

Using AI to Classify Neutron Diffraction Patterns into Bravais Lattices

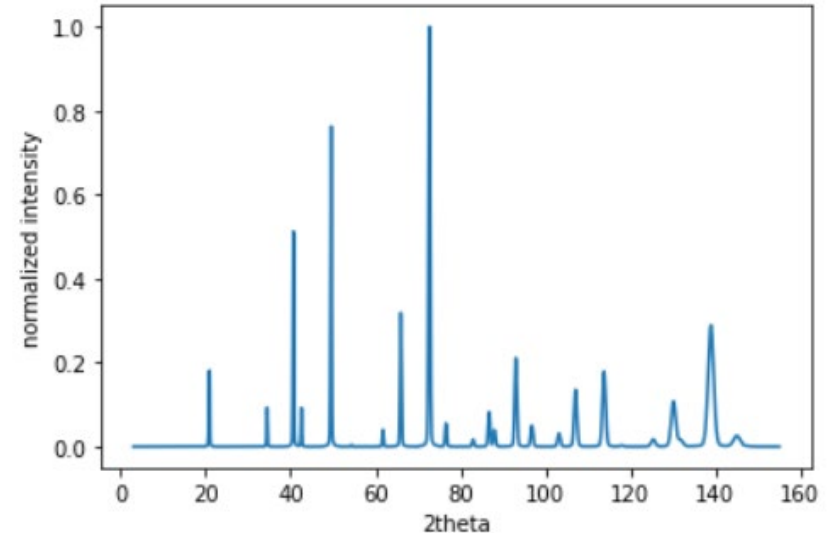
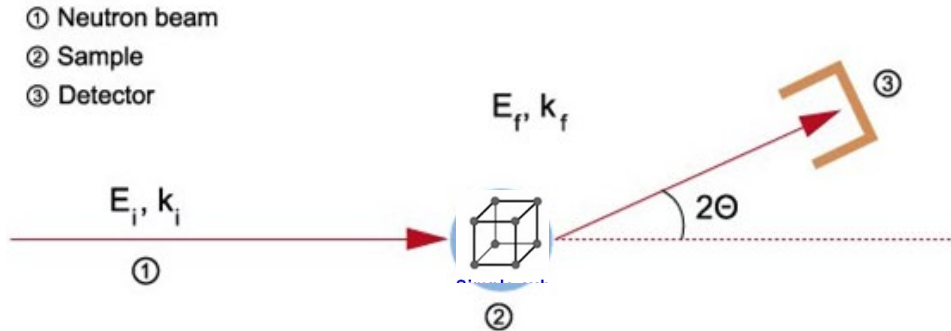
Satvik Lolla
Poolesville HS





Neutron Diffraction

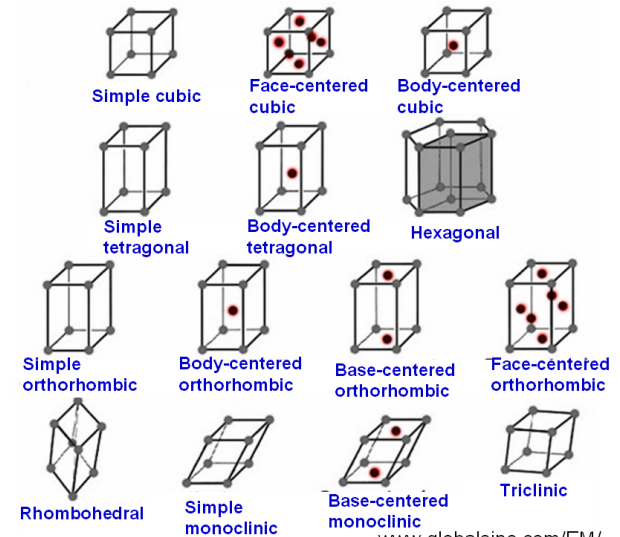
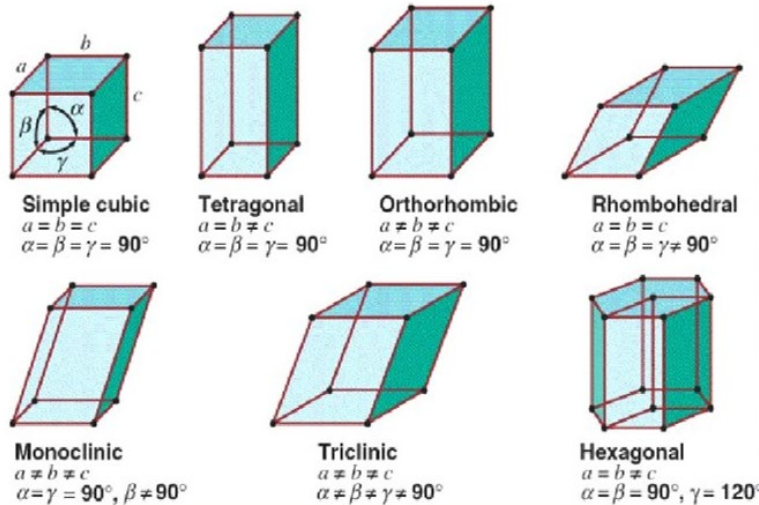
- Determine the atomic structure
- Use powder





