SASNets: Classifying Small Angle Scattering Data Using Convolutional Neural Networks

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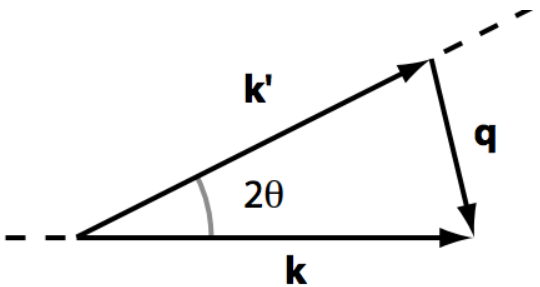
July 31, 2017

Outline

Introduction to SANS

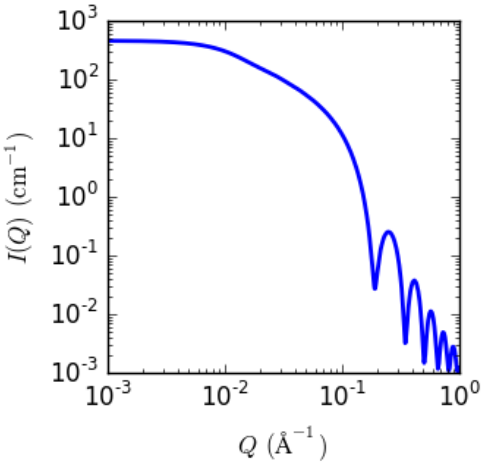
- Probes matter structure with neutrons
- Uses neutron's special properties



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

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

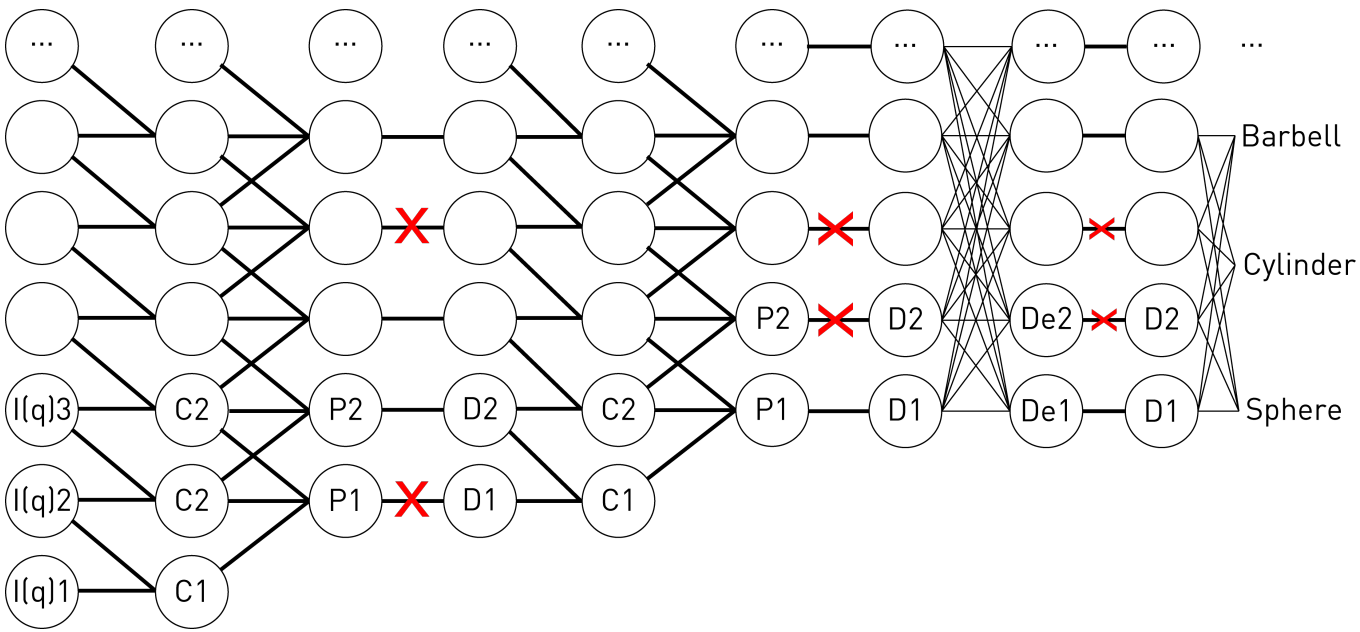
(a) Q vectors[1].



