THEORY-BASED PRINCIPLES FOR BENCHMARKING OPERATOR LEARNING

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ABSTRACT

This talk reviews several recently established theoretical principles regarding generalization error guarantees for operator learning. These principles are united by a common theme of smoothness: smoothness of the problem, smoothness of the training data, and smoothness of the test data. The analysis reveals partial answers to important considerations that are crucial for the design of widely applicable benchmarks in scientific machine learning. For example, if operator learning is used to train a surrogate (e.g., for an expensive scientific simulation), how does one guarantee any robustness of the surrogate under data distribution shifts at prediction time? Moreover, how should the accuracy of operator learning models be evaluated? This question also deserves careful treatment that depends on the application at hand. All of the above influence, in a non-trivial way, how much training data is required to learn an accurate model. Much of the existing work on operator learning follows the traditional computer science "train/validate/test" paradigm. In contrast, the results presented here suggest that operator learning for the physical sciences, where often the data generation procedure is controlled by the user, requires new ideas. Grounded in the above perspectives, this work advocates for several concrete operator learning benchmark problems. Particular emphasis is placed on inverse problems and problems beyond parametric partial differential equations.

REFERENCES

[1] M.V. de Hoop, N.B. Kovachki, N.H. Nelsen, and A.M. Stuart, Convergence Rates for Learning Linear Operators from Noisy Data, *SIAM-ASA J. Uncertain. Quantif.*, 2023.