Case Study: CMS in Next Decade

Solving the quantum many-body problem with artificial neural networks

G. Carleo and M. Tyoer

Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland
Quantum Architectures and Computation Group,
Microsoft Research, Redmond, WA 98052, USA and
Station Q, Microsoft Research, Santa Barbara, CA 93106-6105, USA

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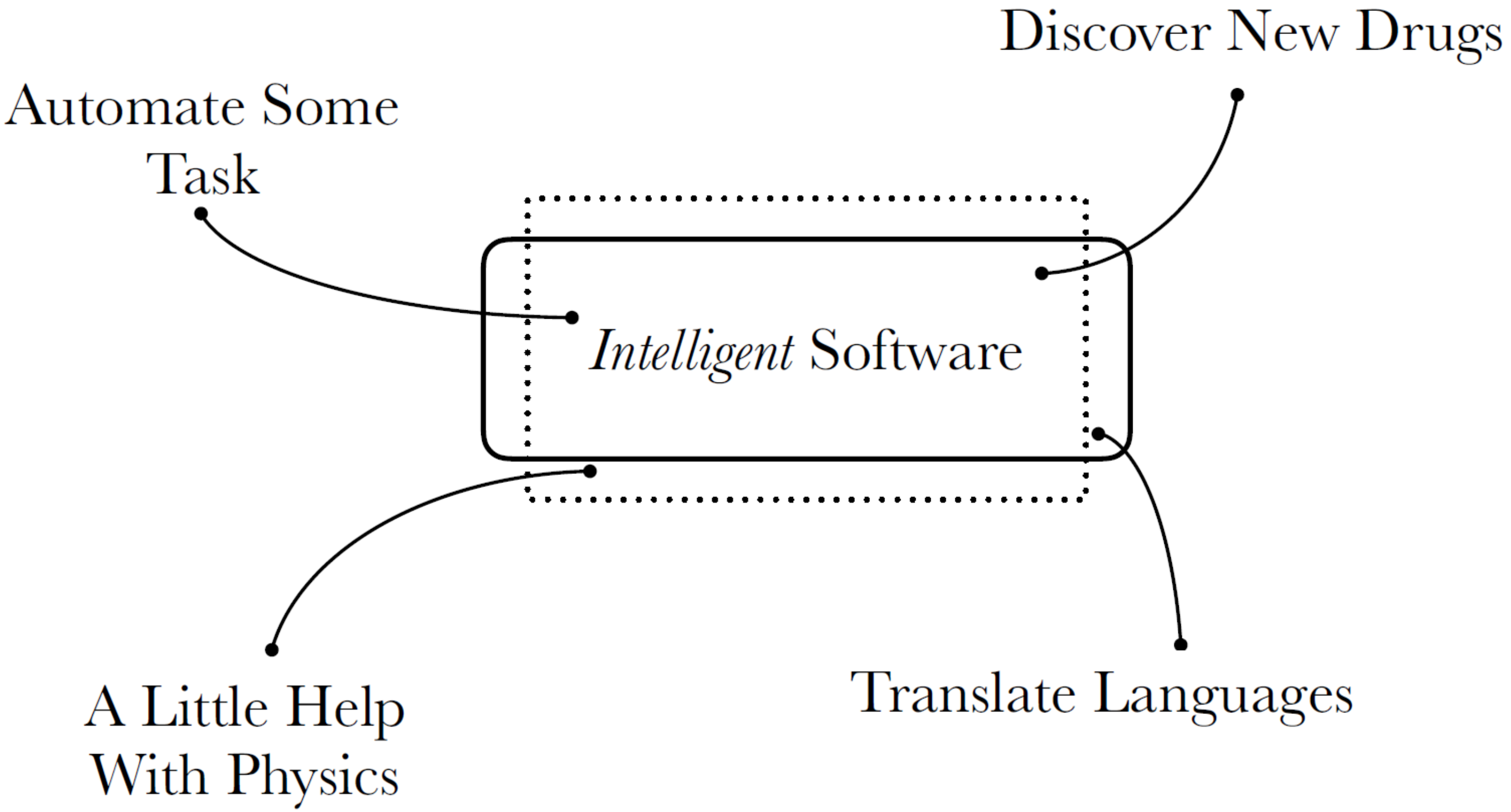
Machine Learning

"A machine that can think"

