

## The Abdus Salam International Centre for Theoretical Physics



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Title: Approximately equivariant graph networks

Abstract: Graph neural networks (GNNs) are commonly described as being permutation equivariant with respect to node relabeling in the graph. This symmetry of GNNs is often compared to the translation equivariance symmetry of Euclidean convolution neural networks (CNNs). However, these two symmetries are fundamentally different: The translation equivariance of CNNs corresponds to symmetries of the fixed domain acting on the image signal

(sometimes known as active symmetries), whereas in GNNs any permutation acts on both the graph signals and the graph domain (sometimes described as passive symmetries). In this work, we focus on the active symmetries of GNNs, by considering a learning setting where signals are supported on a fixed graph. In this case, the natural symmetries of GNNs are the automorphisms of the graph. Since real-world graphs tend to be asymmetric, we relax the notion of symmetries by formalizing approximate symmetries via graph coarsening.

We present a bias-variance formula that quantifies the tradeoff between the loss in expressivity and the gain in the regularity of the learned estimator, depending on the chosen symmetry group. To validate our approach, we conduct extensive experiments on human pose estimation and traffic flow prediction with different choices of symmetries. We show theoretically and empirically that the best generalization performance can be achieved by choosing a suitably larger group than the graph automorphism group, but smaller than the full permutation group.