ULTRA-PINNS: EXPLOITING ULTRAWEAK IMPLEMENTATIONS TO BOOST THE PERFORMANCE OF VARIATIONAL PINNS

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Abstract. We propose UltraPINNs, a method for solving PDEs using NNs that offers two approaches: one based on the ultraweak variational formulation of a PDE, and the other considering its strong or weak formulation. In the latter, we compute the loss function by transferring derivatives from the trial to the test space through repeated integration by parts and assuming suitable regularity in the user-selected test functions. Our characterization of this strategy as an "ultraweak implementation" rather than an "ultraweak formulation" reflects that we retain the consistency between the loss and the error in relevant norms, while eliminating the need for numerical differentiation of the trial function.

Our method showcases two main advantages: (i) Due to the increased regularity of the integrand, using classical quadrature rules yields higher precision without increasing the number of integration points. (ii) Despite the often suboptimal convergence rates of gradient-based optimization algorithms like Adam, it is possible to expedite the convergence by interpreting the neurons in the last hidden layer of the NN as basis functions within the trial space and employing a least-squares (LS) solver to calculate the last-layer weights [**?**]. However, if the construction of the LS matrix requires the calculation of the spatial derivatives of the trial function, then its computational cost becomes dominant and increases linearly with its size. In UltraPINNs, the cost of constructing the LS matrix is significantly lower than in weak-type implementations, resulting in enhanced performance speeds.

We demonstrate the performance of UltraPINNs equipped with a hybrid Adam/LS solver using numerical examples in 1D, 2D, and 3D. We observe meaningful improvements in both convergence rate and computational cost, surpassing the performance of Adam or Adam/LS with weak-type implementations, and improving the integration error.

Keywords: Deep Learning, Physics-informed machine learning, Enhanced optimization algorithms

Mathematics Subject Classifications (2010): 68T05, 65N50

References

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