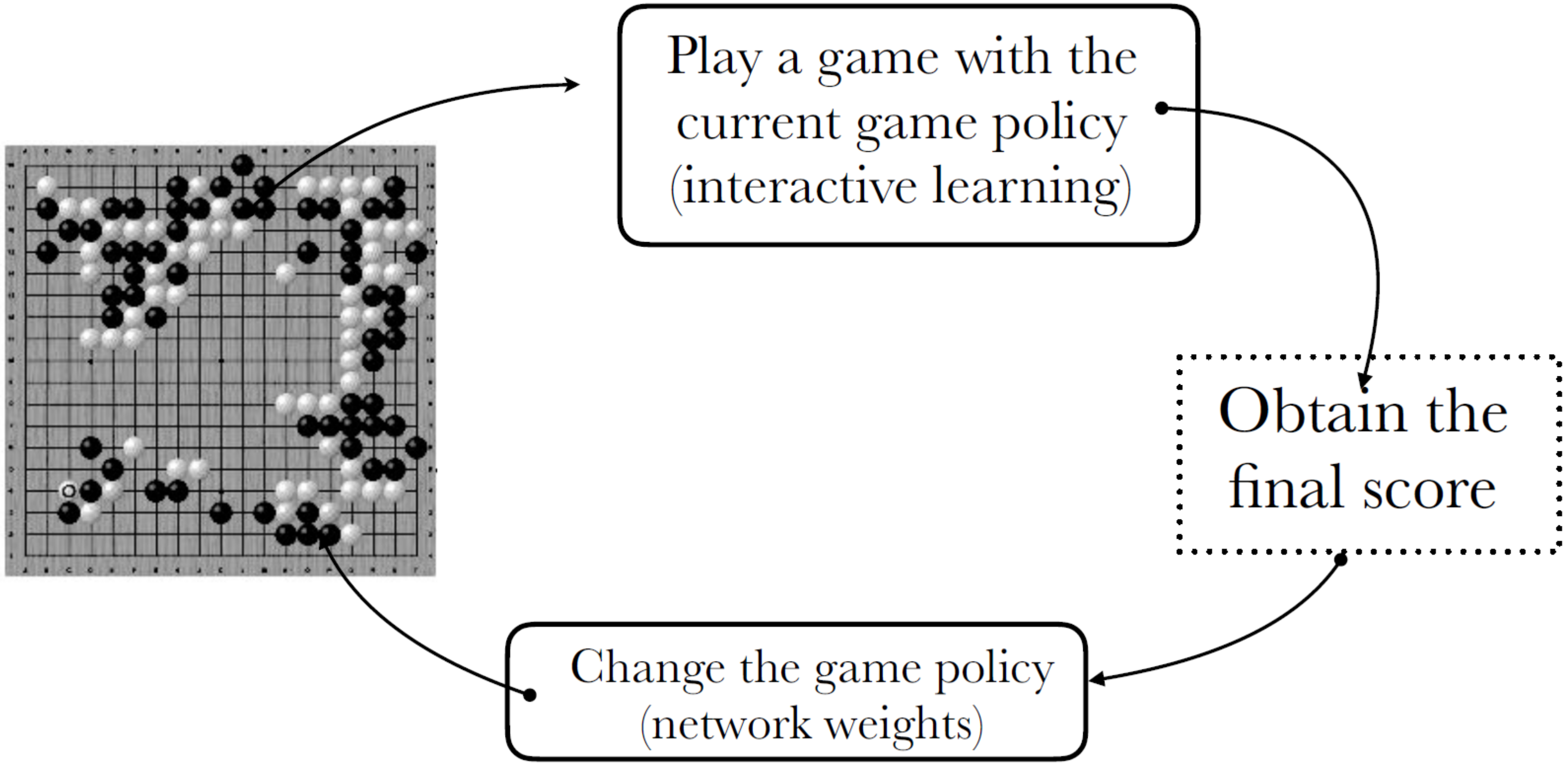
Machine learning is a computational technique dedicated to achieve self-learning and self-improvement with the help of empirical experience (or limited knowledge).



