# Covariant Compositional Networks for Learning Graphs

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## ABSTRACT

In this paper, we propose Covariant Compositional Networks (CCNs), the state-of-the-art generalized convolution graph neural network for learning graphs. By applying higher-order representations and tensor contraction operations that are permutation-invariant with respect to the set of vertices, CCNs address the representation limitation of all existing neural networks for learning graphs in which permutation invariance is only obtained by summation of feature vectors coming from the neighbors for each vertex via well-known message passing scheme.

For an application of learning small-scale molecular graphs, we investigate the efficiency of CCNs in estimating Density Functional Theory (DFT) that is the most successful and widely used approach to compute the electronic structure of matter but significantly expensive in computation. We obtain a very promising result and outperform other state-of-the-art graph learning models in Harvard Clean Energy Project [1] and QM9 [2] molecular datasets.

We also apply CCNs to learn large-scale networks such as Cora & Citeseer [3] in the task of semi-supervised transductive node classification. In addition, we combine CCNs with a scheme of hierarchical pooling to obtain a coarse-grained model that both increases robustness as well as computational saving.

## KEYWORDS

graph neural networks, graph learning, quantum chemistry, network analysis

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