Advanced simulations

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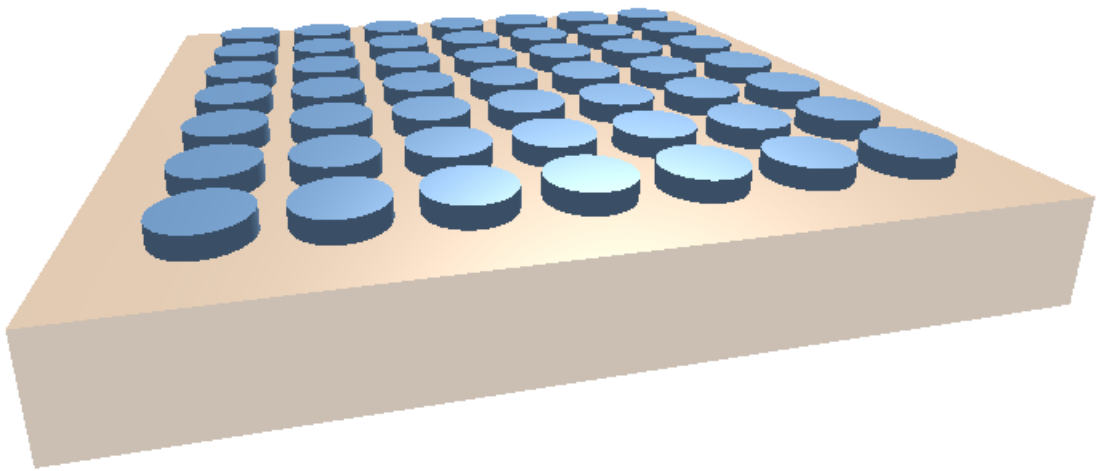
Overview

Rotating square lattice movie

A sample with cylinders in a square lattice arrangement is rotated during the measurement along the z-axis.

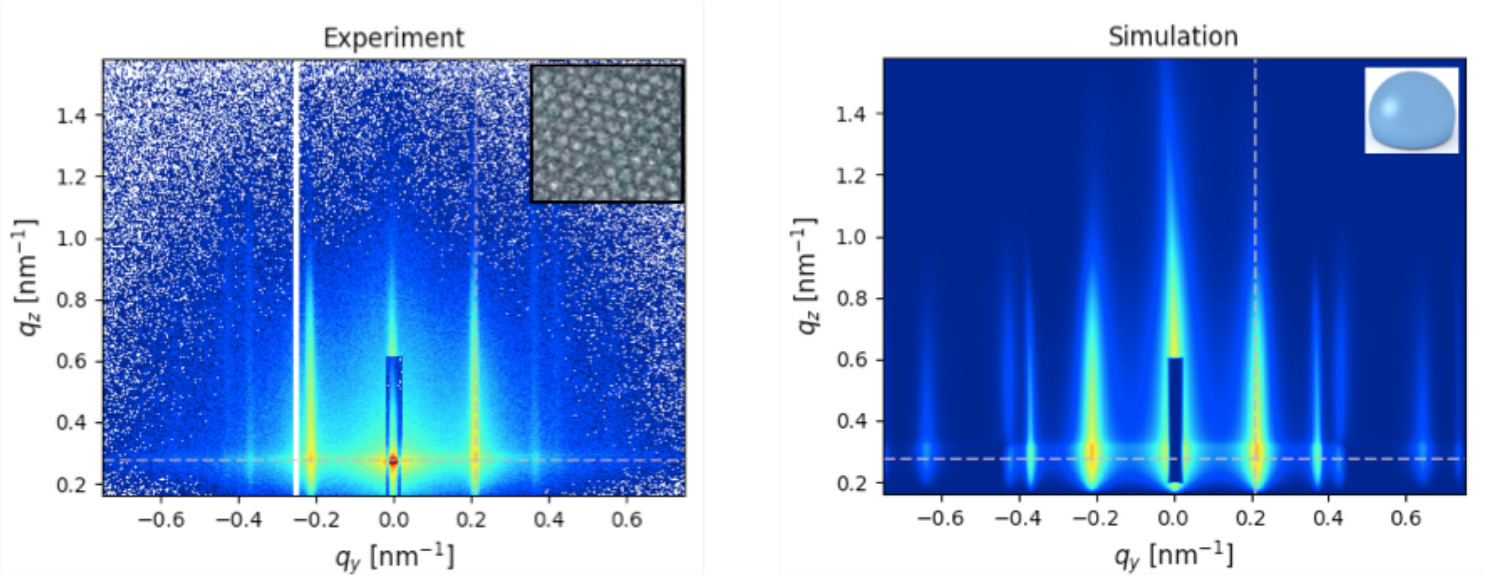


Deep learning with BornAgain

- Motivation
- Neural networks and deep learning
- Data generation
- Training
- Validation

Motivation

Hexagonally arranged $CoFe_2O_4$ nanoparticles.

