Scientific Machine Learning

Student

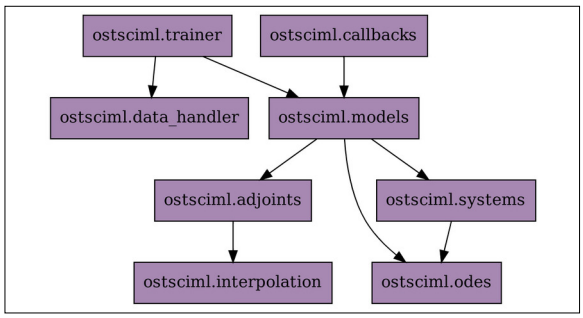
Patrik Müller

Introduction: Scientific machine learning (SciML) stands as an emerging paradigm that melds the strengths of scientific computation and machine learning. This groundbreaking approach offers the potential to bridge the gap between domain-specific insights and data-driven methodologies. This thesis embarks on a journey to harness the power of SciML by deriving, developing, and implementing a comprehensive library that integrates scientific principles with machine learning techniques, thus opening avenues for innovative problem-solving in complex systems.

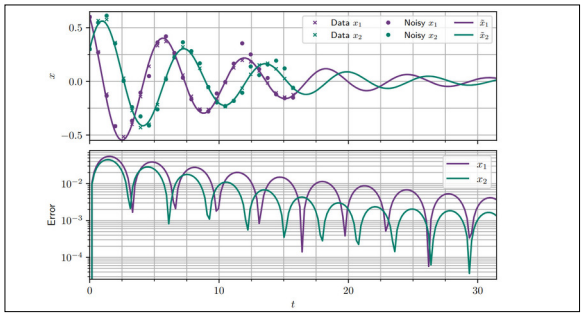
Approach: The core of this work is to build a versatile SciML library for harmonizing domain knowledge and data-driven insights. The architecture of the library is designed to seamlessly integrate various components, including support for differential equation solvers, adjoint methods, model building interfaces, and advanced training programs. This library encompasses the intricacies of scientific modeling and machine learning and is designed to provide researchers and practitioners with a unified tool set to address a wide range of challenges.

Result: This endeavor culminates in an extensive investigation into the theoretical foundations that underpin the intersection of scientific computing and machine learning. The resultant SciML library stands out as a powerful resource that showcases its capacity to harmoniously integrate physics-based modeling with data-driven methodologies. The utility of the library is demonstrated through two illustrative experiments, which illuminate the potential of SciML in extracting insights from intricate systems. Nonetheless, it's crucial to acknowledge that while the results are promising, further exploration and refinement are essential to fully harness the library's potential across a broader spectrum of applications.

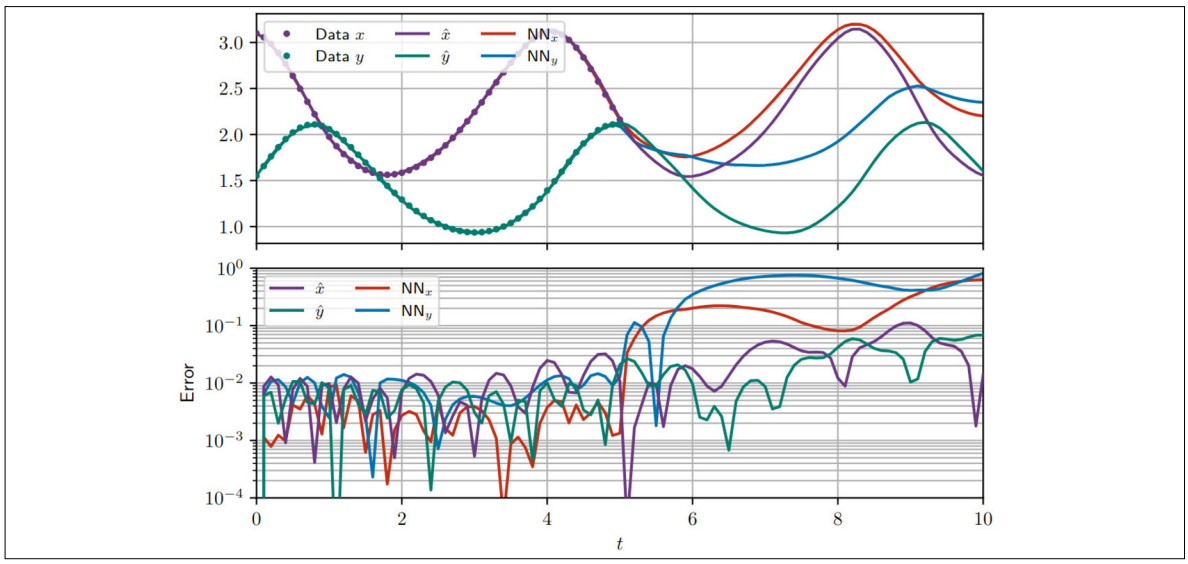
Dependency structure of the implemented SciML library.
Own presentment



Result of fitting a SciML model to a noisy dataset. In the lower plot the absolute error of predictions are plotted.
Own presentment



Result of fitting a SciML model to data of a nonlinear system. The model is compared against a neural network.
Own presentment



Advisor
Hannes Badertscher

Subject Area
Data Science, Computer Science, Software and Systems