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Web Seminar

Scientific Understanding from Machine Learning in Materials Science

Ryo Yoshida

The Institute of Statistical Mathematics., Tokyo, Japan

Abstract

Data-driven science is advancing rapidly and transform the world around us. As such, machine learning has received considerable attention as a key driver to the next frontier of materials science, enabling us to reap substantial time and cost savings in the discovery and development of innovative functional materials. The objective of designing materials is to identify a set of design variables that exhibits desired material properties. Here we apply a two-stage workflow that consists of forward and backward predictions. The objective of the forward problem is to predict the properties of any given design variable. The task of the inverse problem is to identify promising design candidates that exhibit a given set of desired properties by solving the inverse mapping of the forward model. This talk describes a basic concept and some key technologies of machine learning for the inverse materials design, illustrated with practical applications from our recent works on polymer and quasicrystal researches. In particular, I discuss some use cases and strategies for obtaining human-interpretable scientific knowledge from black-box models of machine learning.

[1] Liu et al. Machine learning to predict quasicrystals from chemical compositions, Adv Mater. 33(36):e2102507 (2021).

[2] Wu et al. Machine-learning-assisted discovery of polymers with high thermal conductivity using a molecular design algorithm. npj Comput Mater. 5:66 (2019).

[3] Ju et al. Exploring ultrahigh lattice thermal conductivity crystals via feature-based transfer learning. Phys Rev Mater. 5, 053801 (2021).

[4] Yamada et al. Predicting materials properties with little data using shotgun transfer learning. ACS Cent Sci. 5(10):1717-1730 (2019).
[5] Ikebata et al. Bayesian molecular design with a chemical language model. J Comput Aided Mol Des. 31(4):379-391 (2017).