Deep Learning Methods On Neutron Scattering Data

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Summary

Apply machine learning to scientific data

Convolutional Neuron Network – tools and methods

Results and perspectives

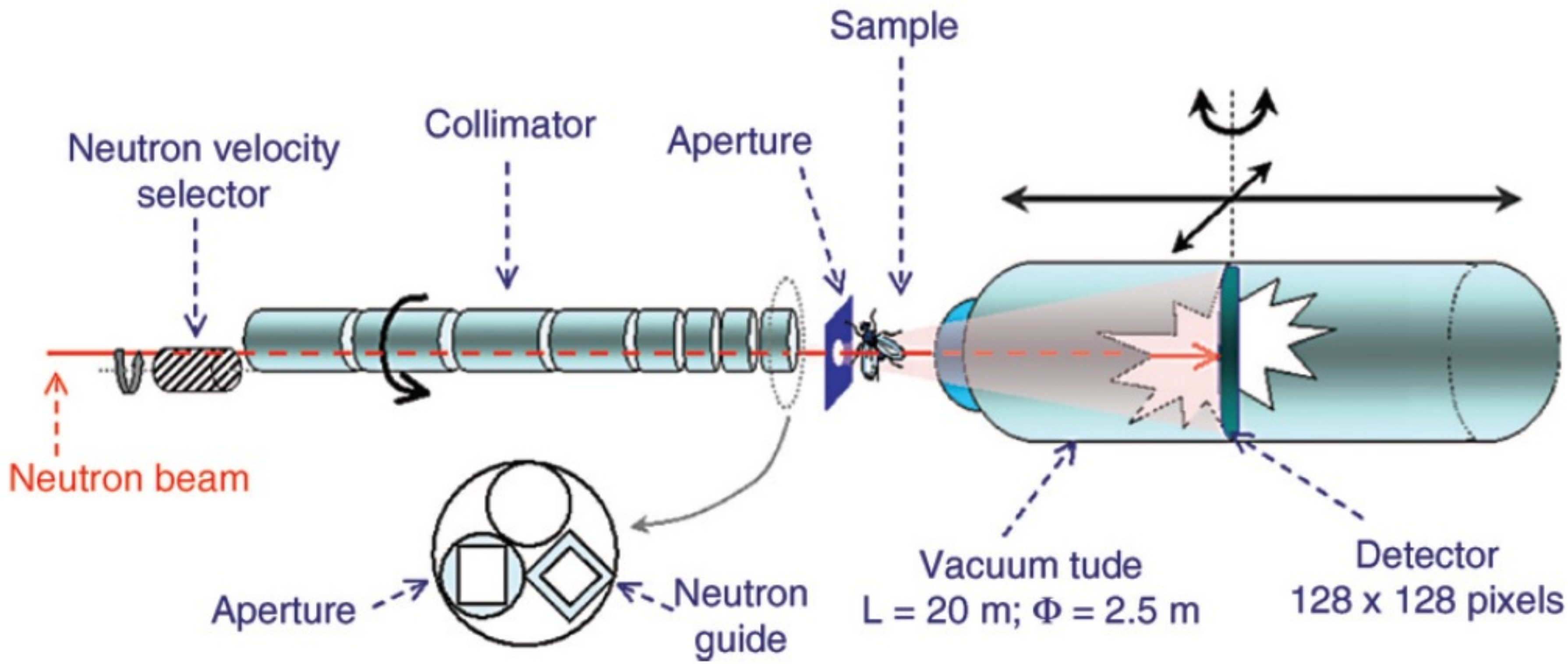
Use Case: Small Angle Neutron Scattering

The Swiss knife of material science: can deliver information on hard and soft matter, from crystals to biological structures

Long setup time but short measurements

Large demand and big variety of users' experience

Schematic Of A SANS Instrument



A Multi-Parameter Space

Instrument parameters
- Detector
- Collimation
- Wavelength

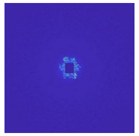
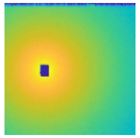
Sample parameters
- Geometry
- Distance
- Organization

Environment parameters
- Temperature
- Magnetic Field
- Pressure
- Angle
- …

Early prediction of material's structure will help optimizing instrument's parameters and increasing beam time productivity

The Project's Workflow

Early experimental scattering image

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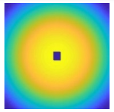
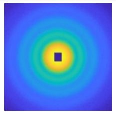
Trained classifier

Recognized structure model (i.e. sphere, cylinder, Bragg glass etc.)

