Supervised Learning of Ising Model
Part I

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02/03/2018

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Machine Learning Phases of Matter

nature physics

LETTERS

PUBLISHED ONLINE: 13 FEBRUARY 2017 | DOI: 10.1038/NPHYS4035

Machine learning phases of matter

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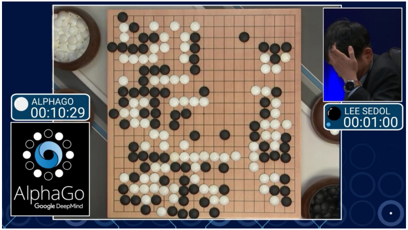
Condensed-matter physics is the study of the collective behaviour of infinitely complex assemblies of electrons, nuclei, magnetic moments, atoms or qubits[1]. This complexity is reflected in the size of the state space, which grows exponentially with the number of particles, reminiscent of the 'curse of dimensionality' commonly encountered in machine learning[2]. Despite this curse, the machine learning community has developed techniques with remarkable abilities to recognize, classify, and characterize complex sets of data. Here, we show that modern machine learning architectures, such as fully connected and convolutional neural networks[3], can identify phases and phase transitions in a variety of condensed-matter Hamiltonians. Readily programmable through modern software libraries[4,5], neural networks can be trained to detect multiple types of order parameter, as well as highly non-trivial states with no conventional order, directly from raw state configurations sampled with Monte Carlo[6,7].

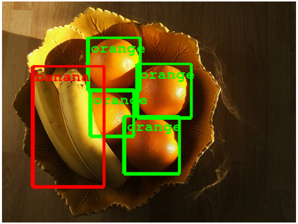
Conventionally, the study of phases in condensed-matter systems

is composed of an input layer with values determined by the spin configurations, a 100-unit hidden layer of sigmoid neurons, and an analogous output layer. When trained on a broad range of data at temperatures above and below T_c, the neural network is able to correctly classify data in a test set. Finite-size scaling is capable of systematically narrowing in on the thermodynamic value of T_c in a way analogous to measurements of the magnetization: a data collapse of the output layer (Fig. 1b) leads to an estimate of the critical exponent $\nu \simeq 1.0 \pm 0.2$, while a size scaling of the crossing temperature T^*/J estimates $T_c/J \simeq 2.266 \pm 0.002$ (Fig. 1c). One can understand the training of the network through a simple toy model involving a hidden layer of only three analytically 'trained' perceptrons, representing the possible combinations of high- and low-temperature magnetic states exclusively on the basis of their magnetization. Similarly, our 100-unit neural network relies on the magnetization of the configurations in the classification task. Details about the toy model, the 100-unit neural network, as well as a low-dimensional visualization of the training data, which may be used

What is Machine Learning?

Machine Learning refers to some kind of algorithms which help a computer to learn.





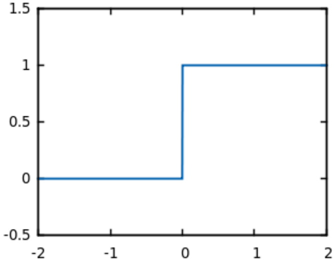
Learning Tasks

- Supervised learning (labeled data)
- Unsupervised learning (unlabeled data)
- Reinforcement learning ('reward' data)

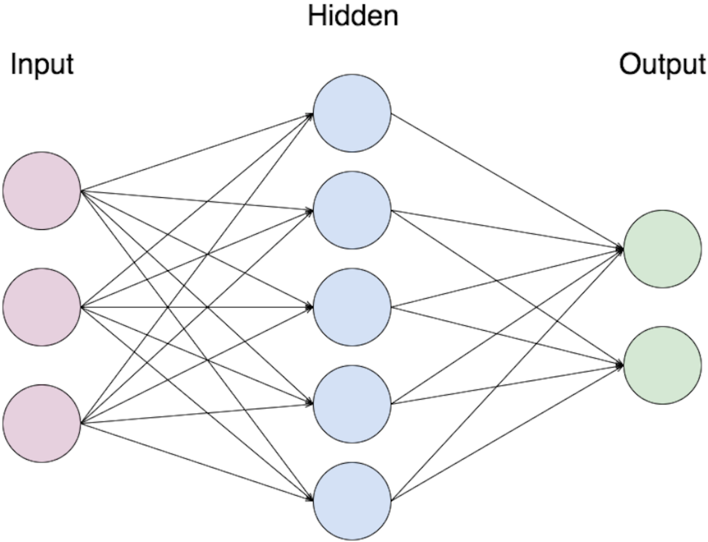
Supervised Learning

There is several models for a supervised learning

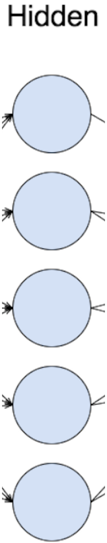
1. The linear model $(f(x) = wx + b)$
2. Kernel learning $(f(x) = w\Phi(x))$
3. Neural Networks $(f(x) = \sigma(wx + b))$



Neural Networks



Hidden Layers



Each hidden layer contains a certain number of nodes called *neurons* which transmit information from the input date.

$$z = f(x) = \sigma(wx + b)$$
$$\sigma(x) = \frac{1}{1 + e^{-x}}.$$

Learning

Given an initial prediction for the input data (1 or 0 depending if the activation of a neuron z overcome some threshold or not) the machine is trained to get an accurate prediction

$$cost = \frac{1}{N}\sum_{j}(f(x_j) - y_j)^2$$

The idea is minimized the cost function and set

$$w = w - \nabla_w cost$$
$$b = b - \nabla_b cost$$

Example: The Flower Problem

Color	Red	Blue	Red	Blue	Red	Blue	Red	Blue	?
Length	3.0	2.0	4.0	3.0	3.5	2.0	5.5	1.0	1.5
Width	1.5	1.0	1.5	1.0	0.5	0.5	1.0	1.0	1.5

Supervised Learning of Ising Model

Parameter diagnostics of phases and phase transition learning by neural networks

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(Dated: February 28, 2018)

We present an analysis of neural network-based machine learning schemes for phases and phase transitions in theoretical condensed matter research, focusing on neural networks with a single hidden layer. Such shallow neural networks were previously found to be efficient in classifying phases and locating phase transitions of various basic model systems. In order to rationalize the emergence of the classification process and for identifying any underlying physical quantities, it is feasible to examine the weight matrices and the convolutional filter kernels that result from the learning process of such shallow networks. Furthermore, we demonstrate how the learning-by-confusing scheme can be used, in combination with a simple threshold-value classification method, to diagnose the learning parameters of neural networks. In particular, we study the classification process of both fully-connected and convolutional neural networks for the two-dimensional Ising model with extended domain wall configurations included in the low-temperature regime. Moreover, we consider the two-dimensional XY model and contrast the performance of the learning-by-confusing scheme and convolutional neural networks trained on bare spin configurations to the case of preprocessed samples with respect to vortex configurations. We discuss these findings in relation to similar recent investigations and possible further applications.

Input data -Monte Carlo Cluster Algorithm-

Hidden Layer

Output Layer

Results