Capturing Long-Range Interactions in GNNs for Interatomic Potentials with Multi-Scale Virtual Nodes

Finn Tillinger [1], **Jacopo Venturin** [1], **Zakariya El-Machachi** [1], **Cecilia Clementi** [1 †]

[1]Department of Physics, Freie Universität Berlin, Arnimallee 12, 14195, Berlin, Germany
†corresponding author's email: cecilia.clementi@fu-berlin.de

Graph neural networks (GNNs) are widely used in molecular physics and materials research as machine-learned interatomic potentials and machine-learned force fields for molecular dynamics simulations. However, their receptive field spans only a few message-passing steps since stacking too many message-passing layers results in oversmoothing and oversquashing [1]. Therefore, these GNNs are inherently local and fail to capture important long-range interactions such as electrostatics or dispersion. Thus, incorporating long-range interactions in GNNs in a computationally efficient way is a research task of great interest.

We introduce ARRANGE, a model-agnostic framework that equips any baseline GNN with virtual nodes on different length scales, which aggregate and broadcast information from and to the atoms using a distance-aware multi-head attention mechanism. The multi-scale nature of the virtual nodes enables the model to learn long-range interactions on different length scales while avoiding unfeasible all-to-all connections or costly Fourier transformations to reciprocal space. Because ARRANGE creates the virtual nodes dynamically for each structure, the framework is scalable with system size and specifically built for large structures. ARRANGE builds on our previous long-range framework for GNNs, RANGE [2], and refines it to be specialized for scaling to larger structures.

We test this approach on four widely used GNNs – SchNet [3], PaiNN [4], SO3KRATES [5], and MACE [6] – as baseline models to which we add the ARRANGE framework. Across all tested datasets, ranging from proteins to amorphous graphene sheets, we achieve significant improvements in accuracy for energy and force prediction over the respective GNN baseline model while only adding small computational overhead. Compared to other state-of-the-art long-range models, ARRANGE is competitive and outperforms them in particular on large atomic structures.

References

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