Required scattering image type



or



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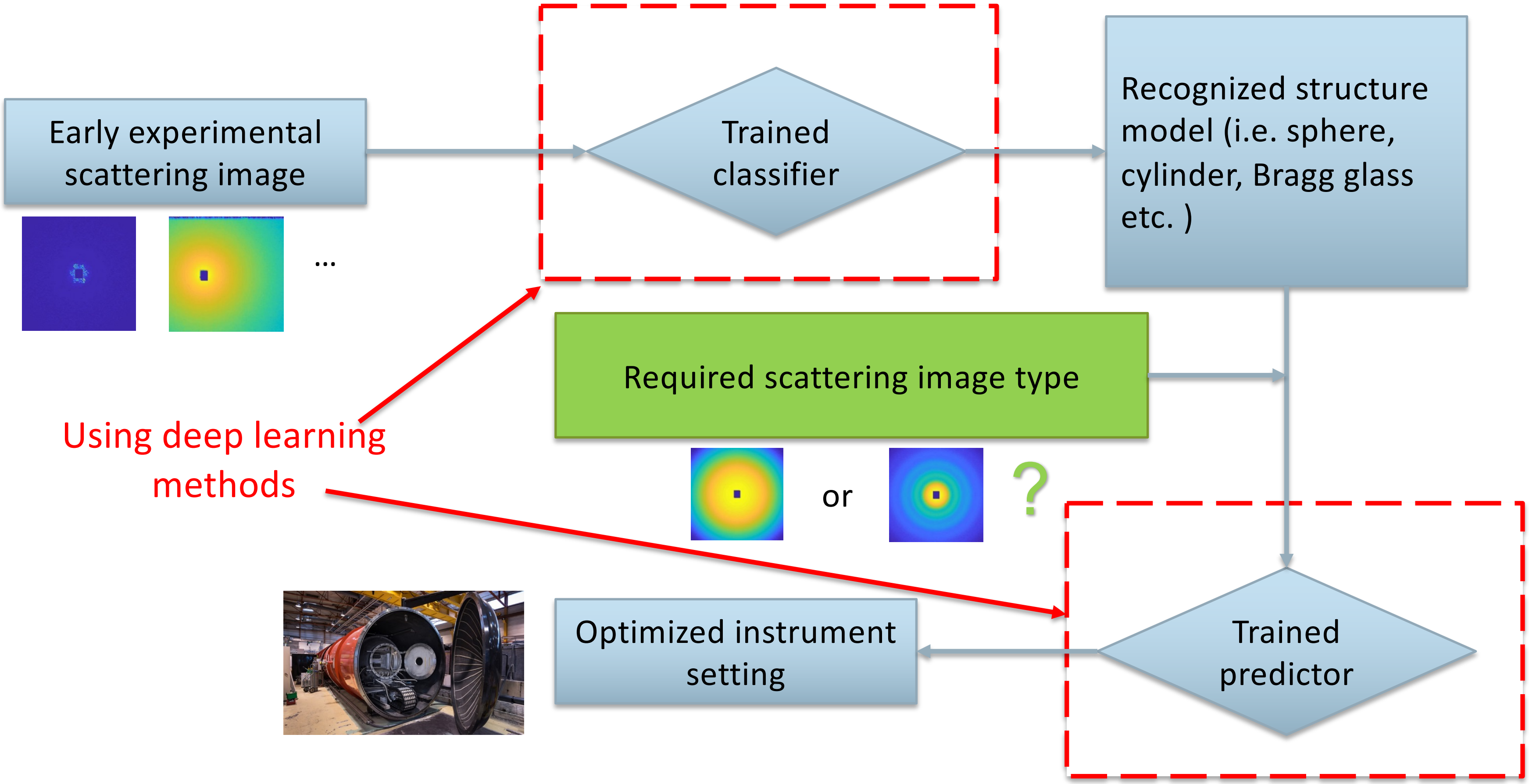
Trained predictor

