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Is the next deep learning disruption in the physical sciences?

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Abstract

A number of fields, most prominently speech, vision and NLP have been disrupted by deep learning technology. A natural question is: "which application areas will follow next?". My prediction is that the physical sciences will experience an unprecedented acceleration by combining the tools of simulation on HPC clusters with the tools of deep learning to improve and accelerate this process. Together, they form a virtuous cycle where simulations create data that feeds into deep learning models which in turn improves the simulations. In a way, this is like building a self-learning computational microscope for the physical sciences. In this talk I will illustrate this using two recent pieces of work from my lab: molecular simulation and PDE solving. In molecular simulation we try to predict molecular properties or digitally synthesize molecules with prescribed properties. We have built a number of equivariant graph neural networks to achieve this. Partial differential equations (PDEs) are the most used mathematical model in natural sciences to describe physical processes. Intriguingly, we find that PDE solvers can be learned from data using graph neural networks as well, which has the added benefit that we can learn a solver that can generalize across PDEs and different boundary conditions. Moreover, it may open the door to ab initio learning of PDEs directly from data.

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