Poster

Applications of isometry invariants on material property prediction

J.Balasingham[1], V. Zamaraev[1], V. Kurlin[1]

[1]University of Liverpool, Ashton Building Liverpool L69 3BX, UK

jbalasin@liverpool.ac.uk

Periodic material or crystal property prediction using machine learning has grown popular in recent years as it provides a computationally efficient replacement for classical simulation methods. A crucial first step for any of these algorithms is the representation used for a periodic crystal. While similar objects like molecules and proteins have a finite number of atoms and their representation can be built based upon a finite point cloud interpretation, periodic crystals are unbounded in size, making their representation more challenging. Isometry invariants offer a consistent way to represent and compare crystal structures. The Pointwise Distance Distribution [1] and Average Minimum Distance [1] have been used to distinguish all (more than 660 thousand) periodic crystals in the Cambridge Structural Database as purely periodic sets of points without atomic types. For machine learning models, the composition of a crystal contains crucial information needed for making accurate predictions. We adapt the Pointwise Distance Distribution to create a graph representation that includes atomic species information that can be utilized by previously developed Graph Neural Networks for material property prediction [2]. We further introduce an encoding method for using the invariants directly in a Transformer model and show its effectiveness on the commonly used Jarvis-DFT and Materials Project datasets [3].

[1] Widdowson, D., & Kurlin, V. (2022). Resolving the data ambiguity for periodic crystals. *Advances in Neural Information Processing Systems*, *35*, 24625-24638.

[2] Balasingham, J., Zamaraev, V. & Kurlin, V. Material Property Prediction Using Graphs Based on Generically Complete Isometry Invariants. *Integr Mater Manuf Innov* (2024). https://doi.org/10.1007/

[3] Balasingham, J., Zamaraev, V. & Kurlin, V. Accelerating material property prediction using generically complete isometry invariants. Sci Rep 14, 10132 (2024). https://doi.org/10.1038/