WESTERN MICHIGAN UNIVERSITY

Project Proposal

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CS 5300

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Project Overview

- Working Title: Studies of Artificial Neural Network Generalization Performance While Training on Materials Physics Research Data

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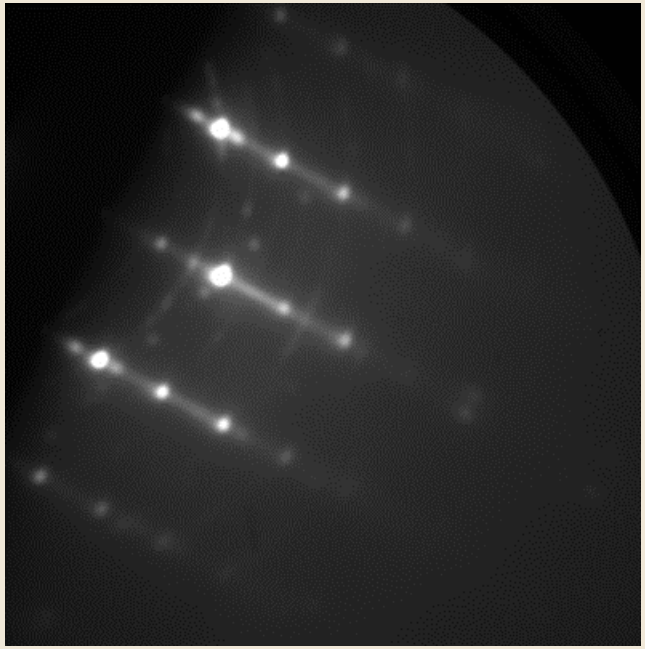
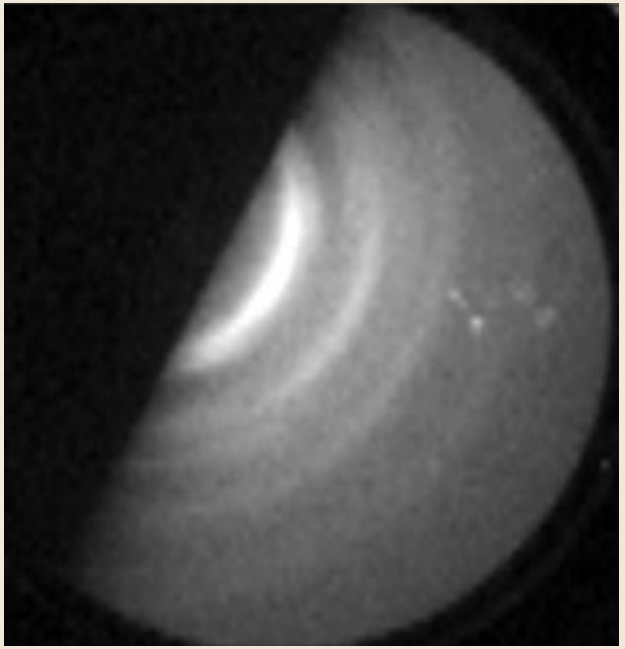
- Aim: Investigate how different (combinations of) regularization techniques influence ANN prediction accuracy on verification data points sampled from real materials research data sets describing various physical systems.

Discrete Data: Binary Classification

Monocrystalline (1)

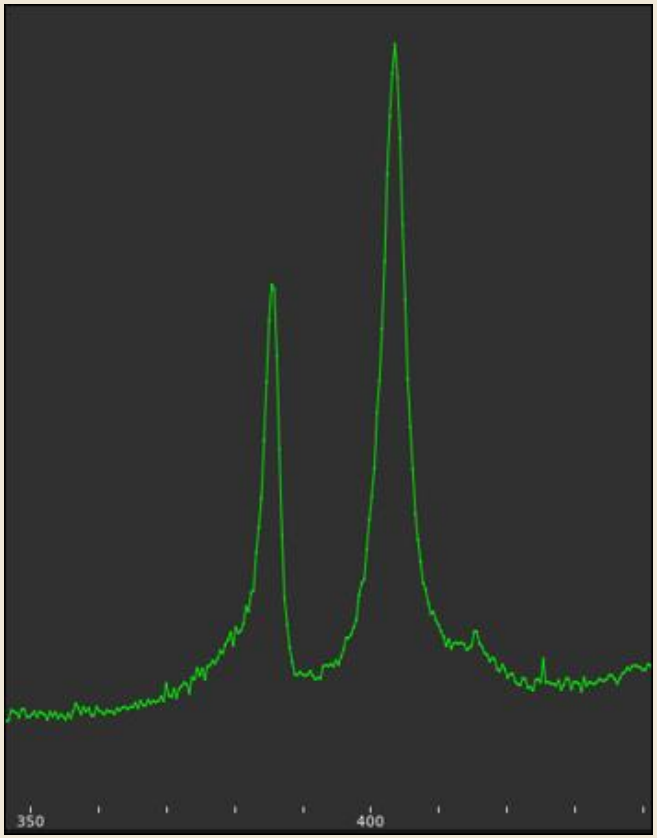


Polycrystalline (0)

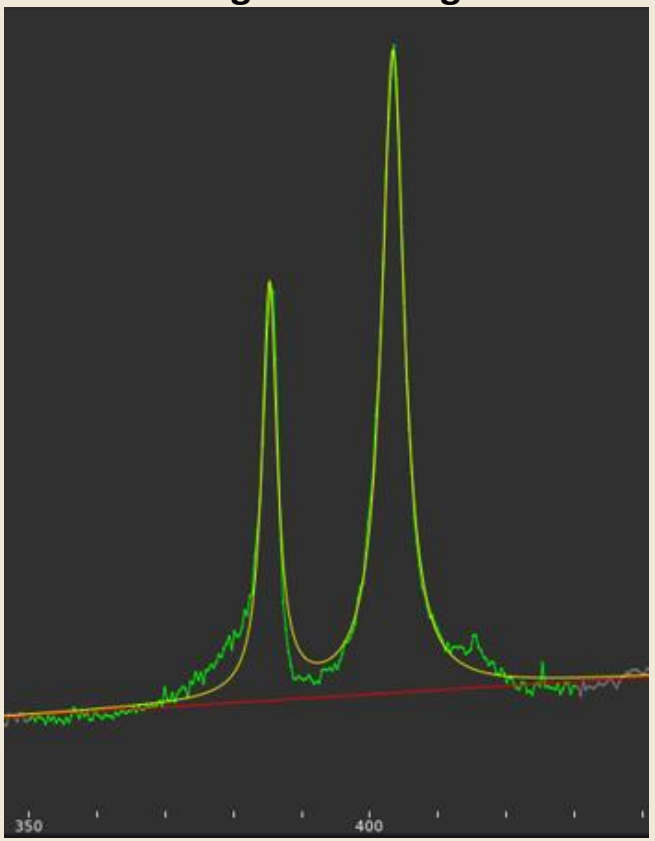


Continuous Data: Regression

Raman Spectrum of MoS_2



Fitting E_{2g} and A_{1g} Modes



Project Outline

1. Finish gathering data (partially completed).
2. Implement artificial neural network algorithms in Python3 via PyTorch, Scikit–Learn, Scikit–Optimize, etc.
3. Survey regularization and other related design optimization techniques for improving ANN generalization performance on the data.
4. Compare the improvements made by the various approaches and use the champion case to generalize and predict a growth space