

SASNets: Classifying Small Angle Scattering Data Using Convolutional Neural Networks

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Outline

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Results

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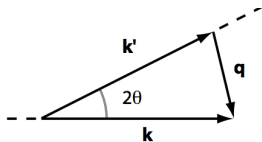
Conclusion

End Matter

End Matter

Introduction to SANS

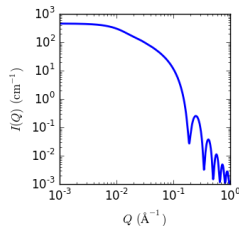
- ▶ Probes matter structure with neutrons
- ▶ Uses neutron's special properties
- ▶ Model → Scattered pattern not invertible



(a) Q vectors¹.

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

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



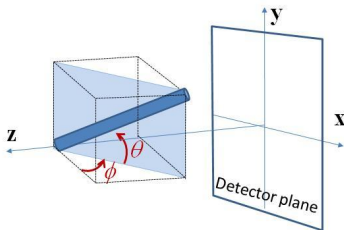
(b) Example SANS result².

¹A. J. Jackson, Introduction to small-angle neutron scattering and neutron reflectometry. 2008.

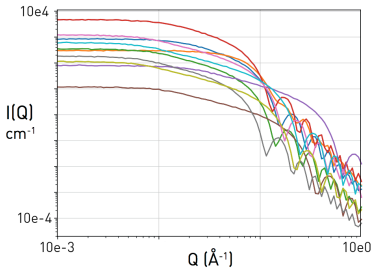
²SASView Documentation.

SANS Data

- 1D pattern is integral over all θ and ϕ



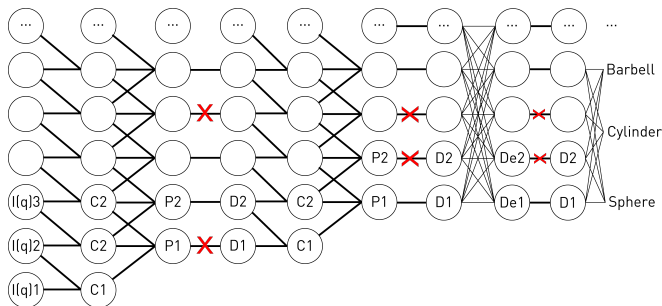
(a) Detector setup.



(b) 10 random cylinder models.

Introduction to Convolutional Neural Networks

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



CNN Example

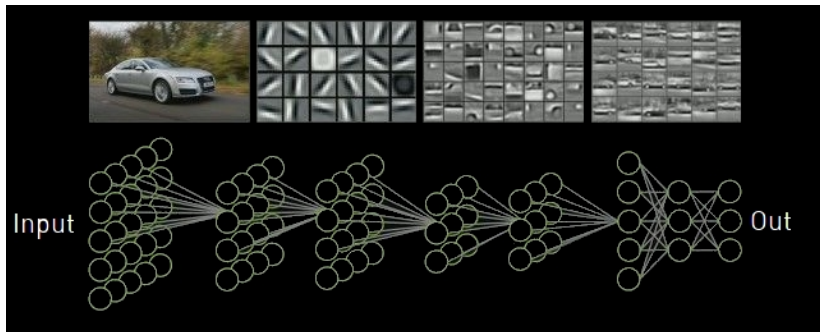
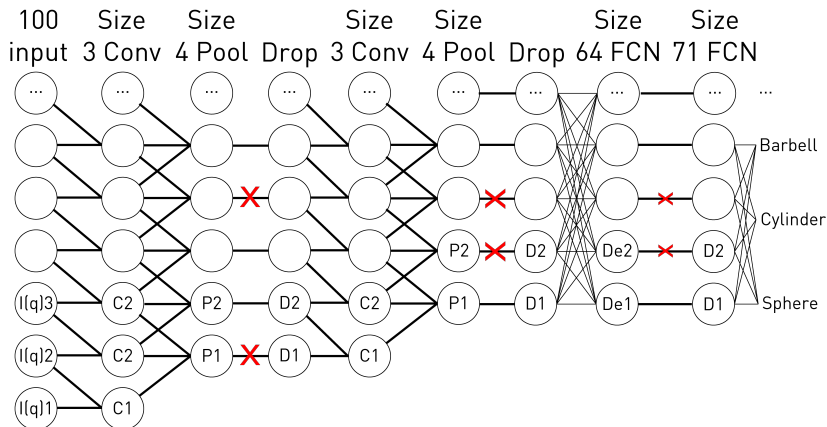
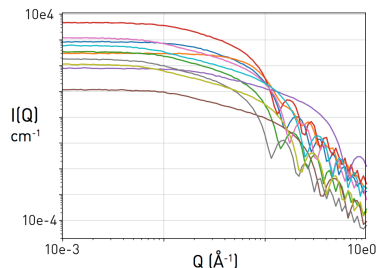
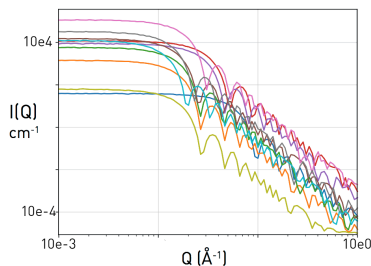


Figure 3: A CNN with features shown.

