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AutoML with Explainable AI Analysis: Optimization and Interpretation of Machine Learning Models for the Prediction of Hysteresis Behavior in Shape Memory Alloys

Dmytro Tymoshchuk and Oleh Yasniy

Department of Artificial Intelligence Systems and Data Analysis, Ternopil Ivan Puluj National Technical University, 46001 Ternopil, Ukraine

INTRODUCTION & AIM

Shape memory alloys (SMAs) belong to a class of smart materials distinguished by their unique properties—the shape memory effect and superelasticity. Due to superelasticity, these materials can withstand large reversible strains (up to 8–10%) and fully recover their original shape after unloading. Under cyclic loading and unloading, reversible phase transformations between martensite and austenite lead to the formation of a hysteresis loop that reflects the material's nonlinear behavior. Predicting this behavior is crucial for assessing the durability of structures. The aim of this study is to develop and evaluate models constructed using the AutoML approach integrated with XAI methods to predict the hysteresis behavior of SMAs. The work focuses on improving the accuracy of strain prediction and achieving interpretability of the results consistent with the physical nature of martensitic–austenitic phase transformations.

METHOD

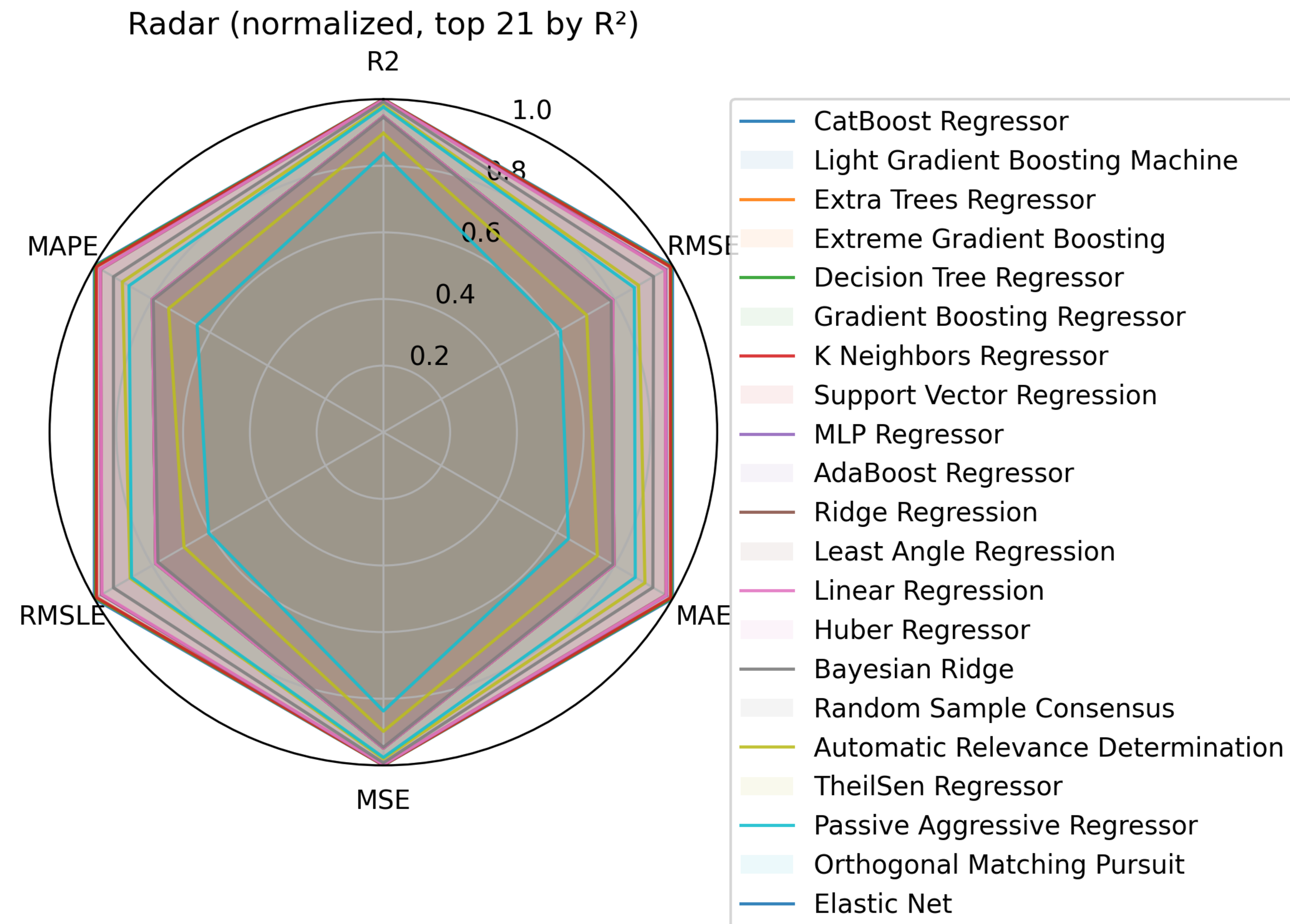
For this study, experimental data were obtained from low-cycle fatigue tests of a wire specimen with a diameter of 1.5 mm and a length of 210 mm, manufactured from a Ni55.8Ti44.2 SMA.

