Locating Peaks in Neutron Diffraction Patterns Using Machine Learning

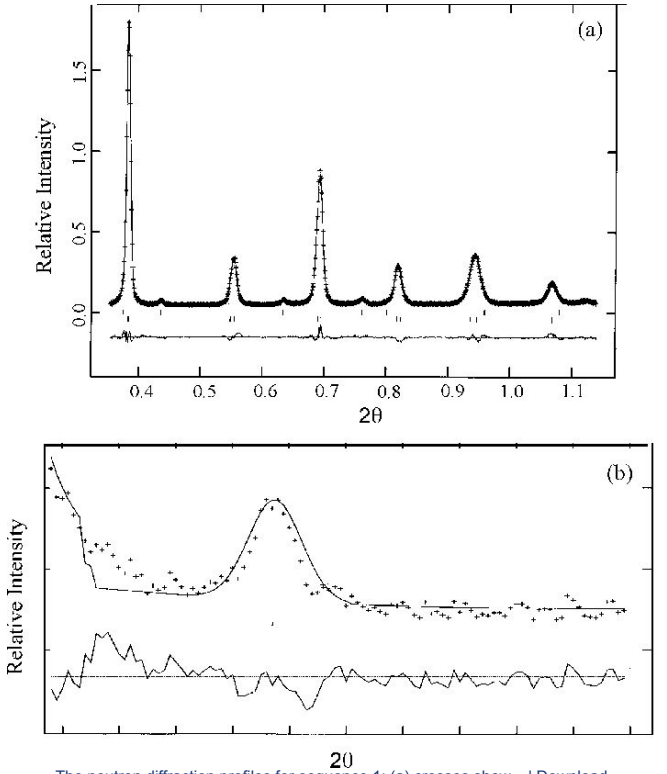
Dylan Zhang

Mentor - Dr. William Ratcliff

Wootton High School

Objective

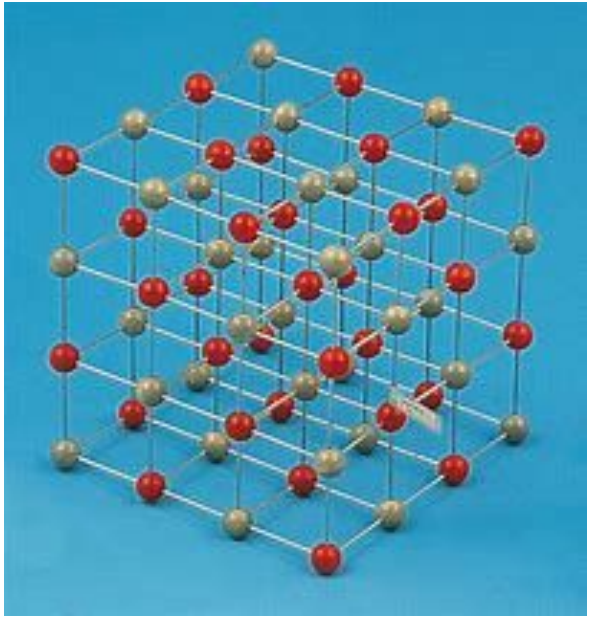
- Build and train a U-net machine learning model to be able to identify peaks on a neutron diffraction graph



The neutron diffraction profiles for sequence 1: (a) crosses show... | Download Scientific Diagram (researchgate.net)

Crystals

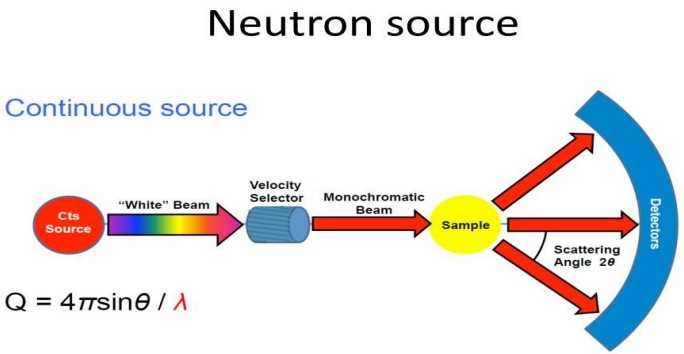
- a type of solid material composed of atoms or groups of atoms that are arranged in a three-dimensional pattern that is very ordered
- Lattice determines the different diffraction patterns



