Machine learning: New tool in the box

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MACHINE LEARNING

New tool in the box

A recent burst of activity in applying machine learning to tackle fundamental questions in physics suggests that associated techniques may soon become as common in physics as numerical simulations or calculus.

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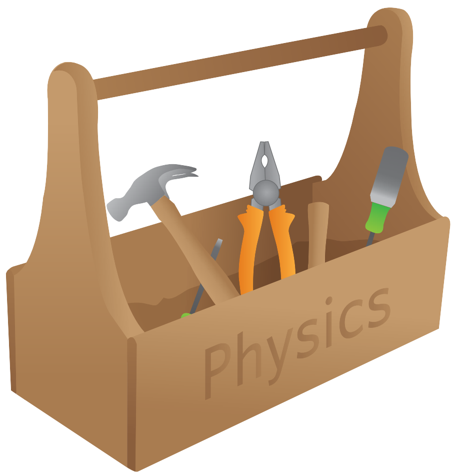
The goal of machine learning, broadly speaking, is to design a computer code — the eponymous machine — capable of discovering meaningful structure in data. The last decade saw a game-changing revolution unfold in this field: with the development of deep neural networks[1], tasks that were considered inaccessible to automated learning became possible. This prompted fierce competition in the artificial intelligence market, but it also brought promise to many areas of data-intensive fundamental science — with physics being no exception. Current machine-learning systems are not yet able to divine the laws of general relativity from planetary data, but they are able to reliably recognize human faces, detect objects in photographs and even beat world champions of Go[2]. And now, writing in *Nature Physics*, two groups have used artificial neural networks to recognize different phases of matter and localize associated phase transitions[3,4].

Juan Carrasquilla and Roger Melko[3] used a type of neural network commonly used to classify images. To illustrate how it works, consider a set of images of cats and dogs, each labelled 1 or 0, respectively. The network then uses this set and the labels to construct a function that takes pixels of each image as an input and returns an output of 1 for cats and 0 for dogs. If this function is later given a previously unseen image, it should return an output corresponding to the presence of a dog or cat in the new image. In Carrasquilla and Melko's study the labels dog and cat were replaced by the low-temperature phase and high-temperature phase of a condensed-matter model. The training set was not given by pixels of an image, but by an equilibrium configuration of the model obtained from Monte Carlo simulations. In another paper, Evert van Nieuwenburg and co-workers[4] showed that if the set of configurations can be ordered on a line — representing the temperature, for example — then these phases can be learned without even knowing the labels. Both works offer an exciting perspective on studying unexplored phases of matter and phase transitions in systems with unknown order parameters.



It should be stressed that saying one applied machine learning to a given problem is about as generic as saying that one used numerical simulations. It is clear to every researcher in physics that there are many kinds of numerical simulations. Depending on the system and the question of interest, it requires insight and experience to find the right numerical simulation and carry it out with sufficient care in order to be able to truly advance our understanding of a given problem. The same is true for applications of tools of machine learning.

A wide range of tools stemming from machine learning have recently been used in physics-related studies. Carrasquilla and Melko represented phases of matter with a two-layer feed-forward neural network. They also showed that in some cases, including Ising lattice gauge theory, this architecture fails, and instead a convolutional neural network succeeds. Van Nieuwenburg *et al.* used a similar two-layer feed-forward neural network, but showed that a much more basic method of principal component analysis succeeds in some of the examples. A different application of machine learning in physics aims at reducing the dimension of a Hilbert space by representing the wavefunction using a restricted Boltzmann machine, with weights obtained through reinforcement

learning[5]. Another group recently showed that a support vector machine can be used to classify which particles in a glassy system are susceptible to rearrangement[6]. Decision forests have been used to classify metals from insulators based on the hybridization function, combined with kernel ridge regression to predict correlation functions in many-body physics[7]. For the quantum systems considered by van Nieuwenburg *et al.*, the neural network was trained on the entanglement spectrum instead of directly on the wavefunction. This is a type of data preprocessing that was exploited in another recent study predicting the quantum energies of molecules, using sparse linear regression on approximated electron densities after preprocessing with the so-called scattering transform[8].

Clearly, this new trend brings with it a host of machine-learning terms that an average physicist encounters only very rarely. We can, however, anticipate that soon all these terms will be taught in undergraduate physics along with Monte Carlo methods and the Fourier transform. When it comes to a new set of tools, it is not only important for the physics community to learn about them, but also for it to build an intuition and understanding of which of the tools are applicable to which question and system. Machine learning is not a magic box — in order to be valuable in physics its results need to be interpreted and validated. So far the first studies have opened up a set of interesting directions with hand-picked examples of successful applications, but systematic studies are needed to better understand the range of validity and applicability of each of the approaches[9]. One might also hope that such a systematic understanding-driven effort will feed back into the machine-learning community where new theoretical insights about various architectures will be welcome. ❐

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