G. Caleo, INT-Seattle presentation, 21/03/2017

Artificial Neural Networks

Mastering the game of Go with deep neural networks and tree search
Silver et al., Nature 529, 484 (2016)



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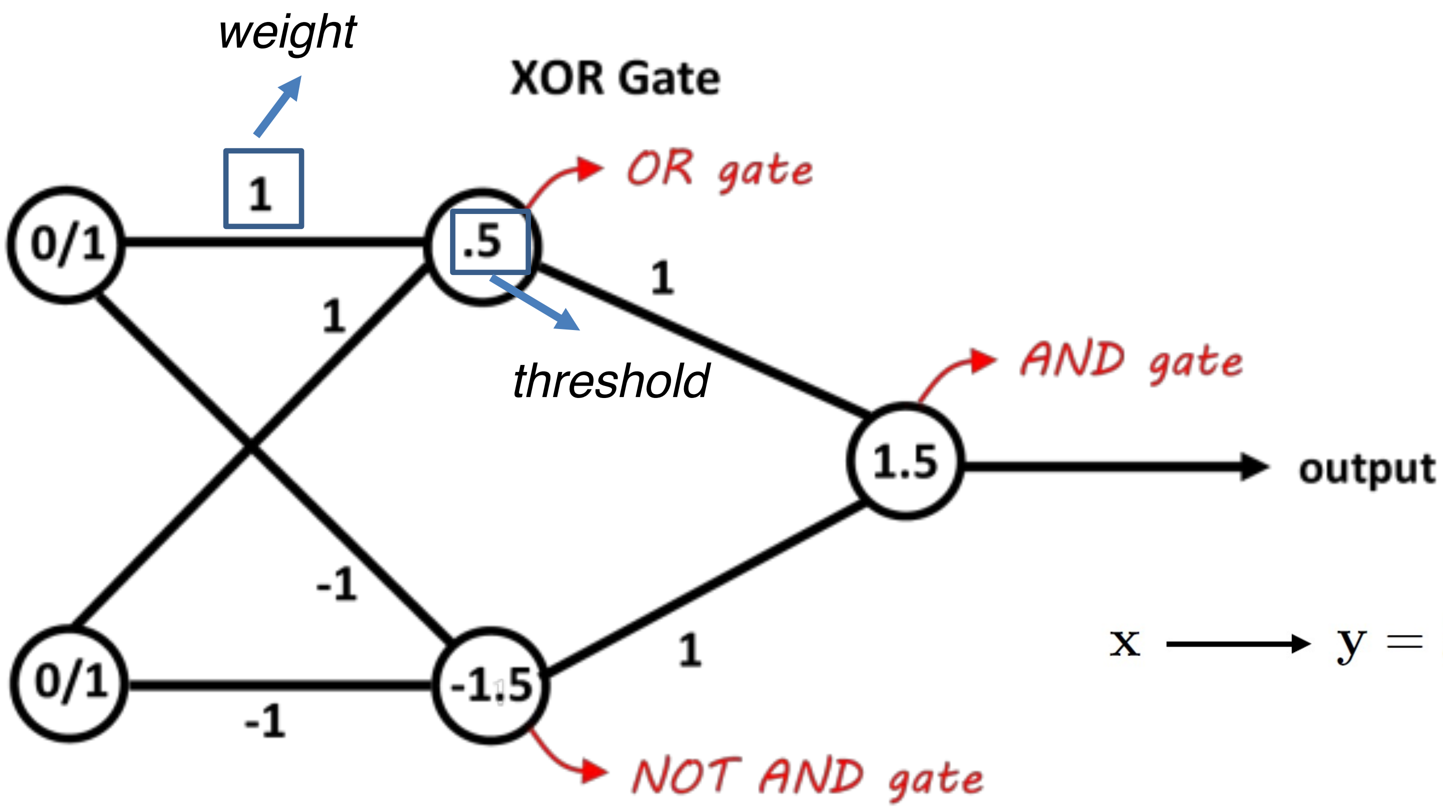
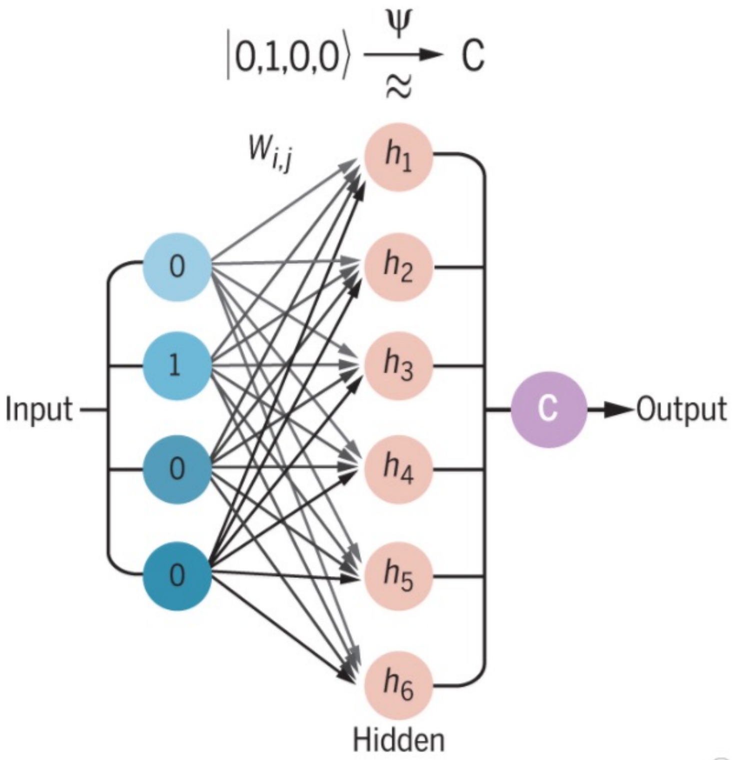
Artificial Neural Networks

