Using AI to Classify Neutron Diffraction Patterns into Bravais Lattices

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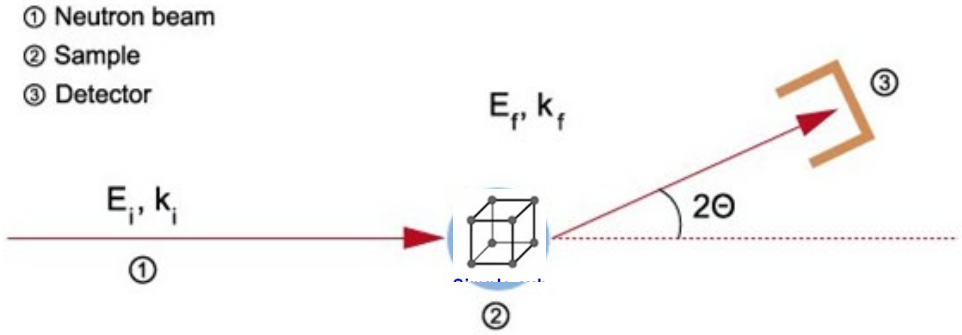
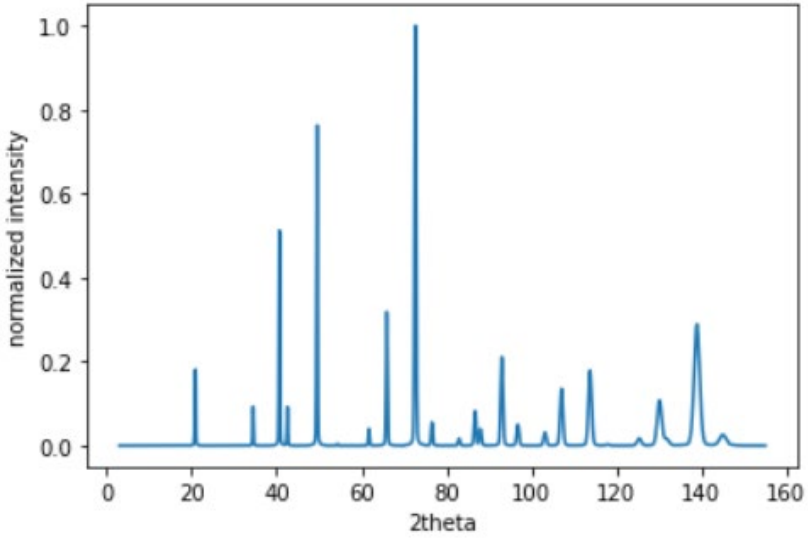
Neutron Diffraction

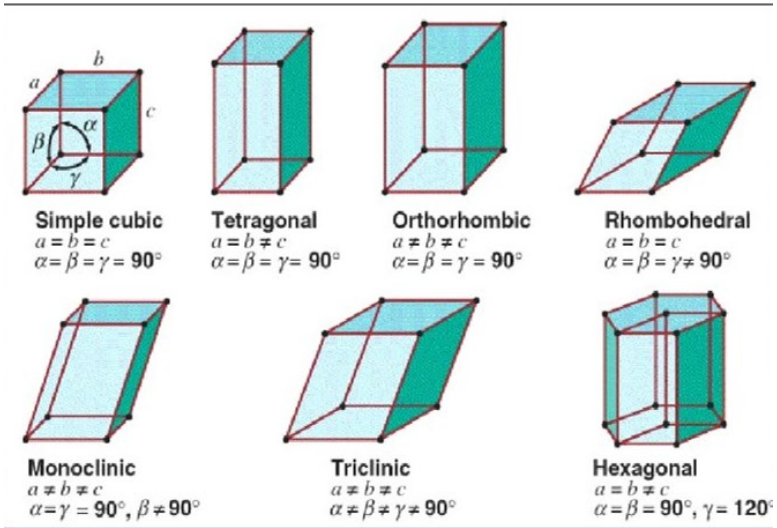
- Determine the atomic structure
- Use powder

