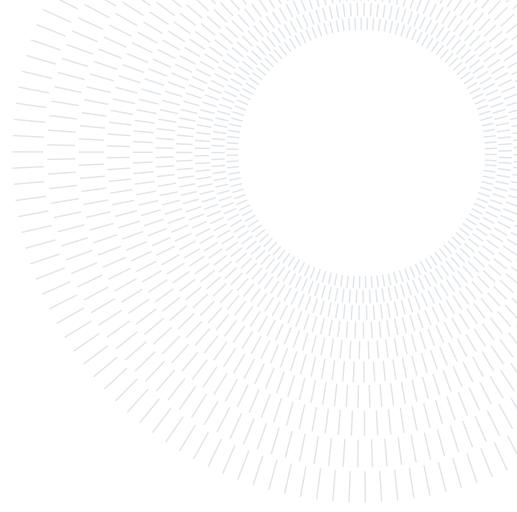




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A fully-comprehensive library for Physics-Informed Deep Learning under uncertainty

Project Report

Advanced Programming for Scientific Computing

Abstract: in this project, we developed a new library implementing several variants of the Bayesian Physics-Informed Neural Networks (B-PINNs) method, a framework to tackle physical problems with Neural Networks that are able to take into account information coming from partial differential equations and quantify the uncertainty around their prediction.

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To implement this strategy, we designed from scratch a modular and flexible pipeline; in our design, indeed, on one hand we wanted to mirror the peculiarities of the network tasks involved in the B-PINN framework into the hierarchy of the classes, while on the other hand we aimed at proposing a structure on which a variety of functionalities for different tasks could be inserted.

In the proposed release, indeed, we provided different variants of the various aspects of the overall process, ranging from data management to training algorithms, among which we implemented Adam, Hamiltonian Monte Carlo, Variational Inference and Stein Variational Gradient Descent.

The library design is also predisposed to further extensions, because the blocks representing the different components that detach from the main skeleton are thought to be defined by few case-specific behaviors and not to have heavy constraints on the functionalities, as validated when implementing algorithms with distinct routines and structures involved or different problems.

Finally, we proposed a showcase of results to highlight the main features of method and library: algorithm comparison, introduction of PDE residuals into Neural Networks, portability to high dimension and quality of results that can be obtained with fine-tuning of model parameters.

Key-words: B-PINNs, Uncertainty Quantification, Scientific Learning

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