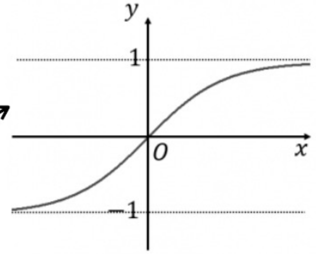
Input layer -> Hidden layer -> Output layer





$$\mathbf{x} \longrightarrow \mathbf{y} = h(\mathbf{x}) \longrightarrow \mathbf{F} = g(\mathbf{y})$$

Activation functions
(tanh, logistic, etc)



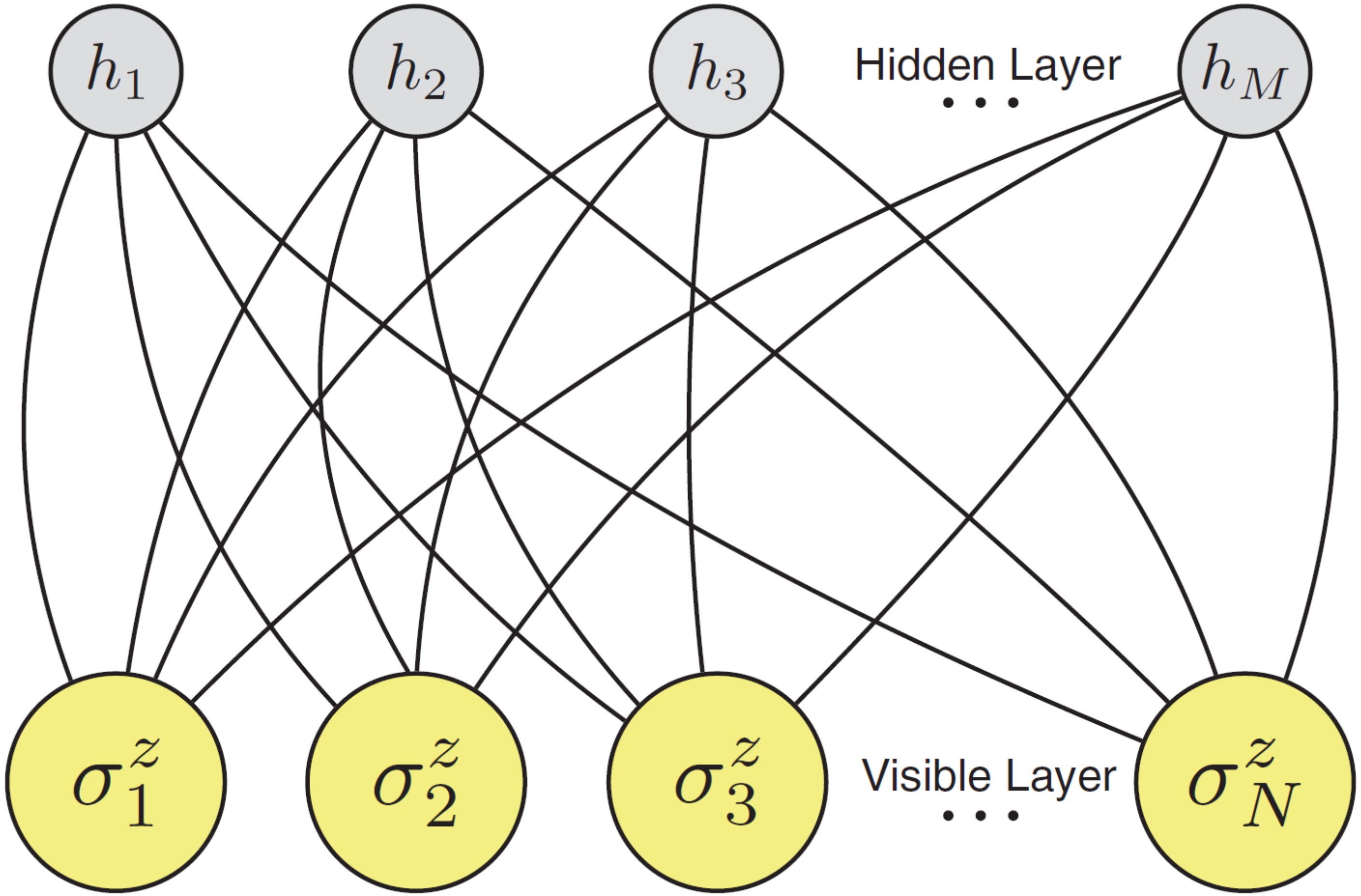
XOR: a logical operation that outputs true only when inputs differ.

