Efficient machine learning for ferromagnetic multilayers by Gaussian data-augmentation method

Mie Univ. [1], NIMS [2], ○Kenji Nawa[1, 2], Katsuyuki Hagiwara[1], Kohji Nakamura[1]

E-mail: nawa@elec.mie-u.ac.jp

Ferromagnetic multilayers potentially exhibit fascinating electronic, magnetic, and optical properties and these properties strongly depend not only on constituent elements and their compositions, but also on the atomic-layer configurations [1]. Search for multi-functional multilayers with optimally controlled atomic-layer configuration is of importance in both fundamental and applied physics perspectives. Neural network (NN), one of machine-learning techniques, has been developed rapidly in recent years and has succeeded to explore desired materials from big database. In contrast, from the first-principles calculations based on density-functional theory (DFT), it is difficult to construct such big database due to the huge computational costs, which limits a learning accuracy of NN training. Thus, an improvement of the learning accuracy from the small database is desired for the NN approach combined with DFT.

Here, we introduce Gaussian data-augmentation (GDA) method to the NN-learning, in which the training input data are augmented by adding Gaussian noises, and apply this method to binary Co-Fe magnetic multilayer system. As a target quantity, we employ the formation energy, E_{Form}, of nine monolayers of $\mathrm{Co}_{1-x}\mathrm{Fe}_x$ on an MgO(001), which corresponds to the number of models, 512 ($=2^9$) atomic-layer configurations [2]. The NN consists of four layers, in which rectified linear and identity functions are employed in the hidden and output layers, respectively. To demonstrate the learning accuracy from small database, we train the network for 30% of all data with size 512 and evaluate the learning accuracy by R^2 score to the test data which accounts for 70% of all data. The NN without the GDA results in small R^2 score (0.215), giving a low prediction accuracy, and the correlation of E_{Form}'s between the DFT and NN results is scattered [Fig. 1(a)]. Contrary, adapting the GDA method significantly improved the learning accuracy up to $R^2 = 0.684$ and the NN-predicted E_{Form}'s reliably follow the DFT results [Fig. 1(b)]. We will present the results applied to the magnetic properties and discuss a role of the GDA in detail.

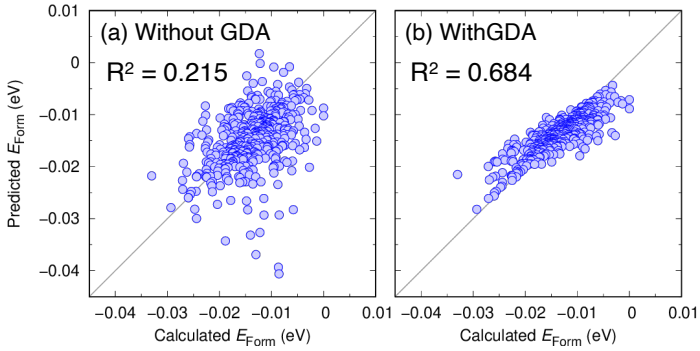

FIG. 1 Correlations between the DFT-calculated and the NN-predicted E_{Form} from (a) without and (b) with GDA.

This work is partly supported by the Tatematsu Foundation and the Data-Science Research Center for Material, Quantum, and Measurement Technologies, Mie University.

[1] K. Hotta et al., PRL **110**, 267206 (2013); K. Nakamura et al., JMMM **537**, 168175 (2021).

[2] 中村浩次, 加藤夕奈, Magnetics Jpn. **15**, 217 (2020).