Optimizing Variational Physics-Informed Neural Networks Using Least Squares

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Abstract: Variational Physics-Informed Neural Networks (VPINNs) [1, 2] often suffer from convergence problems when using gradient-descent-based (GD-based) optimizers. By introducing a Least Squares solver for the weights of the last layer of the neural network [3], we improve the convergence of the loss during training in most practical scenarios. This presentation analyzes the computational cost of the resulting hybrid Least-Squares/Gradient-Descent (LS/GD) optimizer and explains how to implement it efficiently. In particular, we show that a traditional implementation based on backward-mode automatic differentiation leads to a prohibitively expensive algorithm. To remedy this, we propose using either forward-mode automatic differentiation or an ultraweak-type scheme that avoids the differentiation of trial functions in the discrete weak formulation. The proposed alternatives are up to 1,000 times faster than the traditional one, recovering a computational cost-per-iteration similar to that of a conventional GD-based optimizer alone. We derive computational estimates and conduct numerical experiments in one- and two-dimensional problems to support our analysis, monitoring the accuracy and computational cost during training.

References:

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