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Towards instance-dependent approximation guarantees for scientific machine learning using Lipschitz neural networks.

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Neural networks are increasingly used in scientific computing. Indeed, once trained, they can approximate highly complex, non-linear, and high dimensional functions with significantly reduced computational overhead compared to traditional simulation codes based on finite-differences methods. However, unlike conventional simulation whose error can be controlled, neural networks are statistical, data-driven models, for which no approximation error guarantee can be inherently provided. This limitation hinders the use of neural networks on par with finite elements-based simulation codes in scientific computing. In this presentation, we show how to leverage the Lipschitz property of Lipschitz neural networks to establish strict post-training – instance dependent – error bounds given a set of validation points. We show how to derive error bounds using Voronoï diagrams for a Lipschitz neural network approximating a K-Lipschitz function by taking advantage of recent parallel algorithms. Yet, in most scientific computing applications, the Lipschitz constant of the target function remains unknown. Therefore, we explore strategies to adapt and extend these bounds to the case of unknown Lipschitz constant and illustrate them on simple physical simulation test cases.

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