1)/2$

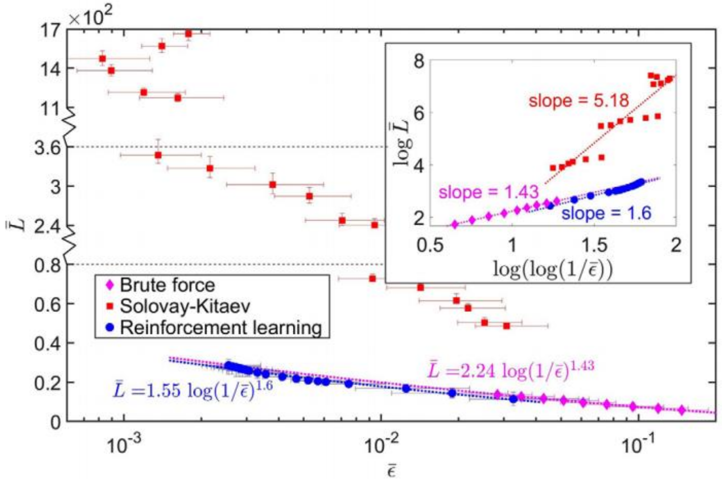
- We prefer to represent the unitary with as much precision with as short a sequence as possible.
  - Brute-force: try out all sequences at a given length, pick the closest unitary
  - Solovay-Kitaev: obtain near-identity unitaries as building block and solve recursively

best length, bad search time
good search time, bad length

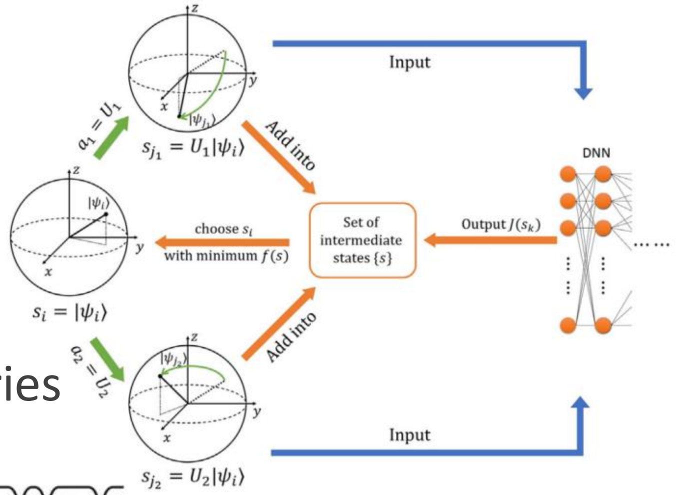
- Reinforcement learning shines where there exists an applicability proof but no optimal strategy.

Reinforcement learning for quantum compiling

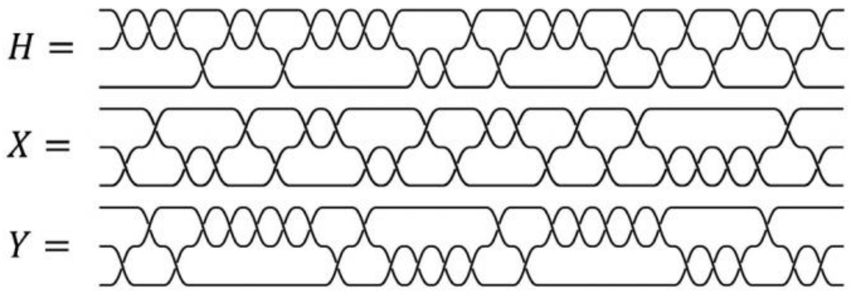
- S: current unitary U, A: applied elementary gate U_i, R: expected distance towards solution within required accuracy threshold
- Application is very time efficient: $S \to S' \to S'' \to \cdots \to$
- Results: comparable sequence length with brute force



General, any single-qubit unitaries



- Selected target unitaries:



all better than $O(10^{-3})$ precision

Yuan-Hang Zhang, Pei-Lin Zheng, YZ, and Dong-Ling Deng*, Phys. Rev. Lett. 125, 170501 (2020).*

Yao's Millionaires' problem

- Possible security of sensitive big data: add (indistinguishable) random noise
- *Secure multi-party computation problem*: for example, two millionaires want to compare their wealth, but refuse to reveal how much money they have, to each other or a trusted third party.
  - Step 1: prepare identical boxed with locks and keys:
  - Step 2: first millionaire puts information about his number inside, lock up all boxes.
  - Step 3: second millionaire chooses the box according to her number, destroy the rest of boxes.
  - Step 4: open the lock on the remaining box to find out the answer.

