Development of prediction models for mechanical properties of polymer composite using various ensemble methods

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In order to be used as a product for various uses in real life, polymer composites must satisfy various physicochemical properties. It is possible to obtain suitable physicochemical properties by optimizing experimental values such as composition ratios and process variables, which takes a lot of time and cost. In this study, predictive models were developed for 7 properties judged as representative mechanical/thermal properties of composite materials. The composition of the polymer composite, the process variables, the polymer descriptor and the inherent properties of the filler and polymer reflecting the composition ratio were used as dependent variables. Various tree-based consensus models (RF, GBT, XGBoost, LightGBM) and deep neural networks were applied as model algorithms. The model's hyperparameter was optimized according to the internal bootstrapping validation, and the performance of the external set that was not used for training was also compared to confirm the predictive ability of the model. The developed model will be an alternative to reduce the time and cost of developing composite materials with desired mechanical/thermal properties.