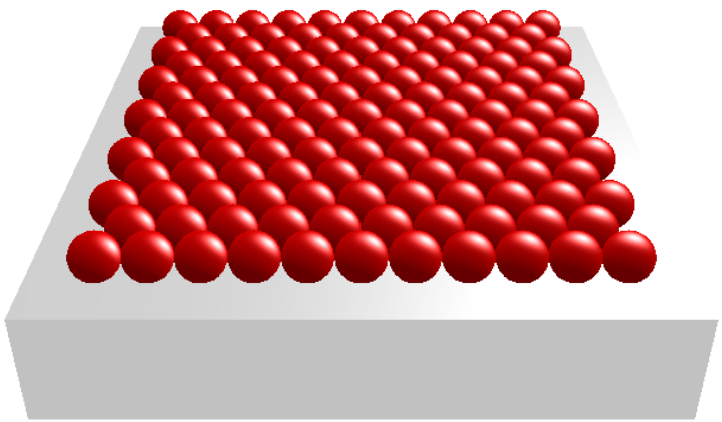


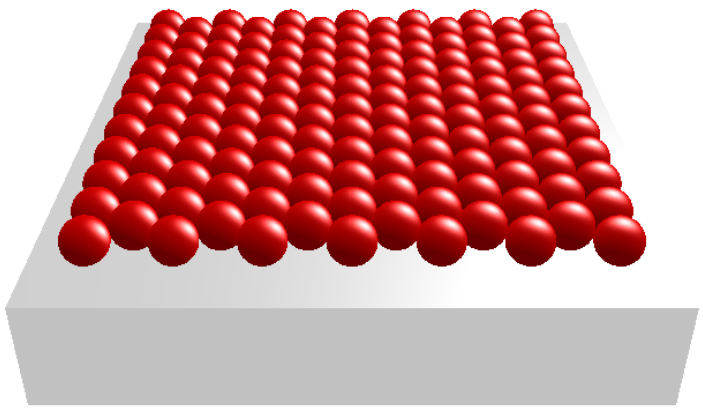
A. Qdemat, E. Kentzinger, G. Portale, M. Ganeva, U. Rücker, Th. Brückel

Despite the good correspondence between data and simulation, it is hard to state that all orientation information is captured by it.

