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Deep Learning for Science: Opening the Pandora Box

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Abstract: Scientists have always attempted to identify and document analytic laws that underlie physical phenomena in nature. The process of finding natural laws has always been a challenge that requires not only experimental data, but also theoretical intuition. Often times, these fundamental physical laws are derived from many years of hard work over many generation of scientists. Automated techniques for generating, collecting, and storing data have become increasingly precise and powerful, but automated discovery of natural laws in the form of analytical laws or mathematical symmetries have so far been elusive. Over the past few years, the application of deep learning to domain sciences –from biology to chemistry and physics is raising the exciting possibility of a data-driven approach to automated science, that makes laborious hand-coding of semantics and instructions that is still necessary in most disciplines seemingly irrelevant. The opaque nature of deep models, however, poses a major challenge. For instance, while several recent works have successfully designed deep models of physical phenomena, the models do not give any insight into the underlying physical laws. This requirement for interpretability across a variety of domains, has received diverse responses. In this talk, I will present our analysis which suggests a surprising alignment between the representation in the scientific model and the one learned by the deep model.

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