# SASNets: Classifying Small Angle Scattering Data Using Convolutional Neural Networks

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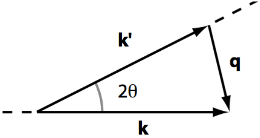
# Outline

# Introduction to SANS

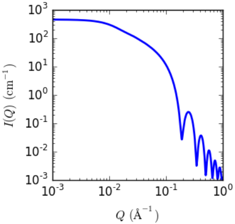
- Probes matter structure with neutrons
- Uses neutron's special properties
- Model → Scattered pattern not invertible




$$\sin\theta = \frac{|\mathbf{q}|}{2}\frac{1}{|\mathbf{k}|}$$

$$q = 2k\sin\theta = \frac{4\pi}{\lambda}\sin\theta$$

(a) Q vectors[1].



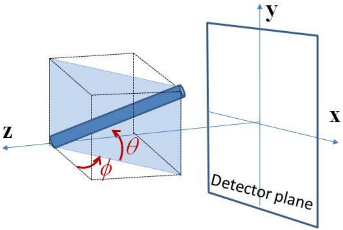

(b) Example SANS result[2].

[2] A. J. Jackson, Introduction to small-angle neutron scattering and neutron reflectometry. 2008.

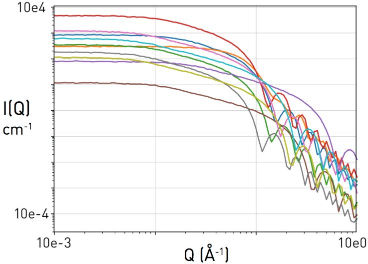
[2] SASView Documentation.

# SANS Data

- 1D pattern is integral over all $\theta$ and $\phi$



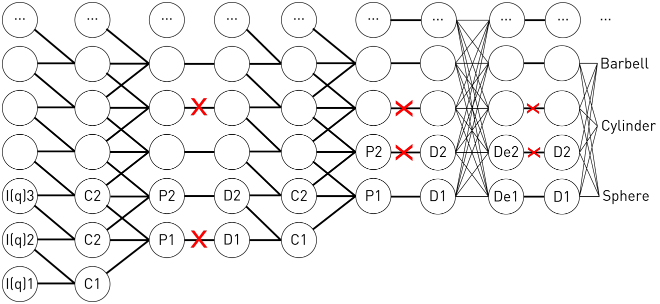

(a) Detector setup.




(b) 10 random cylinder models.

# Introduction to Convolutional Neural Networks

- Network of nodes (axons) and connections (synapses).
- Convolutional operation on input → spatial invariance.



# CNN Example

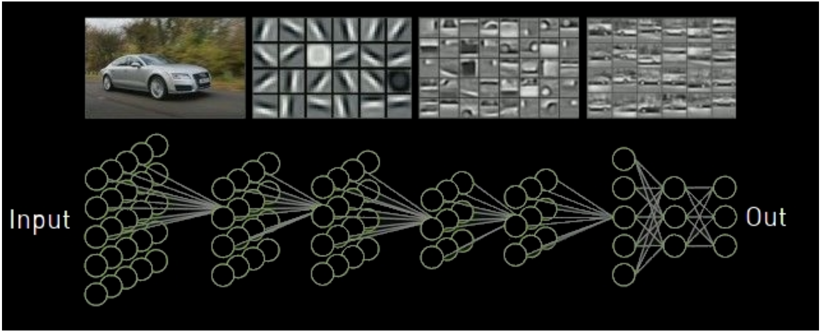
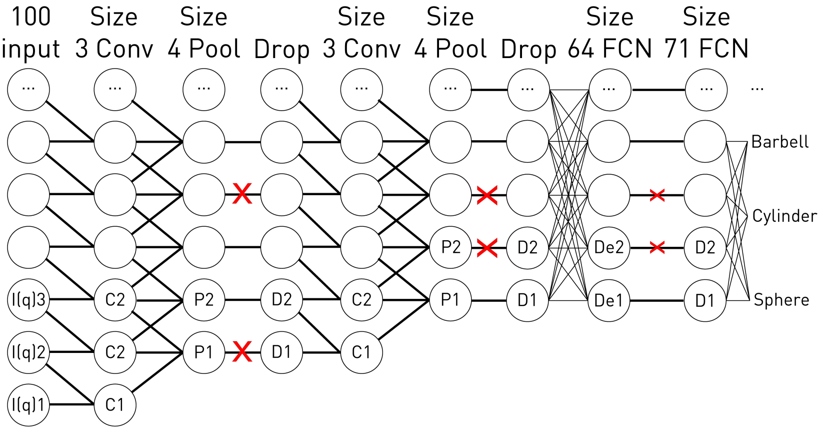
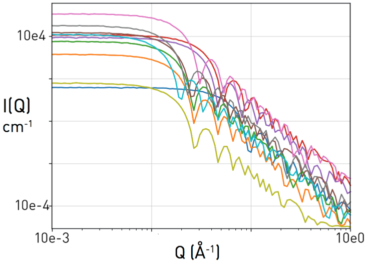



Figure 3: A CNN with features shown.

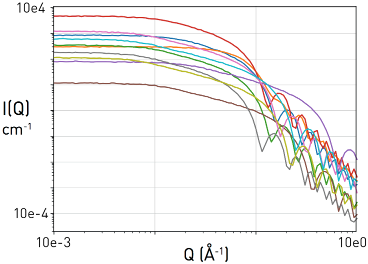
# CNN Design


100 input
Size 3 Conv
Size 4 Pool
Drop
Size 3 Conv
Size 4 Pool
Drop
Size 64 FCN
Size 71 FCN
...
I(q)3
I(q)2
I(q)1
C2
C2
C1
P2
P1
D2
D1
C2
C1
P2
P1
D2
D1
De2
De1
D2
D1
Barbell
Cylinder
Sphere

# Classification Task




(a) 10 random sphere models.




