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UNCERTAINTY QUANTIFICATION IN SCIENTIFIC MACHINE LEARNING: METHODS, METRICS, AND COMPARISONS

Apostolos F Psaros[1], Xuhui Meng[1], Zongren Zou[1], Ling Guo[2], and George Em Karniadakis[1]

[1]Brown University
[2]Normal University, Shanghai

ABSTRACT

Neural networks (NNs) are currently changing the computational paradigm on how to combine data with mathematical laws in physics and engineering in a profound way, tackling challenging inverse and ill-posed problems not solvable with traditional methods. However, quantifying errors and uncertainties in NN-based inference is more complicated than in traditional methods. This is because in addition to aleatoric uncertainty associated with noisy data, there is also uncertainty due to limited data, but also due to NN hyperparameters, overparametrization, optimization and sampling errors as well as model misspecification. Although there are some recent works on uncertainty quantification (UQ) in NNs, there is no systematic investigation of suitable methods towards quantifying the total uncertainty effectively and efficiently even for function approximation, and there is even less work on solving partial differential equations and learning operator mappings between infinite-dimensional function spaces using NNs. In this work, we present a comprehensive framework that includes uncertainty modeling, new and existing solution methods, as well as evaluation metrics and post-hoc improvement approaches. To demonstrate the applicability and reliability of our framework, we present an extensive comparative study in which various methods are tested on prototype problems, including problems with mixed input-output data, and stochastic problems in high dimensions. In the Appendix, we include a comprehensive description of all the UQ methods employed, which we will make available as open-source library of all codes included in this framework.