DEEP REPRESENTATION LEARNING OF SPECTROSCOPIC GRAPHS

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Graph representations of spectroscopic information have been increasing in popularity due to their efficiency and scalability in encoding large volumes of data; simply, energy levels are represented as nodes, and transitions as edges between each level. Thus, all quantum mechanical information pertaining to a molecule can be readily manipulated and transformed using a single data format, allowing computations and visualizations to be performed with ease.

One application of spectroscopic graphs is to assist in the analysis of high resolution spectra of complex mixtures, comprising many observed transitions from an unknown number of molecules. Analysis of such mixtures comprises two coupled tasks: assignment of features to their respective signal carriers, and to decompose the full spectrum into known molecules. Viewing this problem from the perspective of spectroscopic graphs, our task is to fully reconstruct the subgraphs (i.e. molecules) from sparse information obtained with techniques such as AMDOR and MST.

Here, we apply the use of deep graph learning techniques for spectroscopic graph reconstruction. Using convolutional autoencoder architectures, we experiment with the possibility of parameterizing graph neural networks to reproduce complex graphs when given only a limited number of "observed" energy levels and/or transitions. As part of this work, we perform a comprehensive investigation into the successes and challenges of our approach, including the interpretability of learned representations, how they can be manipulated and analyzed, and its applicability in complex mixture analysis.