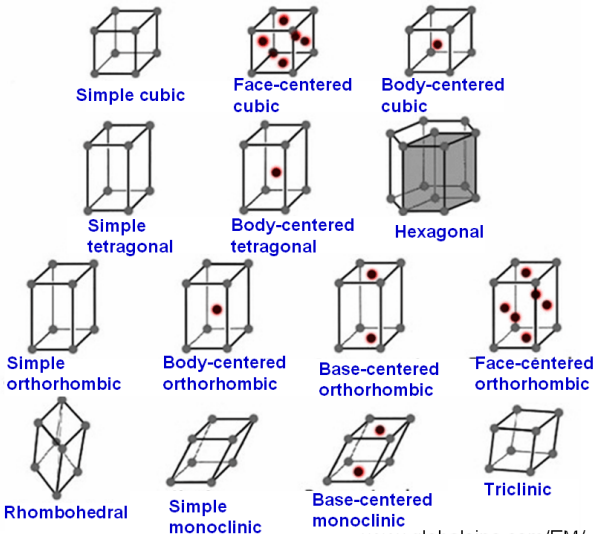




Bravais Lattices

- Build off the 7 crystal systems
- Includes where the crystal is centered





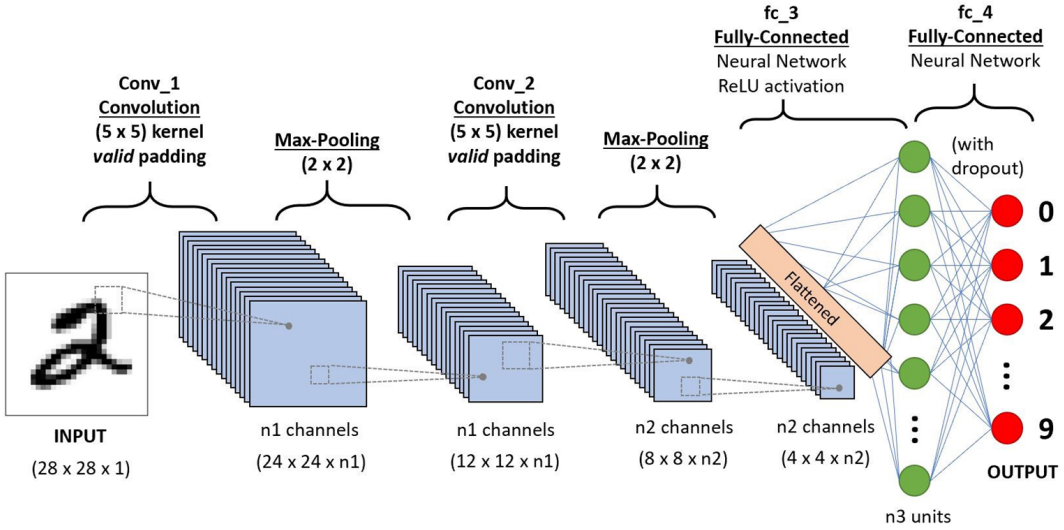
Purpose & Rationale

- Use AI to differentiate between Bravais Lattices
- First step to identifying the position of atoms from diffraction scans
- Automate expensive task

2 Methods

Convolutional Neural Network

- Most commonly used image classification algorithm
- Had 14 outputs



Convolutional Layers

- Apply filter to image
- Extract high level features
- Reduce dimensionality

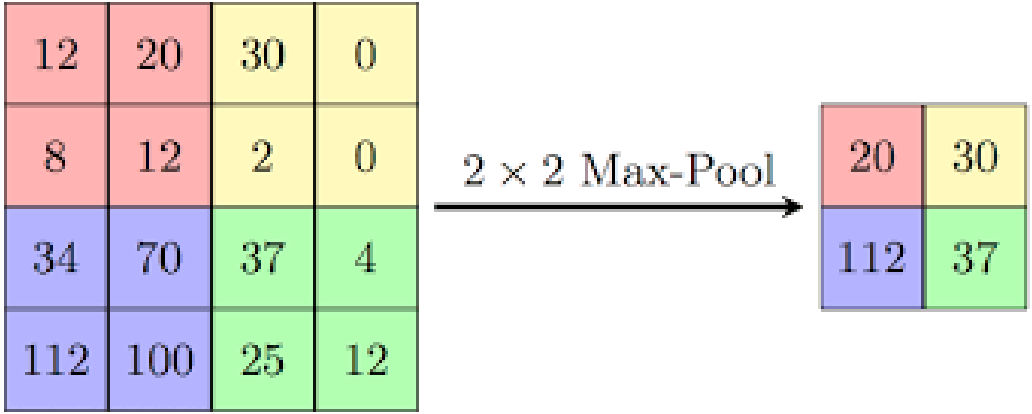
1x1	1x0	1x1	0	0
0x0	1x1	1x0	1	0
0x1	0x0	1x1	1	1
0	0	1	1	0
0	1	1	0	0

4		

Source: https://towardsdatascience.com/pytorch-basics-how-to-train-your-neural-net-intro-to-cnn-26a14c2ea29

