Cartesian encoding graph neural network for crystal structure property prediction: application to thermal ellipsoid estimation

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Abstract

In the diffraction resolution of crystal structures, thermal ellipsoids are a critical parameter that is usually more difficult to determine than atomic positions. These ellipsoids are quantified through Anisotropic Displacement Parameters (ADPs), which provide critical insights into atomic vibrations within crystalline structures. ADPs reflect the thermal behaviour and structural properties of crystal structures. However, traditional methods to compute ADPs are computationally intensive. This paper presents CartNet, a novel graph neural network (GNN) architecture designed to predict properties of crystal structures efficiently by encoding the atomic structural geometry to the Cartesian axes and the temperature of the crystal structure. Additionally, CartNet employs a neighbour equalization technique for message passing to help emphasise the covalent and contact interactions and a novel Cholesky-based head to ensure valid ADP predictions. Furthermore, a rotational SO(3) data augmentation technique has been proposed during the training phase to generalize unseen rotations. To corroborate this procedure, an ADP dataset with over 200 000 experimental crystal structures from the Cambridge Structural Database (CSD) has been curated. The model significantly reduces computational costs and outperforms existing previously reported methods for ADP prediction[1] by 10.87%, while demonstrating a 34.77% improvement over the tested theoretical computation methods[2,3]. Moreover, we have employed CartNet for other already known datasets that included different material properties, such as formation energy, band gap, total energy, energy above the convex hull, bulk moduli, and shear moduli. The proposed architecture outperformed previously reported methods by 7.71% in the JARVIS dataset[4] and 13.16% in the Materials Project dataset[5], proving CarNet's capability to achieve state-of-the-art results in several tasks. The project website with online demo available at: https://www.ee.ub.edu/cartnet

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Figures

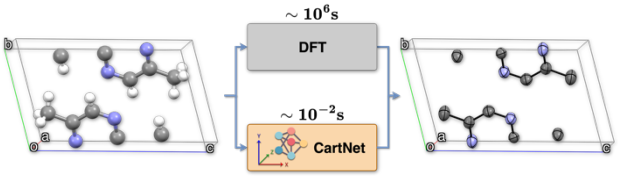

Figure 1. CartNet, a novel graph neural network, efficiently predicts anisotropic displacement parameters (ADPs) for crystal structures, significantly reducing computational costs and outperforming the tested theoretical methods while achieving state-of-the-art accuracy across diverse datasets.