Crystal lattice of NaCl - Crystal lattice models - Structure of crystals - Solid-state physics - Physics Equipment - Physics (leybold-shop.com)

Neutron Diffraction

- Neutron Diffraction is the application of elastic neutron scattering to determine the atomic and magnetic structure of a material
- A sample is placed in a beam of neutrons to obtain a diffraction pattern that provides information about the structure of the sample



PPT - Neutron Diffraction and Scattering in Biology PowerPoint Presentation - ID:2313326 (slideserve.com)

The Problem

- The Neutron diffraction process is largely manual and is extremely time consuming

Why/How

Why

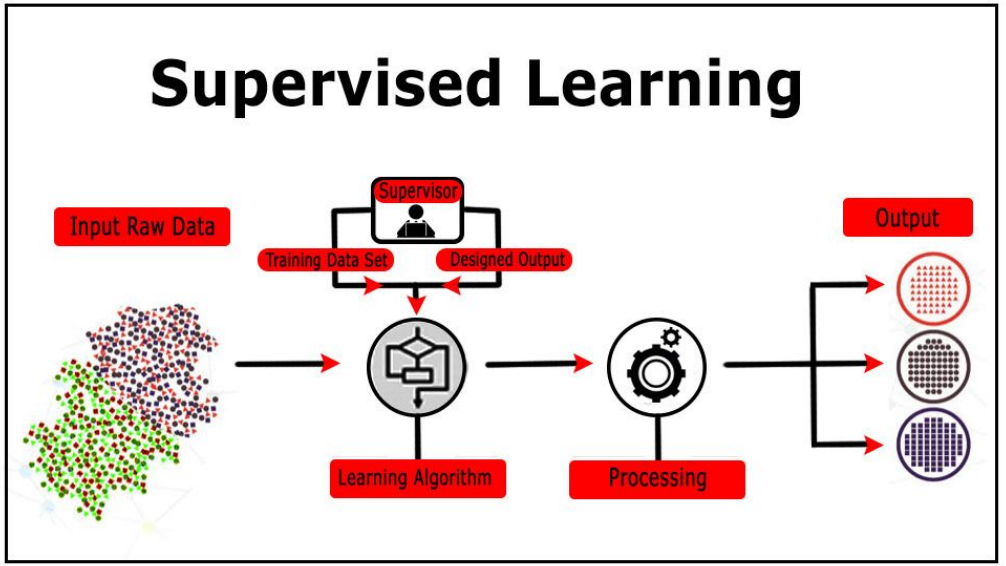
- automate some of the crystallography process
- significant because the position of peaks gives us valuable information on the sample

How

1. Build the U-net model
2. Train the model with graph data and their labels
3. Evaluate/test the model
4. Tune hyperparameters if needed
5. Evaluate again