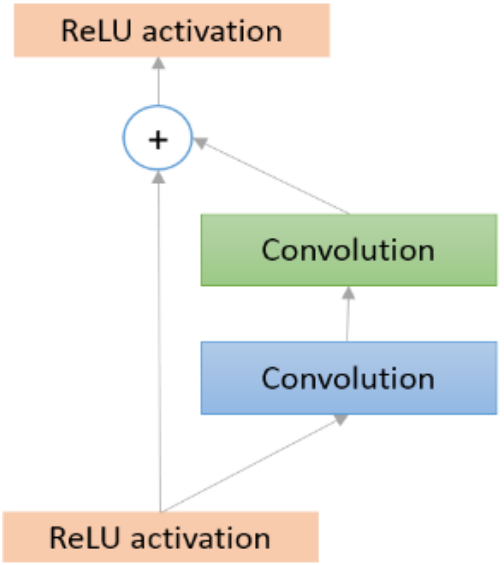
Max Pooling

- Further reduce dimensionality
- Reduce parameters→ reduce training time
- Summarizes features



Model Architecture

- LeNET
  - One of the most basic CNNs
  - Includes 6 layers
- ResNet-34
  - “Skip connections”

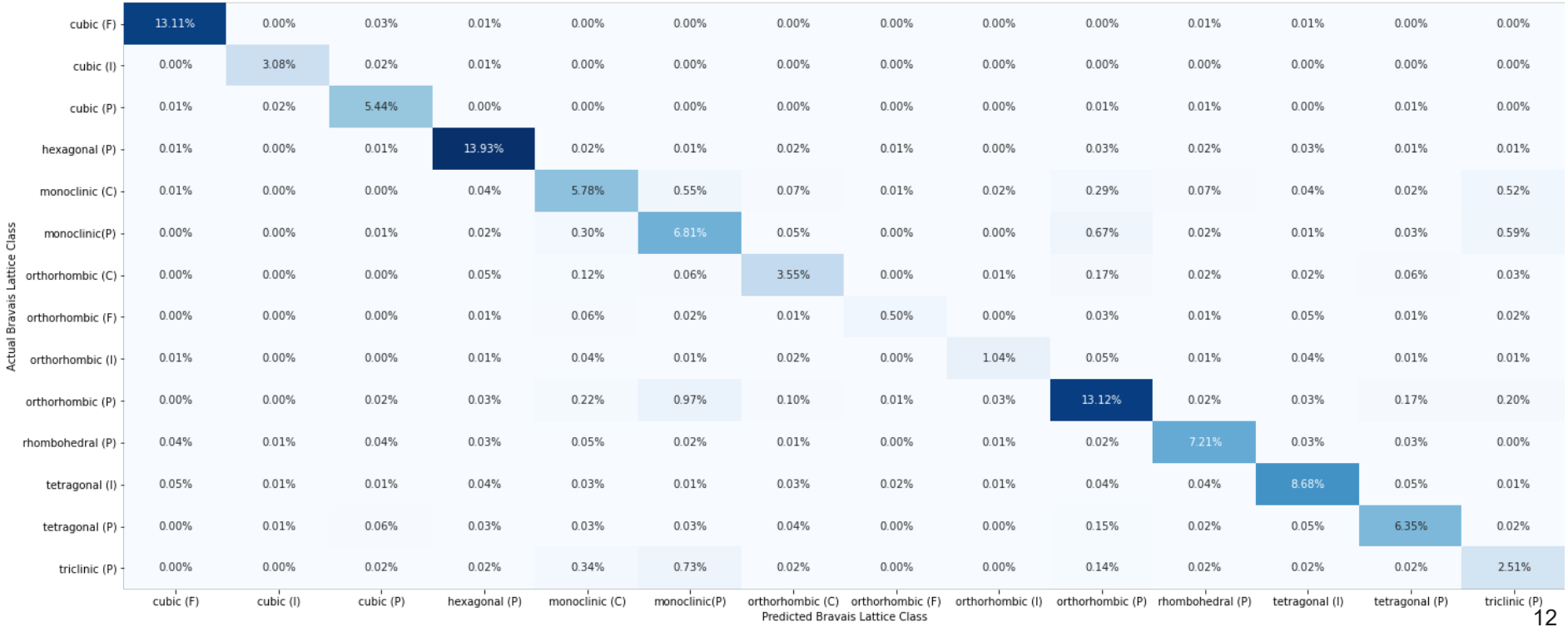


3 Results & Discussion

Results

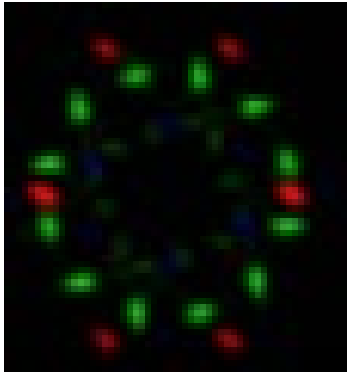
- Accuracy with LeNET: 80.5%
- Accuracy with ResNet: 87.6%