(*Right Up Figure) Michael R. Hush, Science* Vol. 355, Issue 6325, pp. 580, 2017.
All figures after this slide, unless mentioned, are from G. Caleo and M. Troyer, *Science*, Vol. 355, Issue 6325, pp. 602-606, 2017.

Artificial Neural network encoding a many-body quantum state of N spins

Boltzmann machine: an “energy-based” neural network. Visible layer is the input and hidden layer represents the intrinsic behavior of individual visible node.

It gets the name because the probability of a certain state to appear in Boltzmann machine can be expressed in a way analogous to Boltzmann distribution in statistics mechanics.



A restricted **Boltzmann machine** architecture that features a set of N visible artificial neurons (yellow dots) and a set of M hidden neurons (gray dots) is shown.

Algorithm 1: Training the Neural Network

Objective: minimize the energy expectation value $E(W) =< \Psi_M|H|\Psi_M >$ / $< \Psi_M|\Psi_M >$

1 *Initialize network parameters (W, a, b)*

2 *Sample* $|\Psi(S, W_k)|^2$ *for current network parameters*

3 *Stochastic estimates of the average energy and energy gradient is obtained.*

4a *Applying improved gradient descent optimization to obtain updated network parameters.*

4b *The trial wave function is altered to adapt to the new network parameters, back to Step 3.*