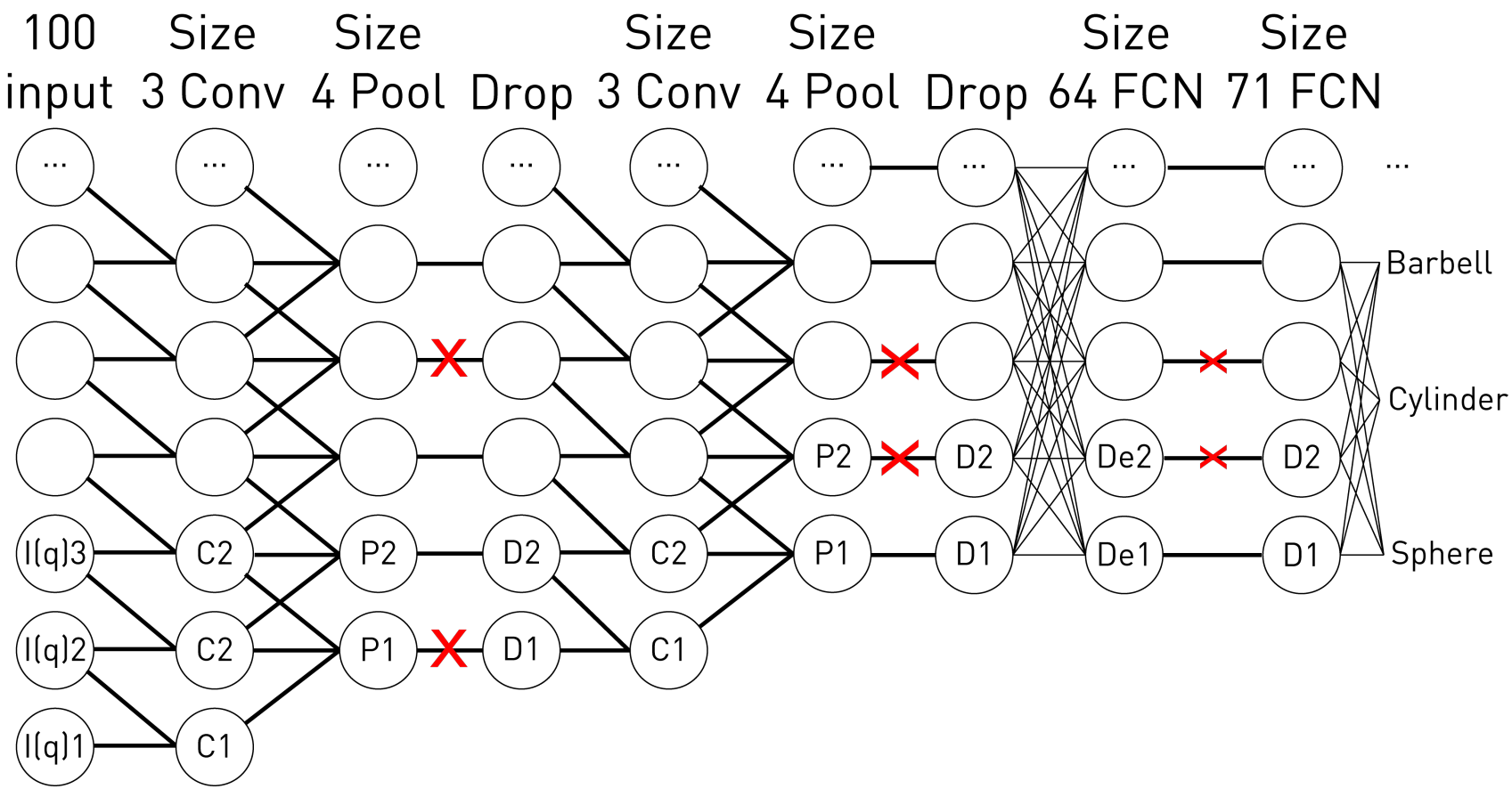
(b) Example SANS result[2].

