SCALABLE AUTOMATED DEEP ENSEMBLE FOR UNCERTAINTY QUANTIFICATION IN SCIENTIFIC MACHINE LEARNING

Prasanna Balaprakash[1], Romain Egele,[2,3], Romit Maulik[3,4], and Krishnan Raghavan[4]

[1]Oak Ridge National Laboratory, USA
[2]Université Paris-Saclay, France
[3]Pennsilvania State University, USA
[4]Argonne National Laboratory USA

ABSTRACT

Data-driven machine learning research has shown remarkable promise in enhancing the predictability and efficiency of various scientific applications. Deep learning-based models have exhibited significant gains in accuracy and time-to-solution over classical methods. However, the widespread adoption of deep learning models remains limited due to their inherent black-box nature, which lacks trustworthiness.

To address this challenge, uncertainty quantification methods have been developed to provide uncertainty estimates alongside model predictions. These methods aim to characterize both data (aleatoric) uncertainty, arising from factors like low-resolution sensors and sparse measurements, and model (epistemic) uncertainty, which stems from the lack of sufficient training data. A promising approach for uncertainty quantification is the use of deep ensembles, wherein a collection of neural networks is trained independently with different methods, resulting in diverse models possessing distinct weights. By aggregating predictions from these diverse models, improved predictions and more accurate uncertainty estimates can be achieved. Nonetheless, manually designing and training diverse high-performing models for the ensemble can be a laborious and costly endeavor.

We present an integrated automated deep ensemble approach that leverages distributed computing to overcome these challenges efficiently. Our proposed method not only discovers high-performing deep learning models but also provides scalable epistemic and aleatoric uncertainty quantification. The key highlights of this work are as follows:

- We demonstrate a unified strategy that efficiently discovers high-performing deep learning models by utilizing distributed computing for scientific machine learning tasks, while quantifying epistemic and aleatoric uncertainties.
- For uncertainty quantification, we employ a variance decomposition approach that separates aleatoric and epistemic uncertainty components, thereby enhancing the interpretability of the uncertainty estimates.
- We validate our proposed approach using real-world, high-dimensional scientific machine learning problems with complex dynamics.

Through extensive experimentation and validation, our integrated automated deep ensemble approach showcases its efficacy in accurately predicting complex systems and providing reliable uncertainty estimates.

REFERENCES

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