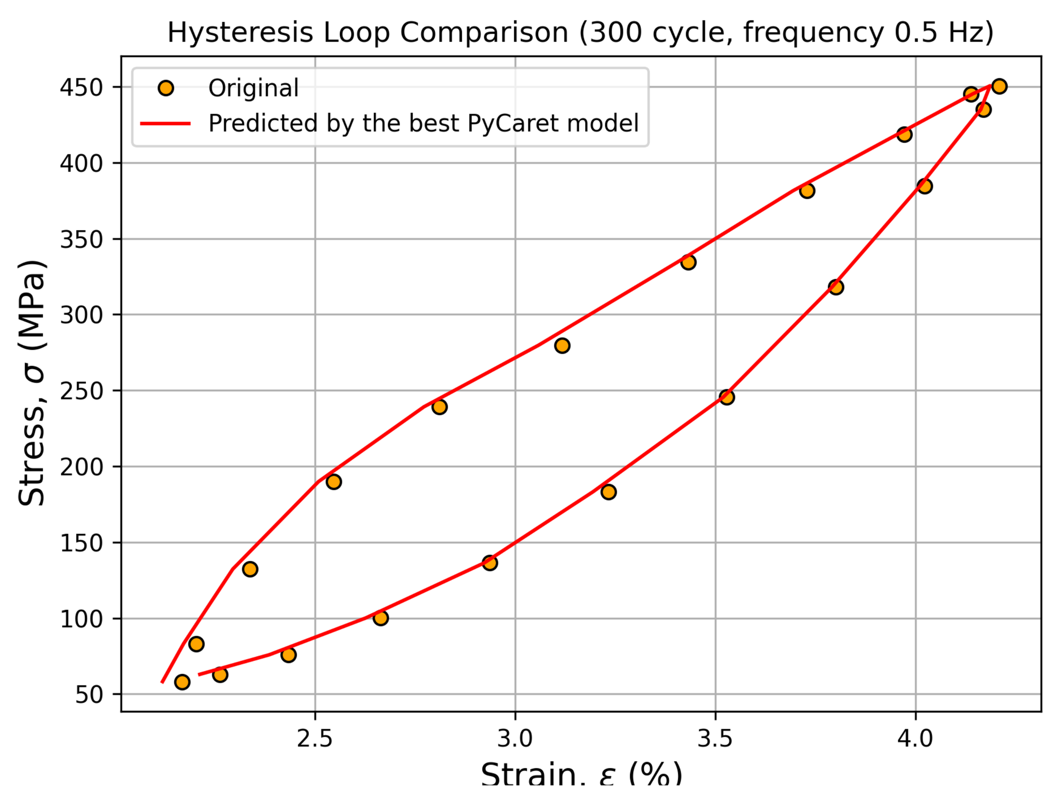
Experimental data were obtained from low-cycle fatigue tests of a wire specimen with a diameter of 1.5 mm and a length of 210 mm, fabricated from a Ni55.8Ti44.2 SMA. The experiments were conducted at room temperature using an STM-100 servo-hydraulic testing machine.

