Stick a PINN in it –

Machine Learning vs. Numerical Simulation in Physics Research

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Do you all have an experience like this? You put a timer on top of the lid of instant noodles, and then when you try to put it back on the wall of the refrigerator, it doesn't stick anymore.

Actually, the phenomenon where heating a magnet weakens its magnetic force can be explained by a simple formulation in physics. When I first saw that formulation, I was deeply impressed and dreamed of becoming a scientist. There are still many physical phenomena in the world that have not yet been formulated. I believe that physics is a discipline that formalizes and elucidates these phenomena around us.

However, it's not enough for the equations in physics to accurately represent the phenomena of the world. For example, an equation with 100 or more terms would likely be impossible to solve, and adding a small term to it probably wouldn't change the description of the phenomenon. Also, even if you formulate a set of conditions to accurately describe only one phenomenon, it may not have much value. Thus, in physics, it's important to find concise and universal laws.

By the way, the problem of whether an equation is solvable is extremely serious. Even the Burgers' equation that is an equation with only three terms is practically impossible for humans to solve, and we have to rely on computers to perform simulations. Here, "solving" usually means seeking how systems change over time (time evolution).

In fact, most equations that arise in research can only be solved through numerical simulations. However, this also incurs costs in terms of time and computational resources.

The fact that even a simple equation with only a few terms could not be solved by hand or with the help of a computer was quite shocking to me. At that time, I heard that machine learning might shed light on it. And that led to the research on Physics-Informed Neural Networks (PINNs) that I am currently conducting.

Now, there has been an AI boom for the past decade. One of the technologies that support AI is machine learning. You might be reading this text using ChatGPT, DeepL Translator, or Google Translate, which are all powered by machine learning. In training of machine learning, adjustments to parameters are made through multiple layers of Neural Networks between inputs and outputs. So the idea of training Neural Networks to output physical quantities and thereby serve as an alternative to numerical simulations doesn't seem far-fetched.

This is the initially conceived Data-Driven method. Here, data at various times was prepared for learning, and parameters were adjusted so that the output matches those values, aiming to create a model adaptable to other times. However, this approach lacks correlations between different times and often requires data calculated through numerical simulations, making it fundamentally similar to traditional methods.

Subsequently, Physics-Informed Neural Networks (PINNs) were devised, a method that uses machine learning to learn the physical simulation itself. In traditional physics simulations, we're given physical laws (update rules), which we strictly follow to determine the system's state at each time step. Conversely, in PINNs, the time evolution is governed by a Neural Network. Parameters are adjusted during training so that the values outputted by the Neural Network satisfy the physical laws, i.e., learn the update rules. It's named physics-informed because it uses physical laws as prior knowledge for learning.

PINNs excel over traditional methods in that, in numerical simulations, to know the information at a certain time t, you start from a reference point (t=0) and go through 0, 1, ..., t-1 to finally get the information at t, whereas PINNs directly learn solutions parameterized by time, enabling direct output at time t. Also, in numerical simulations, errors due to discretizing time into finite steps are unavoidable, but since the time in PINNs is a continuous quantity, this problem is resolved. Additionally, PINNs require only the physical laws for learning; data such as the system's physical quantities at a specific time are not necessary, distinguishing them from numerical simulations.

Thus, the application of machine learning to numerical simulations through PINNs has achieved some success, especially with the advancement in computational power due to the recent machine learning boom. The Burgers' equation based numerical simulations mentioned earlier are often cited as examples. However, there are still hurdles to overcome, such as numerical instability and computational resource issues, and it's not applicable to all physical systems.

Moreover, while PINNs involve humans devising the physical laws themselves and machines taking over their simulation, there is also ambitious research aimed at providing information on the time evolution of systems to machines, enabling them to discover the physical laws themselves. Data-Driven methods can also be considered a type of this. I believe that such research, which combines physics and machine learning, will continue to be active in the future.

Returning to the beginning of the discussion, physics seeks to find concise and widely applicable laws to describe many phenomena. Newton's laws of motion and the Schrödinger equation are prime examples. There may come a day when trained neural networks, which accurately predict the time evolution of any system within their black boxes, replace or supplement these laws, even without being explicitly formulated.

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