

Analysis of X-ray Diffraction by Machine Learning

Thursday 15 September 2022 09:45 (45 minutes)

The long term and sustainable success of the X-ray community essentially depends on its ability to meet growing challenges in handling and analysing data of increasing volume and complexity. Machine Learning (ML) provide a smart solution enabling a dramatic increase in the output of X ray scattering facilities regarding acceleration of data analysis, optimization of beam time usage and, consequently, growth of publication rate. Analysis of scattering data is a very time consuming process as it requires solving an ill-posed inverse problem to infer properties of the imaged object.

During the talk we will be discussing two state-of-the-art methods to solve this task:

- 1) ML-based estimation of the most important parameters of the object in a single step given the experimentally acquired scattering image;
- 2) iterative ML assisted phasing based on automatic differentiation that can be very easily used for fast reconstruction of multiple X-ray scattering modalities such as CDI, mono & polychromatic Ptychography as well as Holography.

Some parameters exhibit low contribution to the acquired data which also hampers reliable predictions and discrimination of these parameters. We show that normalising flows can be used to recover the predictive posterior distribution of these parameters to resolve ambiguous situations and provide information about the reliability of the estimate.

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