Preface: Combining Artificial Intelligence and Machine Learning with Physical Sciences

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This volume contains the contributed papers selected of the AAAI 2020 spring symposium on "Combining Artificial Intelligence and Machine Learning with Physics Sciences." The symposium was held on 23 to 25 March 2020 in a virtual form because of the SARS-CoV-2 virus (Covid-19) outbreak.

This symposium aimed to present the current state of the art and identify opportunities and gaps in AI/ML-based physics modeling and analysis. With recent advances in scientific data acquisition and high-performance computing, Artificial Intelligence (AI) and Machine Learning (ML) have received significant attention from the applied mathematics and physics science community. From successes reported by industry, academia, and the research community at large, we observe that AI and ML hold great potential for leveraging scientific domain knowledge to support new scientific discoveries and enhance the development of physical models for complex natural and engineered systems.

Despite this progress, there are still many open questions. Our current understanding is limited regarding how and why AI/ML work and why they can be predictive. AI has been shown to outperform traditional methods in many cases, especially with high-dimensional, inhomogeneous data sets. Areas where deep learning methods have been demonstrated to outperform traditional numerical schemes include:

- Meshless methods. Deep Neural Networks (DNNs) do not require a grid and can directly map a spatial coordinate (x, y, z) to an output. This is critical in applications where meshing is difficult or the domain of interest is not clearly defined (e.g., for certain inverse modeling problems).
- Global schemes. DNNs allow approximating the solution without resorting to a local scheme based for example on piecewise polynomial approximation methods. In that respect, deep learning is closely related to spectral methods such as the Fourier decomposition.
- High-order and adaptive methods. The depth in DNNs has been associated with highly accurate representations of high-order schemes. For example, deep networks can efficiently represent high-order polynomials using relatively few layers. In addition, DNNs have also shown great accuracy when approximating functions with rapid changes or even discontinuous jumps.
- High-dimensional problems. DNNs are also very effective in representing high-dimensional problems, for example in certain applications in probability which represent the evolution of high-dimensional probability distributions. Applications to high-dimensional parabolic PDEs such as the nonlinear Black–Scholes equation, the Hamilton–Jacobi–Bellman equation, and the Allen–Cahn equation have also been demonstrated.
- Finally, Generative Adversarial Networks offer new avenues to approximate complex probability density functions to model stochastic processes and for uncertainty quantification. They allow going beyond Gaussian process approximations and model more complex dependencies and distributions.

However, a rigorous understanding of when AI/ML is the right approach is largely lacking. That is, for what class of problems, underlying assumptions, available data sets, and constraints are these new methods best suited? The lack of interpretability in AI-based modeling and related scientific theories makes them insufficient for high-impact, safety-critical applications such as medical diagnoses, national security, as well as environmental contamination and remediation. Some of the main limitations include:

- Difficulty to train a network. This requires solving a complex non-convex optimization problem. For example, the accuracy of the solution often depends on the choice of initial conditions.
- Difficulty to assess the accuracy of deep learning predictions. DL is notoriously accurate when the input data resembles similar points in the training data. However, there is less control over the accuracy when the test point moves away from the training set. Quantifying this error and being able to predict the accuracy of DL is currently poorly understood.

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- Tuning a DNN remains an art. Relatively few guidelines exist to determine the architecture of the network and tune the hyperparameters (number of layers, depth, choice of activation function).

With transparency and a clear understanding of data-driven mechanisms, the desirable properties of AI should be best utilized to extend current methods in modeling of physics and engineering problems. At the same time, handling expensive training costs and large memory requirements for ever-increasing scientific data sets is becoming more and more important to guarantee scalable science machine learning.

The symposium focused on challenges and opportunities for increasing the scale, rigor, robustness, and reliability of physics-informed AI necessary for routine use in science and engineering applications. The symposium also discussed bridging AI and engineering research to significantly advance diverse scientific areas and transform the way science is done.

The accepted papers were presented over 3 days with two invited talks each day. The symposium was broadcast live and camera-ready presentations were posted on Youtube.

As editors of the proceedings we are grateful to everyone who contributed to the symposium. We would like to thank the invited speakers:

- Lexing Ying, Stanford University
- Paris Perdikaris, University of Pennsylvania
- Maziar Raissi, University of Colorado, Boulder
- Marco Pavone, Stanford University
- Stefano Ermon, Stanford University
- Kevin Carlberg, University of Washington

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Contents

DeepXDE: A Deep Learning Library for Solving Differential Equations
Lu Lu, Xuhui Meng, Zhiping Mao and George Em Karniadakis

Nonlocal Physics-Informed Neural Networks - A Unified Theoretical and Computational Framework for Nonlocal Models
Marta D'Elia, George E. Karniadakis, Guofei Pang and Michael L. Parks

Permeability Prediction of Porous Media using Convolutional Neural Networks with Physical Properties
Hongkyu Yoon, Darryl Melander and Stephen J. Verzi

Surfzone Topography-informed Deep Learning Techniques to Nearshore Bathymetry with Sparse Measurements
Yizhou Qian, Hojat Ghorbanidehno, Matthew Farthing, Ty Hesser, Peter K. Kitanidis and Eric F. Darve