(b) 10 random cylinder models.

# Implementation

- Implemented random data generation, model training, & model analysis
- Python 2.7, Tensorflow, Keras

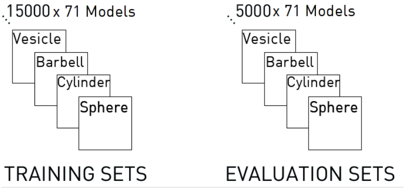



Figure 5: Data used in network.

# Classification Results

- 54.9% validation accuracy on the 71 model set
- Ran for 34 epochs, 2 hours and 30 minutes
- Adam optimizer[3] using multinominal logistic regression[4]

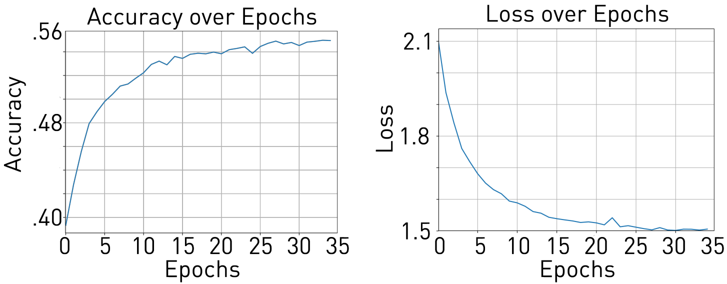
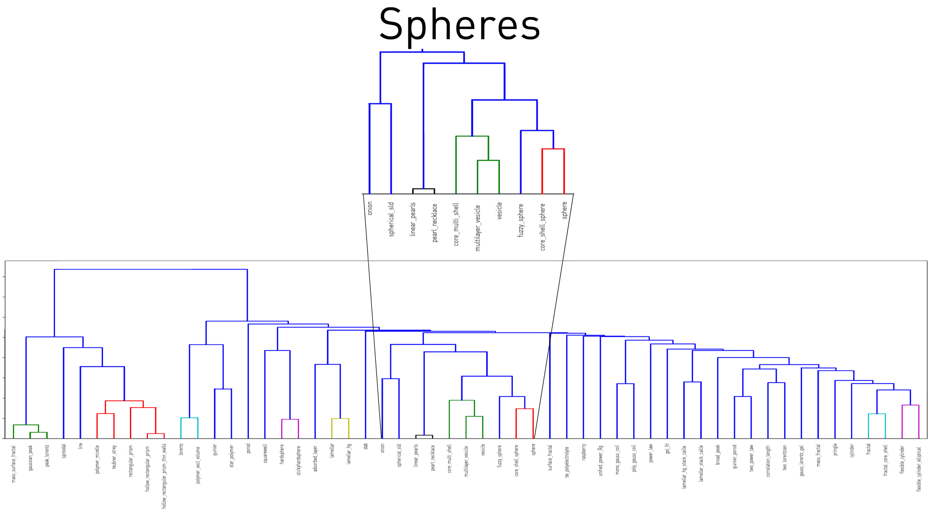



Figure 6: Accuracy and Validation graphs

[3] Kingma and J.Ba, "Adam: A method for stochastic optimization," arXiv preprint.
[4] S. Menard, Applied logistic regression analysis, vol. 106. Sage, 2002.

# Classification Results



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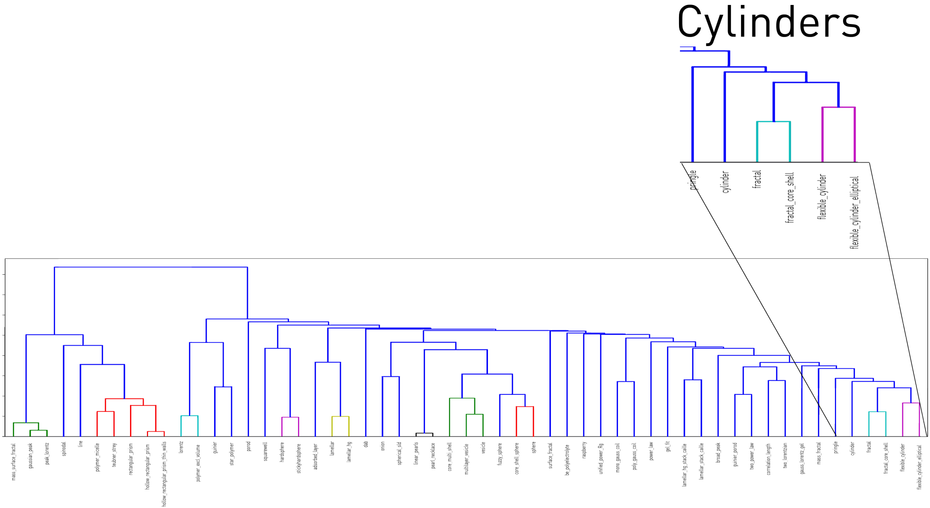

# Conclusion & Next Steps

- Demonstrate CNN can make significant progress on model classification problem
- Implemented network capable of 54.9% accuracy on 71 model set
- Found that network finds groups of models from raw data
- Current data unrealistic, expand model to real data ranges

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- NCNR SHIP Directors
- NSF

# Questions

Any Questions? Thanks for listening!
More information can be found at `sasnets.readthedocs.io`.