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

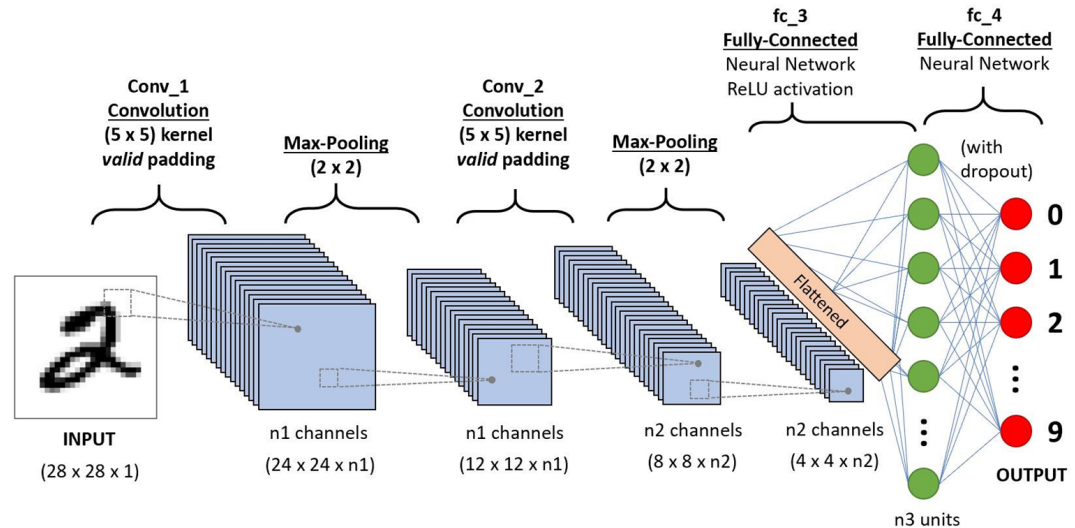
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Methods



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

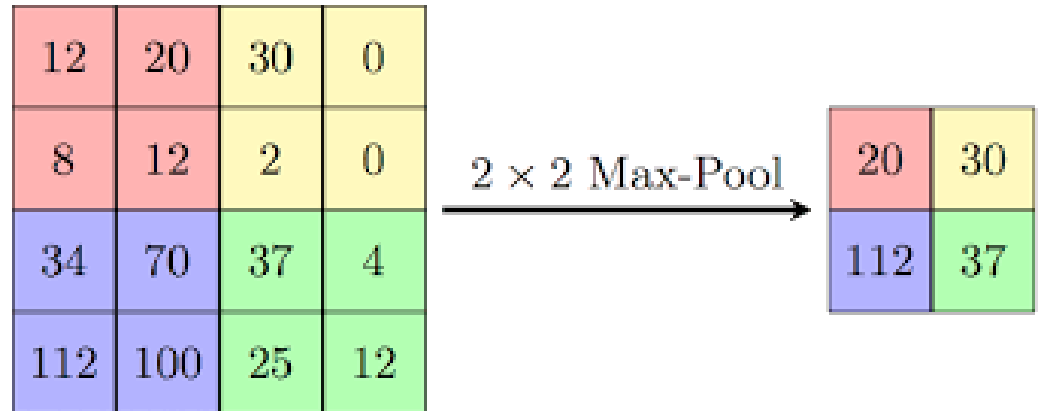
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Source: <https://towardsdatascience.com/pytorch-basics-how-to-train-your-neural-net-intro-to-cnn-26a14c2ea29>



