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A Critical Review of Neural Networks for the Use with Spectroscopic Data

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Abstract

In recent years, neural networks have found increased use in the analysis of crystallographic characterization data, such as X-ray diffraction (XRD) patterns. Previous work has shown that neural networks can successfully identify crystalline phases from XRD patterns and classify their symmetry, even in multiphase mixtures. When compared with classical machine learning methods, such as Support Vector Machines or Decision Trees, CNNs show improved performance in the classification of XRD patterns and can even handle experimental artifacts such as peak shifts caused by strain, whereas the classification models would fail. Such an approach is readily extended to other spectroscopic techniques, including NMR, Raman or NIR. Those network models usually employ a convolutional neural network (CNN) architecture which has been developed for the use with images.

Despite these promising results, our work reveals several key limitations of the CNN architecture with respect to spectroscopic analysis, and we show that these limitations can lead to failed classifications on relatively simple patterns. Convolutional layers are demonstrated to have very little benefit for classification, and their only important contribution comes from the pooling operations that shrink the size of the input while keeping relevant information regarding peak intensities. Those pooling operations compensate for peak shifts, and therefore classical models applied to the shrunken input perform equally well as the presented neural networks. Nonetheless, we show how to adapt various parameters in the neural networks, such as the choice of activation function, to train more robust models with improved accuracy on classification tasks. Based on our findings, we believe that neural networks have their place for use with spectroscopic data but require careful design of their architecture to handle peculiarities inherent to spectral data.