Message Passing Neural Networks and their Applications

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We discuss Message Passing Neural Network (MPNNs) (Gilmer et al., 2017), a framework for Graph Neural Networks (GNN) (Scarselli et al., 2009), and how it is applied to current research. Graph neural networks learn a state embedding which contains information of the neighborhood for each node. By learning the state embedding, the neural network can produce node-level output, such as a label. Several common areas of research that use the MPNN framework are positional graphs, chemical/molecular graphs, natural language processing (NLP), and encoding graphical structures. These applications have made their own adjustments to address limitations in the original framework. The most common limitations that were addressed were that MPNNs fail to capture hierarchical graphical representations and the computational complexity of aggregating all node and neighboring nodes' features. We found that the most common adjustment was the use of sub-graphs to either address complexity or to represent hierarchical representations, or both.