Max Pooling

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





Model Architecture

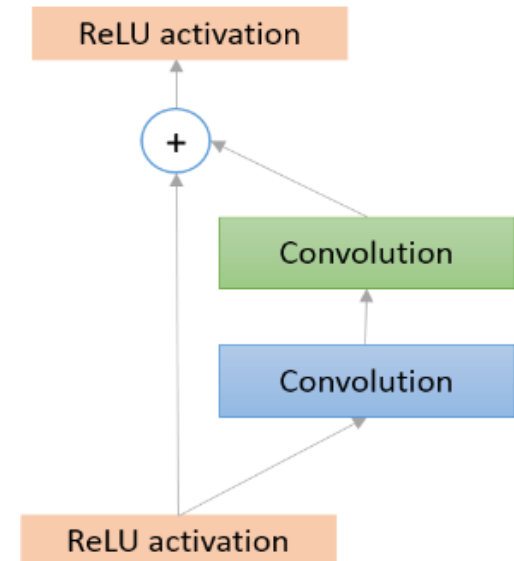


● LeNET

- One of the most basic CNNs
- Includes 6 layers

● ResNet 34

- “Skip connections”



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Results & Discussion



Results

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



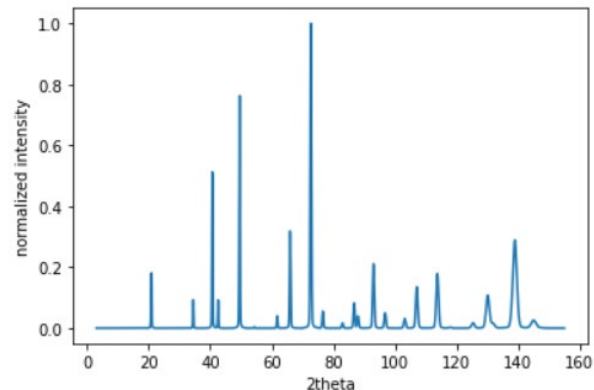
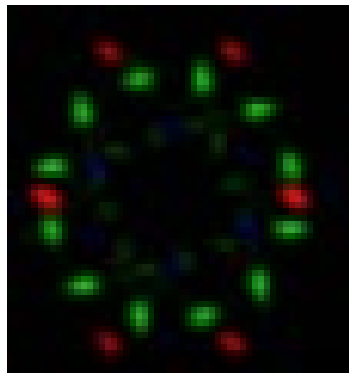
Confusion Matrix