Supervised Learning

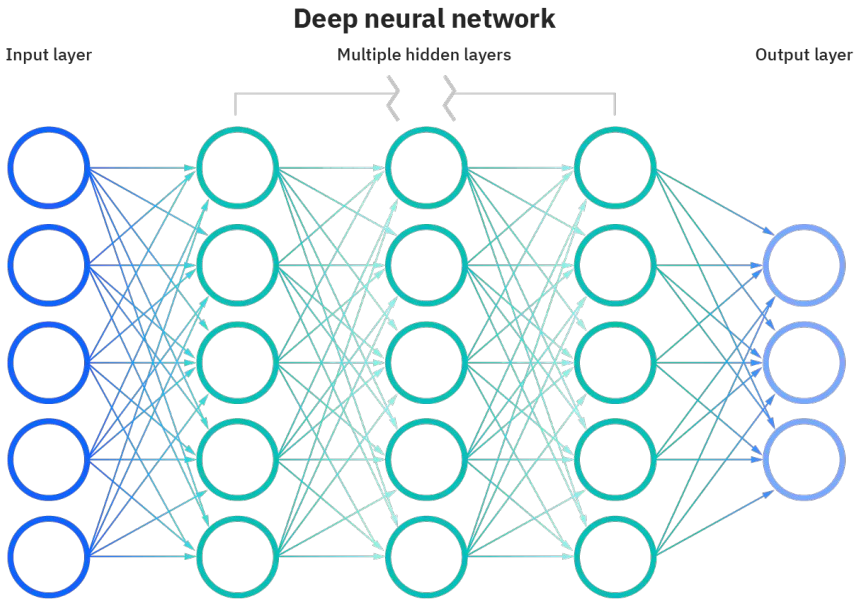
- a subcategory of machine learning
- takes both training data and its associated output
- possible for you to be very specific about the definition of the classes
- supervised learning is a simple process for the supervisor to understand



SUPERVISED MODELS | Data Vedas

Neural Networks

- a computer system modeled on the human brain and nervous system
- comprised of a node layers, containing an input layer, one or more hidden layers, and an output layer
- Each node has an associated weight and threshold

