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Supervised Machine Learning Approach for Phase Identification in Neutron and X-ray Powder Diffraction Experiments

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X-ray and neutron powder diffraction are experimental techniques that allow the determination of structural properties of materials, such as their phase composition (identification and quantification). Machine learning has the potential to efficiently replace the traditional procedural paradigm in phase determination due to its ability to learn data patterns and use them in predictions. In this study, known structures of different phases were obtained from the Crystallography Open Database and the corresponding powder diffraction patterns were calculated. Systematic differences between the measured and calculated diffraction patterns were analysed. A machine learning algorithm was trained and benchmarked against measured data.

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