Actual Bravais Lattice Class	cubic (F)	cubic (I)	cubic (P)	hexagonal (P)	monoclinic (C)	monoclinic (P)	orthorhombic (C)	orthorhombic (F)	orthorhombic (I)	orthorhombic (P)	rhombohedral (P)	tetragonal (I)	tetragonal (P)	triclinic (P)
cubic (F)	13.11%	0.00%	0.03%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.01%	0.01%	0.00%	0.00%
cubic (I)	0.00%	3.08%	0.02%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
cubic (P)	0.01%	0.02%	5.44%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.01%	0.01%	0.00%	0.01%	0.00%
hexagonal (P)	0.01%	0.00%	0.01%	13.93%	0.02%	0.01%	0.02%	0.01%	0.00%	0.03%	0.02%	0.03%	0.01%	0.01%
monoclinic (C)	0.01%	0.00%	0.00%	0.04%	5.78%	0.55%	0.07%	0.01%	0.02%	0.29%	0.07%	0.04%	0.02%	0.52%
monoclinic (P)	0.00%	0.00%	0.01%	0.02%	0.30%	6.81%	0.05%	0.00%	0.00%	0.67%	0.02%	0.01%	0.03%	0.59%
orthorhombic (C)	0.00%	0.00%	0.00%	0.05%	0.12%	0.06%	3.55%	0.00%	0.01%	0.17%	0.02%	0.02%	0.06%	0.03%
orthorhombic (F)	0.00%	0.00%	0.00%	0.01%	0.06%	0.02%	0.01%	0.50%	0.00%	0.03%	0.01%	0.05%	0.01%	0.02%
orthorhombic (I)	0.01%	0.00%	0.00%	0.01%	0.04%	0.01%	0.02%	0.00%	1.04%	0.05%	0.01%	0.04%	0.01%	0.01%
orthorhombic (P)	0.00%	0.00%	0.02%	0.03%	0.22%	0.97%	0.10%	0.01%	0.03%	13.12%	0.02%	0.03%	0.17%	0.20%
rhombohedral (P)	0.04%	0.01%	0.04%	0.03%	0.05%	0.02%	0.01%	0.00%	0.01%	0.02%	7.21%	0.03%	0.03%	0.00%
tetragonal (I)	0.05%	0.01%	0.01%	0.04%	0.03%	0.01%	0.03%	0.02%	0.01%	0.04%	0.04%	8.68%	0.05%	0.01%
tetragonal (P)	0.00%	0.01%	0.06%	0.03%	0.03%	0.03%	0.04%	0.00%	0.00%	0.15%	0.02%	0.05%	6.35%	0.02%
triclinic (P)	0.00%	0.00%	0.02%	0.02%	0.34%	0.73%	0.02%	0.00%	0.00%	0.14%	0.02%	0.02%	0.02%	2.51%



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





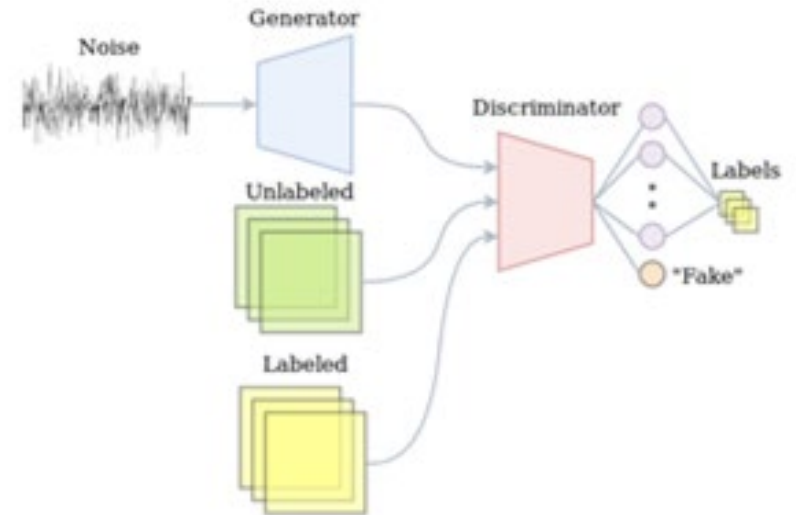
Conclusions

- ◎ 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





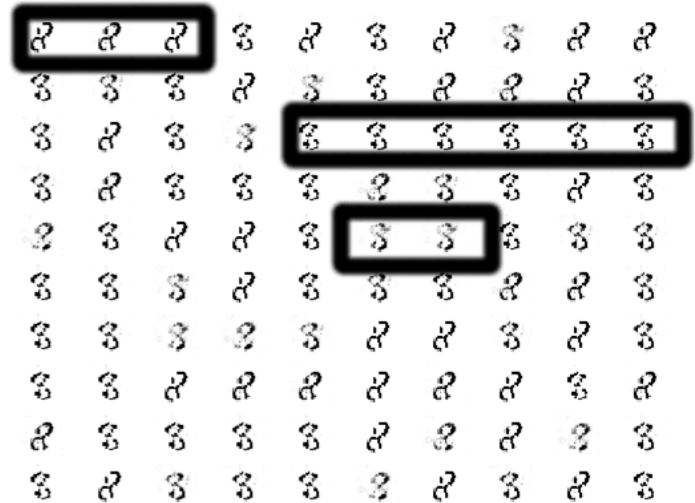
Issues while training GANs

● Mode Collapse

- Generator predicts the same images
- Discriminator never learns

● Vanishing Gradients

- Discriminator is too good
- Generator stops learning





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Thanks!

Any questions ?