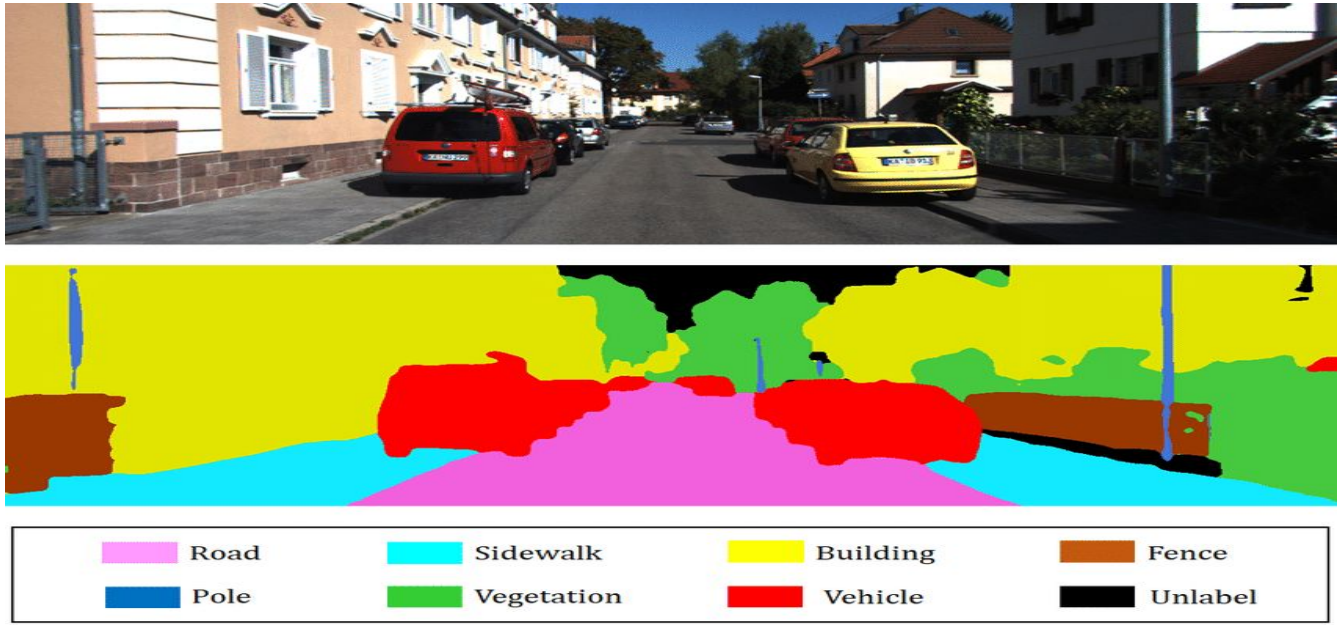


Convolutional Neural Network

- Distinguished from other neural networks by their superior performance with image, speech, or audio signal inputs
- Convolutional layers
  - Main building block
  - Layer where the majority of computation occurs
- pooling layers
  - conducts dimensionality reduction
- fully-connected layers
  - connect every input neuron to every output neuron

Semantic Segmentation

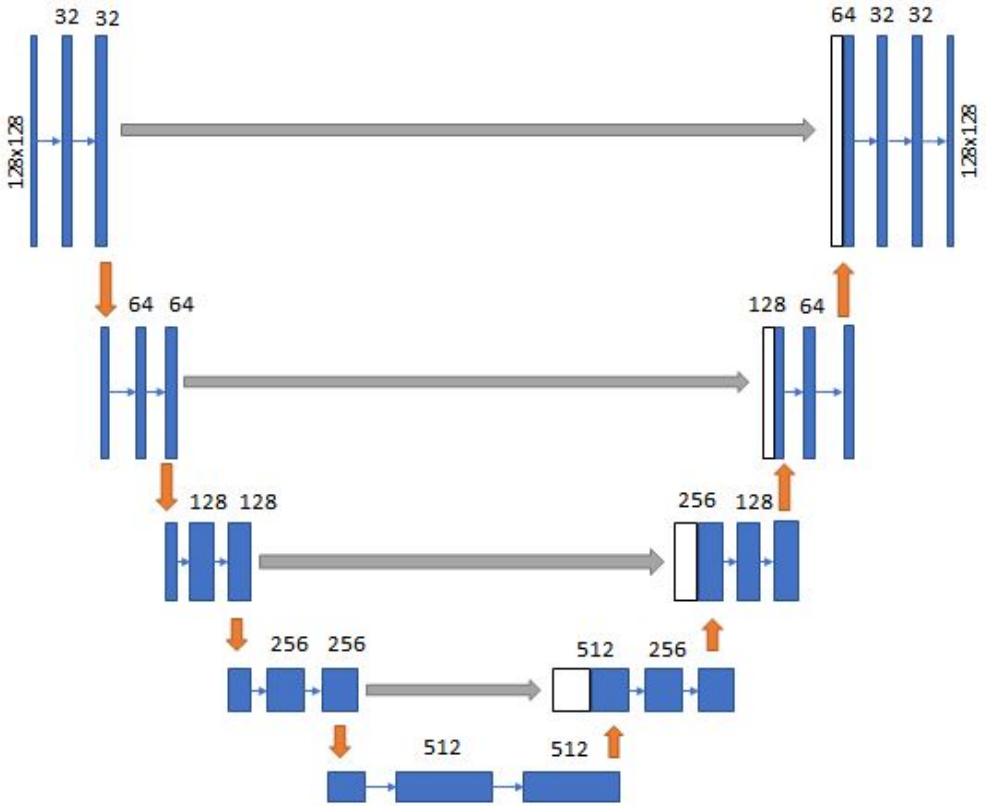
- an image segmentation method that assigns every single pixel in an image belonging to an object



Example of 2D semantic segmentation: (Top) input image (Bottom) prediction. | Download Scientific Diagram (researchgate.net)