Optimized instrument setting

Squeezing out the knowledge and the feeling from the brain of a scientist

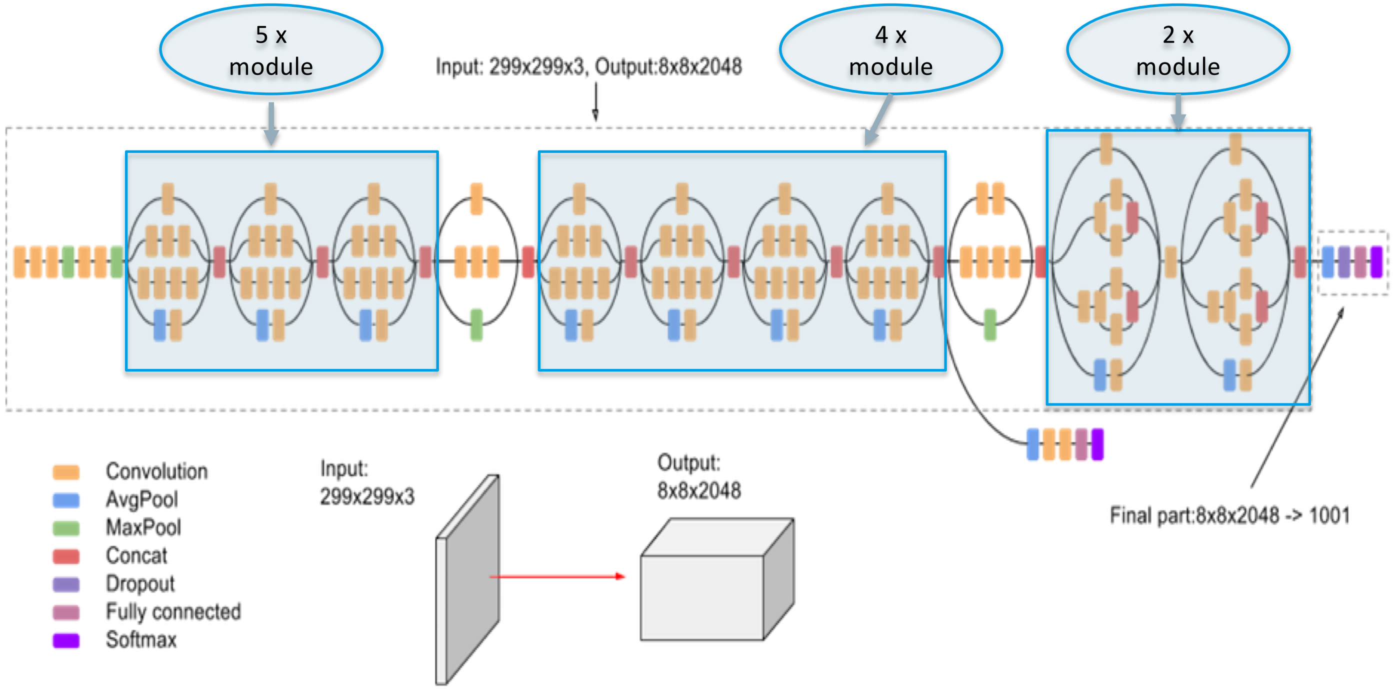
The Project’s Workflow



Inception - V3 Architecture

Published by Google (GoogLeNet)

Fully convolutional, each weight correspond to one multiplication per activation



Reduces the number of connections/parameters without decreasing the network efficiency

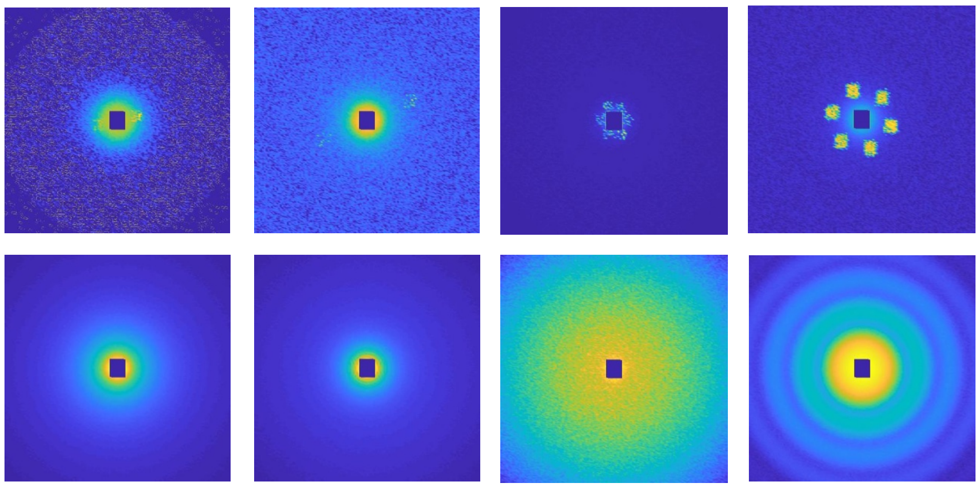
Generating Images For Training

The neuron network is trained using simulated SANS images

Simulation code **GRASP** – mix of analytical and monte-carlo approach

Advantages:

- Include instrument resolution, background and sample environment effects
- Possibility to control all instrument and sample parameters

