

Tutorial "Neural Networks"

Tuesday, 14 September 2021 14:00 (1 hour)

In this tutorial, we discuss a neural network application in materials discovery. More specifically, we will showcase how to accelerate functional high entropy alloy discovery using neural network based generative model and ensemble model for the regression task. Therefore, this tutorial consists of two parts. Firstly, we discuss in detail how to construct an alloy generation scheme based on generative neural network model, attribute classifier, stochastic sampling, and density estimation model. Secondly, we demonstrate a systematic approach to combine Bayesian optimization, neural network and gradient boosting decision tree to achieve a two-stage Ensemble Regression Model (TERM). The first stage concerns composition-based regression models, aiming at fast and large-scale composition inference. The top results from the first-stage model enter a more refined model, where density functional calculations and thermodynamic calculations are included as part of the model input. Finally, the TERM outputs were evaluated based on a rank-based policy.

Primary author: WEI, Ye (Max-Planck-Institut für Eisenforschung GmbH)

Presenter: WEI, Ye (Max-Planck-Institut für Eisenforschung GmbH)

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