Comparison of machine learning methods based on feature importance for predicting mechanical properties of polymer composites

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The process of satisfying the physicochemical properties of polymer composite materials as a material for practical industry requires a lot of money and time to optimize the mixing components, composition ratio, and process. In the study, experimental data on the mechanical properties of composite materials were used to develop models. In order to predict the mechanical properties of polymer composite materials, variables related to the composition, process, material properties and individual properties of polymer descriptors, fillers and polymers are used to optimize physical properties. As a model algorithm, tree-based models (RF, XGBoost, LightGBM) are used. In order to select the variables used in the model, eXplainable Artificial Intelligence (XAI)-based methods and recursive feature elimination methods are combined to proceed with variable selection. The purpose of this study is to see whether the performance improvement effect of the existing model by applying the XAI method to variable selection.