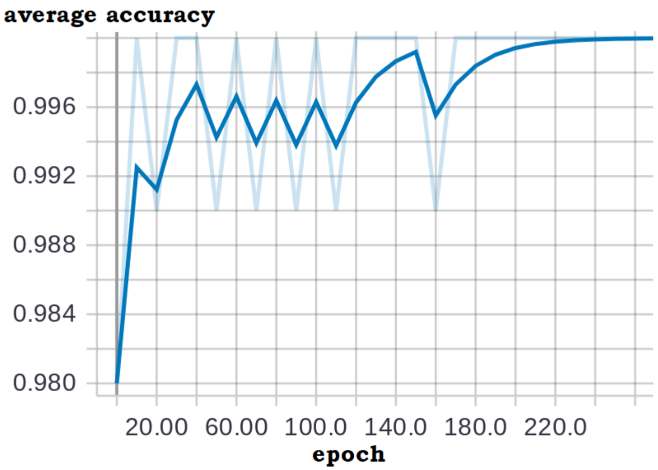


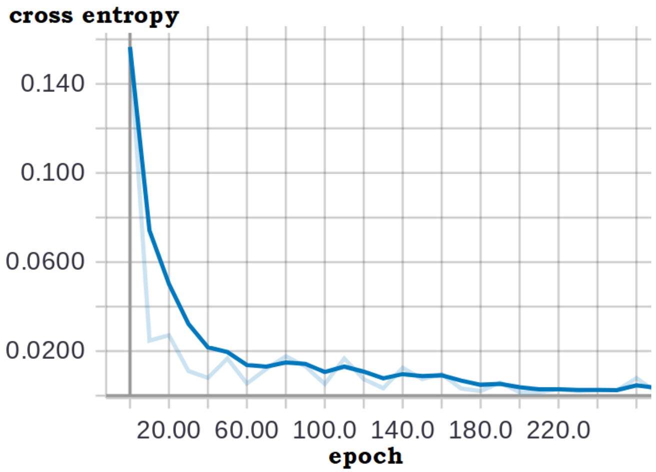
Bragg glass

Sphere

Training The Network

- Training trail begins with the pre-trained model Inception-v3;
- The initial weights are taken from the pre-trained weights based on ImageNet;
- 2000 images per each sample structure
- Initial learning rate is 0.01;
- The model is trained for 300 epochs;
- For each training trail, 80% data are selected randomly for training, 10% data are used for testing and 10% data are used for validation.

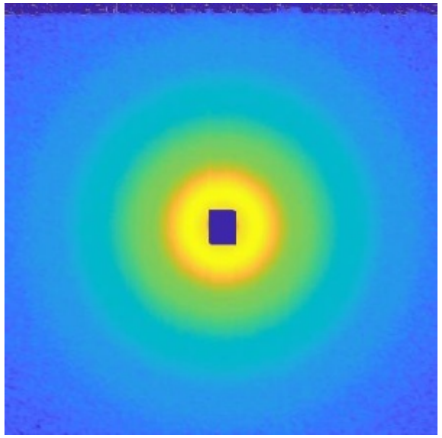




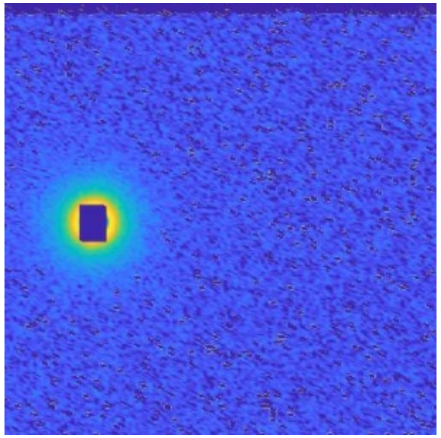
After 200 epochs, the average accuracy is stable to 100%, which indicates all the simulated samples in the dataset are corrected recognized.

Performance On Real Data

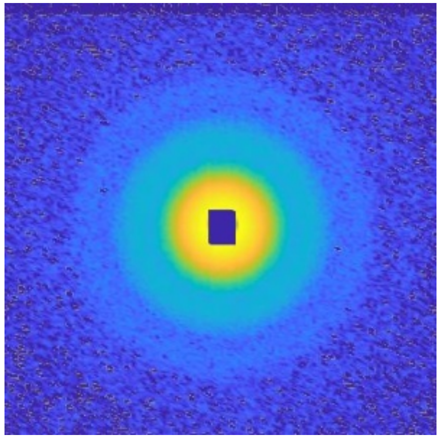
Raw data from silica sample (spherical structure)



