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PSelf-Adaptive Physically-Informed Neural Networks

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It has been recognized that adaptive procedures can improve the convergence of physically-informed neural networks (PINNs). To accomplish that, previous approaches have used various heuristics to define nonadaptive weights in the PINN loss function. Here, we propose Self-Adaptive PINNs (SA-PINNs), a novel family of PINNs that employ fully-trainable weights that work as a self-adaptive mask over the PDE domain, so that the neural network learns by itself which regions of the solution are difficult and is forced to focus on them. The key idea in SA-PINNs is to make the weights increase as the corresponding losses increase, which is accomplished by training the network to simultaneously minimize the losses and maximize the weights, i.e., to find a saddle point in the cost surface. We show that this is formally equivalent to solving a PDE-constrained optimization problem using a penalty-based method, though in a way where the penalty coefficients are trainable. We present numerical experiments with a few benchmarks in which SA-PINNs outperformed other state-of-the-art PINN algorithms in L2 error, while using a smaller number of training epochs. We will also discuss the implementation of SA-PINNs in our open-source TensorDiffEq software. Being currently the only full-fledged PINN software based on Tensorflow 2.x., TensorDiffEq supports the Keras API out-of-the-box and can be easily deployed on multiple GPUs to allow handling high-dimensional and complex problems. Finally, we also intend to describe the activities and ongoing multidisciplinary collaborative efforts at the recently-established Scientific Machine Learning Lab at the Texas A&M Institute of Data Science (TAMIDS).