Motivation

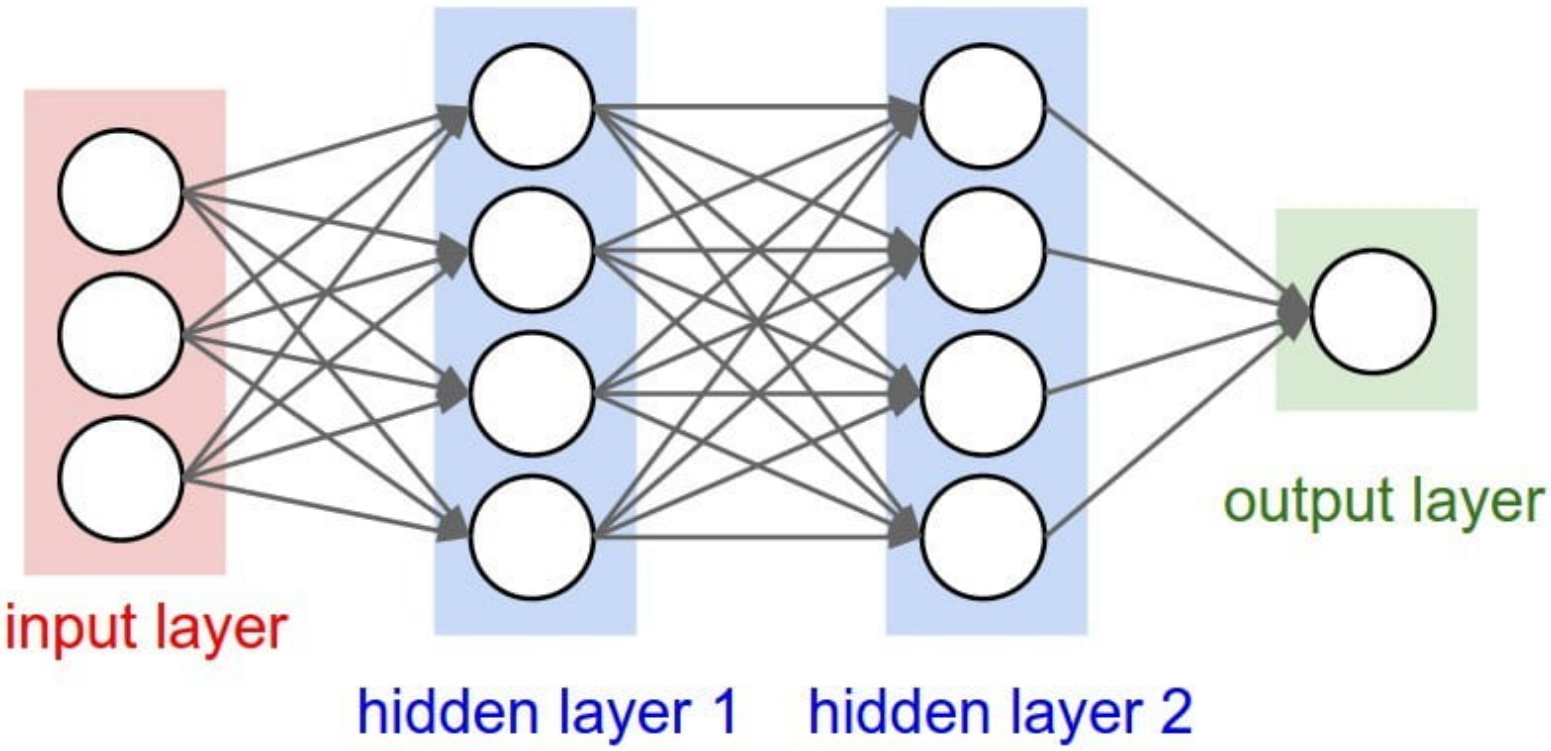
- A 120 parameter fit is unfeasable.
- We investigate if deep learning might help analyzing this type of complex data.





Neural networks

A neural network consists of a succession of layers that combine a linear mapping with some non-linear function.