Andrew C. Yao, SFCS ***1****, 160–164(1982).*

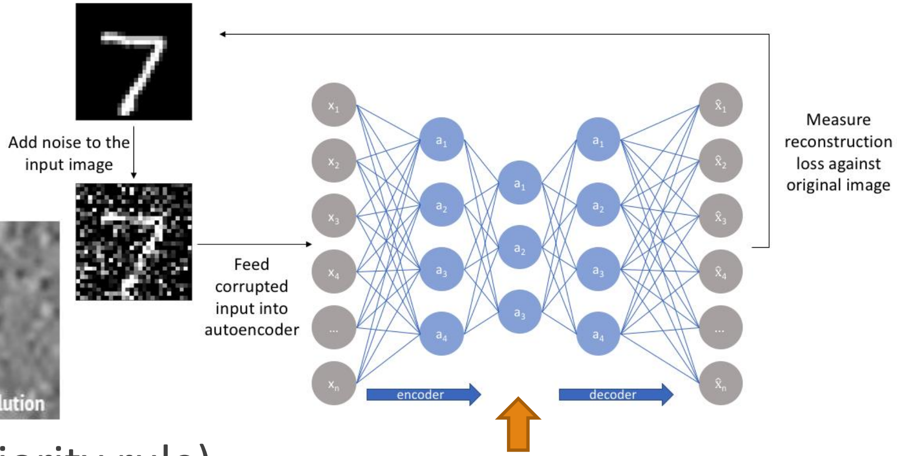
E.g.: double-blind interpretation of experimental/numerical data

Data pooling: the bigger the data, the better machine learning

- *Oblivious transfer*: transfer many messages but is oblivious to which message is used/received.

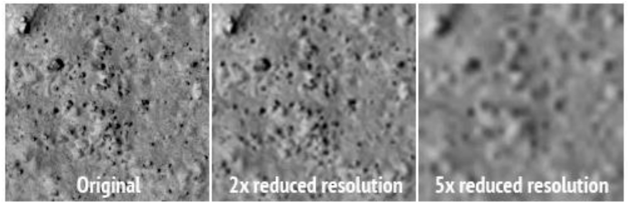
Autoencoder

- Train an ANN with a bottleneck to minimize the reconstruction error $L(\boldsymbol{x}, \widehat{\boldsymbol{x}})$ between the input $\boldsymbol{x}$ and output $\widehat{\boldsymbol{x}}$.
  - Compression: amount of information that can traverse the network is constrained.
  - Dimensional reduction (similar to linear PCA, unsupervised machine learning, to be discussed later)
- The bottleneck should be sufficient to allow to accurately build a reconstruction, but not enough to simply memorize (overfit) the training data.
- Trivia: add noise to the input for the better:



a compressed representation

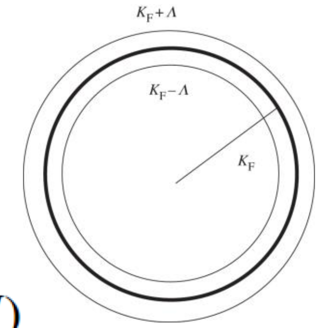
- Idea: representation matters!



