Progressive Layer Enrichment with Guaranteed Error Reduction for Scientific Machine Learning

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Abstract

Developing accurate surrogate models is a central challenge in Scientific Machine Learning. They are widely used to accelerate expensive physical simulations and uncertainty quantification. While deep neural networks have become a popular choice, designing their architecture requires extensive hyperparameter tuning, and their non-convex optimization makes training challenging, often without theoretical guarantees.

In this work, we present a constructive, multi-layer enrichment framework designed to improve the accuracy of an initial surrogate model. Starting from any arbitrary baseline, the proposed method progressively adds layers with polynomial activations. By combining the properties of orthonormal polynomials with a certified optimizer, we provide a theoretical guarantee on strict error reduction with each added layer, while maintaining a controlled complexity throughout the expansion.

Finally, we test the proposed method on several physical benchmark problems. These numerical applications confirm the theoretical error decay in practice and illustrate how the method behaves against standard surrogate models.

References

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