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# An Explainable Pipeline for Machine Learning with Functional Data

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Many machine learning models are considered "black-boxes" because the model parameters do not have a physical meaning in the context of the problem. In recent years, there has been an increase in the development of methods that indirectly provide explanations for predictions made by black-box models. However, the scenario when functional data are used as inputs to a model has received little attention. We propose a pipeline for modeling functional data as inputs to machine learning models that (1) accounts for the functional nature of the data, (2) provides insight into the aspects of the functions that are important to the model for prediction, and (3) is model agnostic. We refer to the approach as the *V*ariable Importance *E*xplainable *E*lastic *S*hape *A*nalysis (*VEESA)* pipeline. The VEESA pipeline transforms the observed functions into principal components (PCs) using the elastic shape analysis framework [1] to appropriately capture the horizontal and/or vertical functional variability. The PCs are used as features in the model, and permutation feature importance (PFI) [2] is used to identify the important PCs. Finally, visualization is used to interpret the important PCs to provide insight into the variability in the functions that is used by the model to make predictions. We apply the VEESA pipeline to a national security example where transparency in predictive modeling is essential: identifying explosive materials from hyperspectral computed tomography scans. Neural networks are used as the model in the pipeline, and the resulting explanations help us gain trust (or distrust) in the models. *SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2022-0417 A.*

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