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Machine Learning-based Auto-indexing of Neutron Diffraction Pattern from China Spallation Neutron Source

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A neutron diffraction pattern auto-indexing algorithm based on machine learning was developed and customed for the diffraction pattern collected from China spallation neutron source (CSNS). Over three hundred thousand crystal structures with different symmetries from the Crystallography Open Database generate the neutron diffraction time-of-flight patterns. In addition, the background and instrument parameters from CSNS modulated the patterns to make them simulate the real-world patterns in CSNS as much as possible. The modulated patterns are the samples composing the training set and evaluation set. The real-world patterns collected from CSNS compose the test set. In this algorithm, the convolutional layers extract the symmetry-related features from samples and the afterward fully connected layers classify samples into different crystal systems and space groups. Based on the prediction result, the algorithm provides several options listed in descending order of likelihood. Apart from symmetry prediction, the algorithm also predicts the lattice parameters and the architecture is still the convolutional neural network. Due to variations in the number and composition of lattice parameters across different crystal systems, each crystal system owns a custom CNN architecture for parameter prediction. The auto-indexing algorithm will be integrated into the CSNS data reduction program.

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