JPEG compression vs reduced resolution (majority rule)

- The extreme limit: phase recognition. Also, CNN’s convolution and pooling

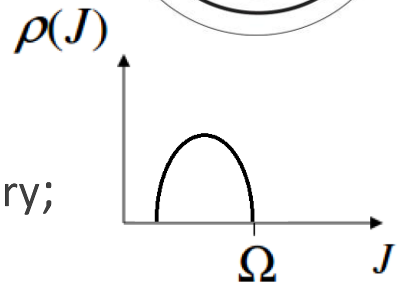
Renormalization group in condensed matter



- Momentum-space RG: e.g. Fermi liquid theory
  - Why electrons with Coulomb interactions commonly behave like non-interacting electron gas?
  - Relevant d.o.f are the momentum shells around the Fermi surface
  - All interactions are irrelevant except (nested) BSC and CDW interaction channels

R. Shankar, Rev. Mod. Phys. ***66****, 129(1994).*

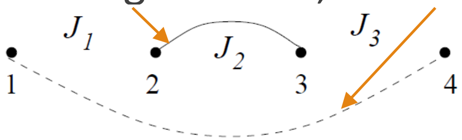
- Real-space RG: e.g. 1D random spin glass



$$\hat{\mathcal{H}} = \sum_i J_i \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1}$$

1. Pick the strongest bond; 2. Eliminate the higher energy d.o.f via perturbation theory;

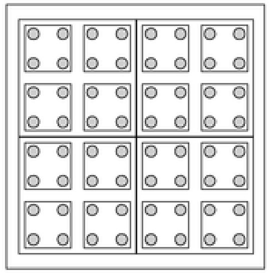
3. iterate.



$\Rightarrow J_{eff} = J_1 J_3 / 2J_2 \qquad J^{typical} \sim \dfrac{\Omega^2}{\Omega_0}$

D. S. Fisher, Phys. Rev. B ***50****, 3799 (1994).*

- Also, block spin RG: $H(T, J)$ describes the system with n.n. coupling J at temperature T: The physics of a 2×2 block is approximately described by $H(T', J')$. $(T, J) \to (T', J') \to \ (T", J") \to \cdots$ long-range behavior after many itineration.



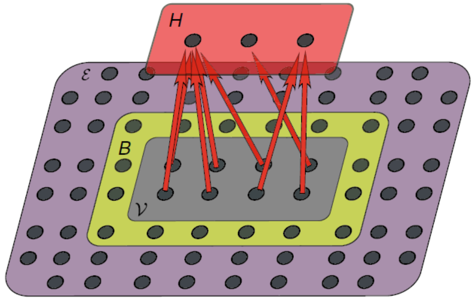
$\Rightarrow$ Fixed points: $T = 0, J \to \infty$; $T = \infty, J \to 0$; $T = T_c, J = J_c$ (unstable, critical).

Leo P. Kadanoff, Physics Physique Fizika. ***2*** *(6), 263(1966).*

Neural network assisted renormalization group

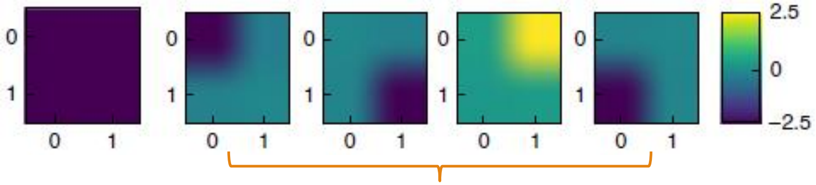
- Mutual information: a measure of the mutual dependence, correlation between two d.o.f

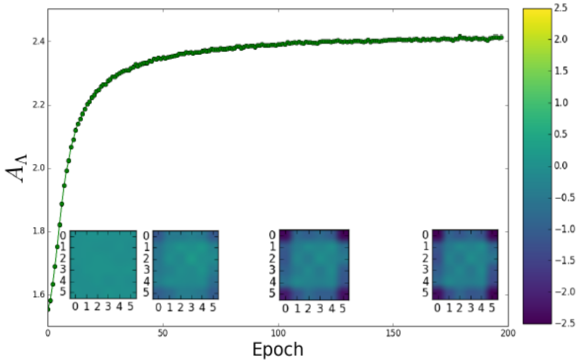
$$I_\Lambda(\mathcal{H}:\mathcal{E}) = \sum_{\mathcal{H},\mathcal{E}} P_\Lambda(\mathcal{E},\mathcal{H}) \log\left(\frac{P_\Lambda(\mathcal{E},\mathcal{H})}{P_\Lambda(\mathcal{H})P(\mathcal{E})}\right)$$