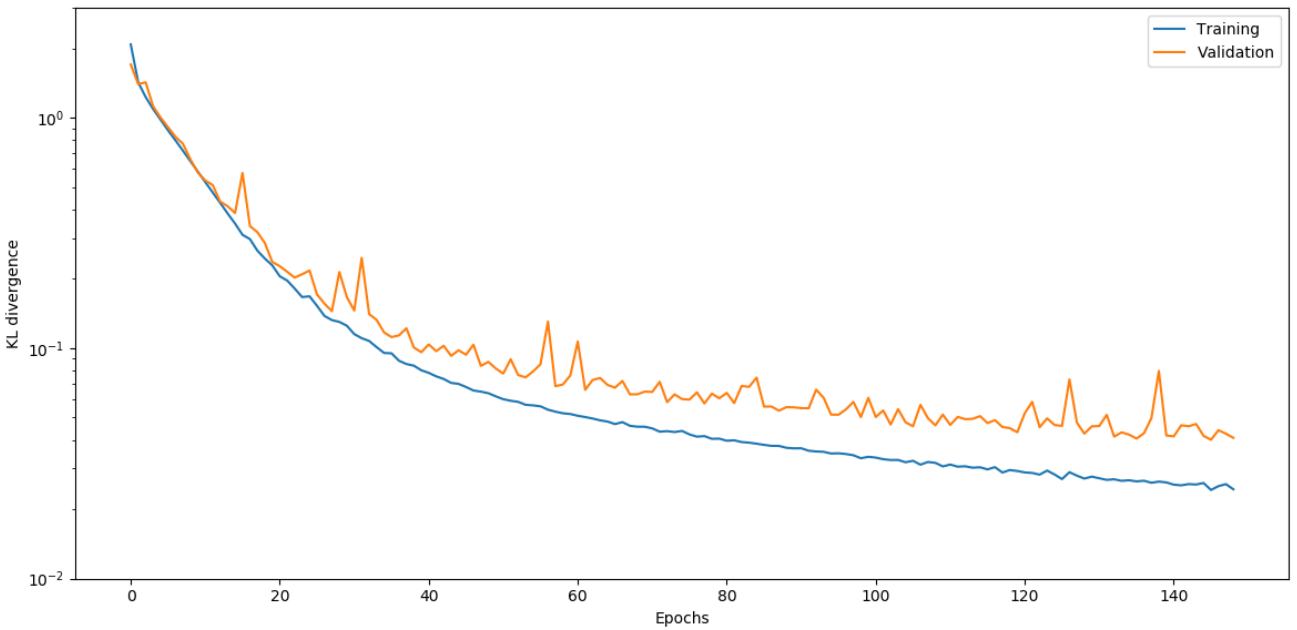
Data generation

Generate data for training/validation:

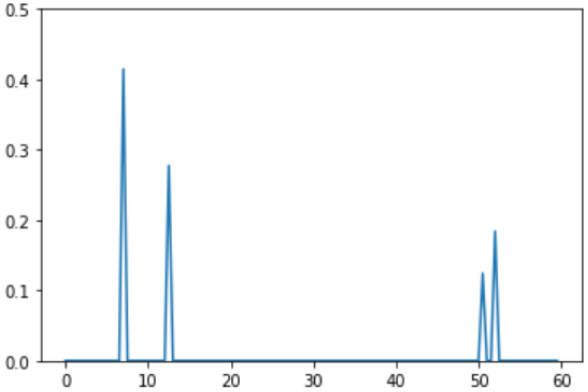
- Input: scattering image
- label: distribution of lattice orientations
- Using BornAgain python API
- 50k training, 10k validation examples
- Fixed: picture size, alignment, lattice lengths, peak shape
- Maximum 5 non-zero probabilities for angles in [0, 0.5, 1.0, ..., 60] degrees
- Input data shifted and rescaled to standard normal distribution

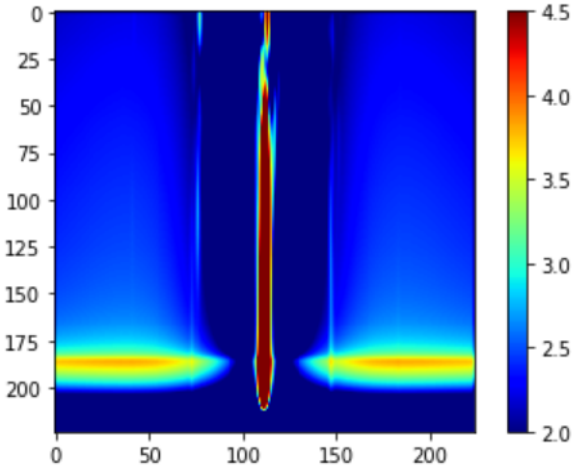
Training

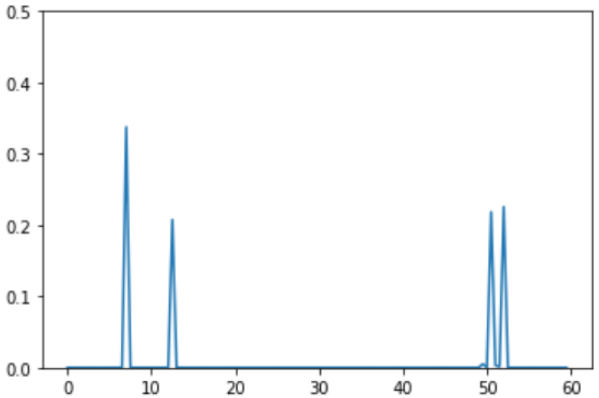
A neural network is trained by minimizing the *difference* between the predicted and the real distribution of lattice orientations.



Validation


0.5
0.4
0.3
0.2
0.1
0.0
0
10
20
30
40
50
60


0
25
50
75
100
125
150
175
200
0
50
100
150
200
4.5
4.0
3.5
3.0
2.5
2.0


0.5
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