

Graph Neural Networks (GNNs) are a powerful tool for handling machine-learning tasks on graph-structured data. Because of the distinct nature of graph data, traditional neural networks are not directly applicable to it. Most GNNs are based on the Weisfeiler-Lehman (WL) algorithm for graph isomorphism. However, just like the WL algorithm, they are incomplete and incapable of distinguishing certain graph structures. In this thesis, we provide an overview of the current state of the art in GNNs, focusing on their application to molecular data. We then present a novel approach to GNNs based on an algorithm for planar graph isomorphism testing, which produces a unique, learnable graph representation. Any sequential model can then use this representation, thus bringing together the fields of GNNs and modern deep-learning techniques. We evaluate the performance of our model on a dataset of molecules and compare it against existing models.