PHYSICS

Machine learning for quantum physics

An artificial neural network can discover the ground state of a quantum many-body system

By **Michael R. Hush**

Machine learning has been used to beat a human competitor in a game of Go (*1*), a game that has long been viewed as the most challenging of board games for artificial intelligence. Research is now under way to investigate whether machine learning can be used to solve long outstanding problems in quantum science. On page 602 of this issue, Carleo and Troyer (*2*) use machine learning on one of quantum science's greatest challenges: the simulation of quantum many-body systems. Carleo and Troyer used an artificial neural network to represent the wave function of a quantum many-body system and to make the neural network "learn" what the ground state (or dynamics) of the system is. Their approach is found to perform better than the current state-of-the-art numerical simulation methods.

Early machine-learning demonstrations were on specific pattern-recognition problems. They have since shown great capability in performing multifaceted tasks, such as playing video games (*3*) or board games (*1*). This capacity to take control of complex systems and achieve difficult goals, in some cases better than human competitors, has recently been used to tackle difficult problems in quantum science. In experimental quantum science, machine learning has been used to design new experiments (*4*), perform automatic optimization (*5*), and improve feedback control (*6*). All of these applications have solved problems that have only recently faced the field.

Due to vast number of complex numbers required to save a complete wave function, the simulation of many-body systems has been an immense challenge in quantum science. For example, consider a many-body system composed of N qubits, the simplest quantum bodies. We must save a complex number for every configuration of this system. Each qubit can be in a state of 0 or 1, so that means we need to save 2^N complex numbers. Even a small number of qubits requires an extreme amount of memory. For example, 26 qubits require around a gigabyte, 46 qubits require a petabyte, and 300 qubits would require more bytes than the number of atoms in the universe. Richard Feynman recognized this problem, which led to his suggestion that quantum computers may have an advantage over conventional computers (*7*) [although we now know that the reason behind the quantum speedup is more nuanced (*8*)].

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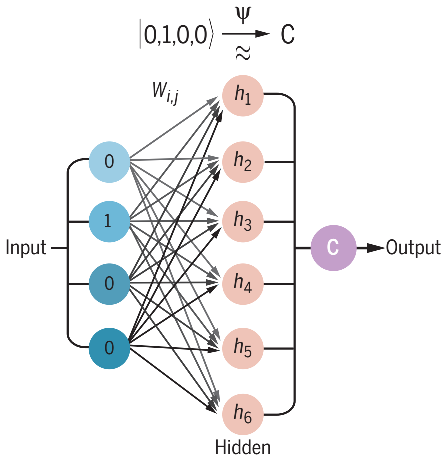
To circumvent this memory requirement issue, a variety of approximate techniques have been developed to solve quantum many-body problems. These involve inventing some compact approximate representation for the wave function. For example, matrix product states are the current state-of-the-art technique for finding ground states of one-dimensional many-body systems (*9*). A set of matrices is used to save the approximate state-of-the-wave function; subsets of these matrices can be multiplied together to get the complex number corresponding to a particular system configuration. Many different representations of the wave function exist, each having advantages in particular physical settings. Discovering new representations for each physical problem has previously required human ingenuity and effort.

Working out a solution

An artificial neural network approximates the wave function of a system composed of 4 qubits. The neural network takes a configuration of the system as an input that is multiplied by a matrix of weights, $W_{i,j}$, added to a set of hidden biases, h_j, and passed through a nonlinear activation function to produce a complex number, C, as an output. The neural network learns what the ground state (or dynamics) of the system is. Increasing the number of hidden biases can improve the accuracy.



Carleo and Troyer suggest using machine learning to automatically discover a compact representation for the wave function appropriate for each physical problem. The wave function can be thought of as a function that takes a system configuration and returns a complex number. They assume that this function can be well approximated with a neural network, made of a set of weights and a single layer of hidden biases (see the figure). Given the Hamiltonian for a particular physical system, they let the neural network learn a compact representation for the wave function of the system's ground state (or dynamics). The learning algorithm they used is adapted from variational Monte Carlo and minimizes the so-called local energy of the system.

Carleo and Troyer found that the neural network is able to discover ground states of quantum many-body systems with a smaller memory footprint than those of competing techniques, such as matrix product states. Furthermore, the accuracy of the neural net estimate can be systematically improved by increasing the number of hidden biases and weights. On the problems they tested, they found the machine-learning algorithm was able to outperform all of the current state-of-the-art numerical techniques.

Carleo and Troyer have currently tested their approach on a few problems that have known solutions. We will not know for certain that machine learning has solved the challenge of simulating many-body quantum systems until more physical systems have been tested. Nevertheless, there is great potential to expand on their work. Carleo and Troyer only considered a single-layer neural net. Deep neural nets, which have multiple layers, have been shown to have the greatest capacity for learning and expression and are yet to be investigated. The work presents a new pathway for physicists to benefit from the rapid developments in the machine-learning community and will hopefully lead to new physical discoveries. ■

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