Automated Crystal Structure Identification from X-ray Diffraction Patterns

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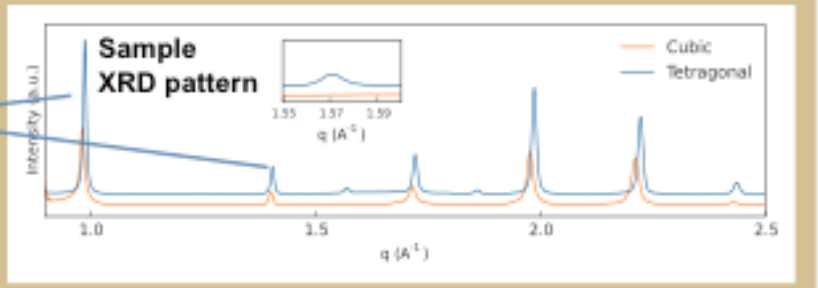
1. Overview

- X-ray diffraction (XRD) detects crystalline structure.
- We implement methods to automatically identify basic crystal structure.

2. Data

Position and **intensity** of peaks give the crystal structure of the material



- We simulate 11000 XRD patterns from known structures in the Inorganic Crystal Structure Database[1]
- 1000 of these are used as the test set

3. Machine Learning methods

Input vector
Intensity at each slice of q (50 – 2000 slices)

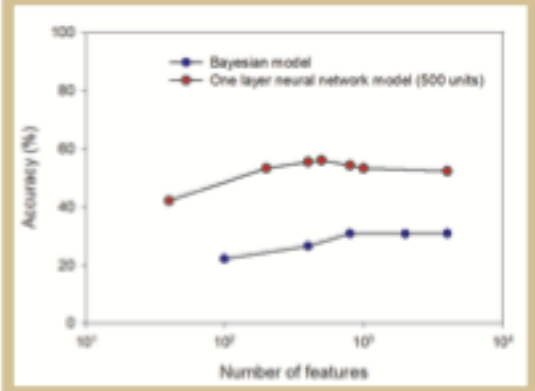
Neural Network
- 1 or 2 hidden fully connected layers
- Sigmoid activation

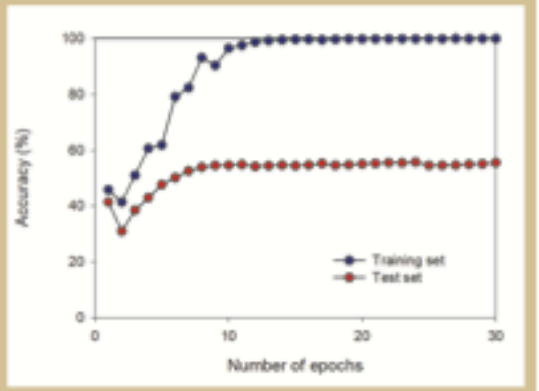
Naïve Bayes
- Assumption of conditionally independent input features

Classification into one of 7 possible crystal systems

4. Results

Method	Training accuracy	Test accuracy
Naïve Bayes	35%	31%
Neural Network	100%	62%





- Regularization improves NN test accuracy from 56% to 62%
- Using 1 or 2 hidden layers shows similar performance.
- Training set and feature set size do not significantly impact error for NN.

5. Outlook

- Neural network outperforms Naïve Bayes due to correlation among input features
- Improving NN architecture could improve performance

1. https://icsd.fiz-karlsruhe.de/