VARIATIONAL PHYSICS-INFORMED NEURAL NETWORKS OPTIMIZED WITH LEAST SQUARES AND ADAPTIVITY IN THE TEST SPACE

MANUELA BASTIDAS, CARLOS URIARTE, JAMIE M. TAYLOR, SERGIO ROJAS, VICTOR M. CALO, AND DAVID PARDO

Abstract. In practical scenarios, Robust Variational Physics-Informed Neural Networks RVPINNs [2] face significant challenges often related to the erratic convergence of the Stochastic Gradient Descent-based optimizers, like Adam. However, an interesting perspective emerges when interpreting the neurons in the last hidden layer of the NN as a basis of the discrete trial space. By doing so, one may boost the perfomance of the optimizer by introducing a least-squares (LS) solver to determine the trainable parameters of the last hidden layer (Cyr et al., [1]).

In the first part of this talk, we discuss the implications of using a hybrid GD/LS solver. In particular, using the discrete weak formulation involves calculating spatial derivatives for functions within the trial space's spanning set. Therefore, the computational cost of each training iteration may vary based on the chosen automatic differentiation strategy for these calculations. On the other hand, it is possible to adopt an ultraweak variational formulation of the PDE, by transferring derivatives from the trial to the test space through repeated integration by parts, assuming suitable regularity in the user-selected test functions. In this scenario, assembling the LS system does not require automatic differentiation of the NN model, leading to improved performance speeds.

In the second part of this talk, we delve into a specific case of RVPINNs known as the Deep Fourier Residual (DFR) method, introduced in [3, 4]. In this method, the loss is equivalent to the dual norm of the error. Moreover, there the calculation of the dual norm relies on the spectrum of the test function space. This representation is well-known only for rectangles in 2D or rectangular cuboids in 3D. Here, we present an extension of the DFR method utilizing adaptive strategies on general polygonal domains. We decompose the PDE domain Ω into overlapping rectangular subdomains, and propose a loss function that is computed as the sum of local loss functions. Employing a Döfler marking algorithm allows us to adaptively refine the initial subdomain decomposition of Ω, enhancing the accuracy of the approximated solution in relevant regions of the domain—essentially, we integrate adaptivity into the test space and mantain the equivalence between the loss and the actual error of the NN aproximate solution.

To demonstrate the effectiveness of the ultraweak implementation of the DFR loss function equipped with a hybrid Adam/LS solver, we provide numerical examples in 1D and 2D. Our results show dramatic improvements in both convergence speed and computational cost, surpassing the performance of Adam or Adam/LS with weak-type implementations. Furthermore, our numerical experiments reveal the generation of quasi-optimal refined meshes in several 1D and 2D problems, including the singular L-shape domain problem.

References

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Universidad Nacional de Colombia, Medellín.
Email address: `mbastidaso@unal.edu.co`

Basque Centre for Applied Mathematics (BCAM), Bilbao, Spain.
University of the Basque Country (UPH/EHU), Leioa, Spain.
Email address: `curiarte@bcamath.org`

CUNEF Universidad, Madrid, Spain.
Email address: `jamie.taylor@cunef.edu`

Pontificia Universidad Católica de Valparaíso, Chile.
Email address: `sergio.rojas.h@pucv.cl`

Curtin University, Perth, WA, Australia
Email address: `victor.calo@curtin.edu.au`

University of the Basque Country (UPH/EHU), Leioa, Spain.
Basque Centre for Applied Mathematics (BCAM), Bilbao, Spain.
Ikerbasque (Basque Foundation For Sciences), Bilbao, Spain.
Email address: `david.pardo@ehu.eus`