Introduction to Convolutional Neural Networks

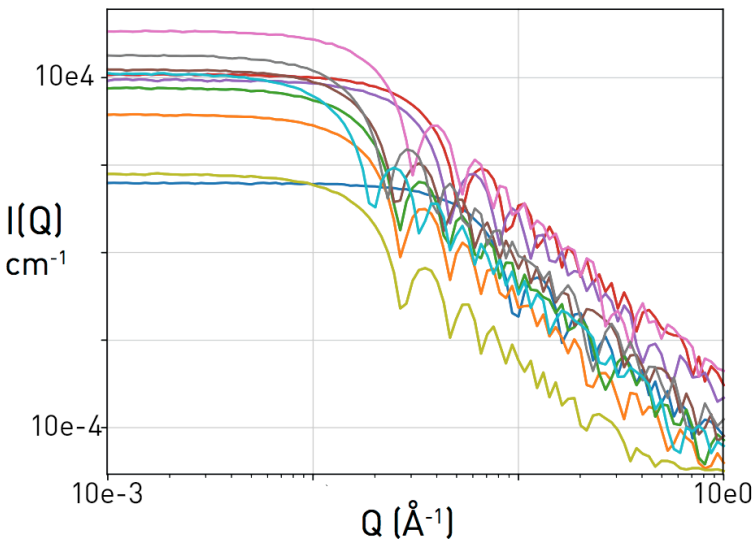
- Network of nodes (axons) and connections (synapses).
- Convolutional operation on input → spatial invariance.



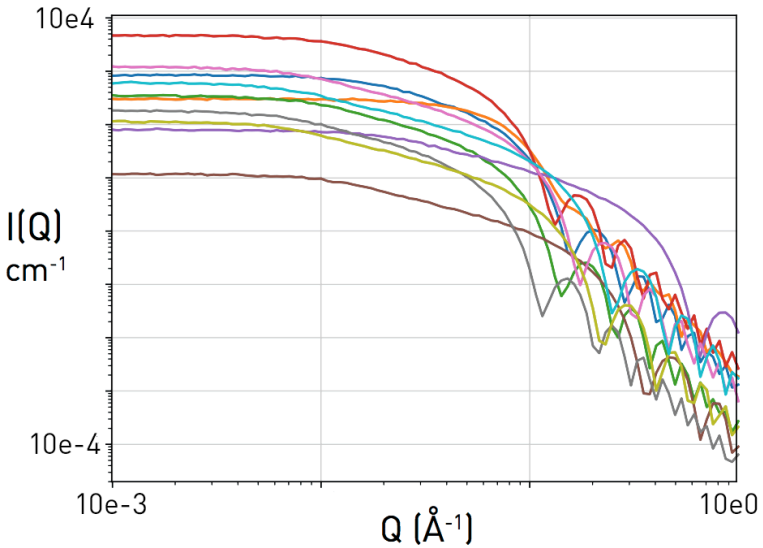
CNN Design


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



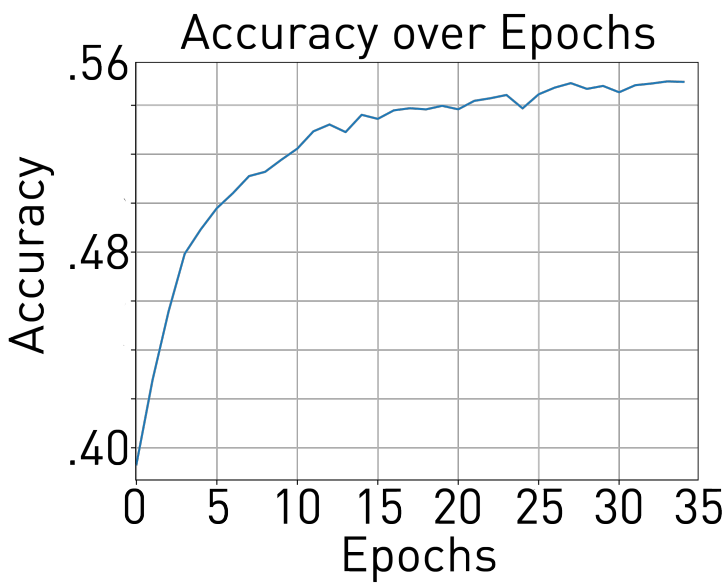
(a) 10 random sphere models.

