Research statment

Towards Robust Machine Learning Model For Scientific Discovery

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Traditional scientific discovery discipline always derives handcraft equations from first principles. Even with expert's carefully mathematical modeling, there are always situations left behind. The recent breakthrough in machine learning algorithms enables us to extract useful information and make useful predictions from data across a wide range of areas, which gives us hope to discover new physic laws from observational data[3,4,10,11,12,13]. Despite the successes, however, several key challenges remain when we apply state-of-the-art models for scientific applications, including physic prediction [3,10,11], medical applications, and climate predictions [3,13]:

- The NN architectural design is still an art and it lacks basic mathematical principles. When applying neural networks to scientific problems, how prior physics knowledge can be integrated into the machine learning system?
- While robustness and reproducibility is the core of scientific research, the state-of-the-art models are discovered to be vulnerable to adversarial perturbations, biased towards spurious relations, and even sensitive to simple domain shift. How to build a robust machine learning systems becomes a crucial challenge faces if we aim to use data-driven discovery for physic law in scientific research.

Previous Research Experience

My previous research lies at the interface of computational physics, statistics, and signal processing, and tends to explore this topic from the following two perspectives:

Encoding Physic Information to the Model. Differential equations play an important role in many disciplines of science and engineering. My research starts from interpreting many effective networks as different numerical discretizations of (stochastic) differential equations [1,2]. Based on this perspective, we are able to combine physic information with the deep neural network system via linking deep learning theory with control theory.

- In [3,4], we present an initial attempt to learn evolution PDEs from data. This approach combines the representation power of the deep neural networks and the transparency of the PDE models which leads to better generalization property towards diverse initial conditions.
- In [5], we apply this idea to inverse problem. With the understanding of the physic behind the task, we additional learn an terminal time for different noise level which leads to better generalization across different noise level and different noise statistics.
- In [6,7], we apply this idea towards understanding the training process of the deep neural networks. The control theory view-point enables us to design 1/4-1/5 times faster algorithm for adversarial training in practice [6] and provide the first convergence proof for stochastic gradient descent training multi-layer networks in mean-field [7].

Building Robust learning Algorithm via Inductive Bias. Overparametraization, *i.e* having more model parameters than necessary, is the core factor behind the success of modern machine learning. However overparametraization also enables the model to fit any noisy signal which makes the model extremely vulnerable. My previous research aims to build robust overparametrized model via understanding the inductive bias.

- In [8], we discussed the how robust overparameterized neural network can be towards croupted label, which is unavoidable when we collect physics signals in experiments. We have shown that although overparameterization can leads to memoryization of all signals, however the discrepancy of convergence speed of different types of information can help us to distinguish signal from the noise. This leads to a theoretical understanding on how distillation algorithm can help in the situation that the supervision signal is noisy

- In [14], the authors have shown that although overparametrization will helps for average-case generalization, but the overparameterized model can't generalize on the worst-case. I aim to understand how overparametrized model effects the worst-case generalization in high dimensional data from the random matrix theory and how meta-learning algorithms can help overparametrized model generalize uniformly.

Research Plan and Goal

The interdisciplinary challenges addressed by this project are representative of our research in general, which seeks to apply state-of-the-art machine learning problem to scientific discovery with a rigorous mathematical theory supporting. The project crosses different domains such as mathematical analysis, computational physics, high dimensional statistics, causal inference and machine learning with their application in time series data occurs in physics experiments and biology researches. The project aims to develop robust, explainable and theoretical guaranteed machine learning tools for scientific research data such as real biological dataset of a metabolic network (Materials and Methods) [12] and NEXRAD climate data[15]. Here is the research plan:

- We have already proposed PDE-Net[3,4] to accurately predict the dynamics of complex systems and to uncover the underlying hidden PDE models at the same time which enables us to infer the source of pollution from the observational data. My first step is to scale up the experiment to noisy real-world climate data. We aim to learn a reduced-order model for climate data with good interpretability which enable us to infer more information than predicting, as an example finding out the pollution source from observational data[3]. The immediate challenge is to generalize our method beyond the regular grid, which needs us to combine our PDE-Net filter with convolutional graph neural networks.
- We also aim to understand the theoretical benefit of encoding prior physic information into deep learning models, including optimization [7], different loss functions [11], representation power [10,16,17], and generalization of the deep neural networks. We hope the theoretical research can help us to derive the original neural network structure, training algorithm, and regularization terms to improve deep learning algorithms for physic, biology problems.
- To causal predict a dynamical system, we need to consider both the stable and predictive structures[12]. In this project, we aim to discover the power of meta-learning to improve the out-of-domain generalization for deep physic models[18]. We hope this approach can break the known trade-off between worst-case generalization and prediction accuracy[13].

Significance of Proposed Work

With the rapid development of sensors, computational power, and data storage in the past decade, huge quantities of data can be easily collected and efficiently stored. Such a vast quantity of data offers new opportunities for the data-driven discovery of physical laws. From experiment design to data analysis, from physics law discovery to make useful predictions, AI can help to make the full process of scientific discovery fully automated. However, the lack of guidance of model design and robustness of the trained model is a clear threat to this area.

To overcome the obstacles mentioned before and make data science become the new scientific discovery discipline beyond the first principle needs interdisciplinary research. As an ICME student, my program enables me to be exposed to knowledge and experts in different areas, varying from basic mathematics to statistics and even physics and biology. Thus, I'm in a pretty good place to adapt the new ideas from the modern machine learning algorithms to different areas and make full use of the information from data to help scientific research in the future. I hope in the near future, physic laws can be discovered from observational data directly and physic law discovered by AI can help scientific researchers to understand the world better.

Reference

My Contribution

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