5 *Process concludes until energy convergence is reached.*

Learning the model

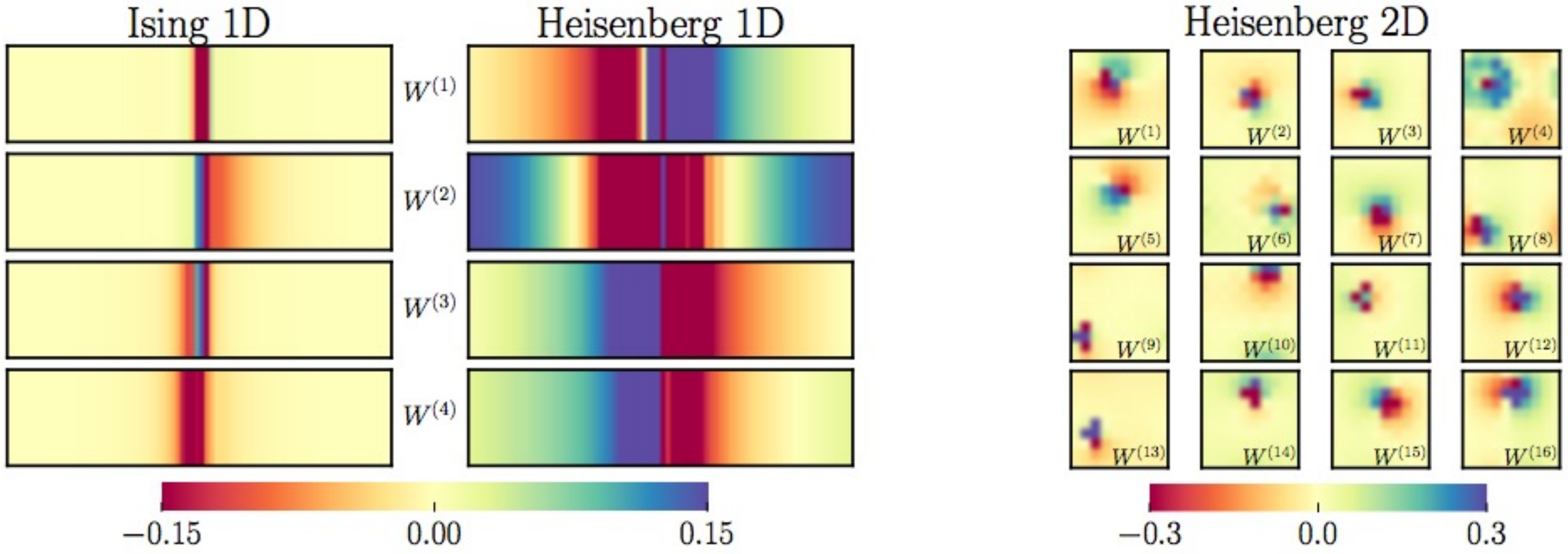
Transverse Field Ising Model

$$\mathcal{H}_{TFI} = -h\sum_i \sigma_i^x - \sum_{ij} \sigma_i^z \sigma_j^z$$

Antiferromagnetic Heisenberg Model

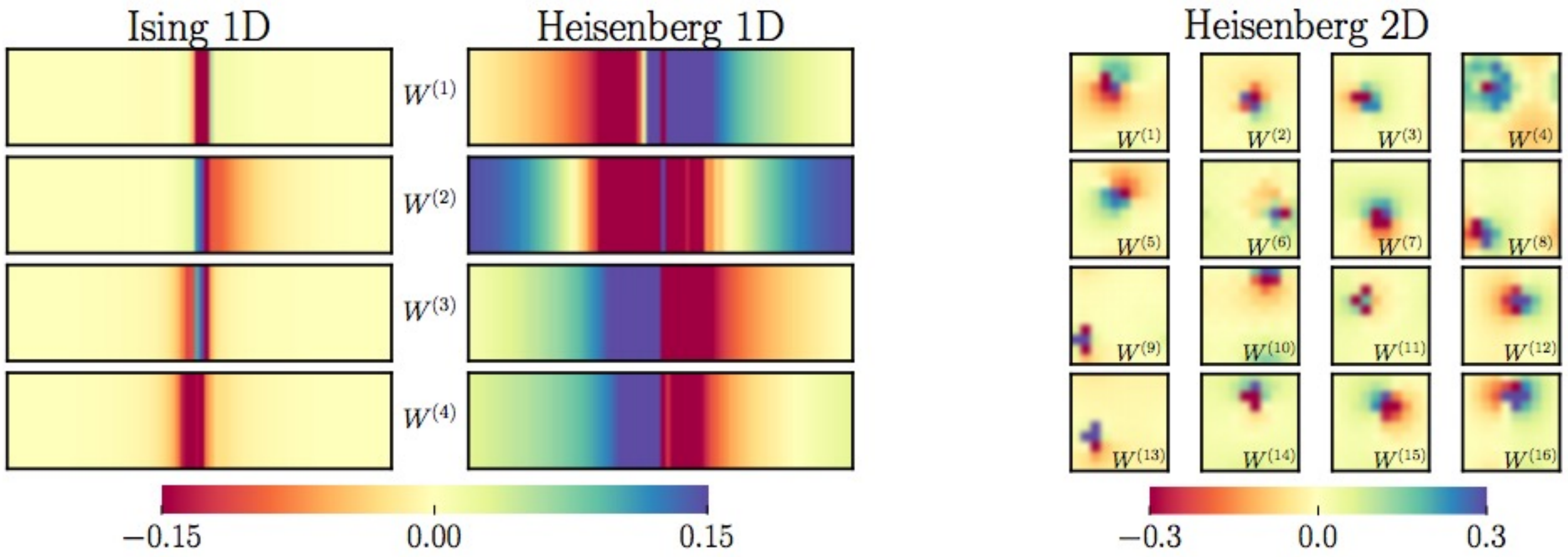
$$\mathcal{H}_{AFH} = \sum_{ij} \sigma_i^x \sigma_j^x + \sum_{ij} \sigma_i^y \sigma_j^y + \sum_{ij} \sigma_i^z \sigma_j^z$$