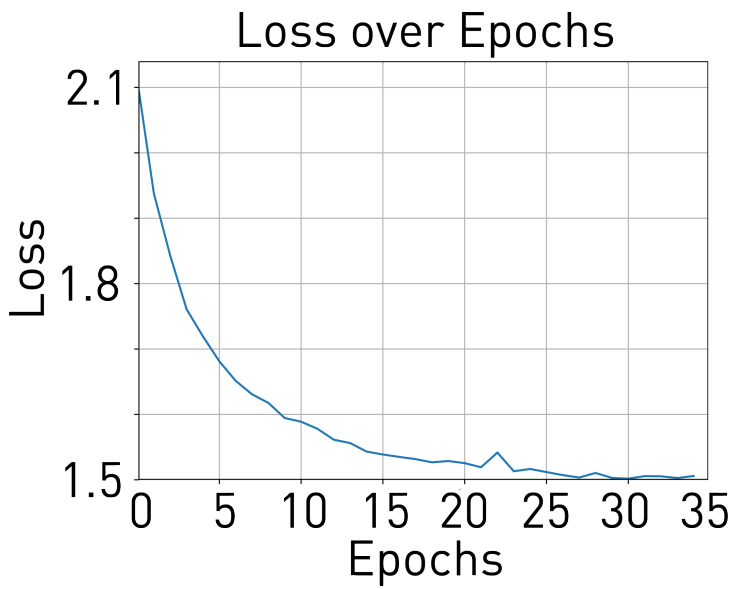


(b) 10 random cylinder models.

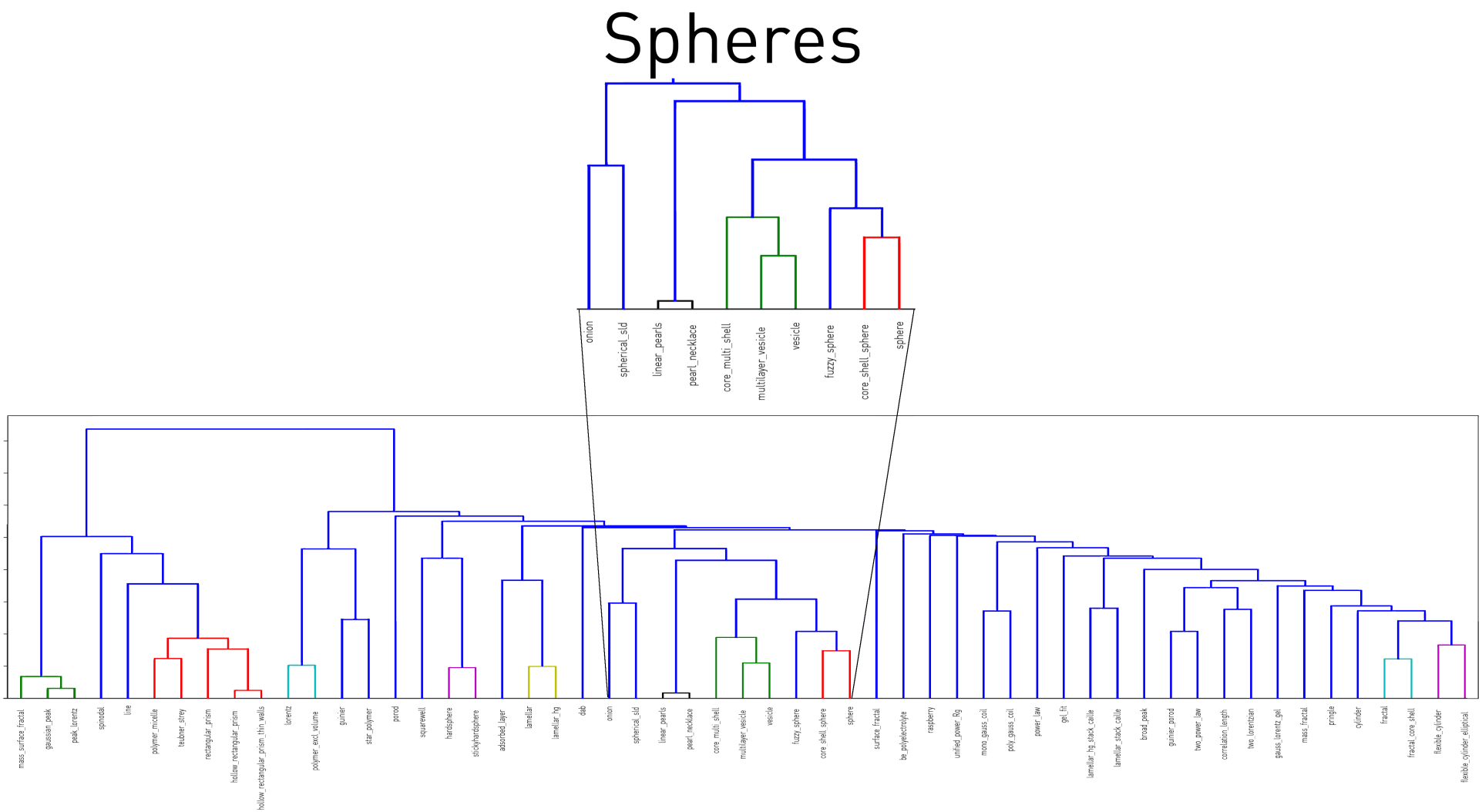
Classification Results

- 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]

