MT 26
International Conference on Magnet Technology
Vancouver, Canada | 2019

Contribution ID: **903** Type: **Poster Presentation**

Mon-Af-Po1.15-08 [40]: Critical Temperature Prediction for a Superconductor: A Bayesian Neural Network Approach

Monday, 23 September 2019 14:30 (2 hours)

Recently, there have been a number of studies using empirical machine learning approaches to extract useful insights on the structure-property relationships of superconductor material. Especially, these approaches are bringing extreme benefits when superconductivity data often come from costly and arduously experimental work. However, this assessment cannot be based solely on an open "black box" machine learning model, which is not fully interpretable, because it can be counter-intuitive to understand why the model gives a particular response to a set of data inputs for superconductivity characteristic analyses e.g. critical temperature, critical current density, and critical fields. This paper aims to present an alternative approach for predicting the superconducting transition temperature Tc from SuperCon database obtained by Japan's National Institute for Materials Science. We address an explainable and reliable machine-learning framework called Bayesian neural network using superconductor's chemical elements and formula to predict Tc. In such a context, the importance of the paper in focus is twofold. First, to improve the interpretability, we use a generative statistical model to capture the mutual correlation of superconductor compounds. Finally, Bayesian optimization is utilized to search for the optimal parameters of Bayesian neural network for an improved performance of the prediction model.

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Session Classification: Mon-Af-Po1.15 - Multiphysics Design and Analysis II