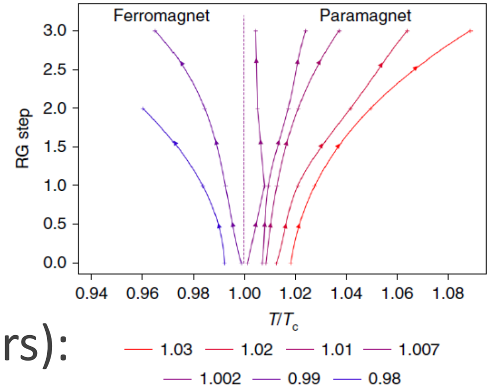
- Choose a subset representation H of V to maximize its *real-space mutual information* with the environment E with a neural network:
  - Example: 2D Ising-model

$$H_\mathrm{I} = \sum_{\langle i,j \rangle} s_i s_j$$





2 × 2 maps to 1   2 × 2 maps to 4   6 × 6 block spin maps to 1

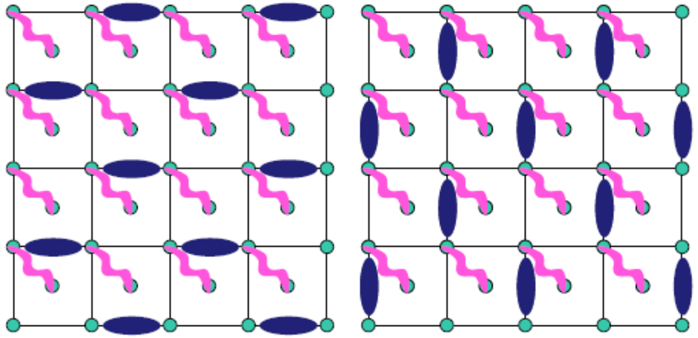


- Itinerate the steps for the RG flows (temperature inferred from correlators):

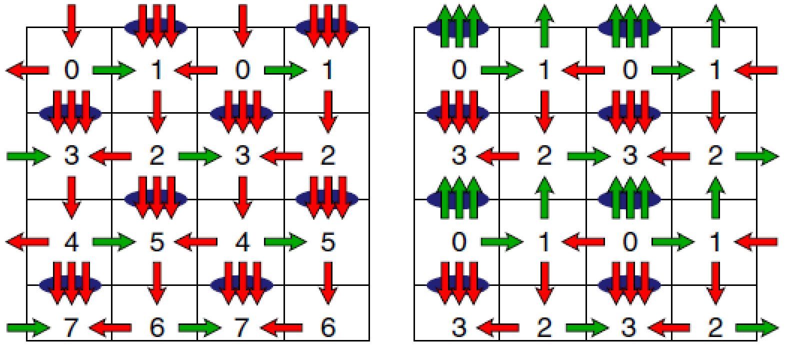
*Maciej Koch-Janusz, Zohar Ringel, Nature Physics **14**, 578–582 (2018).*

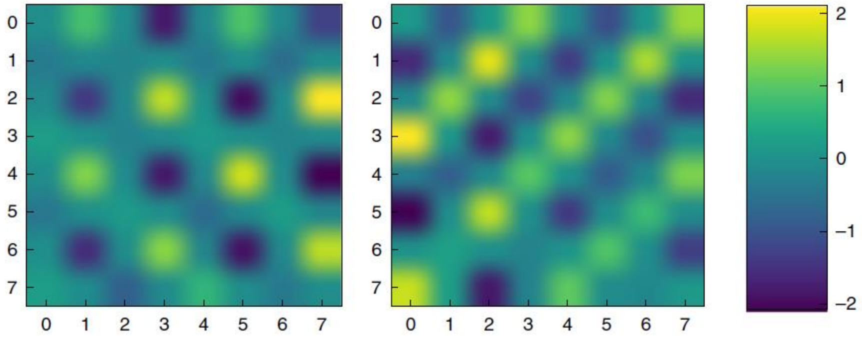
Neural network assisted renormalization group

- Application on dimer model for more nontrivial relevant d.o.f:
  - Also works in the presence of local noises (irrelevant in RG)



- The true degrees of freedom (E fields) are disclosed by ANN:





maps to 2 neurons

Maciej Koch-Janusz, Zohar Ringel, Nature Physics ***14****, 578–582 (2018).*