Visualize the trained network



Color map of weights matrix after training.
To conserve the lattice symmetry, the weight matrix of each hidden node is limited to α possibilities. (α=number of hidden nodes/number of visible nodes)
More hidden nodes means more symmetry can be learned.

Visualize the trained network



Color map of weights matrix after training.
Each color map shows the correlation values that the hidden node imposes on each lattice site.
Physically, these correspond roughly to the common local magnetic structure in the system.

Algorithm 2: Finding the Ground State

Input: Trained network (const network parameters W, a, b and Hamiltonian of a specific model, done in Algorithm 1), Trial spin input S.

(*The hidden layer values are now completely a "black box", their expression have been traced out due to the lack of intralayer interactions.*)

Objective: Find the ground state spin configuration S', and output the ground state energy (as summation from all individual spins).

1 *Initialize all input parameters.*

2 *A random spin is flipped.*

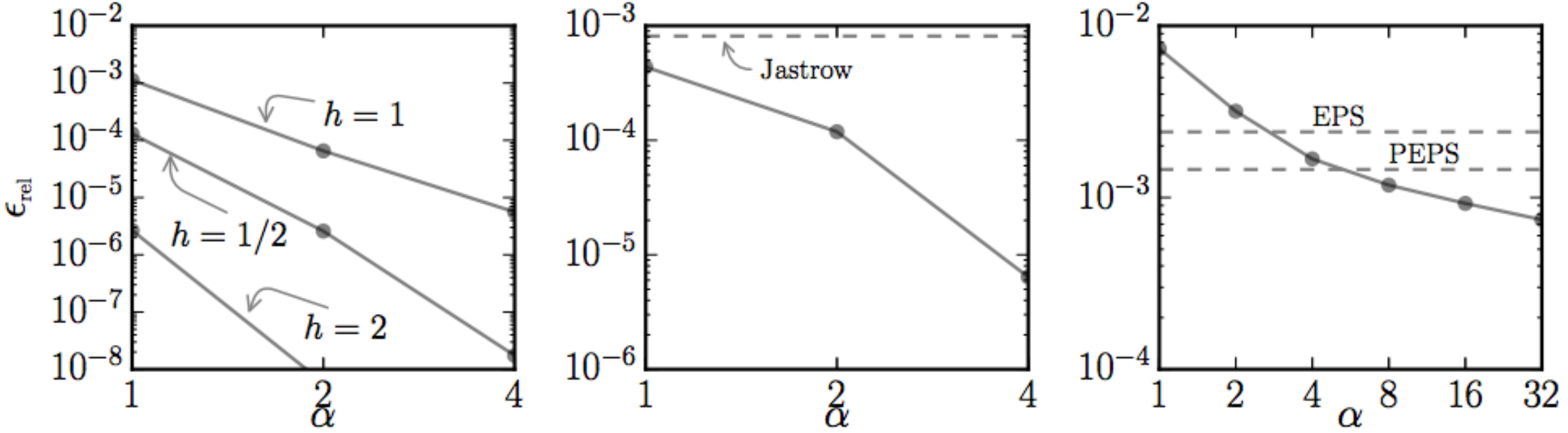
3 *Accept/Reject the change through a simple Metropolis-Hastings algorithm*: Acc = min (1, $|\Psi(S^*)/\Psi(S)|^2$

4 *Back to step 2 until the steplimit (number of sweeps as defined in this paper) is reached.*