To develop the machine learning models, data from 100–250 loading–unloading cycles of the SMA material were used for loading frequencies f=0.3, 0.5, 3, and 5 Hz. The input features included the applied stress σ (MPa), the cycle number N (Cycle parameter), and the indicator of the loading or unloading stage (UpDown). The output feature was the material strain ε (%). The dataset was split in an 80:20 ratio. To automate the model development process, the PyCaret framework implementing the AutoML concept was employed. For interpreting the decisions of the machine learning models, the SHAP method was used. This allowed us to verify the consistency of the model's predictions with the physically grounded mechanisms of phase transformations in SMAs and to increase confidence in the obtained results.

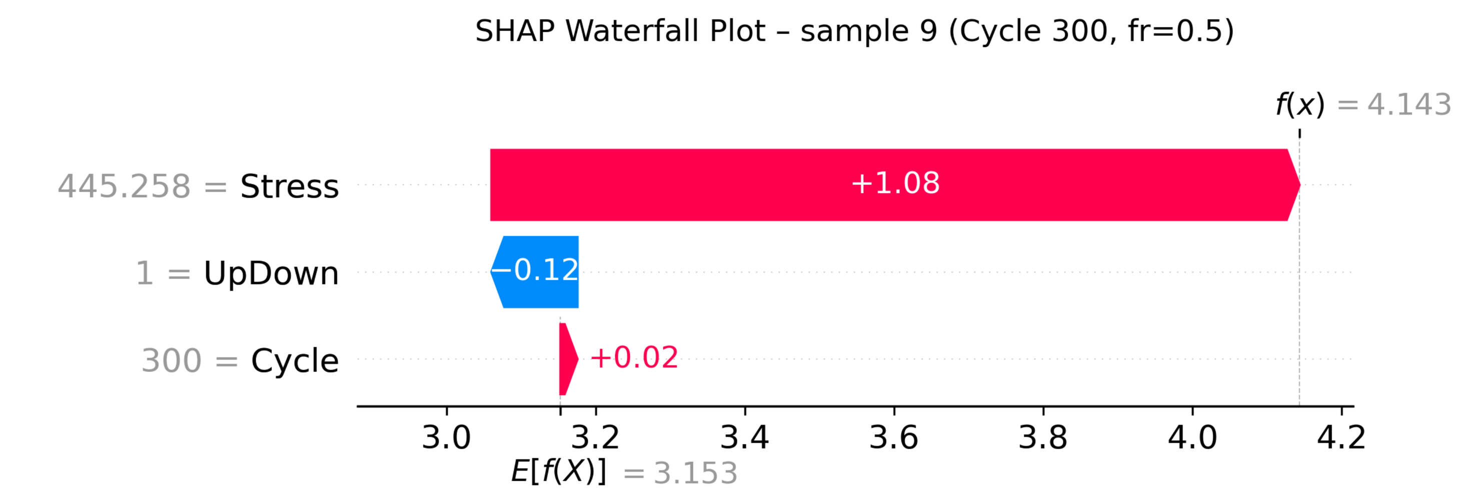
RESULTS & DISCUSSION

Results of selecting the best-performing machine learning model for the 0.5 Hz loading frequency. The coefficient of determination achieved was $R^2 > 0.997$





The generalization capability was evaluated on independent cycles 251, 260, and 300 (outside the 100–250 range). The SHAP analysis results confirm the model's ability to provide a physically meaningful interpretation of its predictions.



For sample #9, the primary contribution to increasing the predicted value comes from the Stress parameter. The UpDown feature reduces the prediction, while the Cycle parameter exhibits a minor positive influence.

CONCLUSION

The models accurately reproduce the complete σ–ε hysteresis loops, demonstrating strong agreement with the experimental data. The SHAP analysis revealed the dominant influence of the Stress parameter, the physically meaningful role of the loading or unloading stage (UpDown), and a gradual increase in the contribution of the Cycle parameter in later cycles, reflecting the effects of fatigue accumulation in the material.