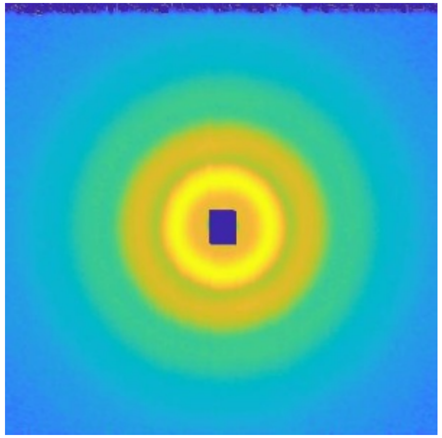
Sphere : 100%
Bragg glass : 0%



Sphere : 98.9%
Bragg glass : 1.1%



Sphere : 99.3%
Bragg glass : 0.7%



Sphere : 100%
Bragg glass : 0%

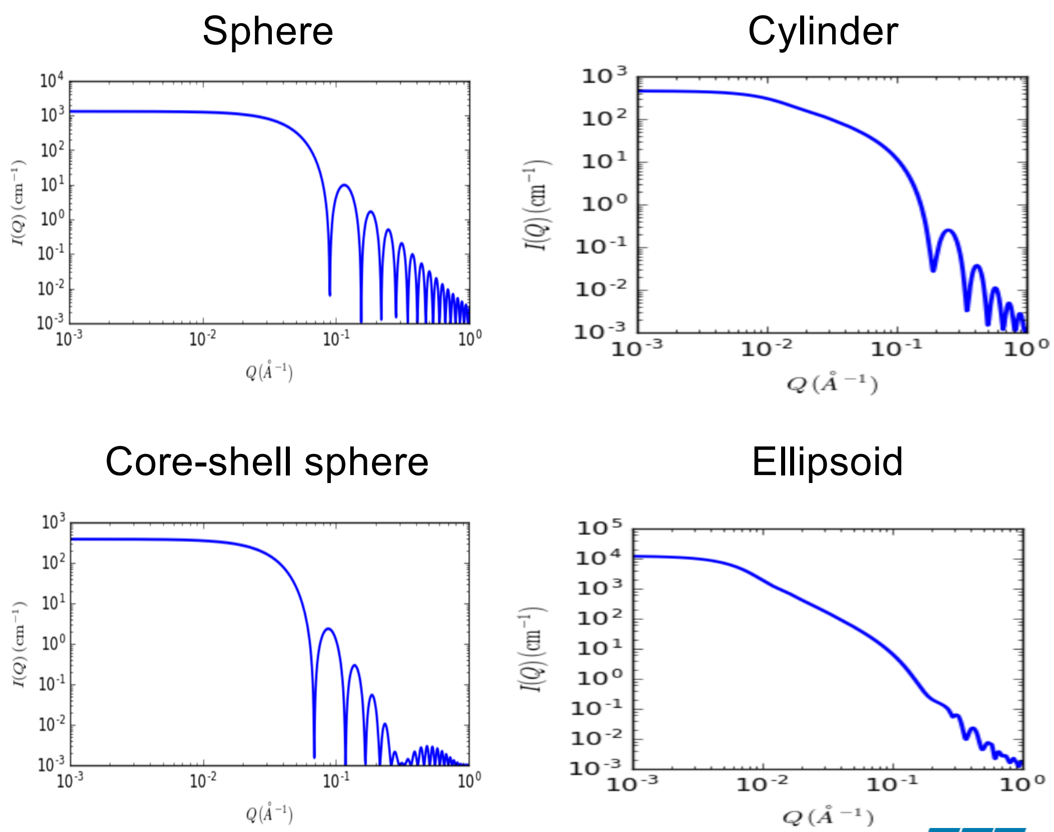
All images are correctly identified with 99% confidence level

Increasing Complexity

Comparison of 4 different structure geometries

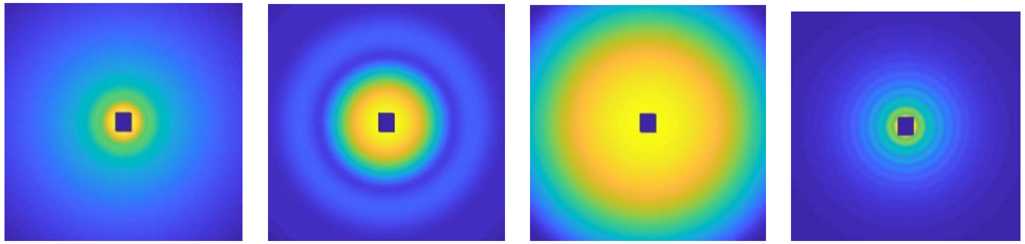
Scattering pattern from sphere, cylinder, core-shell sphere and ellipsoid structures is very similar

Recognition of the structure at an early stage will help a lot in choosing the best instrument setting to obtain a high quality scattering data.

