SASNets: Classifying Small Angle Scattering Data Using Convolutional Neural Networks

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Outline

Introduction
  Introduction to SANS
  Introduction to CNNs

Experimental Setup
  Network Design
  Classification Task

Results
  Results

Conclusion
  Conclusion

End Matter
  End Matter
Introduction to SANS

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

(a) $Q$ vectors\(^1\).

\[
\sin \theta = \frac{|q|}{2|k|} \\
q = 2k \sin \theta = \frac{4\pi}{\lambda} \sin \theta
\]

(b) Example SANS result\(^2\).

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\(^1\) 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 $\rightarrow$ spatial invariance.
CNN Example

Figure 3: A CNN with features shown.
CNN Design

100 input Size 4 Pool Drop Size 4 Pool Drop Size 64 FCN 71 FCN

C2 P2 D2 C2 P1 D1 De2 D2
C2 P1 D1 C1

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

![Diagram of training and evaluation sets with various models]

**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\(^4\)

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**Figure 6:** Accuracy and Validation graphs


Classification Results

Spheres
Classification Results

Cylinders

[Diagram showing classification results with various categories and subcategories, including 'Cylinders', 'Fractal', and 'Flexible cylinder'.]
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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Questions

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