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Artificial neural network hyperparameters optimization for predicting the thermal conductivity of MXene/graphene nanofluids

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Abstract

Background

The critical role of thermal conductivity (TC) as a significant thermo-physical property in MXene/graphene-based nanofluids for photovoltaic/thermal systems has motivated recent research into developing precision predictive models. The multilayer perceptron neural network (MLPNN) has emerged as an eminent AI algorithm for this task.

Methods

This study employs Bayesian optimization, random search (RS), and grid search (GS) to fine-tune MLPNN hyperparameters—hidden layers, neurons, activation functions, standardization, and regularization—to elevate TC modeling efficiency. The proposed methodology unfolds in sequential phases: data analysis, data pre-processing, and introduction of MLPNN, GS, RS, Bayesian approach, and their integration algorithm. The next phase entails developing predictive models and presenting optimal cases. Lastly, the final models undergo statistical evaluation and graphical comparison for a thorough analysis.

Findings

Results manifest that the GS-MLPNN model excels, achieving the lowest testing data error (MAPE = 0.5261%) and high conformity with empirical data (R = 0.99941). Meanwhile, the RS method adjusts hyperparameters with negligible precision loss (MAPE = 0.6046%, R = 0.99887). Contrarily, Bayesian optimization lags, increasing errors (MAPE = 3.1981%) and lower correlation (R = 0.98099), suggesting its relative inefficacy for this specific application. The optimized models provide efficient predictions, significantly reducing the financial/computing costs associated with experimental/numerical analysis.