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Weisfeiler and Lehman Go Topological: Message Passing Simplicial Networks

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The pairwise interaction paradigm of graph machine learning has predominantly governed the modelling of relational systems. However, graphs alone cannot capture the multi-level interactions present in many complex systems and the expressive power of such schemes was proven to be limited. To overcome these limitations, we propose Message Passing Simplicial Networks (MPSNs), a class of models that perform message passing on simplicial complexes (SCs). To theoretically analyse the expressivity of our model we introduce a Simplicial Weisfeiler-Lehman (SWL) colouring procedure for distinguishing non-isomorphic SCs. We relate the power of SWL to the problem of distinguishing non-isomorphic graphs and show that SWL and MPSNs are strictly more powerful than the WL test and not less powerful than the 3-WL test. We deepen the analysis by comparing our model with traditional graph neural networks (GNNs) with ReLU activations in terms of the number of linear regions of the functions they can represent. We empirically support our theoretical claims by showing that MPSNs can distinguish challenging strongly regular graphs for which GNNs fail and, when equipped with orientation equivariant layers, they can improve classification accuracy in oriented SCs compared to a GNN baseline.