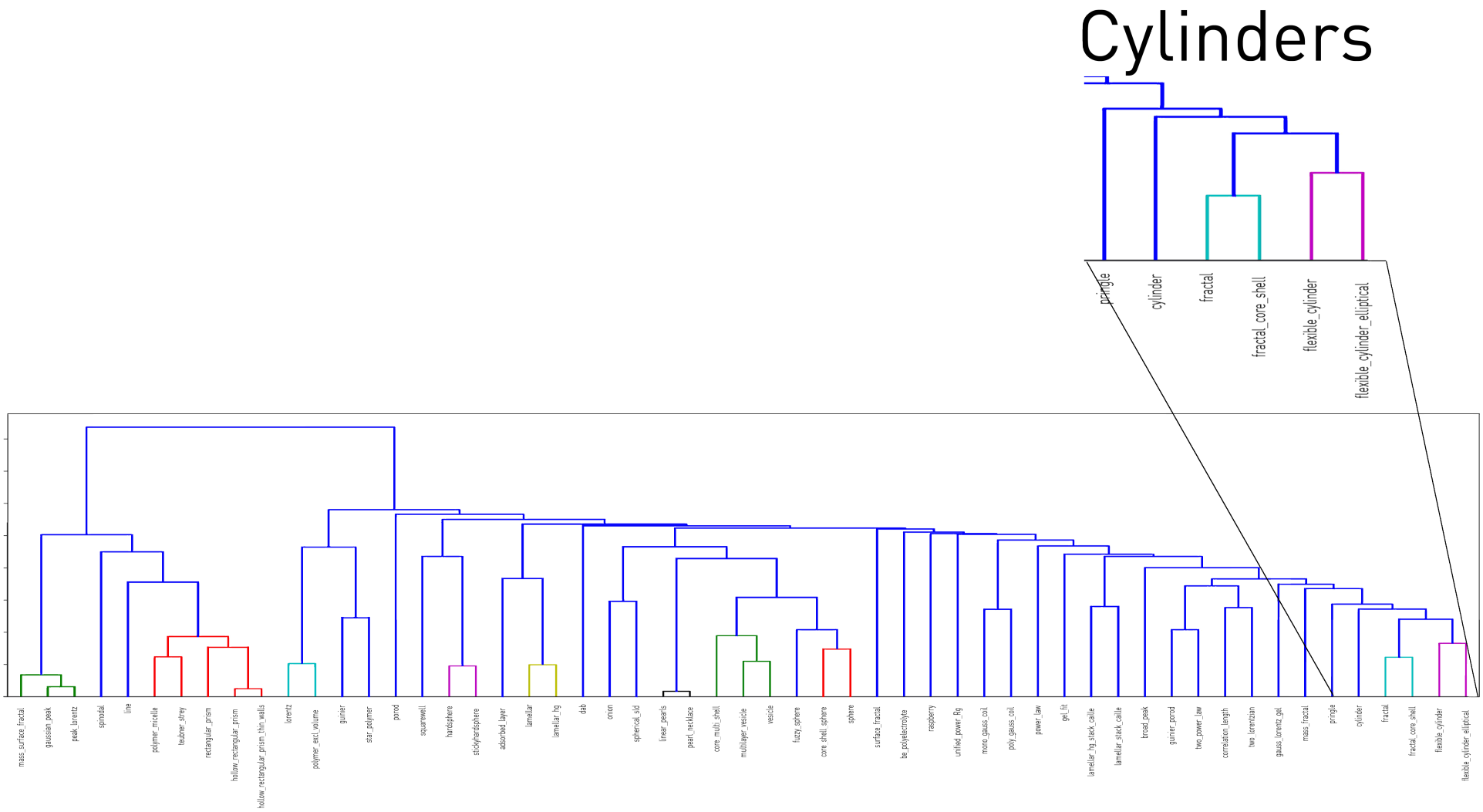




Classification Results



Classification Results



Conclusion & Next Steps

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

References I

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

[2] SASView, "Sasview," 2017.

[3] D. Kingma and J. Ba, "Adam: A method for stochastic optimization," arXiv preprint arXiv:1412.6980, 2014.

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

Acknowledgements

- NIST Centre for Neutron Research and the Centre for High Resolution Neutron Scattering, for funding and material support.
- The SANS Subproject of NSF-funded DANSE DMR-0520547, for SASView and SASModels.
- The many colleagues, for providing data, advice, and material throughout the project.

Questions

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