CNN Design



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

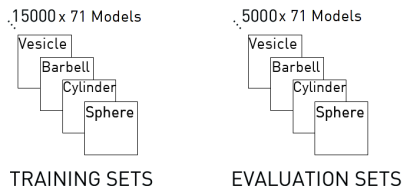


Figure 5: Data used in network.

Classification Results

- ▶ 54.9% validation accuracy on the 71 model set
- ▶ Ran for 34 epochs, 2 hours and 30 minutes
- ▶ Adam optimizer³ using multinomial logistic regression⁴

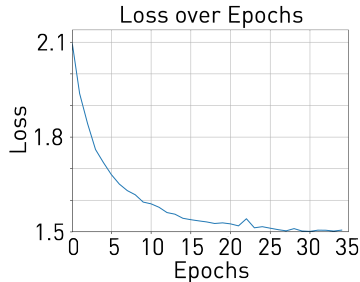
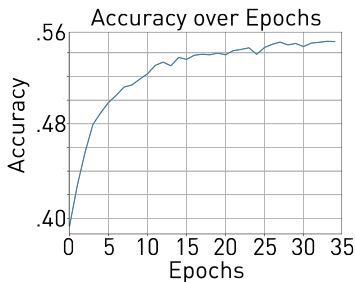
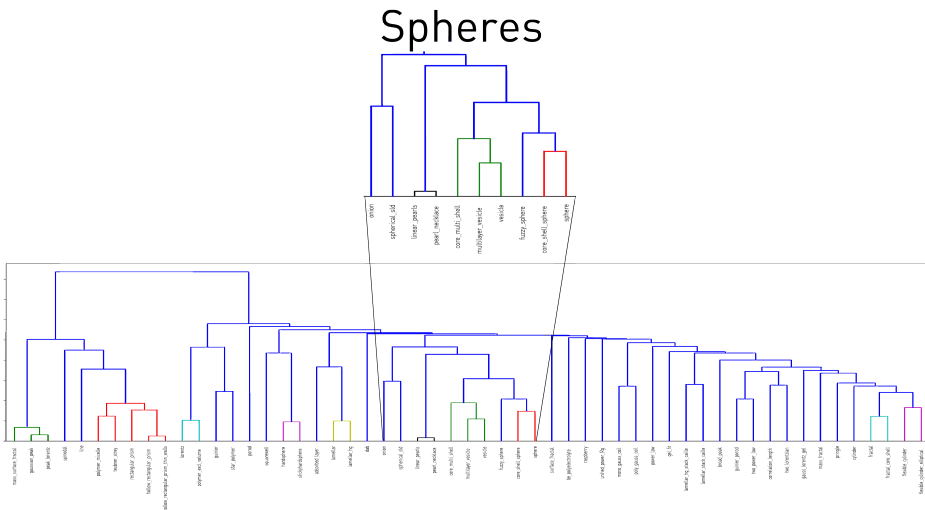


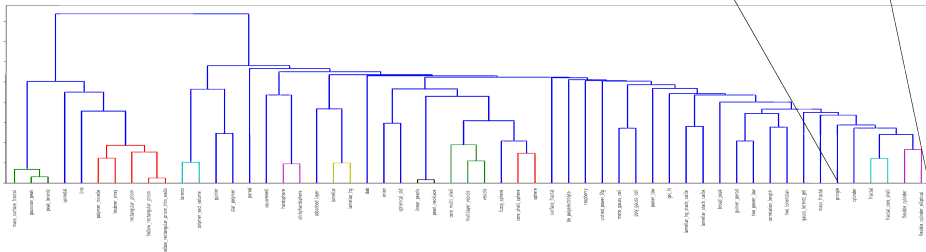
Figure 6: Accuracy and Validation graphs

³Kingma and J.Ba, "Adam: A method for stochastic optimization," arXiv preprint.

⁴S. Menard, Applied logistic regression analysis, vol. 106. Sage, 2002.



Cylinders



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

Acknowledgements

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Questions

Any Questions? Thanks for listening!

More information can be found at sasnets.readthedocs.io.