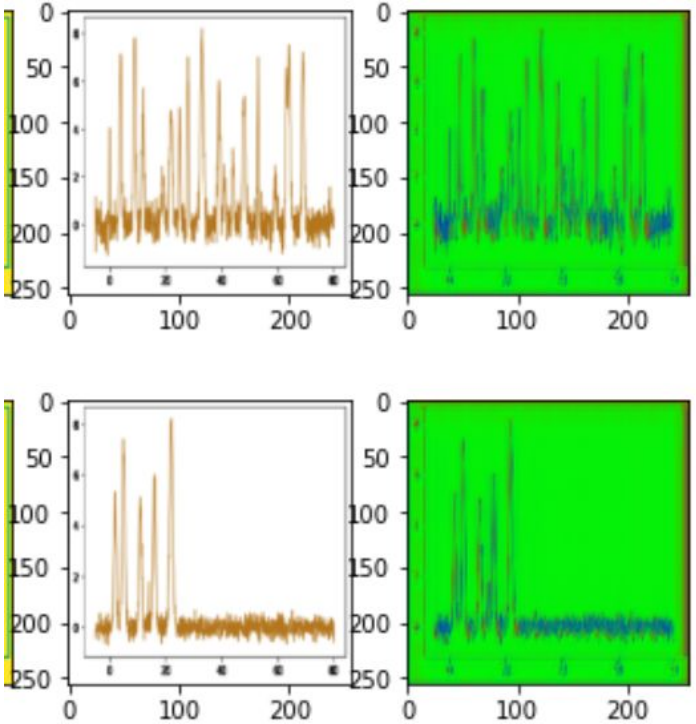
U-net

- Architecture for semantic segmentation
- Computationally efficient
- Trainable with a small data-set
- Trained end-to-end
- great for biomedical image segmentation



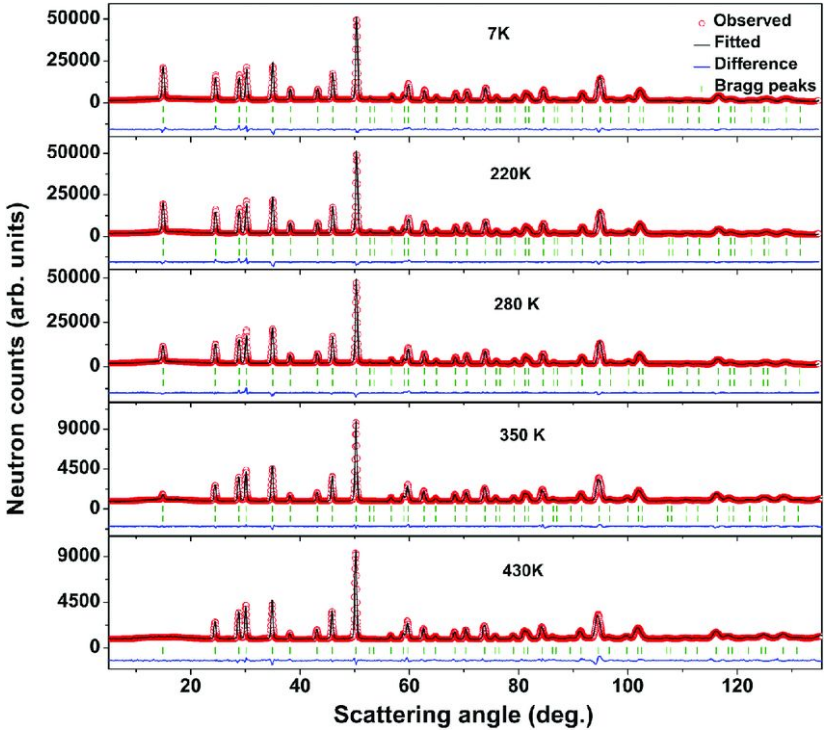
Conclusion

- U-net consistently works well with both simulated data and real data
- Predicts simulated data more accurately



Whats Next

- Use this model to determine which peaks have changed with temperature changes
- Output used to determine where an existing AI program will focus on for temperature measurements



Acknowledgements

- Dr. Ratcliff
- CHRNS
- Dr. Dura
- Dr. Borchers