Convergence and Sketching-Based Efficient Computation of Neural Tangent Kernel Weights in Physics-Based Loss

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Abstract

In multi-objective optimization, multiple loss terms are weighted and added together to form a single objective. These weights are chosen to properly balance the competing losses according to some meta-goal. For example, in physics-informed neural networks (PINNs), these weights are often adaptively chosen to improve the network's generalization error. A popular choice of adaptive weights is based on the neural tangent kernel (NTK) of the PINN, which describes the evolution of the network in predictor space during training [1]. The convergence of such an adaptive weighting algorithm is not clear *a priori*. Moreover, these NTK-based weights would be updated frequently during training, further increasing the computational burden of the learning process. In this talk, we will share results stating that under appropriate conditions, gradient descent enhanced with adaptive NTK-based weights is convergent in a suitable sense. Then addressing the problem of computational efficiency, we will present a randomized algorithm inspired by a predictor-corrector approach and matrix sketching which produces unbiased estimates of the NTK up to an arbitrarily small discretization error. Finally, we will show numerical experiments to support our theoretical findings and to exhibit the efficacy of our randomized algorithm.

References

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