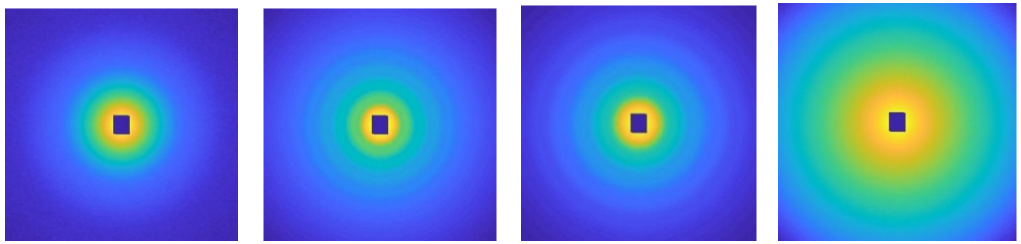


Generating New Datasets

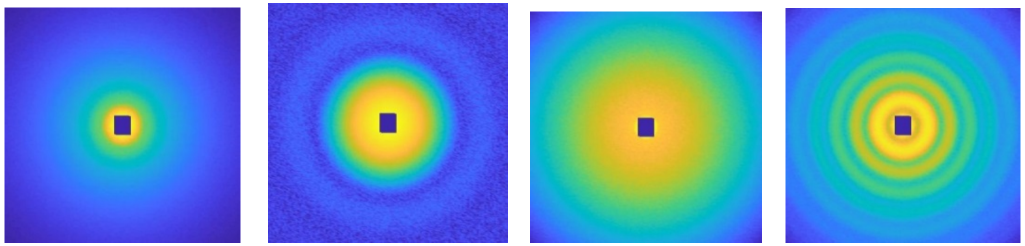
sphere



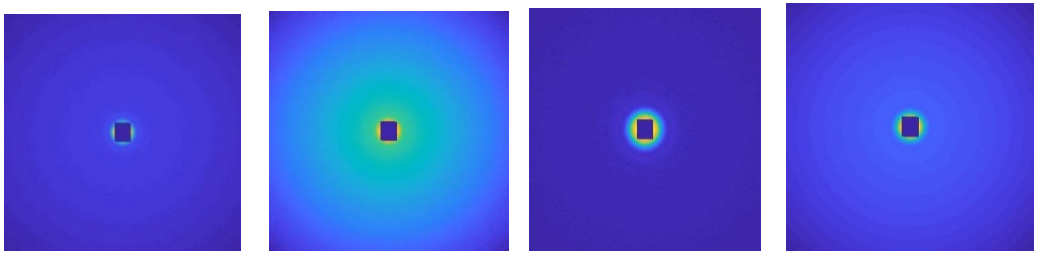
ellipsoid



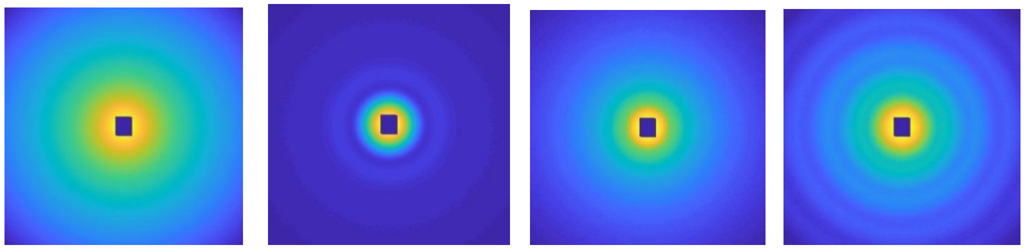
core-shell sphere



unknown



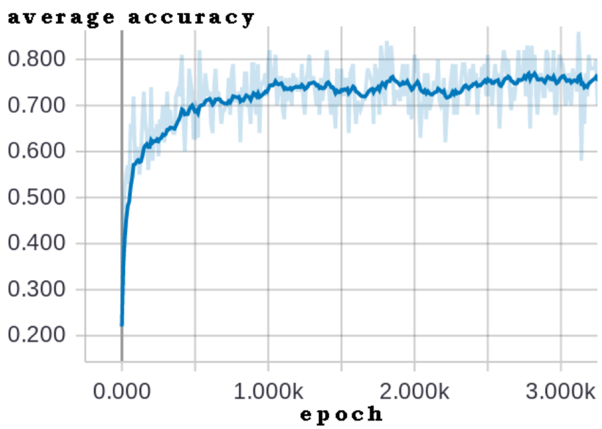
cylinder

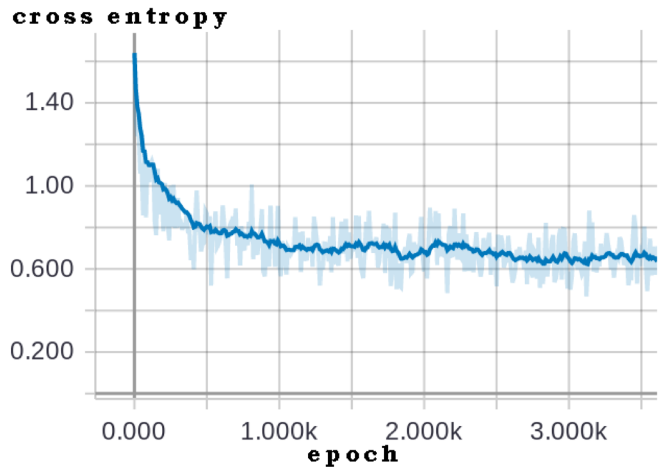


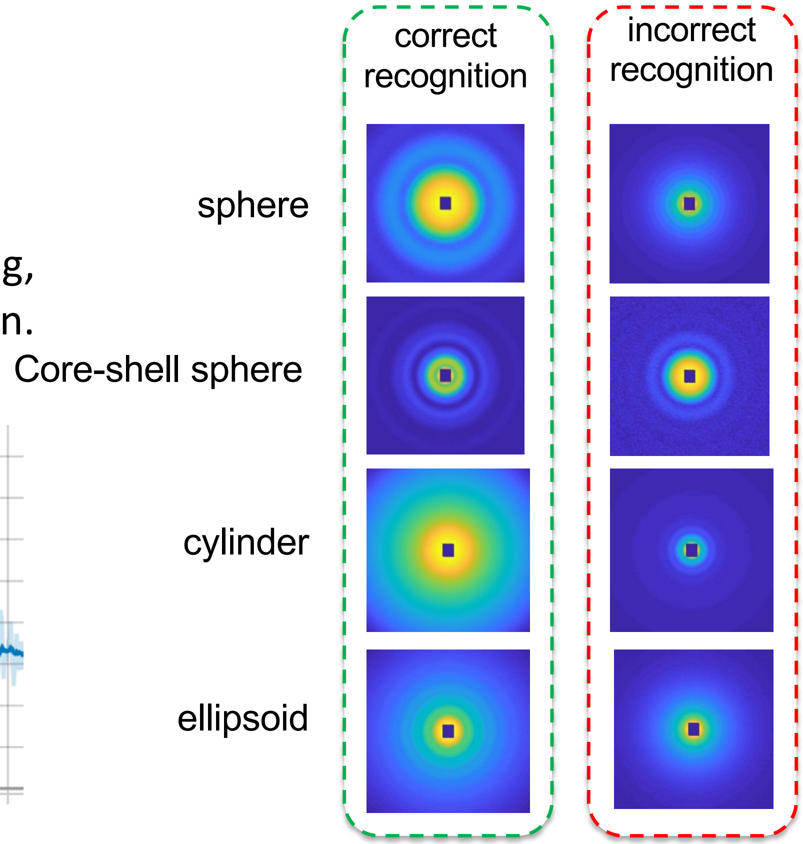
10000 images per structure with random combination of instrument parameters

Results On Simulated Data

- Training trail begins with the pre-trained model Inception-v3;
- Cross-entropy loss function for the training and validation sets;
- Batch size is 100;
- The model is trained for 4000 epochs;
- For each training trail, 80% data are selected randomly for training, 10% data are used for testing and 10% data are used for validation.



