Prediction rigidities for machine learning models in material science

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With the widespread application of machine learning (ML) to material science, it has become ever more crucial to understand how the ML models learn to correlate chemical structures with their properties, and what can be done to improve the training efficiency whilst guaranteeing interpretability and transferability. In this talk, I present the wide utility of *prediction rigidities*, a family of metrics derived from the loss function, in understanding the "robustness" of ML models and their predictions. I comprehensively show that the prediction rigidities allow the assessment of the model not only at the global level [1], but also on the local [2] or the component-wise level [1] at which the "raw" (e.g. atomic, body-ordered, or range-separated) predictions are made by the models. I then demonstrate how these metrics can be leveraged to gain insights to the learning behavior of different ML models, and to guide efficient dataset construction for model training. Finally, I show how the metrics can also be obtained for neural network-based ML models [3] through a set of reasonable approximations.

References

[1] S. Chong, F. Bigi, F. Grasselli, P. Loche, M. Kellner, M. Ceriotti, *Faraday Discuss.*, 256 (2025) 322-344.
[2] S. Chong, F. Grasselli, C. Ben Mahmoud, J. D. Morrow, V. L. Deringer, M. Ceriotti, *J. Chem. Theory Comput.*, 19, 22 (2023) 8020-8031.
[3] F. Bigi, S. Chong, M. Ceriotti, F. Grasselli, *Machine Learn.: Sci. Tech.*, 5, 4 (2024) 045018.

Figures

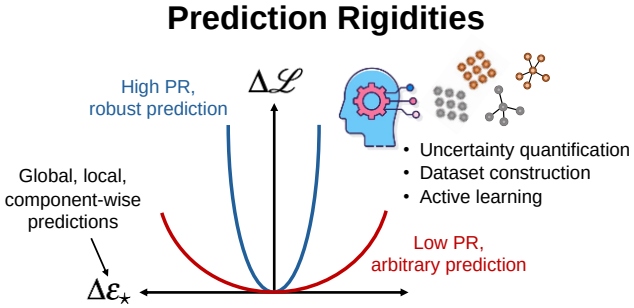

Figure 1. Artwork showing the utilities of prediction rigidities for machine learning models in material science.