5 *Generate output (spin configuration, energy, ...)*

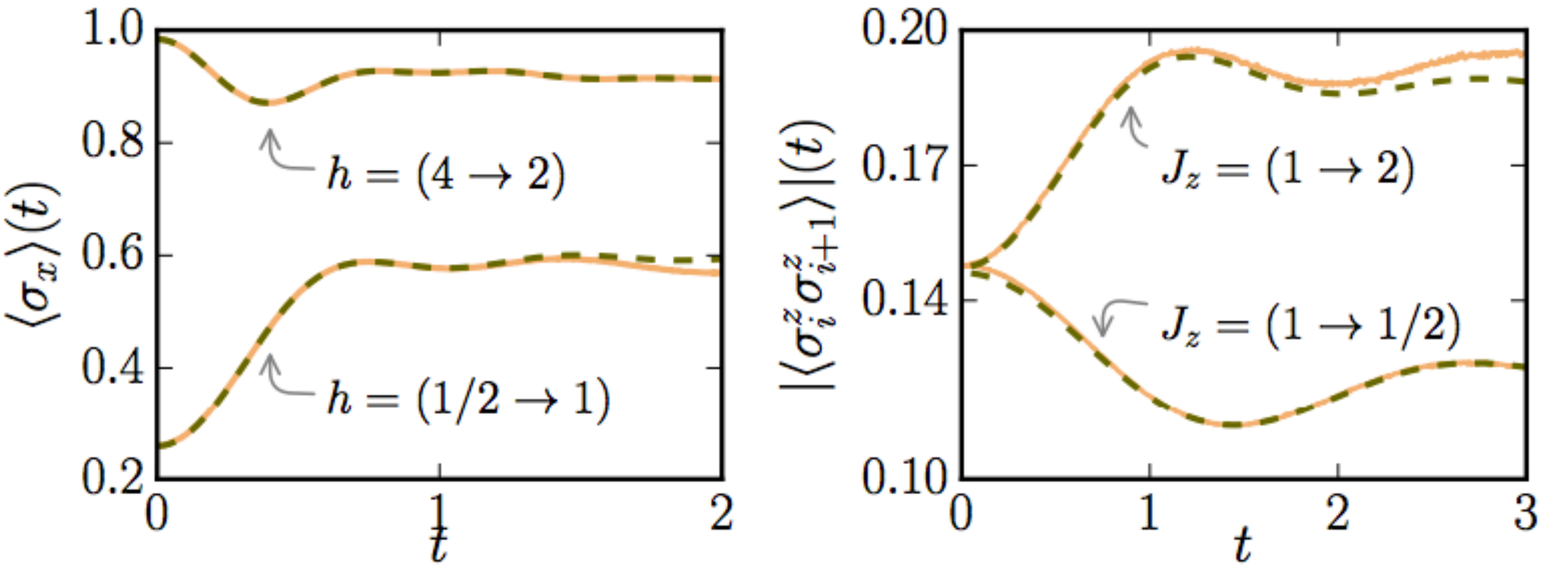
Accuracy of the neural network

Accuracy test vs. exact numerical solution / other theories



Capability to solve time-dependent problems

This artificial neural network can be modified to learn to solve time-dependent problems such as quantum quenching.



Left: Transverse spin polarization vs. time (1D Ising model)
Right: Nearest-neighbor spin correlation vs. time (2D Heisenberg).
Dashed line: exact numerical solution.

Concluding Remarks

- RBM is relatively easy to setup, and achieve comparable high accuracy by comparing with exact solutions. Many paths for research can be envisaged in the near future (the field of machine learning advances very fast. e.g. multi-layer neural network like convolutional neural networks).
- The straightforward approach of NQS can be readily applied in other systems (used to solve more challenging problems).
- NQS can be further modified to represent more compact representations of many-body quantum states.

A C++ code demonstrating Algorithm 2 (Finding the ground state) is provided by the authors and can be found here:
http://science.sciencemag.org/highwire/filestream/690315/field_highwire_adjunct_files/1/aag2302_Code_and_Data_Files.zip

Related Literatures

- **Using machine learning to solve physics (as well as materials) problem:**

- Dong-Ling Deng, Xiaopeng Li, and S. Das Sarma (University of Maryland), Exact Machine Learning Topological States, arXiv:1609.09060v1

- representing quantum topological states with long-range quantum entanglement using artificial neural networks.

- Dong-Ling Deng, Xiaopeng Li, and S. Das Sarma (University of Maryland), Quantum Entanglement in Neural Network States, arXiv:1701.04844v2.

- Li Huang and Lei Wang (IOP, CAS), Accelerated Monte Carlo simulations with restricted Boltzmann machines, Phys. Rev. B 95, 035105 (2017).

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