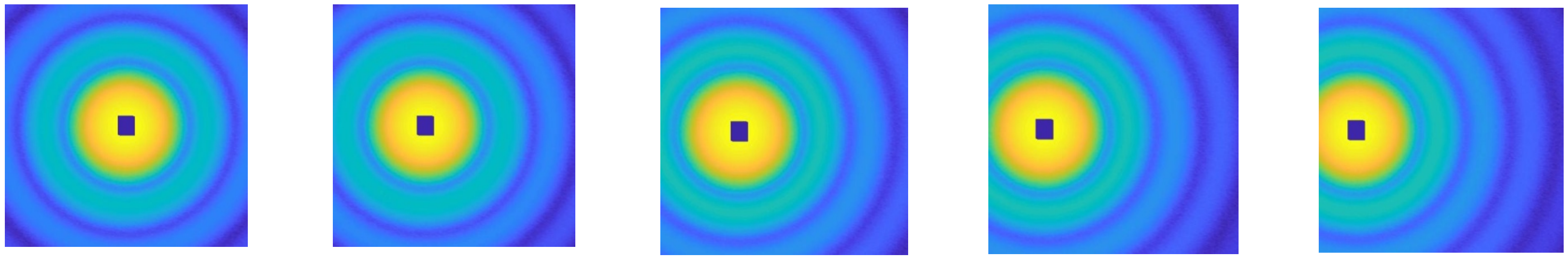




After 1000 epochs, the average accuracy is stable around 73%.

Data Optimization And Fine Tuning

- Data optimization: because of limited field of view of the instrument, in real experiment, sometimes we choose displace the neutron beam with a certain bias from the center, to obtain a larger field of view. 2000 simulated scattering images in this situation are added respectively to each class.

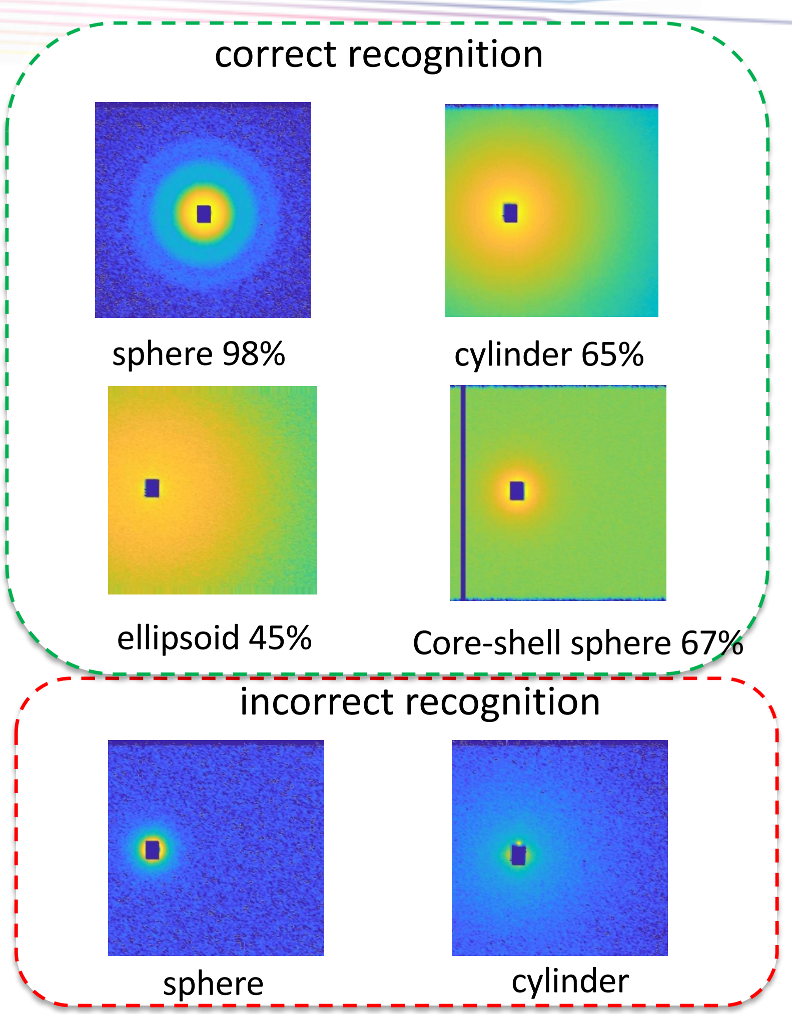


Example of sphere with certain bias from the center

- The model is optimized by stochastic gradient descent optimizer to find an optimal learning rate and batch size.

Performance On Real Data

- 9 silica sphere: 8 image are recognized as sphere with an average confidence value of 92%
- 9 cylinder : 3 images are correctly recognized with an average confidence 63%
- 2 ellipsoid: 2 images are correctly recognized with an average confidence 43%.
- 2 core-shell sphere: 2 images are correctly recognized with an average confidence 67%.



Conclusions

- Recognition accuracy is quite depending on the similarity among the material's structure
- Between models with big difference, high accuracy could be achieved even in low resolution
- Among similar geometrical structures, the accuracy is influenced by the quality of the scattering images and by the field of view
- The classifier trained only on simulated data is effective in recognizing structures from real experimental data
- Once the classifier is trained, the structure recognition is real time