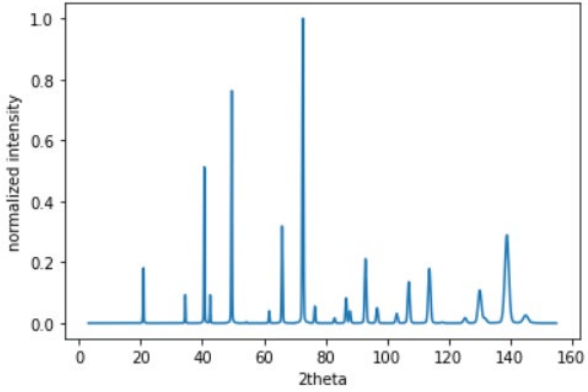
Confusion Matrix



Discussion

- Most studies use 2D networks
  - Obscures data and adds noise
- Highest accuracy with 2D model: 70%
- Highest accuracy with 1D model: 84%
  - Implemented on X-ray data



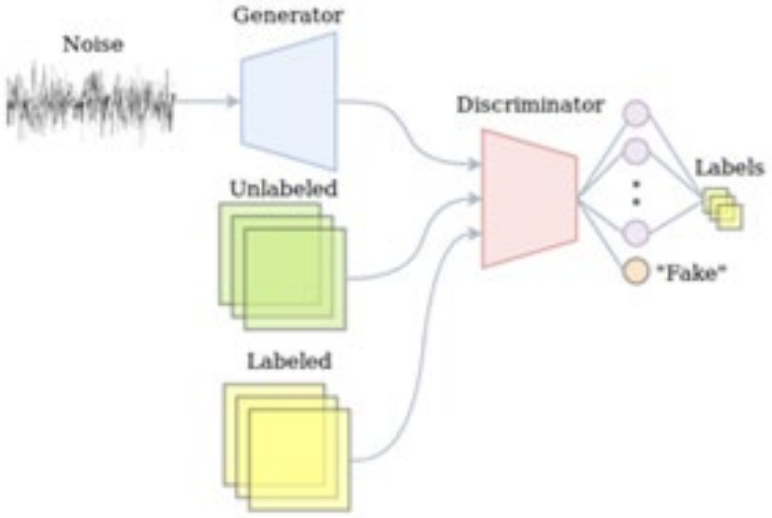


Conclusions

- 1D ResNet model is more accurate than current Bravais Lattice classifiers for neutron data
- Future work
  - More balanced dataset
  - Semi-supervised learning
    - Incorporate unlabeled data in training set

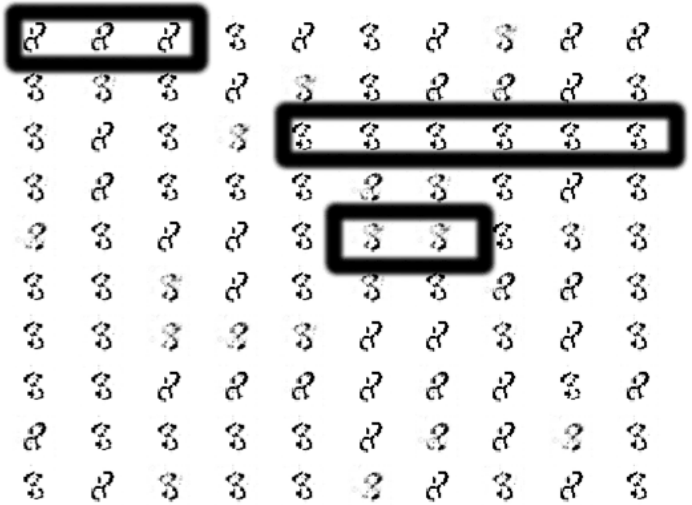
Semi-Supervised GAN

- Uses 2 models: Generator & Discriminator
- Zero sum game
- Labels = Bravais Lattice



Issues while training GANs

- Mode Collapse
  - Generator predicts the same images
  - Discriminator never learns
- Vanishing Gradients
  - Discriminator is too good
  - Generator stops learning



Acknowledgements

- Dr. William Ratcliff (NCNR)
- Dr. Gilad Kusne (MML)
- Dr. Austin McDannald (MML)
- Dr. June Lau (MML)
- Haotong Liang (UMD)

Thanks!

Any questions ?