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Title: Interpretable & Tractable Machine Learning for Natural and Engineering Sciences

Abstract:

Thanks to IT industry push, Machine Learning (ML) capabilities are in a phase of tremendous growth, and there is great opportunity to point these practically powerful tools toward modeling specific to applications, e.g. in natural and engineering sciences. The challenge is to *incorporate domain expertise* from traditional physical and engineering discipline scientific discovery into next-generation ML models. We propose to develop novel **applied & theoretical mathematics and statistics**, computational and algorithmic, that extends cutting-edge ML tools and *merge them with application-specific knowledge* stated in the form of constraints, symmetries, conservation laws, phenomenological assumptions and other examples of domain expertise regarding relevant degrees of freedom. The emerging **Physics Informed Machine Learning** (PIML) methodology will bridge the two complementary poles -- application agnostic modern machine learning (in particular deep learning), computationally efficient but lacking interpretability, and science based tuning, highly interpretable but lacking automatization and implementation efficiency. Different aspects of the PIML methodology are illustrated on the following three enabling examples:

1. Acceleration of Fluid Mechanics Modeling and Simulations with Deep Learning [APS/DFD 2017-18, NIPS 2018 arXiv:1810.07785]

2. Learning Graphical Models [Science 2018/<u>arXiv:1612.05024</u>] and NIPS2016/<u>arXiv:1605.07252</u>]

3. Gauges, Loops, and Polynomials for Partition Functions of Graphical Models [arXiv:1811.04713]