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Deep Learning Framework for Material Design Space Exploration using Active Transfer Learning

Yongtae Kim[1)], Youngsoo Kim[2)], Charles Yang[3)], Kundo Park[1)], Grace X. Gu[3)], *Seunghwa Ryu[1)]

[1]Department of Mechanical Engineering & KI for the NanoCentury, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea
[2]Department of Nature-Inspired System and Application, Korea Institute of Machinery and Materials, Daejeon, (34103) 156, Republic of Korea
[3]Department of Mechanical Engineering, University of California, Berkeley, CA 94720, USA

[1)] yongtae.aug@kaist.ac.kr

ABSTRACT

Neural network-based generative models have been actively investigated as an inverse design method for finding novel materials in a vast design space. However, the applicability of conventional generative models is limited because they cannot access data outside the range of training sets. Advanced generative models that were devised to overcome the limitation also suffer from the weak predictive power on the unseen domain. In this study, we propose a deep neural network-based forward design approach that enables an efficient search for the superior materials far beyond the domain of the initial training set. This approach compensates for the weak predictive power of neural networks on an unseen domain through gradual updates of the neural network with active-transfer learning and data augmentation methods. We demonstrate the potential of our framework with a grid composite optimization problem that has an astronomical number of possible design configurations. Results show that our proposed framework can provide excellent designs close to the global optima, even with the addition of very small dataset corresponding to less than 0.5% of the initial training dataset size.

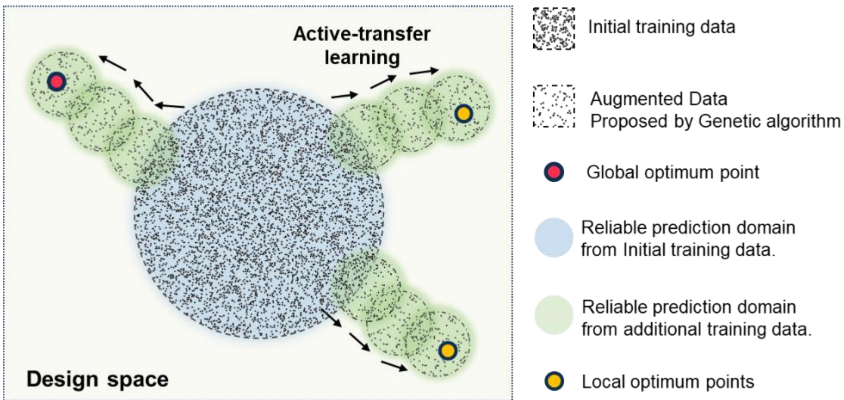

Fig. 1 Schematic of Deep Learning Framework for Material Design Space Exploration.